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STEALTH—A Lagrange Explicit Finite Difference Code for Solids, Structural, and Thermohydraulic Analysis

Volume 1A: User's Manual—Theoretical Background and Numerical Equations

MASTER

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Research Project 307-1

Computer Code Manual, November 1981

Version 4-1A

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For further information about the code described in this report, contact the Electric Power Software Center, University Computing Company, 1930 Hi Line Drive, Dallas, Texas 75207, (214) 655-8883.

Prepared by
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EPRI PERSPECTIVE

PROJECT DESCRIPTION

Through RP307-1, EPRI has made available to utilities and the industry at large the general-purpose and user-oriented explicit finite difference transient continuum mechanics computer code, STEALTH, based on the technology developed and tested in the defense community. As part of the EPRI research program to develop advanced nonlinear analysis methodology and computer codes for nuclear design and licensing analysis, successful completion of the general-purpose version of the STEALTH code has been followed by reduced versions for "specific" applications such as soil-structure interaction, piping flow, and fluid-structure interaction. The current documentation updates expanded capabilities, modeling improvement, and additional qualifications accomplished since the publication of the original STEALTH manuals, EPRI Computer Code Manual NP-260, in 1976.

PROJECT OBJECTIVE

The objective of the project is to develop a general, portable, modular, and machine-independent explicit finite difference code to address transient and quasi-static design situations such as water-hammer, soil-structure interaction, missile impact, piping flow, and fluid-structure interaction. State-of-the-art capabilities are developed, and extensive qualifications are performed. It is intended that, with extensive documentation and user-oriented modeling features, the code can be used by engineers with maximum efficiency and reliability.

PROJECT RESULTS

Since 1976, more than 100 copies of the STEALTH code have been distributed through three releases, to both domestic and foreign organizations, including utilities, vendors, architect-engineering firms, and research institutions. Version 4-1A is the fourth release of the general-purpose STEALTH code, in which three-dimensional capabilities are qualified and documented. In addition to the general-purpose code, special-purpose versions of STEALTH are developed using either mechanical-only or thermal-only subsets for efficient soil-structure interaction, piping flow, and fluid-structure interaction applications. The Introduction and Guide (Volume 0) of the STEALTH manuals provides an overview of the design and documentation structures of the entire STEALTH family codes.

This project has been managed by Conway Chan and H. T. Tang.

H. T. Tang, Project Manager
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ABSTRACT

A useful computer simulation method based on the explicit finite difference technique can be used to address transient dynamic situations associated with nuclear reactor design and analysis.

This volume is divided into two parts. Part A contains the theoretical background (physical and numerical) and the numerical equations for the STEALTH 1D, 2D, and 3D computer codes. Part B contains input instructions for all three codes. The STEALTH codes are based entirely on the published technology of the Lawrence Livermore National Laboratory, Livermore, California, and Sandia National Laboratories, Albuquerque, New Mexico.

ACKNOWLEDGMENTS

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CONTENTS

VOLUME IA

Section . . . Page

1 INTRODUCTION. 1.1

1.1 User's Manual Description. 1.1

1.2 Documentation Updates. 1.3

1.3 Version Numbers. 1.4

1.4 User Comments. 1.6

References for Section 1 . . . . 1.7

2 THE PHYSICS OF CONTINUUM MECHANICS. 2.1

2.1 Derivation of Continuum Mechanics Equations From Fundamental Physical Laws. 2.1

2.1.1 Theoretical Elements of a Physical System . . . 2.1

2.1.2 Conservation Laws 2.2

2.1.3 Boundary Conditions 2.11

2.1.4 Initial Conditions. 2.11

2.1.5 Constitutive Relations. 2.12

2.2 Reduction of the Fundamental Continuum Mechanics Equations to Simpler Forms 2.13

2.2.1 Overview. 2.13

2.2.2 Spatial Simplifications -- Natural Symmetries . 2.13

2.2.3 Temporal Simplifications. 2.15f

2.2.4 Conservation Law Simplifications. 2.15f

2.2.5 Constitutive Simplifications. 2.19

References for Section 2 . . . . 2.28

3 NUMERICAL DIFFERENCE EQUATIONS. 3.1a

3.1 Introduction 3.1a

3.2 Divergence Theorem 3.1b

3.3 One-Dimensional Equations. 3.4

3.4 Two-Dimensional Equations. 3.7

3.5 Three-Dimensional Equations. 3.9

References for Section 3 . . . . 3.28

CONTENTS (continued)

Section Page

4 ONE-DIMENSIONAL LAGRANGIAN FINITE-DIFFERENCE EQUATIONS. 4.1
- 4.1 Introduction 4.1
- 4.2 Displacement Mesh. 4.1
  - 4.2.1 Calculational Sequence. 4.1
  - 4.2.2 Momentum Equation 4.3
  - 4.2.3 Momentum Boundary Conditions. 4.8
  - 4.2.4 Mass Equation 4.12
- 4.3 Stress Mesh. 4.20
  - 4.3.1 Artificial Viscosity. 4.20
  - 4.3.2 Internal Energy Equation. 4.22
  - 4.3.3 Constitutive Equations. 4.23
  - 4.3.4 Simultaneous Solution of Constitutive Equations and Conservation of Energy by a Two-Step Iteration 4.26
- 4.4 Explicit Time Step 4.37
  - 4.4.1 Overview. 4.37
  - 4.4.2 Stable Mechanical Time Steps. 4.37
  - 4.4.3 Stable Thermal Time Steps 4.41
- 4.5 Use of the Developed Equations for Efficient Solution of Non-Transient Cases 4.42
  - 4.5.1 The Problem 4.42
  - 4.5.2 Density Scaling 4.43
  - 4.5.3 Dynamic Relaxation. 4.44
  - 4.5.4 Modulus Scaling 4.46
- References for Section 4 . . . . 4.48

CONTENTS (continued)

Section Page

5 TWO-DIMENSIONAL LAGRANGIAN FINITE-DIFFERENCE EQUATIONS. 5.1

5.1 Introduction 5.1

5.2 Displacement Mesh. 5.1

5.2.1 Calculational Sequence. 5.1

5.2.2 Momentum Equations. 5.3

5.2.3 Momentum Boundary Conditions. 5.12

5.2.4 Mass Equation 5.20

5.3 Stress Mesh. 5.25

5.3.1 Artificial Viscosity. 5.25

5.3.2 Internal Energy Equation. 5.26b

5.3.3 Constitutive Equations. 5.28

5.3.4 Simultaneous Solution of Constitutive Equations and Conservation of Energy by a Two-Step Iteration 5.30

5.4 Explicit Time Step 5.46

5.4.1 Overview. 5.46

5.4.2 Stable Mechanical Time Steps. 5.46

5.4.3 Stable Thermal Time Steps 5.50

5.5 Use of the Developed Equations for Efficient Solution of Non-Transient Cases 5.51

5.5.1 The Problem 5.51

5.5.2 Density Scaling 5.52

5.5.3 Dynamic Relaxation. 5.53

5.5.4 Modulus Scaling 5.56

References for Section 5 . . . . 5.57

This page intentionally left blank.

CONTENTS (continued)

Section Page

6 THREE-DIMENSIONAL LAGRANGIAN FINITE-DIFFERENCE EQUATIONS. . . . 6.1
  6.1 Introduction 6.1
  6.2 Displacement Mesh. 6.1
    6.2.1 Calculational Sequence. 6.1
    6.2.2 Momentum Equations. 6.3
    6.2.3 Momentum Boundary Conditions. 6.18
    6.2.4 Mass Equation 6.29
  6.3 Stress Mesh. 6.113
    6.3.1 Artificial Viscosity. 6.113
    6.3.2 Internal Energy Equation. 6.115
    6.3.3 Constitutive Equations. 6.116
    6.3.4 Simultaneous Solution of Constitutive Equations and Conservation of Energy by a Two-Step Iteration 6.119
  6.4 Explicit Time Step 6.157
    6.4.1 Overview. 6.157
    6.4.2 Stable Mechanical Time Steps. 6.157
    6.4.3 Stable Thermal Time Steps 6.160
  6.5 Use of the Developed Equations for Efficient Solution of Non-Transient Cases 6.162
    6.5.1 The Problem 6.162
    6.5.2 Density Scaling 6.163
    6.5.3 Dynamic Relaxation. 6.165
    6.5.4 Modulus Scaling 6.168
  References for Section 6 . . . . 6.170

VOLUME IB

Section Page

7 INPUT INSTRUCTIONS FOR THE STEALTH COMPUTER PROGRAMS. 7.a
- 7.A Introduction 7.a
  - 7.A.a Record Format 7.a
  - 7.A.b Manual Format 7.e
- 7.B Index Space. 7.g
- 7.C Efficiency Considerations. 7.ℓ
- 7.D Zone Size Criteria and Noise Considerations. 7.o
- 7.E Input Records. 7.x
- Problem Title. 7.y
- References for Section 7 . . . . 7.z
  - 7.0 Problem Specification Phase (PRB) 7.001
  - 7.1 Material Specification Phase (MAT). 7.101
  - 7.2 Grid Points Specification Phase (GPT) 7.201
    - 7.2.1 One-Dimensional Input Blocks 7.203
    - 7.2.2 Two-Dimensional Input Blocks 7.204
    - 7.2.3 Three-Dimensional Input Blocks 7.207
    - 7.2.4 Wall-Point Specification 7.207a
  - 7.3 Zone Specification Phase (ZON). 7.301
    - 7.3.1 Automatic Rezoning 7.302
    - 7.3.2 Restart Alter. 7.305
  - 7.4 Boundary Conditions Specifications Phase (BDY). . 7.401
  - 7.5 Time Specification Phase (TIM). 7.501
  - 7.6 Edit Specification Phase (EDT). 7.601
  - 7.7 End of Input Data Deck (END). 7.701

CONTENTS (continued)

Section Page

APPENDIX BOUNDARY INTERACTION ALGORITHMS (BIA). BIA.1

APPENDIX FILES (FLS). FLS.1

APPENDIX FUNCTIONS (FNC). FNC.1

APPENDIX GLOSSARY (GLS) GLS.1

APPENDIX HYDRODYNAMIC VERSIONS (HYD). HYD.1

APPENDIX IDENTIFIERS (IDS). IDS.1

APPENDIX MATERIAL MODELS (MAT). MAT.1

APPENDIX MAXIMUMS (MAX) MAX.1

APPENDIX MESSAGES (MSG) MSG.1

APPENDIX NOTATION (NTN) NTN.1

APPENDIX OUTPUT (OPT) OPT.1

APPENDIX PHYSICAL UNITS (PHU) PHU.1

This page intentionally left blank.

ILLUSTRATIONS

VOLUME IA

Figure Page

1.1 Documentation Pyramid 1.5
2.1 Volume Element Used to Derive Eulerian Continuum Mechanics Equations 2.2
2.2 Spectrum of Materials in a Non-Plasma Continuum 2.19
3.1 One-Dimensional Lagrange Mesh 3.5
3.2 Two-Dimensional Lagrange Mesh 3.8a
3.3 Two-Dimensional Lagrange Zone 3.8d
3.4 Three-Dimensional Lagrange Mesh 3.10
3.5 Three-Dimensional Tetrahedron Surface Area TLF. 3.11
3.6 Typical Duodecahedron Zone. 3.17
3.7 Front-Top-Left Tetrahedron. 3.25
4.1 One-Dimensional Calculational Cycle 4.2
4.2 Pictorial Representation of Velocity Integration. 4.6
4.3 Pictorial Representation of Displacement Integration. 4.6
4.4 Example of Need for f_{SFR}. 4.40
4.5 Example of Need for f_{GRF}. 4.40
5.1 Two-Dimensional Calculational Cycle 5.2
5.2 Example of Need for f_{SFR} 5.49
5.3 Example of Need for f_{GRF} 5.49
6.1 Three-Dimensional Calculational Cycle 6.2
6.2 Typical Duodecahedron Zone. 6.31
6.3 Example of Need for f_{SFR} 6.159a
6.4 Example of Need for f_{GRF} 6.159a

VOLUME IB

7.1 General Structure of a STEALTH Input Deck 7.b
7.2 Input Record Format 7.d
7.3 Input Record Documentation Format 7.f
7.4 One-Dimensional Index Conventions 7.h
7.5 Two-Dimensional Index Conventions 7.i
7.6 Three-Dimensional Index Conventions 7.k
7.201 Example of Grid Point Generation. 7.208

This page intentionally left blank.

TABLES

VOLUME IA

Table Page

2.1 Theoretical Elements of a Physical System 2.1
2.2 Natural Symmetries. 2.14
2.3 Examples of Some Mass Conservation Simplifications. 2.16
2.4 Examples of Some Momentum Conservation Simplifications. 2.17
2.5 Examples of Some Energy Conservation Simplifications. 2.18

VOLUME IB

7.0 Summary of PRB Phase Input Records and Input Variables. 7.009
7.1 Summary of MAT Phase Input Records and Input Variables. 7.109
7.2 Summary of GPT Phase Input Records and Input Variables. 7.209a
7.3 Summary of ZON Phase Input Records and Input Variables. 7.309
7.4 Summary of BDY Phase Input Records and Input Variables. 7.409a
7.5 Summary of TIM Phase Input Records and Input Variables. 7.509
7.6 Summary of EDT Phase Input Records and Input Variables. 7.609a

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STEALTH DOCUMENTATION REVISIONS

With each release of new or revised STEALTH documentation, the STEALTH user will receive a Newsletter and a set of "REVISIONS" pages, both of which will summarize changes to the documentation. The Newsletter will present general comments, while the REVISIONS pages will include a detailed summary of changes. The REVISIONS pages will be numbered so that they will have a permanent location in an appropriate volume of the STEALTH manuals. The volume number and date of each REVISIONS page will appear in the lower right-hand corner of the page. The format of the REVISIONS page is shown below.

Page	New Rev.#	New Date	COMMENTS	Old Rev.#	Old Date

The "Page" heading refers to the page number of the revised page. The "New" and "Old" headings refer to the information in the lower right-hand corner of each page. (If there is no information in the lower right-hand corner of a page, assume that the page was created on 15 AUG 75 and its revision number is 0.) Under the "COMMENTS" heading, there will be a string of coded letters with the following meanings:

EA = equation(s) added
EC = equation(s) changed
ED = equation(s) deleted

TA = text added
TC = text changed
TD = text deleted

PA = page added
PC = page changed
PD = page deleted

VA = variable(s) added
VC = variable(s) changed
VD = variable(s) deleted

NF = new figure
NT = new table
NE = new equation number
NR = new reference

SC = simple correction (usually correction of typo or spelling)

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
2.5	1	1 DEC 76	SC	0	15 AUG 75
3.2	1	1 DEC 76	EC	0	15 AUG 75
3.3	1	1 DEC 76	SC, EC	0	15 AUG 75
3.6	1	1 DEC 76	TA	0	15 AUG 75
3.8	1	1 DEC 76	SC, EC	0	15 AUG 75
4.7	1	1 DEC 76	EC	0	15 AUG 75
4.32	1	1 DEC 76	EC	0	15 AUG 75
4.38	1	1 DEC 76	TC	0	15 AUG 75
4.41	1	1 DEC 76	TA	0	15 AUG 75
5.3	1	1 DEC 76	TA	0	15 AUG 75
5.4	1	1 DEC 76	SC	0	15 AUG 75
5.6	1	1 DEC 76	EC	0	15 AUG 75
5.7	1	1 DEC 76	EC	0	15 AUG 75
5.10	1	1 DEC 76	EC	0	15 AUG 75
5.14	1	1 DEC 76	EC	0	15 AUG 75
5.39a	1	1 DEC 76	TD	0	15 AUG 75
5.39b	0	1 DEC 76	PA		
5.41	1	1 DEC 76	EC	0	15 AUG 75
5.47	1	1 DEC 76	TC	0	15 AUG 75
5.50	1	1 DEC 76	TA	0	15 AUG 75
6.11	0	1 DEC 76	PA		
6.12	0	1 DEC 76	PA		
6.13	0	1 DEC 76	PA		
7.1	1	1 DEC 76	TA	0	15 AUG 75
7.001	1	1 DEC 76	TA, TC	0	15 AUG 75
7.009	1	1 DEC 76	VA	0	15 AUG 75
7.010a	1	1 DEC 76	VA	0	15 AUG 75
7.010b	1	1 DEC 76	VA	0	15 AUG 75
7.010c	0	1 DEC 76	PA		

---

*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.011	1	1 DEC 76	TA, TC	0	15 AUG 75
7.016b	1	1 DEC 76	TA	0	15 AUG 75
7.109	1	1 DEC 76	VA	0	15 AUG 75
7.110a	1	1 DEC 76	VA	0	15 AUG 75
7.110b	1	1 DEC 76	VA	0	15 AUG 75
7.110c	0	1 DEC 76	PA		
7.112b	1	1 DEC 76	TD	0	15 AUG 75
7.113	1	1 DEC 76	SC	0	15 AUG 75
7.123	1	1 DEC 76	TC	0	15 AUG 75
7.202	1	1 DEC 76	SC	0	15 AUG 75
7.206	1	1 DEC 76	TD	0	15 AUG 75
7.207	1	1 DEC 76	TA	0	15 AUG 75
7.208	0	1 DEC 76	PA, NF		
7.209a	1	1 DEC 76	VA, VC	0	15 AUG 75
7.209b	1	1 DEC 76	VA, VC	0	15 AUG 75
7.210a	1	1 DEC 76	VA	0	15 AUG 75
7.210b	1	1 DEC 76	VA	0	15 AUG 75
7.210c	0	1 DEC 76	PA		
7.212a	1	1 DEC 76	TC, TD	0	15 AUG 75
7.212b	1	1 DEC 76	TD	0	15 AUG 75
7.232	1	1 DEC 76	VC, TC	0	15 AUG 75
7.246a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75
7.246b	1	1 DEC 76	VC, TC	0	15 AUG 75
7.247a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75
7.247b	1	1 DEC 76	VC, TC	0	15 AUG 75
7.256a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75
7.256b	1	1 DEC 76	VC, TC	0	15 AUG 75
7.257a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75
7.257b	1	1 DEC 76	VC, TC	0	15 AUG 75
7.261a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75

---

*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.261b	1	1 DEC 76	VC, TC	0	15 AUG 75
7.262a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75
7.262b	1	1 DEC 76	VC, TC	0	15 AUG 75
7.266a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75
7.266b	1	1 DEC 76	VC, TC	0	15 AUG 75
7.267a	1	1 DEC 76	VC, TC, NF	0	15 AUG 75
7.267b	1	1 DEC 76	VC, TC	0	15 AUG 75
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7.310c	0	1 DEC 76	PA		
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7.331	1	1 DEC 76	TC, VA	0	15 AUG 75
7.341	1	1 DEC 76	TC, VA	0	15 AUG 75
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7.382	0	1 DEC 76	PA		
7.383a	0	1 DEC 76	PA		
7.383b	0	1 DEC 76	PA		
7.383c	0	1 DEC 76	PA		
7.409a	1	1 DEC 76	VA	0	15 AUG 75
7.410a	1	1 DEC 76	VA	0	15 AUG 75
7.410b	1	1 DEC 76	VA	0	15 AUG 75
7.410c	0	1 DEC 76	PA		
7.501	1	1 DEC 76	TC	0	15 AUG 76
7.503	1	1 DEC 76	TA	0	15 AUG 75
7.504	0	1 DEC 76	TA		

---

*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.509	1	1 DEC 76	VA	0	15 AUG 75
7.510a	1	1 DEC 76	VA	0	15 AUG 75
7.510b	1	1 DEC 76	VA	0	15 AUG 75
7.510c	0	1 DEC 76	PA		
7.514	1	1 DEC 76	TC	0	15 AUG 75
7.609a	1	1 DEC 76	VA, VC	0	15 AUG 75
7.609b	0	1 DEC 76	PA, VA		
7.610a	1	1 DEC 76	VA	0	15 AUG 75
7.610b	1	1 DEC 76	VA	0	15 AUG 75
7.610c	0	1 DEC 76	PA		
7.614	1	1 DEC 76	SC	0	15 AUG 75
7.615	0	1 DEC 76	PA		
7.617	0	1 DEC 76	PA		
7.618	0	1 DEC 76	PA		
7.619	1	1 DEC 76	TC	0	15 AUG 75
7.621	1	1 DEC 76	TA	0	15 AUG 75
7.622	1	1 DEC 76	VA, TC	0	15 AUG 75
7.624	0	1 DEC 76	PA		
7.631	1	1 DEC 76	TA	0	15 AUG 75
7.641	1	1 DEC 76	TA	0	15 AUG 75
7.651	1	1 DEC 76	TA	0	15 AUG 75
7.652a	0	1 DEC 76	PA		
7.652b	0	1 DEC 76	PA		
7.653	0	1 DEC 76	PA		
7.654a	0	1 DEC 76	PA		
7.654b	0	1 DEC 76	PA		
7.661	0	1 DEC 76	PA		
7.662	0	1 DEC 76	PA		
7.663	1	1 DEC 76	TC	0	15 AUG 75

---

*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.671	1	1 DEC 76	TA	0	15 AUG 75
7.674b	1	1 DEC 76	TC	0	15 AUG 75
7.675a	1	1 DEC 76	TC	0	15 AUG 75
7.675b	1	1 DEC 76	TC	0	15 AUG 75
7.677	0	1 DEC 76	PA		
FLS.1	1	1 DEC 76	TC, TA	0	15 AUG 75
IDS.1	1	1 DEC 76	TC	0	15 AUG 75
MAT.12	1	1 DEC 76	EC, TC	0	15 AUG 75
MAT.14	1	1 DEC 76	EC, TA	0	15 AUG 75
MAT.15	1	1 DEC 76	EC	0	15 AUG 75
MAT.17	1	1 DEC 76	EC, TC	0	15 AUG 75
MAT.19	1	1 DEC 76	SC, TA	0	15 AUG 75
MAT.21	1	1 DEC 76	SC, TA	0	15 AUG 75
MAX.1	1	1 DEC 76	TC, TA	0	15 AUG 75
OPT.1	1	1 DEC 76	TC, TA	0	15 AUG 75
OPT.2	1	1 DEC 76	TC, TA	0	15 AUG 75
OPT.3	1	1 DEC 76	TC, TA	0	15 AUG 75
OPT.4	1	1 DEC 76	SC	0	15 AUG 75
OPT.7	1	1 DEC 76	TA	0	15 AUG 75
OPT.10	1	1 DEC 76	TD	0	15 AUG 75
OPT.11	1	1 DEC 76	TA	0	15 AUG 75
OPT.13	1	1 DEC 76	TA, SC	0	15 AUG 75
OPT.14	1	1 DEC 76	TA	0	15 AUG 75
OPT.17	1	1 DEC 76	TA	0	15 AUG 75
OPT.18	1	1 DEC 76	TC	0	15 AUG 75
OPT.19	1	1 DEC 76	TC	0	15 AUG 75
OPT.20	1	1 DEC 76	TC	0	15 AUG 75
OPT.21	1	1 DEC 76	TC	0	15 AUG 75
OPT.22	1	1 DEC 76	SC	0	15 AUG 75

---

*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
OPT.23	0	1 DEC 76	PA		
OPT.24	0	1 DEC 76	PA		
OPT.25	0	1 DEC 76	PA		
OPT.26	0	1 DEC 76	PA		
OPT.27	0	1 DEC 76	PA		
OPT.28	0	1 DEC 76	PA		
OPT.29	0	1 DEC 76	PA		
OPT.30	0	1 DEC 76	PA		
OPT.31	0	1 DEC 76	PA		
OPT.32	0	1 DEC 76	PA		
vi	1	1 DEC 76	TA	0	15 AUG 75
xiii	0	1 DEC 76	PA		
xiv	0	1 DEC 76	PA		
xv	0	1 DEC 76	PA		
xvi	0	1 DEC 76	PA		
xvii	0	1 DEC 76	PA		
xviii	0	1 DEC 76	PA		
xix	0	1 DEC 76	PA		

---

*Key to COMMENTS appears on Page xiii.

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REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
1.2	1	15 NOV 77	TA, TC	0	15 AUG 75
2.3	1	15 NOV 77	TC	0	15 AUG 75
2.4	1	15 NOV 77	TA	0	15 AUG 75
2.5	2	15 NOV 77	TA	1	1 DEC 76
2.6	1	15 NOV 77	VC	0	15 AUG 75
2.7	1	15 NOV 77	EC, SC	0	15 AUG 75
2.8	1	15 NOV 77	TC	0	15 AUG 75
2.9	1	15 NOV 77	VC, EC	0	15 AUG 75
2.10	1	15 NOV 77	TC, TA	0	15 AUG 75
2.11	1	15 NOV 77	TC, TA	0	15 AUG 75
2.12	1	15 NOV 77	TC	0	15 AUG 75
2.13	1	15 NOV 77	TC	0	15 AUG 75
2.14	1	15 NOV 77	TC, TA	0	15 AUG 75
2.15a	1	15 NOV 77	TC, TA, EC	0	15 AUG 75
2.15b	0	15 NOV 77	PA		
2.15c	0	15 NOV 77	PA		
2.15d	0	15 NOV 77	PA		
2.15e	0	15 NOV 77	PA		
2.15f	0	15 NOV 77	PA		
2.16	1	15 NOV 77	TC	0	15 AUG 75
2.17	1	15 NOV 77	TD	0	15 AUG 75
2.18	1	15 NOV 77	TD	0	15 AUG 75
2.22	1	15 NOV 77	NE	0	15 AUG 75
2.23	1	15 NOV 77	NE	0	15 AUG 75
2.24	1	15 NOV 77	NE	0	15 AUG 75
2.25	1	15 NOV 77	NE	0	15 AUG 75
2.26	1	15 NOV 77	NE, TC, EC	0	15 AUG 75
2.27	0	15 NOV 77	PA		
3.1a	1	15 NOV 77	TA	0	15 AUG 75
3.1b	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
3.2	2	15 NOV 77	EC, TC	1	1 DEC 76
3.3	2	15 NOV 77	EC, TC	1	1 DEC 76
3.4	1	15 NOV 77	TC	0	15 AUG 75
3.5	1	15 NOV 77	NF	0	15 AUG 75
3.6a	2	15 NOV 77	TA	1	1 DEC 76
3.6b	0	15 NOV 77	PA		
3.6c	0	15 NOV 77	PA		
3.6d	0	15 NOV 77	PA		
3.6e	0	15 NOV 77	PA		
3.6f	0	15 NOV 77	PA		
3.6g	0	15 NOV 77	PA		
3.7	1	15 NOV 77	EC, TC	0	15 AUG 75
3.8a	1	15 NOV 77	NF	0	15 AUG 75
3.8b	0	15 NOV 77	PA		
3.8c	0	15 NOV 77	PA		
3.8d	0	15 NOV 77	PA		
3.8e	0	15 NOV 77	PA		
3.8f	0	15 NOV 77	PA		
3.8g	0	15 NOV 77	PA		
3.8h	0	15 NOV 77	PA		
3.9	0	15 NOV 77	PA		
3.10	0	15 NOV 77	PA		
3.11	0	15 NOV 77	PA		
3.12	0	15 NOV 77	PA		
3.13	0	15 NOV 77	PA		
3.14	0	15 NOV 77	PA		
3.15	0	15 NOV 77	PA		
3.16	0	15 NOV 77	PA		
3.17	0	15 NOV 77	PA		
3.18	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
3.19	0	15 NOV 77	PA		
3.20	0	15 NOV 77	PA		
3.21	0	15 NOV 77	PA		
3.22	0	15 NOV 77	PA		
3.23	0	15 NOV 77	PA		
3.24	0	15 NOV 77	PA		
4.2	1	15 NOV 77	EC	0	15 AUG 75
4.3	1	15 NOV 77	EC, TA	0	15 AUG 75
4.4	1	15 NOV 77	EC	0	15 AUG 75
4.5	1	15 NOV 77	EC	0	15 AUG 75
4.7	2	15 NOV 77	EC	1	1 DEC 76
4.8	1	15 NOV 77	TC	0	15 AUG 75
4.17	1	15 NOV 77	EC, NE	0	15 AUG 75
4.18	1	15 NOV 77	NE	0	15 AUG 75
4.20	1	15 NOV 77	SC, NR	0	15 AUG 75
4.21	1	15 NOV 77	EC	0	15 AUG 75
4.22	1	15 NOV 77	EC, TC	0	15 AUG 75
4.23	1	15 NOV 77	VC, TC	0	15 AUG 75
4.25	1	15 NOV 77	EC	0	15 AUG 75
4.29	1	15 NOV 77	VC	0	15 AUG 75
4.34	1	15 NOV 77	VC	0	15 AUG 75
4.36	1	15 NOV 77	TC	0	15 AUG 75
4.42	0	15 NOV 77	PA		
4.43	0	15 NOV 77	PA		
4.44	0	15 NOV 77	PA		
4.45	0	15 NOV 77	PA		
4.46	0	15 NOV 77	PA		
4.47	0	15 NOV 77	PA		
5.1	1	15 NOV 77	TC	0	15 AUG 75
5.2	1	15 NOV 77	EC	0	15 AUG 75

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
5.3	2	15 NOV 77	EC	1	1 DEC 76
5.4	2	15 NOV 77	EC	1	1 DEC 76
5.5	1	15 NOV 77	EC	1	15 AUG 75
5.6	2	15 NOV 77	EC	1	1 DEC 76
5.7	2	15 NOV 77	EC, TC, TA	1	1 DEC 76
5.8	1	15 NOV 77	EC	0	15 AUG 75
5.10	2	15 NOV 77	EC	1	1 DEC 76
5.14	2	15 NOV 77	EC	1	1 DEC 76
5.17	1	15 NOV 77	TC	0	15 AUG 75
5.19	1	15 NOV 77	TA	0	15 AUG 75
5.20	1	15 NOV 77	EC, TC	0	15 AUG 75
5.22	1	15 NOV 77	TD, TC	0	15 AUG 75
5.24	1	15 NOV 77	TC, EC	0	15 AUG 75
5.25	1	15 NOV 77	EC, TC, NR	0	15 AUG 75
5.26	1	15 NOV 77	EC, VC, TC	0	15 AUG 75
5.27	1	15 NOV 77	NE, TC, VC	0	15 AUG 75
5.31	1	15 NOV 77	EC, TC	0	15 AUG 75
5.37	1	15 NOV 77	VC, TC	0	15 AUG 75
5.39b	1	15 NOV 77	EC	0	1 DEC 76
5.43	1	15 NOV 77	VC	0	15 AUG 75
5.44	1	15 NOV 77	VC	0	15 AUG 75
5.45	1	15 NOV 77	TC	0	15 AUG 75
5.51	0	15 NOV 77	PA		
5.52	0	15 NOV 77	PA		
5.53	0	15 NOV 77	PA		
5.54	0	15 NOV 77	PA		
5.55	0	15 NOV 77	PA		
5.56	0	15 NOV 77	PA		
6.1	0	15 NOV 77	PA		
6.2	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.3	0	15 NOV 77	PA		
6.4	0	15 NOV 77	PA		
6.5	0	15 NOV 77	PA		
6.6	0	15 NOV 77	PA		
6.7	0	15 NOV 77	PA		
6.8	0	15 NOV 77	PA		
6.9	0	15 NOV 77	PA		
6.10	0	15 NOV 77	PA		
6.11	0	15 NOV 77	PA		
6.12	0	15 NOV 77	PA		
6.13	0	15 NOV 77	PA		
6.14	0	15 NOV 77	PA		
6.15	0	15 NOV 77	PA		
6.16	0	15 NOV 77	PA		
6.17	0	15 NOV 77	PA		
6.18	0	15 NOV 77	PA		
6.19	0	15 NOV 77	PA		
6.20	0	15 NOV 77	PA		
6.21	0	15 NOV 77	PA		
6.22	0	15 NOV 77	PA		
6.23	0	15 NOV 77	PA		
6.24	0	15 NOV 77	PA		
6.25	0	15 NOV 77	PA		
6.26	0	15 NOV 77	PA		
6.27	0	15 NOV 77	PA		
6.28	0	15 NOV 77	PA		
6.29	0	15 NOV 77	PA		
6.30	0	15 NOV 77	PA		
6.31	0	15 NOV 77	PA		
6.32	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.33	0	15 NOV 77	PA		
6.34	0	15 NOV 77	PA		
6.35	0	15 NOV 77	PA		
6.36	0	15 NOV 77	PA		
6.37	0	15 NOV 77	PA		
6.38	0	15 NOV 77	PA		
6.39	0	15 NOV 77	PA		
6.40	0	15 NOV 77	PA		
6.41	0	15 NOV 77	PA		
6.42	0	15 NOV 77	PA		
6.43	0	15 NOV 77	PA		
6.44	0	15 NOV 77	PA		
6.45	0	15 NOV 77	PA		
6.46	0	15 NOV 77	PA		
6.47	0	15 NOV 77	PA		
6.48	0	15 NOV 77	PA		
6.49	0	15 NOV 77	PA		
6.50	0	15 NOV 77	PA		
6.51	0	15 NOV 77	PA		
6.52	0	15 NOV 77	PA		
6.53	0	15 NOV 77	PA		
6.54	0	15 NOV 77	PA		
6.55	0	15 NOV 77	PA		
6.56	0	15 NOV 77	PA		
6.57	0	15 NOV 77	PA		
6.58	0	15 NOV 77	PA		
6.59	0	15 NOV 77	PA		
6.60	0	15 NOV 77	PA		
6.61	0	15 NOV 77	PA		
6.62	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.63	0	15 NOV 77	PA		
6.64	0	15 NOV 77	PA		
6.65	0	15 NOV 77	PA		
6.66	0	15 NOV 77	PA		
6.67	0	15 NOV 77	PA		
6.68	0	15 NOV 77	PA		
6.69	0	15 NOV 77	PA		
6.70	0	15 NOV 77	PA		
6.71	0	15 NOV 77	PA		
6.72	0	15 NOV 77	PA		
6.73	0	15 NOV 77	PA		
6.74	0	15 NOV 77	PA		
6.75	0	15 NOV 77	PA		
6.76	0	15 NOV 77	PA		
6.77	0	15 NOV 77	PA		
6.78	0	15 NOV 77	PA		
6.79	0	15 NOV 77	PA		
6.80	0	15 NOV 77	PA		
6.81	0	15 NOV 77	PA		
6.82	0	15 NOV 77	PA		
6.83	0	15 NOV 77	PA		
6.84	0	15 NOV 77	PA		
6.85	0	15 NOV 77	PA		
6.86	0	15 NOV 77	PA		
6.87	0	15 NOV 77	PA		
6.88	0	15 NOV 77	PA		
6.89	0	15 NOV 77	PA		
6.90	0	15 NOV 77	PA		
6.91	0	15 NOV 77	PA		
6.92	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.93	0	15 NOV 77	PA		
6.94	0	15 NOV 77	PA		
6.95	0	15 NOV 77	PA		
6.96	0	15 NOV 77	PA		
6.97	0	15 NOV 77	PA		
6.98	0	15 NOV 77	PA		
6.99	0	15 NOV 77	PA		
6.100	0	15 NOV 77	PA		
6.101	0	15 NOV 77	PA		
6.102	0	15 NOV 77	PA		
6.103	0	15 NOV 77	PA		
6.104	0	15 NOV 77	PA		
6.105	0	15 NOV 77	PA		
6.106	0	15 NOV 77	PA		
6.107	0	15 NOV 77	PA		
6.108	0	15 NOV 77	PA		
6.109	0	15 NOV 77	PA		
6.110	0	15 NOV 77	PA		
6.111	0	15 NOV 77	PA		
6.112	0	15 NOV 77	PA		
6.113	0	15 NOV 77	PA		
6.114	0	15 NOV 77	PA		
6.115	0	15 NOV 77	PA		
6.116	0	15 NOV 77	PA		
6.117	0	15 NOV 77	PA		
6.118	0	15 NOV 77	PA		
6.119	0	15 NOV 77	PA		
6.120	0	15 NOV 77	PA		
6.121	0	15 NOV 77	PA		
6.122	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.123	0	15 NOV 77	PA		
6.124	0	15 NOV 77	PA		
6.125	0	15 NOV 77	PA		
6.126	0	15 NOV 77	PA		
6.127	0	15 NOV 77	PA		
6.128	0	15 NOV 77	PA		
6.129	0	15 NOV 77	PA		
6.130	0	15 NOV 77	PA		
6.131	0	15 NOV 77	PA		
6.132	0	15 NOV 77	PA		
6.133	0	15 NOV 77	PA		
6.134	0	15 NOV 77	PA		
6.135	0	15 NOV 77	PA		
6.136	0	15 NOV 77	PA		
6.137	0	15 NOV 77	PA		
6.138	0	15 NOV 77	PA		
6.139	0	15 NOV 77	PA		
6.140	0	15 NOV 77	PA		
6.141	0	15 NOV 77	PA		
6.142	0	15 NOV 77	PA		
6.143	0	15 NOV 77	PA		
6.144	0	15 NOV 77	PA		
6.145	0	15 NOV 77	PA		
6.146	0	15 NOV 77	PA		
6.147	0	15 NOV 77	PA		
6.148	0	15 NOV 77	PA		
6.149	0	15 NOV 77	PA		
6.150	0	15 NOV 77	PA		
6.151	0	15 NOV 77	PA		
6.152	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.153	0	15 NOV 77	PA		
6.154	0	15 NOV 77	PA		
6.155	0	15 NOV 77	PA		
6.156	0	15 NOV 77	PA		
6.157	0	15 NOV 77	PA		
6.158	0	15 NOV 77	PA		
6.159	0	15 NOV 77	PA		
6.160	0	15 NOV 77	PA		
6.161	0	15 NOV 77	PA		
7.a	1	15 NOV 77	PC	0	15 AUG 75
7.b	1	15 NOV 77	PC	0	15 AUG 75
7.c	1	15 NOV 77	PC	0	15 AUG 75
7.d	1	15 NOV 77	PC	0	15 AUG 75
7.e	1	15 NOV 77	PC	0	15 AUG 75
7.f	1	15 NOV 77	PC	0	15 AUG 75
7.g	1	15 NOV 77	PC, TC	0	15 AUG 75
7.h	1	15 NOV 77	PC	0	15 AUG 75
7.i	1	15 NOV 77	PC	0	15 AUG 75
7.j	1	15 NOV 77	PC, TC, TA	0	15 AUG 75
7.k	0	15 NOV 77	PA		
7.ℓ	1	15 NOV 77	PC	0	1 DEC 76
7.m	1	15 NOV 77	PC, TC	0	1 DEC 76
7.n	1	15 NOV 77	PC, TC	0	1 DEC 76
7.r	2	15 NOV 77	PC	1	1 DEC 76
7.s	1	15 NOV 77	PC	0	15 AUG 75
7.001	2	15 NOV 77	TC, TA	1	1 DEC 76
7.002	1	15 NOV 77	TC	0	15 AUG 75
7.009	2	15 NOV 77	VA	1	1 DEC 76
7.012	1	15 NOV 77	TC	0	15 AUG 75
7.013	1	15 NOV 77	TC	0	15 AUG 75

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.014	1	15 NOV 77	TC, TA	0	15 AUG 75
7.016b	2	15 NOV 77	TC	1	1 DEC 76
7.017	1	15 NOV 77	VA, TA	0	15 AUG 75
7.018a	1	15 NOV 77	VA, TA	0	15 AUG 75
7.018b	0	15 NOV 77	PA		
7.113	2	15 NOV 77	TC, TD	1	1 DEC 76
7.201	1	15 NOV 77	TA, TC	0	15 AUG 75
7.202a	2	15 NOV 77	PC	1	1 DEC 76
7.202b	0	15 NOV 77	PA		
7.202c	0	15 NOV 77	PA		
7.203	1	15 NOV 77	TC	0	15 AUG 75
7.204	1	15 NOV 77	TA, TC	0	15 AUG 75
7.207	2	15 NOV 77	TA, TC	1	1 DEC 76
7.208	1	15 NOV 77	TC	0	1 DEC 76
7.209a	2	15 NOV 77	VA	1	1 DEC 76
7.211	1	15 NOV 77	VC	0	15 AUG 75
7.212b	2	15 NOV 77	TC	1	1 DEC 76
7.221a	1	15 NOV 77	VA	0	15 AUG 75
7.221b	1	15 NOV 77	VA, TC, VC	0	15 AUG 75
7.301	2	15 NOV 77	TA, SC	1	1 DEC 76
7.302a	1	15 NOV 77	TA, TC	0	1 DEC 76
7.302b	0	15 NOV 77	PA		
7.302c	0	15 NOV 77	PA		
7.309	2	15 NOV 77	VC, VA	1	1 DEC 76
7.311a	1	15 NOV 77	VA	0	15 AUG 75
7.311b	1	15 NOV 77	VA, TA	0	15 AUG 75
7.381a	1	15 NOV 77	TC	0	1 DEC 76
7.381b	0	15 NOV 77	PA		
7.382a	1	15 NOV 77	TC	0	1 DEC 76
7.382b	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.382c	0	15 NOV 77	PA		
7.382d**	0	15 NOV 77	PA		
7.388	0	15 NOV 77	PA		
7.389	0	15 NOV 77	PA		
7.401	1	15 NOV 77	TC	0	15 AUG 75
7.402	1	15 NOV 77	TA	0	15 AUG 75
7.403	1	15 NOV 77	TC, TA	0	15 AUG 75
7.409a	2	15 NOV 77	VA	1	1 DEC 76
7.409b	1	15 NOV 77	VA	0	15 AUG 75
7.412c	1	15 NOV 77	TC	0	15 AUG 75
7.422	1	15 NOV 77	TC	0	15 AUG 75
7.423	1	15 NOV 77	TC	0	15 AUG 75
7.431a	1	15 NOV 77	TC	0	15 AUG 75
7.432	1	15 NOV 77	TC	0	15 AUG 75
7.441a	1	15 NOV 77	TC	0	15 AUG 75
7.442	1	15 NOV 77	TC	0	15 AUG 75
7.443a	1	15 NOV 77	TC	0	15 AUG 75
7.444	1	15 NOV 77	TC	0	15 AUG 75
7.445a	0	15 NOV 77	PA		
7.445b	0	15 NOV 77	PA		
7.446	0	15 NOV 77	PA		
7.451a	1	15 NOV 77	TC	0	15 AUG 75
7.452	1	15 NOV 77	TC	0	15 AUG 75
7.461a	1	15 NOV 77	TC	0	15 AUG 75
7.462	1	15 NOV 77	TC	0	15 AUG 75
7.463a	1	15 NOV 77	TC	0	15 AUG 75
7.464	1	15 NOV 77	TC	0	15 AUG 75
7.465a	0	15 NOV 77	PA		
7.465b	0	15 NOV 77	PA		
7.466	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

**Pages 7.383a, 7.383b, and 7.383c are to be removed from the manual.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.481	1	15 NOV 77	VC	0	15 AUG 75
7.482a	1	15 NOV 77	VA, TA	0	15 AUG 75
7.482b	1	15 NOV 77	VA, TA	0	15 AUG 75
7.601	1	15 NOV 77	TA	0	15 AUG 75
7.602	1	15 NOV 77	TC	0	15 AUG 75
7.609a	2	15 NOV 77	VA	1	1 DEC 76
7.609b	1	15 NOV 77	VA	0	1 DEC 76
7.621	2	15 NOV 77	TC	1	1 DEC 76
7.622a	2	15 NOV 77	VA, TC, VC	1	1 DEC 76
7.622b	0	15 NOV 77	PA		
7.624	1	15 NOV 77	TD	0	1 DEC 76
7.631	2	15 NOV 77	TC	1	1 DEC 76
7.632a	1	15 NOV 77	VA	0	15 AUG 75
7.632b	1	15 NOV 77	VC, VA, TA	0	15 AUG 75
7.641	2	15 NOV 77	TC	1	1 DEC 76
7.651	2	15 NOV 77	TC	1	1 DEC 76
7.652a	1	15 NOV 77	VC, VA, TA	0	1 DEC 76
7.652b	1	15 NOV 77	VC, VA, TA	0	1 DEC 76
7.661	1	15 NOV 77	TC	0	1 DEC 76
7.662	1	15 NOV 77	TC	0	1 DEC 76
7.663	2	15 NOV 77	TC	1	1 DEC 76
7.671	2	15 NOV 77	TC	1	1 DEC 76
7.672a	1	15 NOV 77	TC, TA	0	15 AUG 75
7.672b	1	15 NOV 77	TC, TA	0	15 AUG 75
7.674a	1	15 NOV 77	TC, TA	0	15 AUG 75
7.674b	2	15 NOV 77	TC, TA	1	1 DEC 76
7.675a	2	15 NOV 77	VC	1	1 DEC 76
7.677	1	15 NOV 77	TC	0	1 DEC 76

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
BIA.1	0	15 NOV 77	PA		
BIA.2	0	15 NOV 77	PA		
BIA.3	0	15 NOV 77	PA		
BIA.4	0	15 NOV 77	PA		
BIA.5	0	15 NOV 77	PA		
BIA.6	0	15 NOV 77	PA		
BIA.7	0	15 NOV 77	PA		
BIA.8	0	15 NOV 77	PA		
BIA.9	0	15 NOV 77	PA		
BIA.10	0	15 NOV 77	PA		
BIA.11	0	15 NOV 77	PA		
BIA.12	0	15 NOV 77	PA		
BIA.13	0	15 NOV 77	PA		
BIA.14	0	15 NOV 77	PA		
BIA.15	0	15 NOV 77	PA		
BIA.16	0	15 NOV 77	PA		
BIA.17	0	15 NOV 77	PA		
BIA.18	0	15 NOV 77	PA		
BIA.19	0	15 NOV 77	PA		
BIA.20	0	15 NOV 77	PA		
BIA.21	0	15 NOV 77	PA		
BIA.22	0	15 NOV 77	PA		
BIA.23	0	15 NOV 77	PA		
BIA.24	0	15 NOV 77	PA		
FLS.1	2	15 NOV 77	TC	1	1 DEC 76
GLS.2	1	15 NOV 77	TC, TA	0	15 AUG 75
IDS.1	2	15 NOV 77	TA	1	1 DEC 76
MAT.2	1	15 NOV 77	TC	0	15 AUG 75
MAT.3	1	15 NOV 77	TC, TA	0	15 AUG 75
MAT.4	1	15 NOV 77	TC	0	15 AUG 75

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*Key to COMMENTS appears on Page xiii.

REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
MAT.5	1	15 NOV 77	TC	0	15 AUG 75
MAT.7	1	15 NOV 77	TC	0	15 AUG 75
MAT.10	1	15 NOV 77	TA	0	15 AUG 75
MAX.1	2	15 NOV 77	TA, TD, TC	1	1 DEC 76
MSG.1	1	15 NOV 77	TC	0	15 AUG 75
MSG.2	1	15 NOV 77	TA	0	15 AUG 75
NTN.1,2	1	15 NOV 77	VA, VC	0	15 AUG 75
REF.1	1	15 NOV 77	TC	0	15 AUG 75
iii	1	15 NOV 77	TA	0	15 AUG 75
v	1	15 NOV 77	TA, TC	0	15 AUG 75
vi	2	15 NOV 77	TA, TC	1	1 DEC 76
vii	1	15 NOV 77	TA, TC	0	15 AUG 75
viii	1	15 NOV 77	TA, TC	0	15 AUG 75
ix	1	15 NOV 77	TA, TC	0	15 AUG 75
xi	1	15 NOV 77	TC	0	15 AUG 75
xiii	1	15 NOV 77	TA	0	15 AUG 75
xxi	0	15 NOV 77	PA		
xxii	0	15 NOV 77	PA		
xxiii	0	15 NOV 77	PA		
xxiv	0	15 NOV 77	PA		
xxv	0	15 NOV 77	PA		
xxvi	0	15 NOV 77	PA		
xxvii	0	15 NOV 77	PA		
xxviii	0	15 NOV 77	PA		
xxix	0	15 NOV 77	PA		
xxx	0	15 NOV 77	PA		
xxxi	0	15 NOV 77	PA		
xxxii	0	15 NOV 77	PA		
xxxiii	0	15 NOV 77	PA		
xxxiv	0	15 NOV 77	PA		
xxv	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

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REVISIONS

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
i	3	30 SEP 80	TC	2	15 NOV 77
iii	2	30 SEP 80	TC	1	15 NOV 77
v	2	30 SEP 80	TA	1	15 NOV 77
vi	3	30 SEP 80	TA	2	15 NOV 77
vi.a	0	30 SEP 80	PA		
vii	2	30 SEP 80	TA	1	15 NOV 77
viii	2	30 SEP 80	TA, TC	1	15 NOV 77
viii.a	0	30 SEP 80	PA		
ix	2	30 SEP 80	TA, TC	1	15 NOV 77
1.1	1	30 SEP 80	TC, TA	0	15 AUG 75
1.2	2	30 SEP 80	TA, TD	1	15 NOV 77
1.3	0	30 SEP 80	PA		
1.4	0	30 SEP 80	PA		
1.5	0	30 SEP 80	PA		
1.6	0	30 SEP 80	PA		
1.7	0	30 SEP 80	PA		
2.3	2	30 SEP 80	TC	1	15 NOV 77
2.5	3	30 SEP 80	TC	2	15 NOV 77
2.12	2	30 SEP 80	TC	1	15 NOV 77
2.22	2	30 SEP 80	TC	1	15 NOV 77
2.23	2	30 SEP 80	TA, EA	1	15 NOV 77
2.25	2	30 SEP 80	TC, EC	1	15 NOV 77
2.26	2	30 SEP 80	EC	1	15 NOV 77
2.28	0	30 SEP 80	PA		
3.1a	2	30 SEP 80	TC	1	15 NOV 77
3.1b	1	30 SEP 80	TC	0	15 NOV 77
3.3	3	30 SEP 80	EC	2	15 NOV 77
3.7	2	30 SEP 80	TC, EC	1	15 NOV 77
3.8b	1	30 SEP 80	EC	0	15 NOV 77

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
3.8c	1	30 SEP 80	TA	0	15 NOV 77
3.8d	1	30 SEP 80	PC	0	15 NOV 77
3.8e	1	30 SEP 80	PC	0	15 NOV 77
3.8f	1	30 SEP 80	EC	0	15 NOV 77
3.8g	1	30 SEP 80	TC	0	15 NOV 77
3.8i	0	30 SEP 80	PA		
3.8j	0	30 SEP 80	PA		
3.8k	0	30 SEP 80	PA		
3.11	1	30 SEP 80	TC	0	15 NOV 77
3.17	1	30 SEP 80	TC	0	15 NOV 77
3.18	1	30 SEP 80	EC	0	15 NOV 77
3.24	1	30 SEP 80	TC	0	15 NOV 77
3.25	0	30 SEP 80	PA		
3.26	0	30 SEP 80	PA		
3.27	0	30 SEP 80	PA		
3.28	0	30 SEP 80	PA		
4.2	2	30 SEP 80	TC	1	15 NOV 77
4.3	2	30 SEP 80	TC	1	15 NOV 77
4.4	2	30 SEP 80	EC	1	15 NOV 77
4.5	2	30 SEP 80	EC	1	15 NOV 77
4.9	1	30 SEP 80	EC	0	15 AUG 75
4.11	1	30 SEP 80	EC	0	15 AUG 75
4.18	2	30 SEP 80	TC	1	15 NOV 77
4.20	2	30 SEP 80	TC	1	15 NOV 77
4.21	2	30 SEP 80	TC, TA	1	15 NOV 77
4.34	2	30 SEP 80	EC	1	15 NOV 77
4.35	1	30 SEP 80	EC	0	15 AUG 75
4.39	1	30 SEP 80	TA, EC	0	15 AUG 75

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
4.40	1	30 SEP 80	PC, NF	0	15 AUG 75
4.40a	0	30 SEP 80	PA		
4.40b	0	30 SEP 80	PA		
4.41	2	30 SEP 80	EC	1	01 DEC 76
4.45	1	30 SEP 80	TC	0	15 NOV 77
4.48	0	30 SEP 80	PA		
5.2	2	30 SEP 80	TC	1	15 NOV 77
5.3	3	30 SEP 80	TC	2	15 NOV 77
5.9	1	30 SEP 80	TC	0	15 AUG 75
5.18	1	30 SEP 80	TC	0	15 AUG 75
5.19	2	30 SEP 80	TC	1	15 NOV 77
5.24a	0	30 SEP 80	PA		
5.24b	0	30 SEP 80	PA		
5.25	2	30 SEP 80	TC, TA	1	15 NOV 77
5.26	2	30 SEP 80	NE, TA	1	15 NOV 77
5.26a	0	30 SEP 80	PA		
5.26b	0	30 SEP 80	PA		
5.29	1	30 SEP 80	EC, TC	0	15 AUG 75
5.43	2	30 SEP 80	EC	1	15 NOV 77
5.44	2	30 SEP 80	EC	1	15 NOV 77
5.48	1	30 SEP 80	TC, EC	0	15 AUG 75
5.49	1	30 SEP 80	PC, NF	0	15 AUG 75
5.49a	0	30 SEP 80	PA		
5.49b	0	30 SEP 80	PA		
5.50	2	30 SEP 80	EC	1	01 DEC 76
5.53	1	30 SEP 80	NE	0	15 NOV 77
5.54	1	30 SEP 80	EC, TC	0	15 NOV 77
5.57	0	30 SEP 80	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.1	1	30 SEP 80	PC	0	15 NOV 77
6.2	1	30 SEP 80	TC, EA	0	15 NOV 77
6.3	0	15 NOV 77	PA		
6.4	0	15 NOV 77	PA		
6.5	0	15 NOV 77	PA		
6.6	0	15 NOV 77	PA		
6.7	0	15 NOV 77	PA		
6.8	0	15 NOV 77	PA		
6.9	0	15 NOV 77	PA		
6.10	0	15 NOV 77	PA		
6.11	0	15 NOV 77	PA		
6.12	0	15 NOV 77	PA		
6.13	0	15 NOV 77	PA		
6.14	0	15 NOV 77	PA		
6.15	0	15 NOV 77	PA		
6.16	0	15 NOV 77	PA		
6.17	0	15 NOV 77	PA		
6.18	0	15 NOV 77	PA		
6.19	0	15 NOV 77	PA		
6.20	0	15 NOV 77	PA		
6.21	0	15 NOV 77	PA		
6.22	0	15 NOV 77	PA		
6.23	0	15 NOV 77	PA		
6.24	0	15 NOV 77	PA		
6.25	0	15 NOV 77	PA		
6.26	0	15 NOV 77	PA		
6.27	0	15 NOV 77	PA		
6.28	0	15 NOV 77	PA		
6.29	0	15 NOV 77	PA		
6.30	1	30 SEP 80	TC	0	15 NOV 77

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.31	0	15 NOV 77	PA		
6.32	1	30 SEP 80	EC	0	15 NOV 77
6.33	0	15 NOV 77	PA		
6.34	0	15 NOV 77	PA		
6.35	0	15 NOV 77	PA		
6.36	0	15 NOV 77	PA		
6.37	1	30 SEP 80	NE	0	15 NOV 77
6.38	0	15 NOV 77	PA		
6.39	0	15 NOV 77	PA		
6.40	0	15 NOV 77	PA		
6.41	0	15 NOV 77	PA		
6.42	0	15 NOV 77	PA		
6.43	0	15 NOV 77	PA		
6.44	0	15 NOV 77	PA		
6.45	0	15 NOV 77	PA		
6.46	0	15 NOV 77	PA		
6.47	0	15 NOV 77	PA		
6.48	0	15 NOV 77	PA		
6.49	0	15 NOV 77	PA		
6.50	0	15 NOV 77	PA		
6.51	0	15 NOV 77	PA		
6.52	0	15 NOV 77	PA		
6.53	0	15 NOV 77	PA		
6.54	0	15 NOV 77	PA		
6.55	0	15 NOV 77	PA		
6.56	0	15 NOV 77	PA		
6.57	0	15 NOV 77	PA		
6.58	0	15 NOV 77	PA		
6.59	0	15 NOV 77	PA		
6.60	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.61	0	15 NOV 77	PA		
6.62	0	15 NOV 77	PA		
6.63	0	15 NOV 77	PA		
6.64	0	15 NOV 77	PA		
6.65	0	15 NOV 77	PA		
6.66	0	15 NOV 77	PA		
6.67	0	15 NOV 77	PA		
6.68	0	15 NOV 77	PA		
6.69	0	15 NOV 77	PA		
6.70	0	15 NOV 77	PA		
6.71	0	15 NOV 77	PA		
6.72	0	15 NOV 77	PA		
6.73	0	15 NOV 77	PA		
6.74	0	15 NOV 77	PA		
6.75	0	15 NOV 77	PA		
6.76	0	15 NOV 77	PA		
6.77	0	15 NOV 77	PA		
6.78	0	15 NOV 77	PA		
6.79	0	15 NOV 77	PA		
6.80	0	15 NOV 77	PA		
6.81	0	15 NOV 77	PA		
6.82	0	15 NOV 77	PA		
6.83	0	15 NOV 77	PA		
6.84	0	15 NOV 77	PA		
6.85	0	15 NOV 77	PA		
6.86	0	15 NOV 77	PA		
6.87	0	15 NOV 77	PA		
6.88	0	15 NOV 77	PA		
6.89	0	15 NOV 77	PA		
6.90	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.91	0	15 NOV 77	PA		
6.92	0	15 NOV 77	PA		
6.93	0	15 NOV 77	PA		
6.94	0	15 NOV 77	PA		
6.95	0	15 NOV 77	PA		
6.96	0	15 NOV 77	PA		
6.97	0	15 NOV 77	PA		
6.98	0	15 NOV 77	PA		
6.99	0	15 NOV 77	PA		
6.100	0	15 NOV 77	PA		
6.101	0	15 NOV 77	PA		
6.102	0	15 NOV 77	PA		
6.103	0	15 NOV 77	PA		
6.104	0	15 NOV 77	PA		
6.105	0	15 NOV 77	PA		
6.106	0	15 NOV 77	PA		
6.107	0	15 NOV 77	PA		
6.108	0	15 NOV 77	PA		
6.109	0	15 NOV 77	PA		
6.110	0	15 NOV 77	PA		
6.111	0	15 NOV 77	PA		
6.112	0	15 NOV 77	PA		
6.112a	0	30 SEP 80	PA		
6.113	1	30 SEP 80	TC	0	15 NOV 77
6.114	1	30 SEP 80	NE	0	15 NOV 77
6.114a	0	30 SEP 80	PA		
6.114b	0	30 SEP 80	PA		
6.115	0	15 NOV 77	PA		
6.116	0	15 NOV 77	PA		
6.117	0	15 NOV 77	PA		
6.118	1	30 SEP 80	EC	0	15 NOV 77
6.119	0	15 NOV 77	PA		
6.120	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.121	0	15 NOV 77	PA		
6.122	0	15 NOV 77	PA		
6.123	0	15 NOV 77	PA		
6.124	0	15 NOV 77	PA		
6.125	0	15 NOV 77	PA		
6.126	0	15 NOV 77	PA		
6.127	0	15 NOV 77	PA		
6.128	0	15 NOV 77	PA		
6.129	0	15 NOV 77	PA		
6.130	0	15 NOV 77	PA		
6.131	0	15 NOV 77	PA		
6.132	0	15 NOV 77	PA		
6.133	0	15 NOV 77	PA		
6.134	0	15 NOV 77	PA		
6.135	0	15 NOV 77	PA		
6.136	0	15 NOV 77	PA		
6.137	0	15 NOV 77	PA		
6.138	0	15 NOV 77	PA		
6.139	0	15 NOV 77	PA		
6.140	0	15 NOV 77	PA		
6.141	0	15 NOV 77	PA		
6.142	0	15 NOV 77	PA		
6.143	0	15 NOV 77	PA		
6.144	0	15 NOV 77	PA		
6.145	0	15 NOV 77	PA		
6.146	0	15 NOV 77	PA		
6.147	0	15 NOV 77	PA		
6.148	0	15 NOV 77	PA		
6.149	0	15 NOV 77	PA		
6.150	0	15 NOV 77	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
6.151	0	15 NOV 77	PA		
6.152	0	15 NOV 77	PA		
6.153	0	15 NOV 77	PA		
6.154	1	30 SEP 80	EC	0	15 NOV 77
6.155	0	15 NOV 77	PA		
6.156	0	15 NOV 77	PA		
6.157	0	15 NOV 77	PA		
6.158	0	15 NOV 77	PA		
6.159	1	30 SEP 80	TC	0	15 NOV 77
6.159a	0	30 SEP 80	PA		
6.159b	0	30 SEP 80	PA		
6.160	1	30 SEP 80	TC	0	15 NOV 77
6.161	1	30 SEP 80	EC	0	15 NOV 77
6.162	0	30 SEP 80	PA		
6.163	0	30 SEP 80	PA		
6.164	0	30 SEP 80	PA		
6.165	0	30 SEP 80	PA		
6.166	0	30 SEP 80	PA		
6.167	0	30 SEP 80	PA		
6.168	0	30 SEP 80	PA		
6.169	0	30 SEP 80	PA		
6.170	0	30 SEP 80	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.c	2	30 SEP 80	TC, SC	1	15 NOV 77
7.d	2	30 SEP 80	TA	1	15 NOV 77
7.e	2	30 SEP 80	TC, TA	1	15 NOV 77
7.f	2	30 SEP 80	TA	1	15 NOV 77
7.g	2	30 SEP 80	SC	1	15 NOV 77
7.m	2	30 SEP 80	TC, TA	1	15 NOV 77
7.n	2	30 SEP 80	TC, TA	1	15 NOV 77
7.o	0	30 SEP 80	PA		
7.p	0	30 SEP 80	PA		
7.x/7.r	3	30 SEP 80	PA, PD	2	15 NOV 77
7.y/7.s	2	30 SEP 80	PA, PD	1	15 NOV 77
7.z	0	30 SEP 80	PA		
7.001	3	30 SEP 80	TC	2	15 NOV 77
7.011	2	30 SEP 80	TC	1	01 DEC 76
7.012	2	30 SEP 80	TA	1	15 NOV 77
7.013	2	30 SEP 80	TA	1	15 NOV 77
7.014	2	30 SEP 80	TA	1	15 NOV 77
7.016a	1	30 SEP 80	TC	0	15 AUG 75
7.018a	2	30 SEP 80	TA, SC	1	15 NOV 77
7.111a	1	30 SEP 80	SC, TC	0	15 AUG 75
7.112b	2	30 SEP 80	TA	1	01 DEC 76
7.203	2	30 SEP 80	TD	1	15 NOV 77
7.204	2	30 SEP 80	SC	1	15 NOV 77
7.205	1	30 SEP 80	SC, TC, TA	0	15 AUG 75
7.206	2	30 SEP 80	TA	1	01 DEC 76
7.207	3	30 SEP 80	TA	2	15 NOV 77
7.207a	0	30 SEP 80	PA		
7.209a	3	30 SEP 80	TA	2	15 NOV 77
7.209b	2	30 SEP 80	TA	1	01 DEC 76

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*Key to COMMENTS appears on Page xiii.

Page	New Rev. #	New Date	COMMENTS*	Old Rev.#	Old Date
7.211	2	30 SEP 80	TA, SC	1	15 NOV 77
7.221a	2	30 SEP 80	TA	1	15 NOV 77
7.221b	2	30 SEP 80	SC	1	15 NOV 77
7.233a	0	30 SEP 80	PA		
7.233b	0	30 SEP 80	PA		
7.248a	0	30 SEP 80	PA		
7.248b	0	30 SEP 80	PA		
7.249a	0	30 SEP 80	PA		
7.249b	0	30 SEP 80	PA		
7.257a	2	30 SEP 80	TA	1	01 DEC 76
7.271	0	30 SEP 80	PA		
7.301	3	30 SEP 80	TA	2	15 NOV 77
7.302	2	30 SEP 80	TC	1	15 NOV 77
7.303/7.302b	1	30 SEP 80	TC	0	15 NOV 77
7.304/7.302c	1	30 SEP 80	TC	0	15 NOV 77
7.305	0	30 SEP 80	PA		
7.309	3	30 SEP 80	TA	2	15 NOV 77
7.311a	2	30 SEP 80	TA	1	15 NOV 77
7.321	2	30 SEP 80	TA	1	01 DEC 76
7.381a	2	30 SEP 80	SC	1	15 NOV 77
7.382a	2	30 SEP 80	TA	1	15 NOV 77
7.388	1	30 SEP 80	TA	0	15 NOV 77
7.401	2	30 SEP 80	SC	1	15 NOV 77
7.402	2	30 SEP 80	TA	1	15 NOV 77
7.404	1	30 SEP 80	TA, TC	0	15 AUG 75
7.409a	3	30 SEP 80	TA	2	15 NOV 77
7.409b	2	30 SEP 80	TA	1	15 NOV 77
7.411a	1	30 SEP 80	TC, TA	0	15 AUG 75
7.412a	1	30 SEP 80	TC, TA	0	15 AUG 75
7.412b	1	30 SEP 80	TA	0	15 AUG 75
7.412c	2	30 SEP 80	TA	1	15 NOV 77

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.413a	0	30 SEP 80	PA		
7.413b	0	30 SEP 80	PA		
7.414a	0	30 SEP 80	PA		
7.414b	0	30 SEP 80	PA		
7.421b	1	30 SEP 80	TA	0	15 AUG 75
7.422	2	30 SEP 80	TA, TD	1	15 NOV 77
7.423	2	30 SEP 80	TA, TD	1	15 NOV 77
7.451b	1	30 SEP 80	SC	0	15 AUG 75
7.482a	2	30 SEP 80	TA	1	15 NOV 77
7.482b	2	30 SEP 80	TA, SC	1	15 NOV 77
7.483b	1	30 SEP 80	SC	0	15 AUG 75
7.484b	1	30 SEP 80	SC	0	15 AUG 75
7.503	2	30 SEP 80	TA	1	01 DEC 76
7.513a	1	30 SEP 80	TA	0	15 AUG 75
7.514	2	30 SEP 80	TA	1	01 DEC 76
7.609a	3	30 SEP 80	TA	2	15 NOV 77
7.610a	2	30 SEP 80	TC	1	01 DEC 76
7.616	1	30 SEP 80	TA	0	15 AUG 75
7.623	1	30 SEP 80	TC	0	15 AUG 75
7.624	2	30 SEP 80	TA	1	15 NOV 77
7.625	0	30 SEP 80	PA		
7.631	3	30 SEP 80	SC	2	15 NOV 77
7.641	3	30 SEP 80	SC	2	15 NOV 77
7.651	3	30 SEP 80	SC	2	15 NOV 77
7.653	1	30 SEP 80	TA, TD	0	01 DEC 76
7.654a	1	30 SEP 80	TA, TC	0	01 DEC 76
7.661	2	30 SEP 80	SC	1	15 NOV 77
7.663	3	30 SEP 80	SC	2	15 NOV 77
7.674a	2	30 SEP 80	TA, SC	1	15 NOV 77
7.674b	3	30 SEP 80	TA, TC	2	15 NOV 77
7.674c	0	30 SEP 80	PA		
7.675a	3	30 SEP 80	TA, TC	2	15 NOV 77
7.675b	2	30 SEP 80	TA	1	01 DEC 76

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
7.677	2	30 SEP 80	SC	1	15 NOV 77
BIA.1	1	30 SEP 80	TC	0	15 NOV 77
BIA.5	1	30 SEP 80	TC	0	15 NOV 77
BIA.9	1	30 SEP 80	TA	0	15 NOV 77
BIA.25	0	30 SEP 80	PA		
BIA.26	0	30 SEP 80	PA		
BIA.27	0	30 SEP 80	PA		
BIA.28	0	30 SEP 80	PA		
BIA.29	0	30 SEP 80	PA		
BIA.30	0	30 SEP 80	PA		
BIA.31	0	30 SEP 80	PA		
BIA.32	0	30 SEP 80	PA		
FLS.1	3	30 SEP 80	TA, TC	2	15 NOV 77
GLS.1	1	30 SEP 80	SC	0	15 AUG 75
GLS.2	2	30 SEP 80	TA	1	15 NOV 77
GLS.2a	0	30 SEP 80	PA		
GLS.3	1	30 SEP 80	TD	0	15 AUG 75
GLS.4	1	30 SEP 80	TA	0	15 AUG 75
GLS.6	1	30 SEP 80	TA	0	15 AUG 75
GLS.7	1	30 SEP 80	TA	0	15 AUG 75
GLS.8	1	30 SEP 80	TA	0	15 AUG 75
HYD.1	0	30 SEP 80	PA		
HYD.2	0	30 SEP 80	PA		
HYD.3	0	30 SEP 80	PA		
HYD.4	0	30 SEP 80	PA		
HYD.5	0	30 SEP 80	PA		
HYD.6	0	30 SEP 80	PA		
HYD.7	0	30 SEP 80	PA		
HYD.8	0	30 SEP 80	PA		
HYD.9	0	30 SEP 80	PA		
HYD.10	0	30 SEP 80	PA		

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
HYD.11	0	30 SEP 80	PA		
HYD.12	0	30 SEP 80	PA		
HYD.13	0	30 SEP 80	PA		
HYD.14	0	30 SEP 80	PA		
HYD.15	0	30 SEP 80	PA		
HYD.16	0	30 SEP 80	PA		
HYD.17	0	30 SEP 80	PA		
HYD.18	0	30 SEP 80	PA		
HYD.19	0	30 SEP 80	PA		
HYD.20	0	30 SEP 80	PA		
HYD.21	0	30 SEP 80	PA		
HYD.22	0	30 SEP 80	PA		
IDS.1	3	30 SEP 80	TA, TC	2	15 NOV 77
MAT.2	2	30 SEP 80	TC	1	15 NOV 77
MAT.7	2	30 SEP 80	TA	1	15 NOV 77
MAT.7a	0	30 SEP 80	PA		
MAT.7b	0	30 SEP 80	PA		
MAT.7c	0	30 SEP 80	PA		
MAT.7d	0	30 SEP 80	PA		
MAT.8	1	30 SEP 80	TA	0	15 AUG 75
MAT.9	1	30 SEP 80	TC	0	15 AUG 75
MAT.11	1	30 SEP 80	TA	0	15 AUG 75
MAT.14	2	30 SEP 80	TA	1	01 DEC 76
MAT.16	1	30 SEP 80	TA	0	15 AUG 75
MAT.18	1	30 SEP 80	TA	0	15 AUG 75
MAT.19	2	30 SEP 80	TA	1	01 DEC 76
MAT.21	2	30 SEP 80	TA	1	01 DEC 76
MAX.1	3	30 SEP 80	TC, TA	2	15 NOV 77
MSG.1	2	30 SEP 80	TA	1	15 NOV 77
MSG.2	2	30 SEP 80	TA	1	15 NOV 77
MSG.3	1	30 SEP 80	TA	0	15 AUG 75

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*Key to COMMENTS appears on Page xiii.

Page	New Rev.#	New Date	COMMENTS*	Old Rev.#	Old Date
NTN.1	2	30 SEP 80	TC	1	15 NOV 77
NTN.2	2	30 SEP 80	TA	1	15 NOV 77
NTN.3	0	30 SEP 80	PA		
OPT.4	2	30 SEP 80	TA	1	01 DEC 76
OPT.5	1	30 SEP 80	TC	0	15 AUG 75
OPT.6	1	30 SEP 80	TC	0	15 AUG 75
OPT.6a	0	30 SEP 80	PA		
OPT.6b	0	30 SEP 80	PA		
OPT.7	2	30 SEP 80	TC	1	01 DEC 76
OPT.8	1	30 SEP 80	TC	0	15 AUG 75
OPT.9	1	30 SEP 80	TC	0	15 AUG 75
OPT.10	2	30 SEP 80	TC	1	01 DEC 76
OPT.10a	0	30 SEP 80	PA		
OPT.11	1	30 SEP 80	TC	0	01 DEC 76
OPT.11a	0	30 SEP 80	PA		
OPT.16	1	30 SEP 80	TA	0	15 AUG 75
OPT.18	2	30 SEP 80	TA	1	01 DEC 76
OPT.21	2	30 SEP 80	TC	1	01 DEC 76
OPT.22	2	30 SEP 80	TC	1	01 DEC 76
OPT.23	1	30 SEP 80	TA	0	01 DEC 76
OPT.25	1	30 SEP 80	TD	0	01 DEC 76
OPT.26	1	30 SEP 80	TD	0	01 DEC 76
OPT.28	1	30 SEP 80	TC	0	01 DEC 76
OPT.29	0	01 DEC 76	PD		
OPT.30	0	01 DEC 76	PD		
OPT.31	0	01 DEC 76	PD		
OPT.32	0	01 DEC 76	PD		
PHU.1	1	30 SEP 80	TC	0	15 AUG 75
PHU.2	0	30 SEP 80	PA		
REF.1	1	15 NOV 77	PD		

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*Key to COMMENTS appears on Page xiii.

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SECTION 1

INTRODUCTION

1.1 USER'S MANUAL DESCRIPTION

The STEALTH User's Manual is intended to be a relatively complete but expandable document for users of general-purpose STEALTH* 1D, 2D and 3D, and ADAPRO*. The User's Manual is Volume 1 of a four-volume set. The STEALTH volumes are titled as follows:

Volume 1	STEALTH User's Manual
	Part A Theoretical Background and Numerical Equations
	Part B Input Instructions
Volume 2	STEALTH Example and Verification Problems
Volume 3	STEALTH Programmer's Manual
Volume 4	GRADIS* Manual

The STEALTH User's Manual is divided into seven sections. Page numbers in Sections 1 through 6 and the first part of Section 7 are of the form S.n, where S is the section number and n is a unique sequential page number. This convention was adopted to permit future addition of pages to a section without the necessity of changing page numbers of any other section.

The portion of Section 7 which contains the input record pages uses the following convention for page numbering: page numbers are of the form S.iii, where S is the section number and iii is the input record type. If the input record type is numeric, this is used for the page number. If the input record type is an alphabetic one or if the page contains general information, then the iii is a specified three-digit number different from any possible numeric input record type.

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*STEALTH (Solids and Thermal hydraulics codes for EPRI Adapted from Lagrange TOODY and HEMP), ADAPRO (Archive DAta PROcessor), and GRADIS (GRAphic DISplay) were developed under EPRI Contract RP-307.

The pagination convention for the Appendixes is different from Section conventions. Page numbers in the Appendixes are of the form AAA.n, where AAA is a three-letter mnemonic identifying the appendix and n is a unique sequential page number. Appendixes are in alphabetical order by three-letter mnemonic.

Volume 1 contains the following sections and appendixes:

Section	Title
1	Introduction
2	The Physics of Continuum Mechanics
3	Numerical Difference Equations
4	One-Dimensional Lagrangian Finite-Difference Equations
5	Two-Dimensional Lagrangian Finite-Difference Equations
6	Three-Dimensional Lagrangian Finite-Difference Equations
7	Input Instructions for the STEALTH Computer Programs

Appendixes	Title
FLS	Files
FNC	Functions
GLS	Glossary
IDS	Identifiers
HYD	Hydrodynamic Versions
MAT	Material Models
MAX	Maximums
MSG	Messages
NTN	Notation
OPT	Output
PHU	Physical Units

Sections 1 through 6 are published as Part A, while Section 7 and the Appendixes are published as Part B.

1.2 DOCUMENTATION UPDATES

STEALTH documentation will be updated periodically to correct typographical errors and omissions, to supplement or expand existing documentation, and to describe new capabilities. The procedure for all STEALTH documentation is as follows:

- Whenever changes are made to the documentation, a solid black vertical bar will appear at the right edge of the page to indicate where changes have been made. The revision number and the revision date will be changed to reflect how many times the page has been changed and when the last change was made.

- New pages will be added in sequence behind existing pages. The page number of the page before the addition will be given a lower case alphabetic character, and the new page(s) that follow will use the page number of the previous page, with alphabetic characters in increasing order. New pages will be noted as "Rev. 0" and will include the date of the addition.

- A revision summary page called "REVISIONS" will be included to describe all revised pages, whether these pages are new or corrected. The revision summary page will have a page number which will follow the Table of Contents and List of Figures. Revision summary pages will be sequentially numbered so that a user can tell if any revision summary pages are missing.

The STEALTH code system and documentation actively support three levels of users. The first level includes the occasional user who runs problems which involve only the standard options. The second level includes users who make runs that require special coding in the user-supplied subroutines. The third level involves users who want to make major changes to the STEALTH logic in order to perform very non-standard calculations. Figure 1.1 displays the STEALTH documentation pyramid that has been designed to address all three user levels. The documentation pyramid is made up of several volumes of EPRI NP-2080 (References 1.1-1.8). At the top of the pyramid is "Introduction and Guide". The next level (Volumes 1-3) contains detailed information about the general-purpose versions. Volumes 1-3 include a user's manual, example problems, and a programmer's manual. The third level (Volumes 5-9) contains documentation on the special-purpose versions. The latter volumes rely heavily on information in the general-purpose documentation. All versions of the STEALTH codes use the GRADIS graphics system, which is documented in Volume 4.*

1.3 VERSION NUMBERS

In general, STEALTH version numbers are composed of three characters. The first character on the left is the "generic version number", and is always numeric. The middle character is separated from the left character by a hyphen. It is also always numeric. It represents the "re-sequencing code". The third character, the one on the right, is always alphabetic. It designates the "correction level" or "bug fix level" for a particular generic version number and re-sequencing code.

The correction level character changes most often and identifies levels of changes which are supposed to be transparent to all users. The re-sequencing code digit changes next most often and is supposed to be transparent to users not updating the code. Users who are updating the code will have to change their update sequence numbers when the middle character of the version number changes. A change in the generic version

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*Volume 4 is not up to date for Version 4-1A of STEALTH. However, all STEALTH plot input is adequately documented in Volume 1.

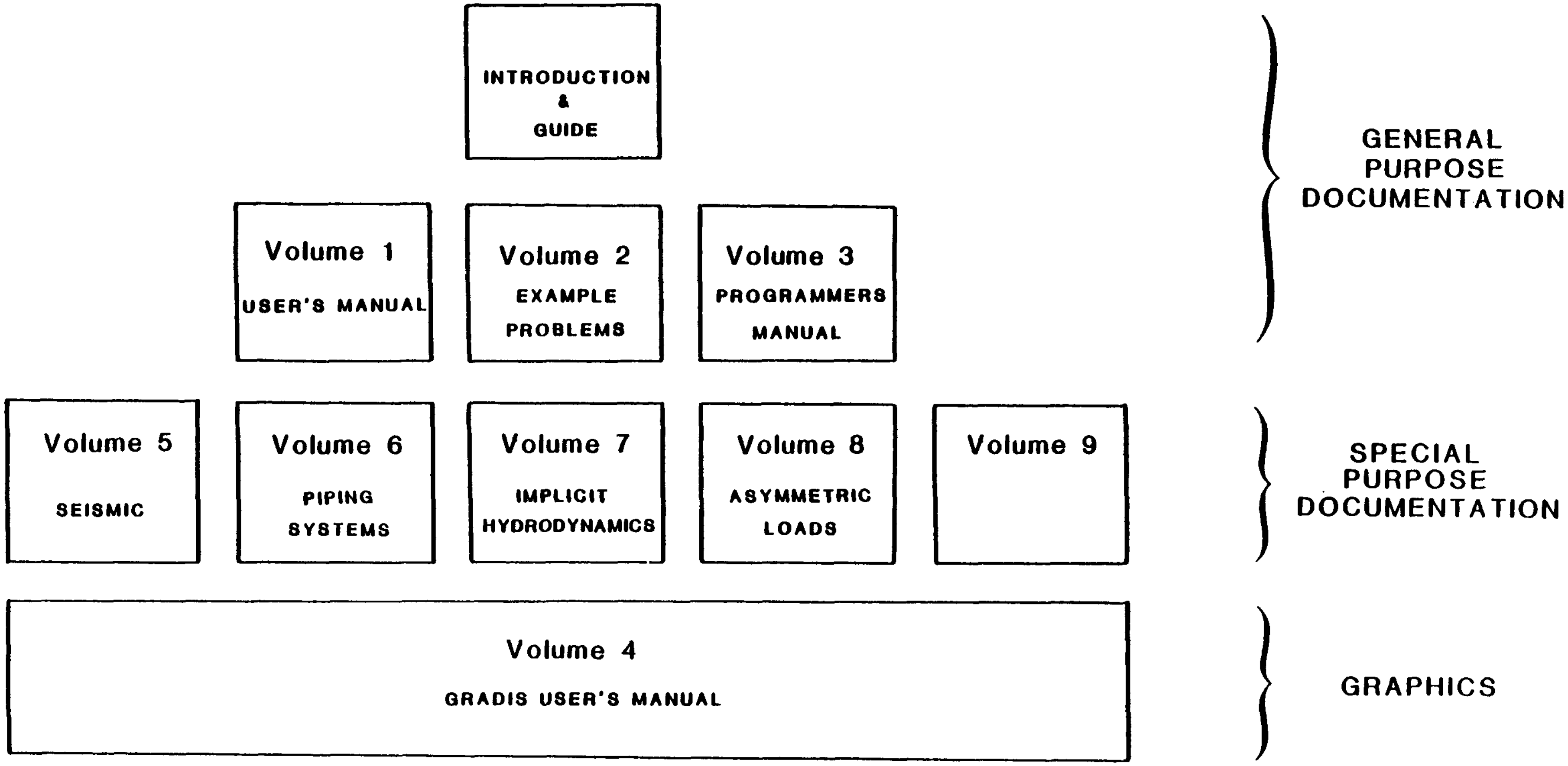

Figure 1.1. Documentation pyramid.

number, however, is a change that is not transparent to any user. A change in the generic version number usually means that a format has changed, i.e., the format of the restart tape or archive tape has changed, common blocks are different, etc.

Users of STEALTH should not feel that they have to keep up with the most current version of the code. Newer versions of the code may contain options not necessarily needed by a user dealing with an older version. It is hoped that information in the STEALTH Newsletter that accompanies each version of STEALTH will be sufficient to allow one to make the choice as to whether to hang a new version of the code. The Newsletter will attempt to explore the options for the user and make recommendations based on the changes that are being presented.

1.4 USER COMMENTS

In order to insure clear documentation and systematic bug elimination, it is necessary to have constant feedback from active users. At the end of this section are two forms which may be copied and filled out. The first, "STEALTH Suspected Error Report", is intended for reporting errors in the documentation and/or coding. Evidence supporting the discovered bug or annotated copies of misleading documentation should be included with a description of the problem. The second form, "STEALTH Reader's Comment Form", is intended to encourage general comments on the documentation.

REFERENCES FOR SECTION 1

1.1 Ronald Hofmann, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. User's Manual", EPRI NP-2080 (formerly NP-260), Vol. 1, Electric Power Research Institute, Palo Alto, California, November 1981. Prepared by Science Applications, Inc., San Leandro, California.

1.2 Ronald Hofmann, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. Sample and Verification Problems", EPRI NP-2080 (formerly NP-260), Vol. 2, Electric Power Research Institute, Palo Alto, California, December 1981. Prepared by Science Applications, Inc., San Leandro, California.

1.3 Ronald Hofmann, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. Programmer's Manual", EPRI NP-2080 (formerly NP-260), Vol. 3, Electric Power Research Institute, Palo Alto, California, November 1981. Prepared by Science Applications, Inc., San Leandro, California.

1.4 Bence I. Gerber, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. GRADIS Manual", EPRI NP-260, Vol. 4, Electric Power Research Institute, Palo Alto, California, August 1976. Prepared by Science Applications, Inc., San Leandro, California.

1.5 Ronald Hofmann, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. Seismic Versions", EPRI NP-2080, Vol. 5, Electric Power Research Institute, Palo Alto, California. Prepared by Science Applications, Inc., San Leandro, California. (To be published.)

1.6 Ronald Hofmann, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. Piping Models", EPRI NP-2080, Vol. 6, Electric Power Research Institute, Palo Alto, California. Prepared by Science Applications, Inc., San Leandro, California. (To be published.)

1.7 Ronald Hofmann, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. Implicit Hydrodynamics", EPRI NP-2080, Vol. 7, Electric Power Research Institute, Palo Alto, California. Prepared by Science Applications, Inc., San Leandro, California. (To be published.)

1.8 Ronald Hofmann, "STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis. Asymmetric Loads", EPRI NP-2080, Vol. 8, Electric Power Research Institute, Palo Alto, California. Prepared by Science Applications, Inc., San Leandro, California. (To be published.)

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STEALTH SUSPECTED ERROR REPORT

Please complete this form and return to:

Nuclear Safety and Analysis Dept., Attn: Dr. H. T. Tang
Electric Power Research Institute
3412 Hillview Avenue
P.O. Box 10412
Palo Alto, California 94304

STEALTH 1D ☐ 2D ☐ 3D ☐ Version No. ____________________

Machine ______________________________ System ________________________

Name: ______________________________ Telephone ____________________

Address ______________________________

____

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Description: (Please be complete. Append relevant decks, listings, core dumps, etc.)

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STEALTH

READER'S COMMENT FORM

Please complete this form and return to:

Nuclear Safety and Analysis Dept., Attn: Dr. H. T. Tang
Electric Power Research Institute
3412 Hillview Avenue
P.O. Box 10412
Palo Alto, California 94304

Your comments and suggestions about this computer code manual may help to improve its usefulness; this form will be sent to the author for appropriate action. Possible topics for comment are: clarity; accuracy; completeness; organization; index; figures; examples; legibility.

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SECTION 2

THE PHYSICS OF CONTINUUM MECHANICS

2.1 DERIVATION OF CONTINUUM MECHANICS EQUATIONS FROM FUNDAMENTAL PHYSICAL LAWS

2.1.1 Theoretical Elements of a Physical System. The mathematical description of a physical event is always derived from the conservation laws of physics. These laws apply to all phenomena and can be applied to any physical system. The external boundaries of the physical system may be chosen to encompass any volume of space. Usually, the choice is made partly from considerations based on the region of interest of the physical event and partly because of certain difficulties in describing some boundary values. Boundary values must be known for certain dependent variables at every point on the external boundaries. The fundamental conservation principles may be written as mathematical equations in any frame of reference and using any set of convenient coordinates. These mathematical equations are theoretically solvable for any geometric shape (symmetric or asymmetric) when constitutive equations and initial conditions are supplied.

Table 2.1 summarizes the theoretical elements necessary to analyze the physical response of any system. The resulting partial differential

TABLE 2.1. THEORETICAL ELEMENTS OF A PHYSICAL SYSTEM

● Conservation laws	physical principles governing all motion
● Boundary conditions	geometric constraints and boundary values
● Initial conditions	initial state of things
● Constitutive relations	material models

equations are time-dependent and nonlinear. They are hyperbolic in form and are sometimes referred to as the "nonlinear wave equation." In this section, these equations will be limited to mechanical and thermal effects and will henceforth be called the fundamental continuum mechanics equations -- or just "continuum mechanics equations."

2.1.2 Conservation Laws. Derivation of the fundamental, non-symmetric, continuum mechanics equations is accomplished by applying the conservation laws to a small volume element in space. The volume element may be in any frame of reference. For mechanical and thermal problems, a non-relativistic (inertial) frame is required. For the purposes of demonstration, a volume element fixed in space (i.e., laboratory frame), described by Cartesian coordinates (x,y,z), will be used to derive the Eulerian continuum mechanics equations. The resulting mathematical equations are written in fixed (Eulerian) coordinates. Figure 2.1 shows a typical non-moving, fixed volume element in this frame.

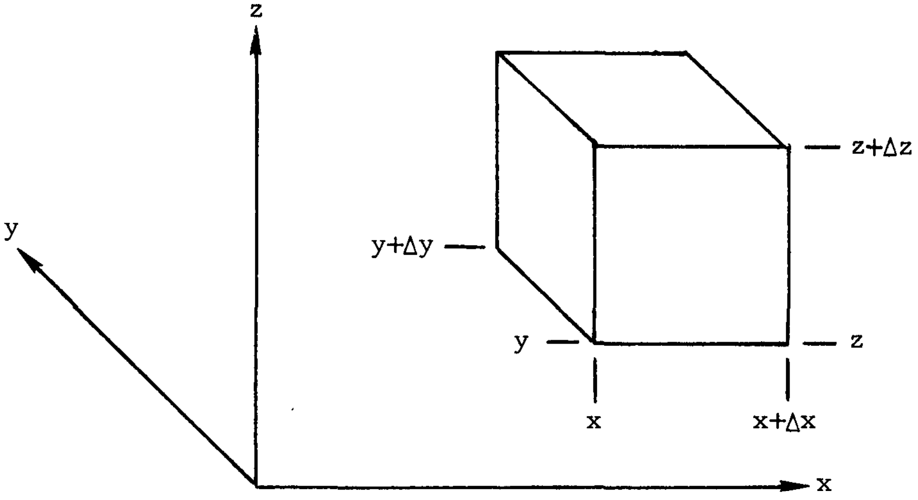

Figure 2.1. Volume element used to derive Eulerian continuum mechanics equations.

The conservation laws are a direct application of the Divergence Theorem and may be summarized as follows (Reference 2.1):

(1) Law of Conservation of Mass

$$\left\{\begin{array}{l}\text{Rate of }\underline{\text{increase}}\\ \text{of mass within}\\ \text{volume element}\end{array}\right\} = \left\{\begin{array}{l}\text{Rate of mass}\\ \text{flowing }\underline{\text{into}}\\ \text{volume element}\end{array}\right\} - \left\{\begin{array}{l}\text{Rate of mass}\\ \text{flowing }\underline{\text{out of}}\\ \text{volume element}\end{array}\right\} ;$$

(2) Law of Conservation of Momentum

$$\left\{\begin{array}{l}\text{Rate of }\underline{\text{increase}}\\ \text{of } i^{th} \text{ component}\\ \text{momentum within}\\ \text{the volume element}\end{array}\right\} = \left\{\begin{array}{l}\text{Rate of momentum}\\ \text{flowing }\underline{\text{into}}\text{ the}\\ \text{volume element}\\ \text{in } i^{th} \text{ direction}\end{array}\right\} - \left\{\begin{array}{l}\text{Rate of momentum}\\ \text{flowing }\underline{\text{out of}}\text{ the}\\ \text{volume element}\\ \text{in } i^{th} \text{ direction}\end{array}\right\}$$

$$+ \left\{\begin{array}{l}\text{Sum of the}\\ \underline{\text{surface}}\text{ forces}\\ \text{acting on the}\\ \text{volume element}\\ \text{in } i^{th} \text{ direction}\end{array}\right\} + \left\{\begin{array}{l}\text{Sum of the}\\ \underline{\text{body}}\text{ forces}\\ \text{acting on the}\\ \text{volume element}\\ \text{in } i^{th} \text{ direction}\end{array}\right\} ;$$

(3) Law of Conservation of Energy

$$\left\{\begin{array}{l}\text{Rate of }\underline{\text{increase}}\text{ of}\\ \text{energy}^{*}\text{ within the}\\ \text{volume element}\end{array}\right\} = \left\{\begin{array}{l}\text{Rate of energy}\\ \text{convected }\underline{\text{into}}\\ \text{the volume element}\end{array}\right\} - \left\{\begin{array}{l}\text{Rate of energy}\\ \text{convected }\underline{\text{out of}}\\ \text{the volume element}\end{array}\right\}$$

$$+ \left\{\begin{array}{l}\text{Rate of energy}\\ \underline{\text{added}}\text{ by work on}\\ \text{volume element}\end{array}\right\} + \left\{\begin{array}{l}\text{Rate of energy}\\ \underline{\text{added}}\text{ to volume element}\\ \text{by conduction \& radiation}\end{array}\right\} .$$

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[*] "energy" includes internal and kinetic energies; potential energy due to gravity is a work term.

Applying the law of conservation of mass to Figure 2.1 results in the following equation,

$$\frac{\partial}{\partial t}(\rho\,\Delta x\,\Delta y\,\Delta z) = \left\{\begin{array}{l} +\ \rho v_x\big|_{x}\ \Delta y\,\Delta z \\ \\ +\ \rho v_y\big|_{y}\ \Delta x\,\Delta z \\ \\ +\ \rho v_z\big|_{z}\ \Delta x\,\Delta y \end{array}\right\} - \left\{\begin{array}{l} +\ \rho v_x\big|_{x+\Delta x}\ \Delta y\,\Delta z \\ \\ +\ \rho v_y\big|_{y+\Delta y}\ \Delta x\,\Delta z \\ \\ +\ \rho v_z\big|_{z+\Delta z}\ \Delta x\,\Delta y \end{array}\right\} \qquad (2.1)$$

where*

v = velocity of material relative to the fixed volume element

ρ = mass density

$(\Delta x\,\Delta y\,\Delta z)$ = the volume of the element

$$\left.\begin{array}{l}(v_x\,\Delta y\,\Delta z)\\(v_y\,\Delta x\,\Delta z)\\(v_z\,\Delta x\,\Delta y)\end{array}\right\} = \text{volume rates of flow through the element.}$$

Dividing Eq.(2.1) by $(\Delta x\,\Delta y\,\Delta z)$ and rearranging, yields

$$\frac{\partial}{\partial t}\rho = -\left[\frac{\rho v_x\big|_{x+\Delta x} - \rho v_x\big|_{x}}{\Delta x}\right] - \left[\frac{\rho v_y\big|_{y+\Delta y} - \rho v_y\big|_{y}}{\Delta y}\right] - \left[\frac{\rho v_z\big|_{z+\Delta z} - \rho v_z\big|_{z}}{\Delta z}\right] . \qquad (2.2)$$

Taking the limit of Eq.(2.2) as $\Delta x \to 0$, $\Delta y \to 0$, and $\Delta z \to 0$, results in

$$\frac{\partial}{\partial t}\rho = -\frac{\partial}{\partial x}(\rho v_x) - \frac{\partial}{\partial y}(\rho v_y) - \frac{\partial}{\partial z}(\rho v_z) \ . \qquad (2.3)$$

Equation (2.3) is known as the Eulerian "continuity equation" in component

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*All symbols and notation are defined in Appendix NTN.

form. It is the mathematical representation of the law of conservation of mass in Cartesian coordinates in a fixed frame of reference. Equation (2.3) may be written in vector notation*,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \underline{v}) , \tag{2.3a}$$

and in tensor notation*,

$$\boxed{\frac{\partial \rho}{\partial t} = - \frac{\partial}{\partial x_j}(\rho v_j)} \cdot \tag{2.3b}$$

Applying the law of conservation of momentum to Figure 2.1 in the x-direction yields

$$\frac{\partial}{\partial t}(\rho v_x) = - \frac{\partial}{\partial x}(\rho v_x v_x) - \frac{\partial}{\partial y}(\rho v_x v_y) - \frac{\partial}{\partial z}(\rho v_x v_z)$$

$$+ \frac{\partial}{\partial x} s_{xx} + \frac{\partial}{\partial y} s_{yx} + \frac{\partial}{\partial z} s_{zx} - \frac{\partial}{\partial x} p + \rho g_x , \tag{2.4}$$

where

s = deviatoric stress (tension is positive)
p = hydrostatic pressure (compression is positive)
$s - p \equiv \sigma$ = total stress**
g = acceleration of gravity.

Equation (2.4) is the Eulerian, x-component "equation of motion." Similar equations can be written for the y- and z-components of momentum. All three components of the momentum equation may be written in vector notation as

$$\frac{\partial}{\partial t}(\rho \underline{v}) = -(\nabla \cdot \rho \, \underline{v} \, \underline{v}) + (\nabla \cdot \underline{\underline{s}}) - (\nabla p) + \rho \, \underline{g} , \tag{2.4a}$$

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[*] Conventions used are from Appendix A of Reference 2.1.

[**] This sign convention assumes that pressure is positive in compression and stress and stress deviator are positive in tension.

and in tensor notation as

$$\boxed{\frac{\partial}{\partial t}(\rho v_i) = -\frac{\partial}{\partial x_j}(\rho v_j v_i) + \frac{\partial}{\partial x_j} s_{ji} - \frac{\partial}{\partial x_j} p\delta_{ij} + \rho g_i} \qquad (2.4b)$$

(where δ_{ij} is the Kronecker delta).

Applying the law of conservation of energy to Figure 2.1 yields

$$\begin{aligned}
\frac{\partial}{\partial t}\left(\rho\hat{u} + \frac{1}{2}\rho v^2\right) = &- \frac{\partial}{\partial x}\left[v_x\left(\rho\hat{u} + \frac{1}{2}\rho v^2\right)\right] - \frac{\partial}{\partial y}\left[v_y\left(\rho\hat{u} + \frac{1}{2}\rho v^2\right)\right] - \frac{\partial}{\partial z}\left[v_z\left(\rho\hat{u} + \frac{1}{2}\rho v^2\right)\right] \\
&- \frac{\partial}{\partial x}\dot{h}''_x - \frac{\partial}{\partial y}\dot{h}''_y - \frac{\partial}{\partial z}\dot{h}''_z \\
&+ \frac{\partial}{\partial x}(s_{xx}v_x + s_{xy}v_y + s_{xz}v_z) + \frac{\partial}{\partial y}(s_{yx}v_x + s_{yy}v_y + s_{yz}v_z) \\
&+ \frac{\partial}{\partial z}(s_{zx}v_x + s_{zy}v_y + s_{zz}v_z) - \frac{\partial}{\partial x}(pv_x) - \frac{\partial}{\partial y}(pv_y) - \frac{\partial}{\partial z}(pv_z) \\
&+ \rho(v_x g_x + v_y g_y + v_z g_z) + \dot{U}''' \,. \qquad (2.5)
\end{aligned}$$

where

$\hat{u}$ = internal energy per unit mass

$\dot{h}''$ = conduction energy flux

$\dot{U}'''$ = energy source or sink rate per unit volume.

Equation (2.5) is the Eulerian energy equation in component notation. Equation (2.5) may be written in vector notation,

$$\frac{\partial}{\partial t}\left(\rho\hat{u} + \frac{1}{2}\rho v^2\right) = -\nabla\cdot\underline{v}\left(\rho\hat{u} + \frac{1}{2}\rho v^2\right) - \nabla\cdot\underline{\dot{h}}'' + \nabla\cdot(\underline{\underline{s}}\cdot\underline{v}) - \nabla\cdot p\underline{v} + \rho\underline{v}\cdot\underline{g} + \dot{U}''' \,. \qquad (2.5a)$$

or tensor notation,

$$\boxed{\frac{\partial}{\partial t}\left(\rho\hat{u}+\frac{1}{2}\rho v^2\right) = -\frac{\partial}{\partial x_i}v_i\left(\rho\hat{u}+\frac{1}{2}\rho v^2\right) - \frac{\partial}{\partial x_i}\dot{h}''_i + \frac{\partial}{\partial x_i}s_{ji}v_j - \frac{\partial}{\partial x_i}pv_i + \rho v_i g_i + \dot{U}'''} \quad . \tag{2.5b}$$

Equations (2.3a), (2.4a), and (2.5a) are the general mechanical and thermal equations of change in vector notation assuming an Eulerian point of view. Equations (2.3b), (2.4b), and (2.5b) are the same equations, respectively, in tensor notation. These five equations may be converted into moving coordinates (Lagrangian frame of reference) by realizing the following consequences of fixed and moving coordinates. The Eulerian point of view requires that volume elements are fixed in space. Lagrange coordinates, on the other hand, require volume elements which can move and distort in space. In the former, mass in an element is variable, while in the latter, mass is fixed. A transformation between the two frames follows directly from the law of conservation of mass. In the Eulerian system, mass is transported from volume element to volume element. Associated with the transported mass is an amount of momentum and energy that is also carried from cell to cell. In the Lagrange system, fixed mass units translate, rotate, compress, expand, and distort. Momentum is associated with the motion of the mass and internal energy is fixed to the mass unit.

Equation (2.4b) is referenced to fixed coordinates. To obtain the form of the momentum equations for moving coordinates, rearrange Eq.(2.4b) in the following way:

$$\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\rho v_j v_i) = +\frac{\partial}{\partial x_j}s_{ji} - \frac{\partial}{\partial x_j}p\delta_{ij} + \rho g_i \ . \tag{2.6}$$

The left side of Eq. (2.6) may be expanded,

$$\rho\frac{\partial}{\partial t}v_i + v_i\frac{\partial}{\partial t}\rho + \rho v_j\frac{\partial}{\partial x_j}v_i + \rho v_i\frac{\partial}{\partial x_j}v_j + v_i v_j\frac{\partial}{\partial x_j}\rho \ , \tag{2.7a}$$

and then rearranged,

$$\rho\left[\frac{\partial}{\partial t}v_i + v_j\frac{\partial}{\partial x_j}v_i\right] + v_i\left[\frac{\partial}{\partial t}\rho + v_j\frac{\partial}{\partial x_j}\rho\right] + \rho v_i\frac{\partial}{\partial x_j}v_j \ . \tag{2.7b}$$

Using the definition of the "material" derivative,

$$\frac{D}{Dt}(\ ) \equiv \frac{\partial}{\partial t}(\ ) + v_j\frac{\partial}{\partial x_j}(\ ) \ ;$$

the left side of Eq.(2.6) may be written as

$$\rho\frac{D}{Dt}v_i + v_i\frac{D}{Dt}\rho + \rho v_i\frac{\partial}{\partial x_j}v_j \ . \tag{2.7c}$$

But from Eq.(2.3b), conservation of mass for a fixed mass may be shown to be

$$\boxed{\frac{D}{Dt}\rho = -\rho\frac{\partial}{\partial x_j}v_j} \ . \tag{2.8}$$

Substituting Eq.(2.8) into the expression (2.7c) and plugging the result into Eq.(2.6), yields

$$\boxed{\rho\frac{D}{Dt}v_i = +\frac{\partial}{\partial x_j}s_{ji} - \frac{\partial}{\partial x_j}p\delta_{ij} + \rho g_i} \ . \tag{2.9}$$

The Lagrangian motion equations, Eqs.(2.9), are a composite of the conservation of mass and momentum principles.

A similar approach may be taken to convert the Eulerian energy equation, (2.5b), to the Lagrange frame of reference. Forming the scalar product of the fixed volume (Eulerian) momentum equation with material velocity $\underline{v}$, yields, in vector notation

$$\underline{v} \cdot \frac{\partial}{\partial t}(\rho \underline{v}) = -\underline{v} \cdot (\nabla \cdot \rho\, \underline{v}\, \underline{v}) + \underline{v} \cdot (\nabla \cdot \underline{\underline{s}}) - (\underline{v} \cdot \nabla p) + \underline{v} \cdot \rho \underline{g} \,, \tag{2.10a}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho v^2\right) = -\left(\nabla \cdot \frac{1}{2}\rho v^2 \underline{v}\right) - (\underline{\underline{s}}:\nabla \underline{v}) + (\nabla \cdot (\underline{\underline{s}} \cdot \underline{v})) + p(\nabla \cdot \underline{v}) - (\nabla \cdot p\underline{v}) + \rho \underline{v} \cdot \underline{g} \,. \tag{2.10b}$$

This equation is called the Eulerian "mechanical" energy equation. It is not a fundamental equation, only a form of the momentum principle. Subtracting it from the equation (2.5b) leaves the Eulerian "internal" energy equation,

$$\frac{\partial}{\partial t}(\rho \hat{u}) = -\nabla \cdot \rho \hat{u} \underline{v} - \nabla \cdot \underline{\dot{h}}'' + (\underline{\underline{s}}:\nabla \underline{v}) - p(\nabla \cdot \underline{v}) + \dot{U}''' \,, \tag{2.11a}$$

or in tensor notation,

$$\frac{\partial}{\partial t}(\rho \hat{u}) = -\frac{\partial}{\partial x_i}\rho \hat{u} v_i - \frac{\partial}{\partial x_i}\dot{h}''_i + s_{ij}\frac{\partial}{\partial x_j}v_i - p\frac{\partial}{\partial x_i}v_i + \dot{U}''' \,. \tag{2.11b}$$

Equation (2.11b) is referenced to fixed coordinates. To obtain the form of the equation of internal energy conservation for moving coordinates, rearrange Eq.(2.11b) in the following way,

$$\frac{\partial}{\partial t}(\rho \hat{u}) + \frac{\partial}{\partial x_i}(\rho \hat{u} v_i) = -\frac{\partial}{\partial x_i}\dot{h}''_i + s_{ij}\frac{\partial}{\partial x_j}v_i - p\frac{\partial}{\partial x_i}v_i + \dot{U}''' \,. \tag{2.12}$$

The left side may be expanded,

$$\rho\frac{\partial}{\partial t}\hat{u} + \hat{u}\frac{\partial}{\partial t}\rho \quad + \quad \rho\hat{u}\frac{\partial}{\partial x_i}v_i + \rho v_i\frac{\partial}{\partial x_i}\hat{u} + \hat{u}v_i\frac{\partial}{\partial x_i}\rho \ , \tag{2.13a}$$

rearranged,

$$\rho\left[\frac{\partial}{\partial t}\hat{u} + v_i\frac{\partial}{\partial x_i}\hat{u}\right] + \hat{u}\left[\frac{\partial}{\partial t}\rho + v_i\frac{\partial}{\partial x_i}\rho\right] + \rho\hat{u}\frac{\partial}{\partial x_i}v_i \ , \tag{2.13b}$$

and converted to "material" derivative form,

$$\rho\frac{D}{Dt}\hat{u} + \hat{u}\frac{D}{Dt}\rho + \rho\hat{u}\frac{\partial}{\partial x_i}v_i \ . \tag{2.13c}$$

But again, Eq.(2.8) may be substituted into Eq.(2.13c) and the result applied to Eq.(2.12) to yield

$$\boxed{\rho\frac{D}{Dt}\hat{u} = -\frac{\partial}{\partial x_i}\dot{h}_i'' + s_{ij}\frac{\partial}{\partial x_j}v_i - p\frac{\partial}{\partial x_i}v_i + \dot{U}'''} \ . \tag{2.14}$$

The Lagrangian internal energy equation, Eq.(2.14), is a composite of the conservation of mass and energy principles.

Equations (2.8), (2.9), and (2.14) are the Lagrangian equivalents of Eqs.(2.3b), (2.4b), and (2.5b), respectively. (The Euler set has been expressed in component form in Cartesian coordinates (x,y,z).) Any other spatial coordinates (e.g., r,z,θ) would have worked, but for the general non-symmetric equations, Cartesian coordinates are the most convenient. Symmetric equations are often more conveniently written in other spatial coordinates. The five Lagrangian equations (three components of momentum, the internal energy equation, and the Lagrangian form of conservation of mass, sometimes called conservation of volume) express the same physical principles of mechanical and thermal motion as the five Eulerian equations which include an explicit form of continuity. Conservation of mass is inherent in the Lagrangian formulation, i.e., $\rho(x,y,z,t)$ is computed on that basis. In either case, the number of equations so far derived is less than the number of variables. To obtain a unique solution of either set of equations for a particular problem requires more equations (physical relationships called constitutive equations), proper boundary conditions, and correct initial values.

2.1.3 Boundary Conditions. Boundary conditions may be divided into two distinct categories: geometric constraints and boundary values. The geometric constraints define the location of physical or conveniently chosen external boundaries as well as internal material interfaces and voids. The boundary values are values of certain dependent variables used in the conservation equations at the external boundaries. Typically, the momentum equations require that components of stress or velocity be given for all boundary points and the energy equation requires temperature or heat flux boundary values. In the Eulerian frame, the continuity equation needs mass flux boundary values while in the Lagrange frame, mass flux is always zero.

There are two ways in which boundary values are obtained, i.e., by prescription or by interaction. By prescription means that boundary values are provided as time histories for an entire event; by interaction means that an algorithm for calculating values is provided. The latter case is typically required when two or more materials interact at a common interface.

2.1.4 Initial Conditions. Initial values must be given for all time-dependent variables in the space. That is, the initial thermodynamic state and geometry must be known. The initial values give the current state of things prior to any motion.

Initial values may be divided into thermodynamically intensive and extensive parts. The intensive group includes scalar and tensor variables such as pressure, internal energy, density, stress deviators, etc. The extensive initial values refer to the vector components of the conservation equations such as the initial velocity field (i.e., kinetic energy).

2.1.5 Constitutive Relations. The additional equations (physical relationships) that are necessary to completely describe a system come from a knowledge of the inherent response characteristics of each portion of the space enclosed by the external boundaries. These response characteristics form a set of equations which are called the constitutive relations. As an example, the mechanical and thermal response model of an isotropic material may be divided into three classes of equations which completely describe the appropriate equilibrium material response characteristics of a physical space. These classes are:

(1) The mean stress or pressure equation-of-state model,

$$p = p(\hat{u}, \rho);$$

(2) The deviatoric stress model,

$$s_{ij} = s(J'_i, Y)$$

where J'_i are elastic stress deviator invariants and Y is the yield stress,

$$Y = Y(\hat{u}, \rho);$$

(3) The heat flux model,

$$\dot{h}''_i = h(T)$$

where T is the temperature,

$$T = T(\hat{u}, \rho) .$$

The forms of these equations will depend on the material and on the boundary conditions. The lack of material (void) may be described by a set of trivial constitutive equations or by correct boundary conditions.

This particular model is a convenient one for modeling complex response characteristics of an isotropic material. It is by no means unique. For example, simple mechanical material response characteristics need not make the distinction between mean stress and deviatoric stress. In the case of nonisotropic materials, the mean stress or pressure cannot even be measured in a thermodynamically meaningful way. In either case, the notion of stress invariants and yield stress, Y, can be replaced by a completely different theory, e.g., Endochronic Theory (Reference 2.2).

2.2 REDUCTION OF THE FUNDAMENTAL CONTINUUM MECHANICS EQUATIONS TO SIMPLER FORMS

2.2.1 Overview. The conservation and constitutive equations coupled to appropriate boundary and initial conditions form the necessary and sufficient mathematical data required to theoretically analyze a physical system. An analytic solution of the continuum mechanics equations for arbitrary constitutive properties, complex boundary conditions, and non-simple initial conditions is not available. Simplified or reduced versions of the continuum mechanics equations can be solved using analytic techniques. Typically, the simplifications that make these equations more analytically convenient are those that lead to linear ordinary differential equations or elliptic or parabolic partial differential equations with constant coefficients.

Simplifications may be conveniently separated into several distinct types of physical assumptions. Mathematically, all assumptions are always achieved by selectively or globally invoking some form of the conditions $\nabla(\ ) = 0$ and/or $\frac{\partial}{\partial t}(\ ) = 0$. Fundamental physical assumptions relate to spatial and temporal variables, (x_i, t) and require that $\nabla(\ ) = 0$ or $\frac{\partial}{\partial t}(\ ) = 0$ be invoked globally; that is, all dependent variables are affected by the conditions $\nabla(\ ) = 0$ or $\frac{\partial}{\partial t}(\ ) = 0$. These assumptions are considered fundamental because (x_i, t) are the independent variables. All other physical assumptions are mathematical subsets of these, and are, therefore, not fundamental. The mathematical conditions, $\nabla(\ ) = 0$ and $\frac{\partial}{\partial t}(\ ) = 0$, in this case are used selectively rather than globally to eliminate specific physical mechanisms. Thus, assumption of ideal material response characteristics, simple geometric shapes and boundary values, and/or quiet initial values, merely becomes a specific application of $\nabla(\ ) = 0$ and $\frac{\partial}{\partial t}(\ ) = 0$.

2.2.2 Spatial Simplifications -- Natural Symmetries. There are always three spatial variables (e.g., $x_i = x,y,z$). However, the number of independent spatial variables can be reduced if the physical system exhibits a "natural" symmetry. There are three one-dimensional and two two-dimensional natural symmetries. They are summarized in Table 2.2.

TABLE 2.2. NATURAL SYMMETRIES

Number of independent spatial variables	Name and mathematical constraint for dependent spatial variables for five symmetries*	
1. x_1 is independent, $\dot{x}_2 = \dot{x}_3 = 0$, (one-dimensional)	plane (x,y,z)	$\frac{\partial}{\partial y}(\ ) = 0$, $\frac{\partial}{\partial z}(\ ) = 0$
	cylindrical (r,θ,z)	$\frac{\partial}{\partial \theta}(\ ) = 0$, $\frac{\partial}{\partial z}(\ ) = 0$
	spherical (r,θ,φ)	$\frac{\partial}{\partial \theta}(\ ) = 0$, $\frac{\partial}{\partial \varphi}(\ ) = 0$
2. x_1 and x_2 are independent, $\dot{x}_3 = 0$, (two-dimensional)	translational (x,y,z)	$\frac{\partial}{\partial z}(\ ) = 0$
	axial (r,θ,z)	$\frac{\partial}{\partial \theta}(\ ) = 0$
3. x_1, x_2, and x_3 are independent (three-dimensional)	asymmetric (x,y,z)	not symmetric

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*( ) means any and all dependent variables.

Many physical problems exhibit symmetrical characteristics. To solve the reduced equations which take advantage of these symmetries does not compromise the fundamental continuum mechanics equations, since these simplifications refer only to the symmetric qualities of the problem. However, when symmetry does exist, the computational cost of solving a problem is lower because the number and length of the continuum mechanics equations are reduced. One-dimensional symmetries involve only three continuum mechanics equations instead of five, and each equation contains fewer terms. For example, the momentum and internal energy equations for one-dimensional planar symmetry are derived by applying $\frac{\partial}{\partial y}(\ ) = 0$ and $\frac{\partial}{\partial z}(\ ) = 0$ to the Cartesian form of Eqs. (2.8), (2.9), and (2.14). From Eqs.(2.9) and (2.14),

$$\rho \ddot{x} = + \frac{\partial}{\partial x} \sigma_{xx} + \rho g_x , \tag{2.15a}$$

$$\rho \hat{u} = - \frac{\partial}{\partial x} \dot{h}''_x - p \frac{\partial}{\partial x} v_x + s_{xx} \frac{\partial}{\partial x} v_x + \dot{U}''' \tag{2.15b}$$

where $\ddot{x} \equiv \frac{D}{Dt} v_x$, $\hat{u} \equiv \frac{D}{Dt} \hat{u}$, and $\frac{\partial}{\partial x} v_x \equiv \dot{\epsilon}_{xx}$.

$\dot{\epsilon}_{xx}$ is the principal strain rate. Conservation of mass, Eq.(2.8), defines the rate of cubical dilation ($\dot{\Delta}$) to be the rate of volume change, i.e., the gradient of the velocity field,

$$\dot{\Delta} \equiv \frac{\partial}{\partial x} v_x . \tag{2.15c}$$

Equations (2.15a), (2.15b), and (2.15c) are the general continuum mechanics equations for a three-dimensional space exhibiting no spatial gradients in two directions and no divergence in the direction of the independent space variable, x.

The remaining one-dimensional symmetric equations may be derived similarly. The cylindrically symmetric forms of momentum and internal energy are derived from the (r,θ,z) forms of Eqs.(2.9) and (2.14). Due to symmetry, the θ and z components of momentum are zero (thus, $\dot\theta$ and $\dot z$ are zero) and the r component of momentum becomes

$$\rho\ddot r = \frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rr}) - \frac{\sigma_{\theta\theta}}{r}$$

or, expanded,

$$\rho\ddot r = \frac{\partial}{\partial r}\sigma_{rr} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} \quad , \tag{2.16a}$$

while the internal energy equation reduces to

$$\rho\hat{u} = -\frac{1}{r}\frac{\partial}{\partial r}(r\dot h''_r) - p\,\frac{1}{r}\frac{\partial}{\partial r}(rv_r) + s_{rr}\frac{\partial}{\partial r}v_r + s_{\theta\theta}\frac{v_r}{r} + \dot U''' \ . \tag{2.16b}$$

The rate of cubical dilation is calculated directly from the rate of volume change and is equal to

$$\begin{aligned}\dot\Delta &= \frac{1}{r}\frac{\partial}{\partial r}(rv_r)\\ &= \frac{\partial}{\partial r}v_r + \frac{v_r}{r}\\ &= \dot\epsilon_{rr} + \dot\epsilon_{\theta\theta} \ .\end{aligned} \tag{2.16c}$$

$\dot\epsilon_{rr}$ is the radial strain rate and $\dot\epsilon_{\theta\theta}$ is the circumferential strain rate.

The spherically symmetric momentum and internal energy equations are derived from (r,θ,φ) coordinate versions of Eqs.(2.9) and (2.14). They are, respectively,

$$\rho\ddot r = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\sigma_{rr}) - 2\left[\frac{\sigma_{\theta\theta}}{r}\right]$$

or, expanded,

$$\rho \ddot{r} = \frac{\partial}{\partial r} \sigma_{rr} + 2\left[\frac{\sigma_{rr} - \sigma_{\theta\theta}}{r}\right] \tag{2.17a}$$

and

$$\rho \dot{\hat{u}} = - \frac{1}{r^2} \frac{\partial}{\partial r}(r^2 \dot{h}'') - p \frac{1}{r^2} \frac{\partial}{\partial r}(r^2 v_r) + s_{rr} \frac{\partial}{\partial r} v_r + 2\left[s_{\theta\theta} \frac{v_r}{r}\right] + \dot{U}''' . \tag{2.17b}$$

The rate of cubical dilation is

$$\begin{aligned} \dot{\Delta} &= \frac{1}{r^2} \frac{\partial}{\partial r}(r^2 v_r) \\ &= \frac{\partial}{\partial r} v_r + 2 \frac{v_r}{r} \\ &= \dot{\epsilon}_{rr} + 2 \dot{\epsilon}_{\theta\theta} . \end{aligned} \tag{2.17c}$$

From symmetry considerations, $s_{\theta\theta} = s_{\varphi\varphi}$ in Eq.(2.17b) and $\dot{\epsilon}_{\theta\theta} = \dot{\epsilon}_{\varphi\varphi}$ in Eq.(2.17c).

The two-dimensional translational symmetry equations are derived from Cartesian coordinates. The momentum components are

$$\begin{aligned} \rho \ddot{x} &= \frac{\partial}{\partial x} \sigma_{xx} + \frac{\partial}{\partial y} \sigma_{xy} + \rho g_x , \\ \rho \ddot{y} &= \frac{\partial}{\partial x} \sigma_{xy} + \frac{\partial}{\partial y} \sigma_{yy} + \rho g_y , \end{aligned} \tag{2.18a}$$

Rev. 0
15 NOV 77

and the internal energy equation is

$$\rho\dot{\hat{u}} = -\frac{\partial}{\partial x}(\dot{h}''_x) - \frac{\partial}{\partial y}(\dot{h}''_y) - p\left(\frac{\partial}{\partial x} v_x + \frac{\partial}{\partial y} v_y\right)$$

$$+ s_{xx}\frac{\partial}{\partial x} v_x + s_{yy}\frac{\partial}{\partial y} v_y + s_{xy}\left(\frac{\partial}{\partial y} v_x + \frac{\partial}{\partial x} v_y\right) + \dot{U}''' \ , \qquad (2.18b)$$

where

$$\frac{\partial}{\partial x} v_x \equiv \dot{\epsilon}_{xx} \ ,$$

$$\frac{\partial}{\partial y} v_y \equiv \dot{\epsilon}_{yy} \ ,$$

$$\frac{\partial}{\partial y} v_x + \frac{\partial}{\partial x} v_y \equiv \dot{\epsilon}_{xy} \ .$$

The rate of cubical dilatation is

$$\dot{\Delta} \equiv \dot{\epsilon}_{xx} + \dot{\epsilon}_{yy} \ . \qquad (2.18c)$$

The two-dimensional axially symmetric momentum and internal energy equations are derived from (r,θ,z) coordinate versions of Eqs.(2.9) and (2.14). Momentum relations are

$$\rho\ddot{r} = \frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rr}) + \frac{\partial}{\partial z}\sigma_{rz} - \frac{\sigma_{\theta\theta}}{r} \ ,$$

$$\rho\ddot{z} = \frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rz}) + \frac{\partial}{\partial z}\sigma_{zz} + \rho g_z \ ,$$

or, in expanded form,

$$\begin{aligned} \rho\ddot{r} &= \frac{\partial}{\partial r}\sigma_{rr} + \frac{\partial}{\partial z}\sigma_{rz} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} , \\ \rho\ddot{z} &= \frac{\partial}{\partial r}\sigma_{rz} + \frac{\partial}{\partial z}\sigma_{zz} + \frac{\sigma_{rz}}{r} + \rho g_z , \end{aligned} \qquad (2.19a)$$

while internal energy is

$$\begin{aligned} \rho\dot{\hat{u}} = &- \frac{1}{r}\frac{\partial}{\partial r}(r\dot{h}''_r) - \frac{\partial}{\partial z}(\dot{h}''_z) - p\left[\frac{1}{r}\frac{\partial}{\partial r}(rv_r) + \frac{\partial}{\partial z}v_z\right] \\ &+ s_{rr}\frac{\partial}{\partial r}v_r + s_{\theta\theta}\frac{v_r}{r} + s_{zz}\frac{\partial}{\partial z}v_z + s_{rz}\left(\frac{\partial}{\partial z}v_r + \frac{\partial}{\partial r}v_z\right) + \dot{U}''' , \end{aligned} \qquad (2.19b)$$

where

$$\frac{\partial}{\partial r}v_r \equiv \dot{\epsilon}_{rr} ,$$

$$\frac{\partial}{\partial z}v_z \equiv \dot{\epsilon}_{zz} ,$$

$$\frac{\partial}{\partial z}v_r + \frac{\partial}{\partial r}v_z \equiv \dot{\epsilon}_{rz} .$$

The term $\frac{1}{r}\frac{\partial}{\partial r}(rv_r) + \frac{\partial}{\partial z}v_z$ is the volumetric strain rate, $\dot{\Delta}$. Expanding the volumetric strain rate,

$$\begin{aligned} \dot{\Delta} &= \frac{\partial}{\partial r}v_r + \frac{v_r}{r} + \frac{\partial}{\partial z}v_z \\ &= \dot{\epsilon}_{rr} + \dot{\epsilon}_{\theta\theta} + \dot{\epsilon}_{zz} . \end{aligned} \qquad (2.19c)$$

2.2.3 Temporal Simplifications. Time simplifications are not as easy to classify as spatial symmetries. Physically, time dependency varies from static (no time dependence) at one extreme, to dynamic (full time dependence) at the other extreme. In between, there are various degrees of time dependence. Mathematically static problems are specified by $\frac{\partial}{\partial t}(\ ) = 0$, whereas fully dynamic problems are given by $\frac{\partial}{\partial t}(\ ) \neq 0$. Steady-state momentum problems are given by $\dot{v}_i = 0$.

A simple example of the static condition exists when $\frac{\partial}{\partial t}(\ ) = 0$ is applied to the one-dimensional, plane symmetry equations. The resulting equations are the static overburden equations for a one-dimensional column of material. The momentum equation becomes a familiar static balance,

$$\frac{\partial}{\partial x} \sigma_{xx} = -\rho g_x ,$$

$$\Delta\sigma_{xx} = -\rho g_x \Delta x ,$$

while the energy equation is indeterminant.

2.2.4 Conservation Law Simplifications. The most common simplifications are those that result from assumptions that eliminate physical mechanisms and interactions from the conservation equations. Mathematically, these assumptions are invoked by specifying that the conditions $\nabla(\ ) = 0$ and $\frac{\partial}{\partial t}(\ ) = 0$ apply selectively to certain of the dependent variables. Since there are only a few primary dependent variables, only a small number of possible physical assumptions is anticipated. (The primary dependent variables are ρ, v_i, s_{ij}, p, $\hat{u}$, $\dot{h}_i''$.) However, many convenient secondary dependent variables (e.g., impulse, momentum, etc.) may be defined,

Rev. 0
15 NOV 77

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leading to the possibility of non-primary physical assumptions. In general, these assumptions are combinations of primary physical assumptions.

Tables 2.3, 2.4, and 2.5 summarize some of the most obvious mechanistic simplifications. Table 2.3 deals with mass; Table 2.4 deals with momentum; and Table 2.5 deals with internal energy.

TABLE 2.3. EXAMPLES OF SOME MASS CONSERVATION SIMPLIFICATIONS

Basic equation:

$$\frac{D}{Dt}\rho = -\rho\left(\frac{\partial}{\partial x_j} v_j\right)$$

Simplifications:

$$\left.\begin{aligned} \frac{D}{Dt}\rho &= 0 \\ \frac{\partial}{\partial x_j} v_j &= 0 \end{aligned}\right\}$$ implies incompressible, from the condition that $\rho = \text{constant} \neq 0$

The assumption of incompressibility applied to a viscous fluid reduces the wave equation to the Diffusion equation (i.e., hyperbolic partial differential equations are reduced to parabolic equations). The pressure (mean stress) is therefore made indeterminate because bulk modulus is now infinite. Sound speed is also infinite. Thus, for viscous fluids, this assumption is valid only for small amplitude pressure waves.

TABLE 2.4. EXAMPLES OF SOME MOMENTUM CONSERVATION SIMPLIFICATIONS

Basic Equation:

$$\rho \frac{D}{Dt} v_i = + \frac{\partial}{\partial x_j} s_{ji} - \frac{\partial}{\partial x_j} p\delta_{ij} + \rho g_i$$

Simplifications:

$$\frac{D}{Dt} v_i = 0 \quad \text{implies} \quad \begin{cases} \text{no acceleration, no} \\ \text{inertial force, i.e.,} \\ \text{steady state or static} \end{cases}$$

a. if $v_i = 0$, implies static

b. if $v_i = \text{constant}$, implies steady state

$$\left.\begin{array}{l} \dfrac{\partial}{\partial x_j} s_{ij} = 0 \quad \text{implies } s_{ij} = \text{constant} \\[2em] \dfrac{\partial}{\partial x_j} p\delta_{ij} = 0 \quad \text{implies } p = \text{constant} \end{array}\right\} \text{implies external forces do no work}$$

$g_i = 0$ implies no gravitational forces.

Inertial assumptions are the most common momentum equation simplifications. For example, a problem involving no motion (static equilibrium) becomes a boundary value problem rather than an initial value problem. Further, the continuum equations become elliptic rather than hyperbolic.

Constant external forces which imply that no work is done yield equations of motion which are integrable in a straightforward manner. The form of the resulting equations is the same as those used to describe particle motion.

TABLE 2.5. EXAMPLES OF SOME ENERGY CONSERVATION SIMPLIFICATIONS

Basic equation:

$$\rho \frac{D}{Dt}\hat{u} = - \frac{\partial}{\partial x_i} \dot{h}_i'' + s_{ij} \frac{\partial}{\partial x_j} v_i - p \frac{\partial}{\partial x_i} v_i + \dot{U}'''$$

Simplifications:

$\frac{D}{Dt}\hat{u} = 0$	implies no change in internal energy
$\dot{h}_i'' = 0$	implies no heat flux (i.e., adiabatic)
$\frac{\partial}{\partial x_i} v_i = 0$	implies no volumetric expansion or compression (i.e., incompressible)
$s_{ij} = 0$	implies no distortional work
$U''' = 0$	implies no sources or sinks.

Energy equation simplifications imply different types of thermodynamic processes. Eliminating effects of irreversibility due to frictional heat loss or distortion can directly reduce the mathematical complexity of the energy equation. Similarly, assumptions relating to adiabatic, isothermal, isobaric, etc., processes can indirectly simplify the equations to be solved because of concomitant constitutive assumptions.

2.2.5 Constitutive Simplifications. Constitutive (material description) simplifications for a continuum response model are among the easiest types of simplifications to categorize once the proper perspective has been achieved. Figure 2.2 consists of a diagram that is intended to help establish this perspective. Presented side by side are the fundamental forms of matter and a more detailed breakdown of the forms of matter for continuum mechanics material modeling. The order in which the forms of matter are listed is extremely important. For example, properties such as mass density, strength, stiffness (inverse of compressibility), and thermal conductivity decrease as matter changes from rigid solid to rarefied gas, while thermal radiation becomes more of a factor as mass density decreases.

Continuum Mechanics Forms of Matter	Fundamental Forms of Matter
Rigid solid Small strain solid Large strain solid	Solid
Very deformable solid Dense liquid	Solid-fluid transition
Liquid Dense gas Gas	Fluid
Rarefied gas Ionized gas	Fluid-plasma transition

Figure 2.2. Spectrum of materials in a non-plasma continuum.

Constitutive models in continuum mechanics ultimately must describe the relationships between total stress, total strain, and internal energy because a relationship between these properties constitutes a complete mechanical and thermal model.* Data which are used to develop the forms of these relationships do not come from a single convenient experiment. Instead, a variety of experiments is used in which different but related properties are measured. For example, strength data may come from uniaxial tension tests, triaxial compression tests, Hugoniot experiments, etc. Each type of experiment supplies different stress-strain data. In uniaxial tension, for example, only one component of strain is measured from one component of stress. Thus, only a partial picture of material strength is described. Caloric properties come from Joule-Thompson experiments, throttling calorimeters, electron beam experiments, etc., each again supplying only part of the energy picture.

Constitutive simplifications result from special relationships between stress, strain, and internal energy. For example, the stress tensor will vary from material to material. However, there are classes of materials for which model stress tensors have the same functional form. The fluids' stress tensor (more often called the viscous stress tensor) is normally a function of velocity gradients (strain rates). If the functional form is a linear combination of velocity gradients, then the tensor is termed Newtonian. If the functional form has nonlinear terms, the tensor is called non-Newtonian. The solids' stress tensor is normally a function of displacement gradients (strains). For linearly related stresses and strains the stress tensor is called elastic. Nonlinear forms include the strain hardening tensor as an example.

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*From a mathematical point of view, these relationships constitute the additional, independent equations needed to solve the fundamental equations of continuum mechanics.

The linear isotropic fluids' stress tensor and the linear isotropic solids' stress tensor are developed below to show the similarity of these two constitutive models. The only information necessary to write down the explicit relationships is provided by the principle of conservation of angular momentum. That is, it can be shown that the stress tensor must be symmetric, i.e.,

$$\sigma_{ij} = \sigma_{ji} .$$

This fact reduces the number of independent tensor components from nine to six and in the case of the Newtonian fluids the only symmetric linear combinations of velocity gradients are

$$\frac{\partial}{\partial x_i} v_j + \frac{\partial}{\partial x_j} v_i$$

and

$$\left(\frac{\partial}{\partial x_i} v_i\right) \delta_{ij} .$$

Thus,

$$\sigma_{ij} = a\left(\frac{\partial}{\partial x_i} v_j + \frac{\partial}{\partial x_j} v_i\right) + b\left(\frac{\partial}{\partial x_i} v_i\right)\delta_{ij}$$

where a and b have no indices if the fluid is assumed isotropic. To be consistent with the definition of viscosity from Newton's law of viscosity

$$a = -\zeta$$

where ζ is the coefficient of viscosity. To be consistent with kinetic theory of gases (Reference 2.3),

$$b = \frac{2}{3}\zeta ,$$

but for dense gases or liquids a correction must be applied such that

$$b = \frac{2}{3}\zeta - \kappa$$

where κ is called the dilatational viscosity. Notice that $\kappa = 0$ for an ideal gas. Finally, one can write for the Newtonian viscous stress tensor

$$\sigma_{ij} = -\zeta\left(\frac{\partial}{\partial x_i} v_j + \frac{\partial}{\partial x_j} v_i\right) + \left(\frac{2}{3}\zeta - \kappa\right)\left(\frac{\partial}{\partial x_i} v_i\right)\delta_{ij} . \qquad (2.20)$$

In component form

$$\sigma_{xx} = -2\zeta \frac{\partial v_x}{\partial x} + \left(\frac{2}{3}\zeta - \kappa\right)\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right)$$

$$= -2\zeta \dot{\epsilon}_{xx} + \left(\frac{2}{3}\zeta - \kappa\right)\frac{\dot{V}}{V} \qquad (2.20a)$$

$$\sigma_{yy} = -2\zeta \frac{\partial v_y}{\partial y} + \left(\frac{2}{3}\zeta - \kappa\right)\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right)$$

$$= -2\zeta \dot{\epsilon}_{yy} + \left(\frac{2}{3}\zeta - \kappa\right)\frac{\dot{V}}{V} \qquad (2.20b)$$

$$\sigma_{zz} = -2\zeta \frac{\partial v_z}{\partial z} + \left(\frac{2}{3}\zeta - \kappa\right)\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right)$$

$$= -2\zeta \dot{\epsilon}_{zz} + \left(\frac{2}{3}\zeta - \kappa\right)\frac{\dot{V}}{V} \qquad (2.20c)$$

$$\sigma_{xy} = \sigma_{yx} = -\zeta \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right)$$

$$= -\zeta\, \dot{\epsilon}_{xy} \qquad (2.20d)$$

$$\sigma_{yz} = \sigma_{zy} = -\zeta \left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right)$$

$$= -\zeta\, \dot{\epsilon}_{yz} \qquad (2.20e)$$

$$\sigma_{zx} = \sigma_{xz} = -\zeta \left(\frac{\partial v_z}{\partial x} + \frac{\partial v_x}{\partial z} \right)$$

$$= -\zeta\, \dot{\epsilon}_{zx} \quad . \qquad (2.20f)$$

Similar arguments lead to the isotropic elastic stress tensor,

$$\sigma_{ij} = G\left(\frac{\partial}{\partial x_i} d_j + \frac{\partial}{\partial x_j} d_i \right) + \left(K - \frac{2}{3} G \right) \left(\frac{\partial}{\partial x_i} d_i \right) \delta_{ij} \qquad (2.21)$$

where G is the shear modulus and K is the bulk modulus; d_i is the displacement in the i-direction. The isotropic elastic constants G and K are related to the Young's modulus, E, and Poisson's ratio, ν, as follows:

$$G = \frac{E}{2(1+\nu)} \; ; \qquad K = \frac{E}{3(1-2\nu)} \quad .$$

Other relationships between isotropic elastic constants are summarized in Reference 2.4. If the material is not isotropic, G and K must be subscripted. Notice the similarities in form between the linear-solid and linear-fluid stress tensors, Eqs.(2.20) and (2.21). Notice the difference in sign convention. In component form, the solid stress tensor is

$$\sigma_{xx} = 2G\epsilon_{xx} + \lambda\Delta \tag{2.21a}$$

$$\sigma_{yy} = 2G\epsilon_{yy} + \lambda\Delta \tag{2.21b}$$

$$\sigma_{zz} = 2G\epsilon_{zz} + \lambda\Delta \tag{2.21c}$$

$$\sigma_{xy} = \sigma_{yx} = G\epsilon_{xy} \tag{2.21d}$$

$$\sigma_{yz} = \sigma_{zy} = G\epsilon_{yz} \tag{2.21e}$$

$$\sigma_{zx} = \sigma_{xz} = G\epsilon_{zx} \tag{2.21f}$$

where $\lambda \equiv K - \frac{2}{3}G$ and

$$\epsilon_{xx} \equiv \frac{\partial d_x}{\partial x}, \qquad \epsilon_{yy} \equiv \frac{\partial d_y}{\partial y}, \qquad \epsilon_{zz} \equiv \frac{\partial d_z}{\partial z},$$

$$\Delta \equiv \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz} = \frac{\partial}{\partial x_i} d_i \, \delta_{ij} ,$$

$$\epsilon_{xy} \equiv \left(\frac{\partial d_y}{\partial x} + \frac{\partial d_x}{\partial y}\right), \quad \epsilon_{yz} \equiv \left(\frac{\partial d_z}{\partial y} + \frac{\partial d_y}{\partial z}\right), \quad \epsilon_{zx} \equiv \left(\frac{\partial d_x}{\partial z} + \frac{\partial d_z}{\partial x}\right) .$$

The properties ζ, κ, G, and K may be functions of any two thermodynamic variables. Generally, they are reported as functions of temperature and pressure. Temperature is the dominant thermodynamic variable with pressure (or density) only becoming important at phase changes.

Because of the manner in which constitutive data are gathered, it is convenient to decompose the relationship between stress, strain, and internal energy into "component" relationships. For example, for an isotropic material, strength data and hydrostatic equation-of state data are derived from completely unrelated experiments. Strength is a function of the deviatoric processes only, while equation-of-state data are related to the hydrostatic (mean) values. Thus, to use these data it is convenient to divide the symmetric total stress tensor into two symmetric parts -- one part is the trace (a diagonal tensor), called the mean stress tensor, $p\delta_{ij}$; the other part, which has diagonal and off-diagonal terms, is the deviatoric stress tensor, s_{ij}. This is written as

$$\sigma_{ij} = s_{ij} - p\delta_{ij} ,$$

where s_{ij} has the same sign convention as σ_{ij} and $p\delta_{ij}$ has the opposite sign convention. The strain tensor must also be decomposed analogously into the mean strain tensor and the deviatoric strain tensor,

$$\epsilon_{ij} = e_{ij} - \frac{\Delta V}{3} \delta_{ij} ,$$

where e_{ij} are deviatoric strain components with the same sign convention as ϵ_{ij}.* The mean stress tensor represents the pressure or hydrostatic stress, while the mean strain tensor represents dilatancy or volumetric strain. Using Eq.(2.21) as a convenient example, the deviatoric stress formula becomes

$$s_{ij} = G\left(\frac{\partial}{\partial x_i} d_j + \frac{\partial}{\partial x_j} d_i - \frac{2}{3} \frac{\partial}{\partial x_i} d_i \delta_{ij}\right) , \qquad (2.22)$$

while the mean stress formula is

$$p = K \frac{\partial}{\partial x_i} d_i . \qquad (2.23)$$

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*ΔV is the change in relative volume.

A more general mean stress (equation-of-state) model is given by the polynomial function,

$$p = b_1 + b_2\mu + b_3\mu^2 + b_4\mu^3 + u(b_8 + b_9\mu) \ . \tag{2.24}$$

Equation (2.24) is a general relationship between mean stress (p), internal energy density (u), and mass density (ρ) where $\mu \equiv \frac{\rho}{\rho^o} - 1$ and ρ^o is a convenient constant called reference density. b_i are material coefficients. Equation (2.23) is a simple subset of Eq.(2.24) where

$$b_2 = K = \text{bulk modulus} \neq 0.0,$$

$$b_1 = b_3 = b_4 = b_8 = b_9 = 0.0 \ ,$$

and

$$\mu = \frac{\partial}{\partial x_i} d_i \ .$$

The same equation-of-state model, Eq.(2.24), can be used for fluids as well as for solids because the mean stress (or pressure) terms are essentially the same in Eqs.(2.17) and (2.18). An ideal gas may be defined in the following way,

$$b_8 = b_9 = \gamma - 1,$$

where γ is the ratio of specific heat capacities $\neq 0.0$, and

$$b_1 = b_2 = b_3 = b_4 = 0.0 \ .$$

The equation of state, Eq.(2.24), becomes

$$p = (\gamma - 1)\frac{u}{V} \ . \tag{2.25}$$

Strength models, heat transfer relationships, and other equations of state can be categorized similarly. Inviscid fluids require that G be zero in the deviatoric stress formula, Eq.(2.22). Plastic flow in solids can be modeled by limiting the values of stress deviators in Eq.(2.22) by invoking "flow rules" based on stress invariants.

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SECTION 3

NUMERICAL DIFFERENCE EQUATIONS

3.1 INTRODUCTION

The mathematical equations, Eqs.(2.8), (2.9), and (2.14), that represent the Lagrange partial differential equations of continuum mechanics cannot be solved analytically for arbitrary boundary and initial conditions and nonlinear constitutive relations. Therefore, they must be solved numerically.

A numerical method well suited to solve these equations is the explicit finite-difference approach. The explicit approach is ideal for solving time-dependent equations because it preserves the notion of time sequence and path dependence. An explicit scheme has two identifying characteristics:

(1) "Unknowns (are computed) directly in terms of the known quantities" (Reference 3.1); e.g., values calculated for a new time (n+1) need only use data from the old, or previous, time (n).

(2) Physical phenomena can propagate only one spatial discretization in one calculated step; e.g., the calculated response at a particular location is only dependent upon the data at nearest neighbor locations.

Implicit methods, on the other hand, result in the solution of a set of simultaneous equations in which time is no longer an independent variable.

The characteristics of an explicit method may be written mathematically as a stability requirement. For example, the requirement for mechanical stability is

$$\frac{c_\ell \Delta t}{\Delta \ell} \leq 1 \tag{3.1}$$

where c_ℓ is the local longitudinal sound speed (i.e., the largest mechanical signal speed), Δt is a stable time step, and $\Delta \ell$ is an appropriately chosen characteristic discretization length, usually in the direction of maximum acceleration. Equation (3.1) is commonly referred to as the "Courant Criterion", based on a 1928 paper (Reference 3.2) by Courant, Friedrichs, and Lewy which introduced the concept of stability. Equation (3.1) is sometimes called the "von Neumann condition" from John von Neumann's work on shock waves (Reference 3.3). Specific formulas for choosing stable mechanical (and thermal) time steps will be derived later.

The choice of using a finite-difference representation for the spatial derivatives in Eqs.(2.8), (2.9), and (2.14) instead of a finite element formulation is somewhat arbitrary. Either approach can be numerically explicit. However, the finite-difference method described in this section has some distinct advantages when the problem to be solved involves transient, high amplitude, large strain response. The explicit finite-difference method has no stiffness matrix to re-form as constitutive properties change; there is no need for multiple formulations of elements to handle different geometric situations; momentum and thermal transport effects do not have to be solved separately; and there is no need to be concerned with different convergence criteria for problems with different characteristic lengths and time scales. The explicit finite-difference formulation results in algebraic constitutive equations, geometric accuracy which depends only on spatial discretization, thermodynamically consistent processes for coupled thermomechanical transport, and, finally, stability criteria which are applicable to a wide range of problems. Furthermore, the finite-difference equations require little mathematical sophistication -- the entire scheme is based on the same fundamental principle as the conservation laws, the Divergence Theorem.

3.2 DIVERGENCE THEOREM

The finite-difference equations for spatial derivatives (gradients) are based on the Divergence Theorem,

$$\iiint_{\mathcal{V}} (\nabla \cdot \underline{A})\, d\mathcal{V} = \iint_{S} (\underline{A} \cdot \underline{n})\, dS \,, \tag{3.2}$$

where the surface, S, encloses the volume, $\mathcal{V}$, and $\underline{n}$ is the positive (outward)

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normal to S. $\underline{A}$ is a vector function of position with continuous derivatives that can be written as

$$\underline{A} \equiv A_x \underline{i} + A_y \underline{j} + A_z \underline{k}$$

where $\underline{i}$, $\underline{j}$, $\underline{k}$ are unit vectors for the Cartesian coordinate system, x, y, z, respectively. A_x, A_y, and A_z are the respective x, y, and z magnitudes of $\underline{A}$. Solving Eq.(3.2) for the divergence of $\underline{A}$ yields

$$\nabla \cdot \underline{A} = \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S (\underline{A} \cdot \underline{n}) dS , \qquad (3.3)$$

where

$$\underline{n} \equiv n_x \underline{i} + n_y \underline{j} + n_z \underline{k} .$$

In component form, Eq.(3.3) becomes

$$\begin{aligned}
\nabla \cdot A_x \underline{i} &= \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S A_x \underline{i} \cdot \underline{n}\, dS = \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S A_x n_x\, dS , \\
\nabla \cdot A_y \underline{j} &= \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S A_y \underline{j} \cdot \underline{n}\, dS = \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S A_y n_y\, dS , \qquad (3.4) \\
\nabla \cdot A_z \underline{k} &= \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S A_z \underline{k} \cdot \underline{n}\, dS = \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S A_z n_z\, dS .
\end{aligned}$$

An analogous derivation may be made for a scalar field.

Equations (3.4) can be put in integral operator form as follows,

$$\nabla \cdot (\ ) = \lim_{\Delta \mathcal{V} \to 0} \frac{1}{\Delta \mathcal{V}} \iint_S (\ ) \cdot \underline{n}\, dS . \qquad (3.5)$$

Equation (3.5) is a general formula for partial derivatives of either a vector or scalar field. This is a direct result of the fact that

$$\frac{\partial}{\partial \underline{x}}(\ ) \equiv \nabla \cdot (\ ) \ . \tag{3.6}$$

In component form, Eqs.(3.4) become

$$\begin{aligned}
\frac{\partial}{\partial x}(\ ) &= \lim_{\Delta\mathcal{V}\to 0} \frac{1}{\Delta\mathcal{V}} \iint_S (\ ) \cdot n_x \, dS \ , \\
\frac{\partial}{\partial y}(\ ) &= \lim_{\Delta\mathcal{V}\to 0} \frac{1}{\Delta\mathcal{V}} \iint_S (\ ) \cdot n_y \, dS \ , \\
\frac{\partial}{\partial z}(\ ) &= \lim_{\Delta\mathcal{V}\to 0} \frac{1}{\Delta\mathcal{V}} \iint_S (\ ) \cdot n_z \, dS \ .
\end{aligned} \tag{3.7}$$

Equations (3.7) may be written in finite-difference form as follows:

$$\begin{aligned}
\frac{\partial}{\partial x}(\ ) &\approx \frac{1}{\mathcal{V}} \sum_{\ell=1}^{\ell_{max}} \Big[(\ ) \times S_x\Big]_\ell \ , \\
\frac{\partial}{\partial y}(\ ) &\approx \frac{1}{\mathcal{V}} \sum_{\ell=1}^{\ell_{max}} \Big[(\ ) \times S_y\Big]_\ell \ , \\
\frac{\partial}{\partial z}(\ ) &\approx \frac{1}{\mathcal{V}} \sum_{\ell=1}^{\ell_{max}} \Big[(\ ) \times S_z\Big]_\ell \ ,
\end{aligned} \tag{3.8}$$

where the index ℓ counts the number of surface elements, S, that enclose the volume, $\mathcal{V}$. These formulas can be used directly to derive specific numerical equations for any spatial symmetry involving Cartesian coordinates. In particular, they are immediately useful for one-dimensional planar, two-dimensional translational, and three-dimensional asymmetric geometries. Equation (3.7) may be rewritten in (r,θ,z) coordinates for one-dimensional cylindrical and two-dimensional axial equations. For one-dimensional spherical equations, Eq.(3.7) must be formulated in (r,θ,φ) coordinates.

3.3 ONE-DIMENSIONAL EQUATIONS

One-dimensional numerical equations are by far the easiest equations to derive because the computational mesh is simply a colinear string of mesh points. Volume is a function of the distance between mesh points and surface area is defined perpendicular to the direction of the mesh points. In plane infinite slab symmetry, Eqs.(2.15a,b,c), the surface areas are the same for all values of the Cartesian coordinate x, and zone volume equals the distance between mesh points times the surface area at the center of the zone. In cylindrical and spherical symmetries, Eqs.(2.16a,b,c) and (2.17a,b,c), the surface area at each mesh point (or zone center) increases with increasing radius, while zone volume increases as the differences of the squares and cubes of mesh point radii, respectively.

Figure 3.1 displays five consecutive interior mesh points in a typical one-dimensional Lagrange mesh, no matter what symmetry is used. The mesh points divide the space into discrete entities known as zones. Momentum-related variables (vectors) are calculated from equations centered at mesh points. Energy-related variables (scalars and tensors) are calculated from equations centered at zone interiors.* For Lagrange zones, conservation of mass is automatically satisfied because the zones have fixed mass.

In the equations that follow, time and space dependence of physical variables is noted by superscripts and subscripts, respectively; n is the temporal index, while i is the one-dimensional spatial index.

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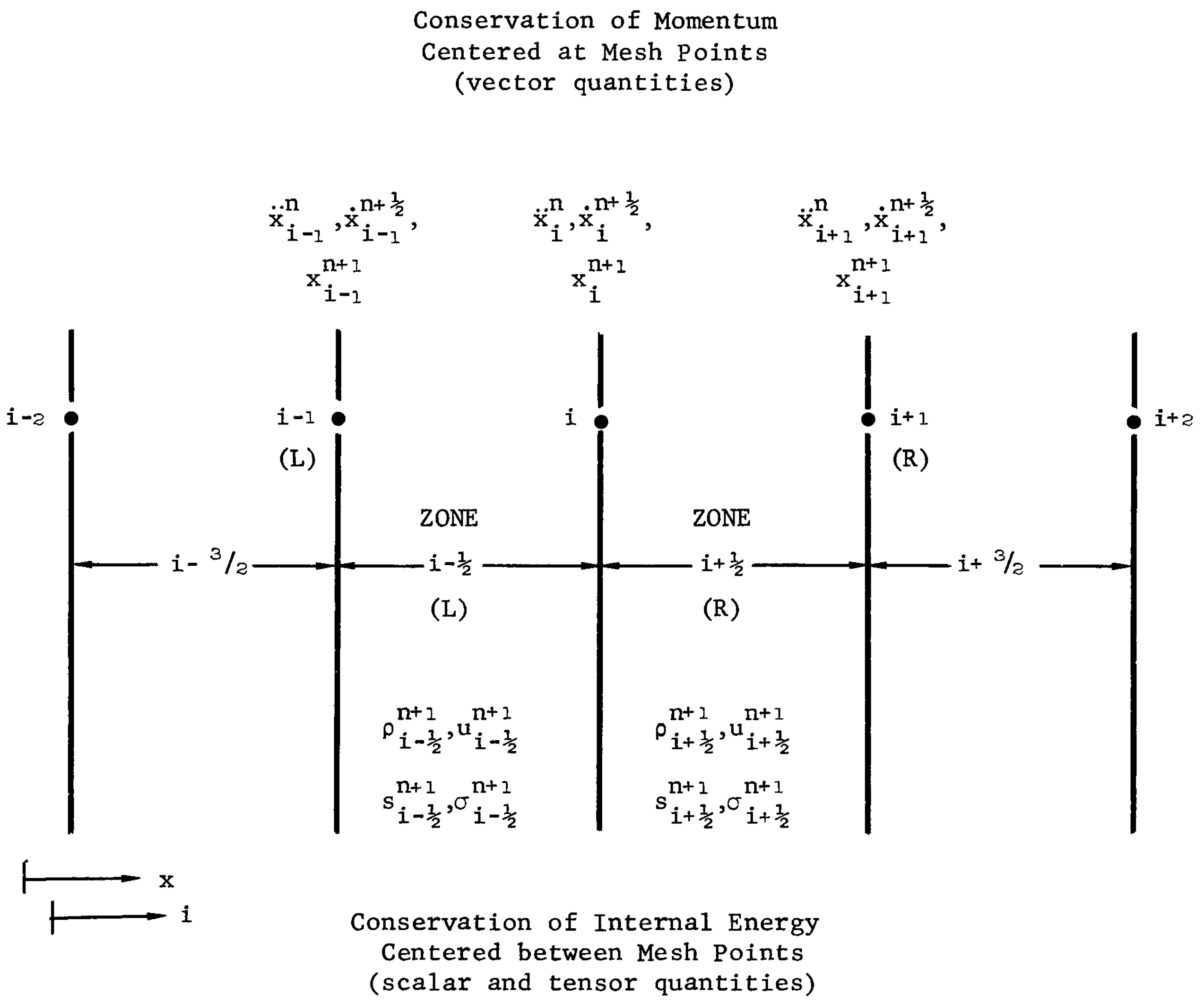
*These spatial conventions result in a second-order accurate numerical scheme. The notion of overlapping meshes is described later.



L = left
R = right

Figure 3.1. One-dimensional Lagrange mesh.

Using the x-component equation from Eqs.(3.8) to represent partial derivatives in one-dimensional symmetry (the y- and z-components are eliminated by symmetry), the following simplified form for the gradient at point i at time n is derived,

$$\frac{\partial}{\partial x}(\ )_i^n = \frac{(\ )_{i+\frac{1}{2}}^n S_{i+\frac{1}{2}}^n - (\ )_{i-\frac{1}{2}}^n S_{i-\frac{1}{2}}^n}{\mathcal{V}_i^n} . \tag{3.9}$$

The values at i+½ and i-½ are average values which apply to the entire zone or, equivalently, are the values that act at the center of the zone. In Eq.(3.9), the contributions from the front and back surfaces cancel each other by symmetry, as do the top and bottom surfaces. $\mathcal{V}_i^n$ is the grid point volume.

In plane infinite slab symmetry, the surface areas $S_{i+\frac{1}{2}}^n$ and $S_{i-\frac{1}{2}}^n$ are equal and can be taken to be unity. The grid point volume is the distance between the centers of adjacent zones multiplied by the average surface area (which in this case is equal to 1). Thus, for one-dimensional slab symmetry, Eq.(3.9) becomes

$$\frac{\partial}{\partial x}(\ )_i^n = \frac{(\ )_{i+\frac{1}{2}}^n - (\ )_{i-\frac{1}{2}}^n}{x_{i+\frac{1}{2}}^n - x_{i-\frac{1}{2}}^n} . \tag{3.10}$$

Equation (3.10) may be used to represent the term $\frac{\partial}{\partial x}\sigma_{xx}$ in Eq.(2.15a).

The coordinates $x_{i-\frac{1}{2}}^n$ and $x_{i+\frac{1}{2}}^n$ in Eq.(3.10) are the locations of zone centers. They are computed from known grid point locations as follows,

$$x_{i-\frac{1}{2}}^n \equiv \frac{x_i^n + x_{i-1}^n}{2} ; \qquad x_{i+\frac{1}{2}}^n \equiv \frac{x_{i+1}^n + x_i^n}{2} . \tag{3.10a}$$

Rev. 2
15 NOV 77

The formula for the gradient at the center of a one-dimensional zone (say, $i-\frac{1}{2}$) is

$$\frac{\partial}{\partial x}(\ )^n_{i-\frac{1}{2}} = \frac{(\ )^n_i S^n_i - (\ )^n_{i-1} S^n_{i-1}}{\mathcal{V}^n_{i-\frac{1}{2}}} \ , \tag{3.11}$$

where S^n_i and S^n_{i-1} are grid point surface areas and $\mathcal{V}^n_{i-\frac{1}{2}}$ is the zone volume. For planar symmetry, Eq.(3.11) becomes

$$\frac{\partial}{\partial x}(\ )^n_{i-\frac{1}{2}} = \frac{(\ )^n_i - (\ )^n_{i-1}}{x^n_i - x^n_{i-1}} \ . \tag{3.12}$$

Equation (3.12) may be used to compute $\frac{\partial}{\partial x} v_x$ in Eq.(2.15b).

Finite-difference formulas for one-dimensional cylindrical and spherical symmetries may be derived from (r,θ,z) and (r,θ,φ) versions of Eq.(3.5), respectively. The radial component of the (r,θ,z) equations is

$$\frac{1}{r}\frac{\partial}{\partial r}\Big[r \cdot (\ )\Big] = \frac{1}{\mathcal{V}} \sum_{\ell=1}^{\ell_{max}} \Big[(\ ) \times S_r\Big] \ . \tag{3.13}$$

The one-dimensional version of Eq.(3.13) analogous to Eq.(3.9) is

$$\frac{1}{r}\frac{\partial}{\partial r}\Big[r \cdot (\ )\Big]^n_i = \frac{(\ )^n_{i+\frac{1}{2}} S^n_{i+\frac{1}{2}} - (\ )^n_{i-\frac{1}{2}} S^n_{i-\frac{1}{2}}}{\mathcal{V}^n_i} \ . \tag{3.14}$$

For cylindrical symmetry, S is the surface area per unit height,

$$S^n_{i+\frac{1}{2}} = 2\pi\, r^n_{i+\frac{1}{2}}$$

$$S^n_{i-\frac{1}{2}} = 2\pi\, r^n_{i-\frac{1}{2}} \ , \tag{3.14a}$$

$\mathcal{V}$ is the volume per unit height,

$$\mathcal{V}^n_i = \pi \left[\left(r^n_{i+\frac{1}{2}} \right)^2 - \left(r^n_{i-\frac{1}{2}} \right)^2 \right] \ , \tag{3.14b}$$

and, letting the variable x be used in place of r, Eq.(3.14) becomes

$$\frac{1}{x}\frac{\partial}{\partial x}\Big[x \cdot (\ ) \Big]^n_i = 2 \left[\frac{(\ )^n_{i+\frac{1}{2}} x^n_{i+\frac{1}{2}} - (\ )^n_{i-\frac{1}{2}} x^n_{i-\frac{1}{2}}}{\left(x^n_{i+\frac{1}{2}} \right)^2 - \left(x^n_{i-\frac{1}{2}} \right)^2} \right] . \tag{3.15}$$

The radial component of the (r,θ,φ) equations is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\Big[r^2 \cdot (\ ) \Big] = \frac{1}{\mathcal{V}} \sum_{\ell=1}^{\ell_{max}} \Big[(\ ) \times S_r \Big] . \tag{3.16}$$

The one-dimensional form of Eq.(3.16) is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\Big[r^2 \cdot (\ ) \Big]^n_i = \frac{(\ )^n_{i+\frac{1}{2}} S^n_{i+\frac{1}{2}} - (\ )^n_{i-\frac{1}{2}} S^n_{i-\frac{1}{2}}}{\mathcal{V}^n_i} . \tag{3.17}$$

In spherical symmetry, the surface area, S, is

$$S^n_{i+\frac{1}{2}} = 4\pi\left(r^n_{i+\frac{1}{2}}\right)^2$$

$$S^n_{i-\frac{1}{2}} = 4\pi\left(r^n_{i-\frac{1}{2}}\right)^2 , \qquad (3.17a)$$

and the volume, $\mathcal{V}$, is

$$\mathcal{V}^n_i = \frac{4}{3}\pi\left[\left(r^n_{i+\frac{1}{2}}\right)^3 - \left(r^n_{i-\frac{1}{2}}\right)^3\right] . \qquad (3.17b)$$

Substituting Eqs.(3.17a) and (3.17b) into Eq.(3.17) and letting r be replaced by the variable x,

$$\frac{1}{x^2}\frac{\partial}{\partial x}\left[x^2 \cdot (\ )\right]^n_i = 3\left[\frac{(\ )^n_{i+\frac{1}{2}}\left(x^n_{i+\frac{1}{2}}\right)^2 - (\ )^n_{i-\frac{1}{2}}\left(x^n_{i-\frac{1}{2}}\right)^2}{\left(x^n_{i+\frac{1}{2}}\right)^3 - \left(x^n_{i-\frac{1}{2}}\right)^3}\right] . \qquad (3.18)$$

Equations (3.15) and (3.18) may be used to describe gradients at grid points of radially diverging quantities. Equations analogous to Eqs.(3.11) and (3.12) can be derived for each symmetry.

Another approach can be used to compute the gradients of diverging quantities. First, expand the radial gradients as follows,

$$\frac{1}{r}\frac{\partial}{\partial r}\left[r \cdot (\ )\right] \equiv \frac{\partial}{\partial r}(\ ) + \frac{(\ )}{r} ,$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 \cdot (\ )\right] \equiv \frac{\partial}{\partial r}(\ ) + 2\frac{(\ )}{r} . \qquad (3.19)$$

Then, a cylindrical equation which is equivalent to Eq.(3.15) can be derived from Eq.(3.10),

$$\frac{1}{x}\frac{\partial}{\partial x}\Big[x\cdot(\;)\Big]_i^n = \frac{(\;)^n_{i+\frac{1}{2}} - (\;)^n_{i-\frac{1}{2}}}{x^n_{i+\frac{1}{2}} - x^n_{i-\frac{1}{2}}} + \frac{(\;)^n_i}{x^n_i}\;, \tag{3.20}$$

and a spherical equation equivalent to Eq.(3.18) may also be derived from Eq.(3.10),

$$\frac{1}{x^2}\frac{\partial}{\partial x}\Big[x^2\cdot(\;)\Big]_i^n = \frac{(\;)^n_{i+\frac{1}{2}} - (\;)^n_{i-\frac{1}{2}}}{x^n_{i+\frac{1}{2}} - x^n_{i-\frac{1}{2}}} + 2\,\frac{(\;)^n_i}{x^n_i}\;. \tag{3.21}$$

In both Eqs.(3.20) and (3.21),

$$(\;)^n_i \equiv \frac{(\;)^n_{i+\frac{1}{2}} + (\;)^n_{i-\frac{1}{2}}}{2}\;. \tag{3.22}$$

For all three symmetries, a common form of the one-dimensional gradient at a grid point is obtained by combining Eqs.(3.10), (3.20), and (3.21),

$$\boxed{\nabla(\;)^n_i = \frac{(\;)^n_{i+\frac{1}{2}} - (\;)^n_{i-\frac{1}{2}}}{x^n_{i+\frac{1}{2}} - x^n_{i-\frac{1}{2}}} + f\left[\frac{(\;)^n_i}{x^n_i}\right]}\;. \tag{3.23}$$

where f = 0 for plane symmetry, f = 1 for cylindrical symmetry, and f = 2 for spherical symmetry. Equation (3.23) may be interpreted as computing the planar gradient and adding an appropriate correction for divergent symmetries. Equation (3.23) may be used to compute gradients of stress in Eqs.(2.16a), (2.17a), and (2.18a).

For gradients at zone centers, the finite-difference formula analogous to Eq.(3.23) is

$$\boxed{\nabla(\;)^n_{i-\frac{1}{2}} = \frac{(\;)^n_i - (\;)^n_{i-1}}{x^n_i - x^n_{i-1}} + f\left[\frac{(\;)^n_{i-\frac{1}{2}}}{x^n_{i-\frac{1}{2}}}\right]} \quad . \tag{3.24}$$

Equation (3.24) may be used to compute gradients of velocity in Eqs.(2.16b), (2.17b), and (2.18b).

In Eqs.(3.23) and (3.24), it was possible to eliminate the grid point and zone volume terms. However, it is necessary to calculate the zone volume so that the mass of each Lagrange zone can be computed. The formulas for zone true volume are derived for each symmetry as follows:

- Zones in plane symmetry are one-dimensional, variable-thickness slabs of specified cross-sectional area. The Lagrange coordinate is perpendicular to the unit cross section. The true volume of a zone is

  $$\mathcal{V} \equiv \text{(slab thickness)} \times \text{(cross section)}.$$

  When the cross-sectional area is constant for all zones, the slab symmetry is called planar; when the cross-sectional area is variable, it is called "planar-flume" or "planar duct" symmetry or simply one-dimensional pipe flow geometry. The true volume formula at time n for a constant cross-sectional area slab symmetry is

  $$\mathcal{V}^n_{i-\frac{1}{2}} = \left(x^n_i - x^n_{i-1}\right) \times (1) \; . \tag{3.25a}$$

  Equation (3.25a) assumes a unit cross-sectional area;

however, any constant may be used, since it will affect all equations in the same way and cancel out.*

- Zones in cylindrical symmetry are concentric cylindrical shells of constant height and finite thickness. The Lagrange coordinate is the radius of the cylindrical shells, always beginning at the point of concentricity (i.e., the center) and directed outward. The true volume at time n comes from the difference in circular cross-sectional areas multiplied by the cylinder height,

$$\mathcal{V}^n_{i-\frac{1}{2}} = \pi\left[\left(x^n_i\right)^2 - \left(x^n_{i-1}\right)^2\right] \times (1) . \tag{3.25b}$$

Equation (3.25b) assumes a unit constant height.** As in the plane slab geometry, any constant may be used. A geometry analogous to pipe flow geometry will result from variable heights. This symmetry is a one-dimensional divergent flow between a variably separated plate geometry.

- Zones in spherical symmetry are finite, concentric spherical shells. The Lagrange coordinate begins at the point of concentricity and is directed outward. The true volume at time n is

$$\mathcal{V}^n_{i-\frac{1}{2}} = \frac{4}{3}\pi\left[\left(x^n_i\right)^3 - \left(x^n_{i-1}\right)^3\right] . \tag{3.25c}$$

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*The volume formula for planar flume (where y is the flume radius) is

$$\mathcal{V}^n_{i-\frac{1}{2}} = \frac{\pi}{3}\left(x^n_i - x^n_{i-1}\right)\left[\left(y^n_i\right)^2 + y^n_i\, y^n_{i-1} + \left(y^n_{i-1}\right)^2\right] .$$

**The volume formula for non-constant height cylindrical symmetry is

$$\mathcal{V}^n_{i-\frac{1}{2}} = 2\pi\left\{m^n_{i-\frac{1}{2}}\left[\left(x^n_i\right)^3 - \left(x^n_{i-1}\right)^3\right] + \frac{1}{2}\left[y^n_{i-1} + m^n_{i-\frac{1}{2}}\, x^n_{i-1}\right]\left[\left(x^n_i\right)^2 - \left(x^n_{i-1}\right)^2\right]\right\}$$

where $m^n_{i-\frac{1}{2}} = \left(y^n_i - y^n_{i-1}\right)/\left(x^n_i - y^n_{i-1}\right)$ and y is the height.

3.4 TWO-DIMENSIONAL EQUATIONS

Two-dimensional gradient equations for a grid point (i,j) denoted by P in Figure 3.2 are derived from the x- and y-components of Eq.(3.8). The surface integral is defined along the diamond-shaped path LTRBL, shown in Figure 3.2, leading to the difference equations,

$$\frac{\partial}{\partial x}(\ )^n_P = \frac{(\ )^n_{TL}\ S^n_{TL_x} + (\ )^n_{TR}\ S^n_{TR_x} + (\ )^n_{BR}\ S^n_{BR_x} + (\ )^n_{BL}\ S^n_{BL_x}}{\mathcal{V}^n_P} ,$$

$$\frac{\partial}{\partial y}(\ )^n_P = \frac{(\ )^n_{TL}\ S^n_{TL_y} + (\ )^n_{TR}\ S^n_{TR_y} + (\ )^n_{BR}\ S^n_{BR_y} + (\ )^n_{BL}\ S^n_{BL_y}}{\mathcal{V}^n_P} . \tag{3.26}$$

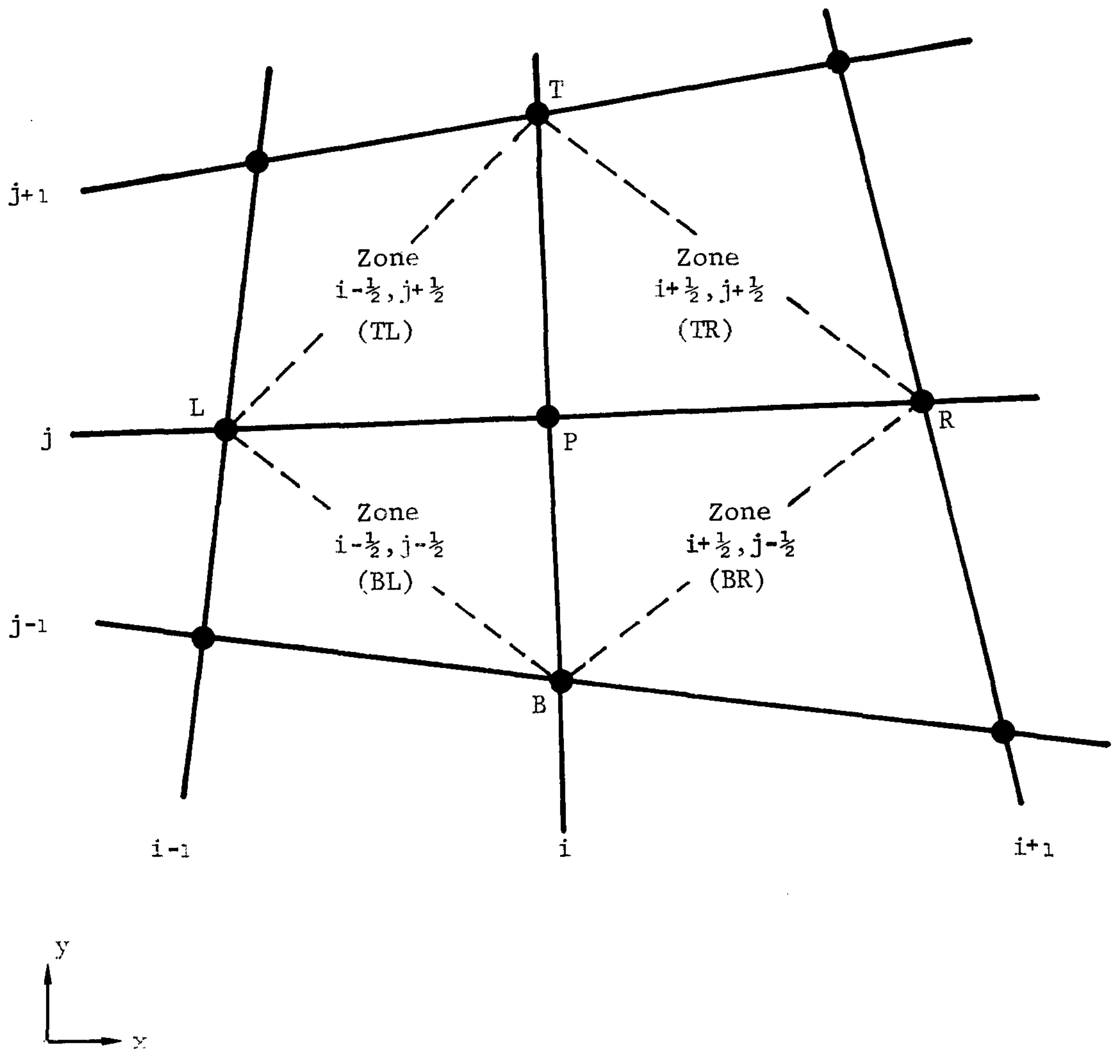
The values at TL_x and TL_y are the x- and y-component average values which apply to the entire top left zone or equivalently, to the center of the top left zone. Similar definitions for TR (top right zone), BR (bottom right zone), and BL (bottom left zone) may be made. The grid point volume, $\mathcal{V}^n_p$, is the volume which is enclosed by the surface with the cross-sectional area defined by LBRTL. In two-dimensional equations, contributions from front and back surfaces cancel each other, leading to four instead of six terms in the numerators of Eqs.(3.26).

For two-dimensional translational slab symmetry, there is a constant slab depth, which leads Eq.(3.26) to be reduced to

$$\frac{\partial}{\partial x}(\ )^n_P = - \frac{(\ )^n_{TL}\ (y_T - y_L)^n + (\ )^n_{TR}\ (y_R - y_T)^n + (\ )^n_{BR}\ (y_B - y_R)^n + (\ )^n_{BL}\ (y_L - y_B)^n}{A^n_P} ,$$

$$\frac{\partial}{\partial y}(\ )^n_P = \frac{(\ )^n_{TL}\ (x_T - x_L)^n + (\ )^n_{TR}\ (x_R - x_T)^n + (\ )^n_{BR}\ (x_B - x_R)^n + (\ )^n_{BL}\ (x_L - x_B)^n}{A^n_P} . \tag{3.27}$$

The grid point area, A^n_P, is the area which is enclosed by the closed contour LBRTL.



P = Point being calculated, (i,j)

L = Left of point P in index space, (i-1,j)

B = Bottom of point P in index space, (i,j-1)

R = Right of point P in index space, (i+1,j)

T = Top of point P in index space, (i,j+1)

Figure 3.2. Two-dimensional Lagrange mesh.

Rev. 1
15 NOV 77

Equations (3.27) may be used to compute grid-point centered gradients in Eq.(2.18a). In terms of the index notation shown in Figure 3.2, Eqs. (3.27) become

$$\begin{aligned}
\frac{\partial}{\partial x}(\ )^n_{i,j} = -\Big[\ & (\ )^n_{i-\frac{1}{2},j+\frac{1}{2}}\,(y^n_{i,j+1} - y^n_{i-1,j}) \\
&+ (\ )^n_{i+\frac{1}{2},j+\frac{1}{2}}\,(y^n_{i+1,j} - y^n_{i,j+1}) \\
&+ (\ )^n_{i+\frac{1}{2},j-\frac{1}{2}}\,(y^n_{i,j-1} - y^n_{i+1,j}) \\
&+ (\ )^n_{i-\frac{1}{2},j-\frac{1}{2}}\,(y^n_{i-1,j} - y^n_{i,j-1})\Big] \Big/ A^n_{i,j}\ , \\[1ex]
\frac{\partial}{\partial y}(\ )^n_{i,j} = \Big[\ & (\ )^n_{i-\frac{1}{2},j+\frac{1}{2}}\,(x^n_{i,j+1} - x^n_{i-1,j}) \\
&+ (\ )^n_{i+\frac{1}{2},j+\frac{1}{2}}\,(x^n_{i+1,j} - x^n_{i,j+1}) \\
&+ (\ )^n_{i+\frac{1}{2},j-\frac{1}{2}}\,(x^n_{i,j-1} - x^n_{i+1,j}) \\
&+ (\ )^n_{i-\frac{1}{2},j-\frac{1}{2}}\,(x^n_{i-1,j} - x^n_{i,j-1})\Big] \Big/ A^n_{i,j}\ .
\end{aligned} \qquad (3.28)$$

$A^n_{i,j}$, which is the quadrilateral area enclosed by LBRTL, is computed from the sum of the triangular areas,

$$A^n_{i,j} = A^n_{LBRTL} \equiv A^n_{PLBP} + A^n_{PBRP} + A^n_{PRTP} + A^n_{PTLP}\ .$$

The formula for the area of a triangle, say A^n_{PLBP}, is determined from analytic geometry as follows,

$$A^n_{PLBP} \equiv \frac{1}{2} \left| \underline{\ell}_{LB} \times \underline{\ell}_{LP} \right|$$

$$= \frac{1}{2} \begin{vmatrix} 0 & 0 & 1 \\ x^n_B - x^n_L & y^n_B - y^n_L & 0 \\ x^n_P - x^n_L & y^n_P - y^n_L & 0 \end{vmatrix}$$

$$= \frac{1}{2} \left[\left(x^n_B - x^n_L\right) \left(y^n_P - y^n_L\right) - \left(x^n_P - x^n_L\right) \left(y^n_B - y^n_L\right) \right]$$

$$= \frac{1}{2} \left[x^n_B \left(y^n_P - y^n_L\right) + x^n_P \left(y^n_L - y^n_B\right) + x^n_L \left(y^n_B - y^n_P\right) \right] . \qquad (3.29a)$$

Equation (3.29a) can be written in index notation as follows,

$$A^n_{PLBP} = \frac{1}{2} \left[x^n_{i,j-1} \left(y^n_{i,j} - y^n_{i-1,j}\right) + x^n_{i,j} \left(y^n_{i-1,j} - y^n_{i,j-1}\right) + x^n_{i-1,j} \left(y^n_{i,j-1} - y^n_{i,j}\right) \right] . \qquad (3.29b)$$

Similar formulas may be derived for triangles PBRP, PRTP, and PTLP.

A formula for translationally symmetric gradients at the center of a zone (say, $i-\frac{1}{2}, j-\frac{1}{2}$)* can be derived similarly to Eqs.(3.27) with the help of Figure 3.3, using the surface integration path TL - BL - BR - TR - TL. Equation (3.26)

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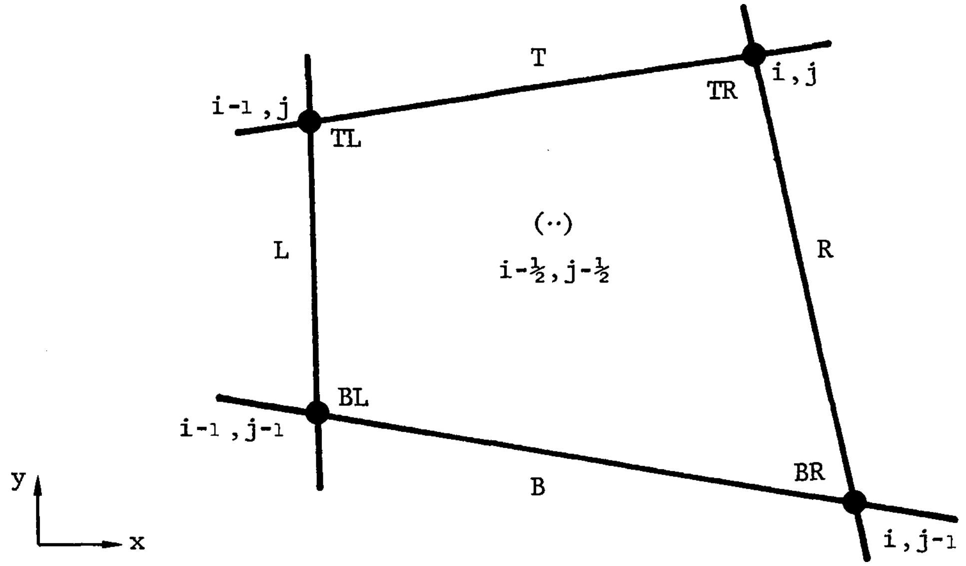
*Zone ($i-\frac{1}{2}, j-\frac{1}{2}$) is defined by the grid points (i,j), (i-1,j), (i-1,j-1), and (i,j-1).



(··) = zone being calculated $(i-\frac{1}{2}, j-\frac{1}{2})$

T = top side of zone in index space

L = left side of zone in index space

B = bottom side of zone in index space

R = right side of zone in index space

TL = top left corner of zone in index space

TR = top right corner of zone in index space

BL = bottom left corner of zone in index space

BR = bottom right corner of zone in index space

Figure 3.3. Two-dimensional Lagrange zone.

becomes

$$\frac{\partial}{\partial x}(\ )^n_{(\cdot\cdot)} = \frac{(\ )^n_T\ S^n_{T_x} + (\ )^n_L\ S^n_{L_x} + (\ )^n_B\ S^n_{B_x} + (\ )^n_R\ S^n_{R_x}}{\mathcal{V}^n_{(\cdot\cdot)}} ,$$

$$\frac{\partial}{\partial y}(\ )^n_{(\cdot\cdot)} = -\frac{(\ )^n_T\ S^n_{T_y} + (\ )^n_L\ S^n_{L_y} + (\ )^n_B\ S^n_{B_y} + (\ )^n_R\ S^n_{R_y}}{\mathcal{V}^n_{(\cdot\cdot)}} . \tag{3.30}$$

Equation (3.27) is

$$\frac{\partial}{\partial x}(\ )^n_{(\cdot\cdot)} = \Big[(\ )^n_T\ (y^n_{i,j} - y^n_{i-1,j}) + (\ )^n_L\ (y^n_{i-1,j} - y^n_{i-1,j-1})$$
$$+ (\ )^n_B\ (y^n_{i-1,j-1} - y^n_{i,j-1}) + (\ )^n_R\ (y^n_{i,j-1} - y^n_{i,j})\Big] / A^n_{(\cdot\cdot)} ,$$

$$\frac{\partial}{\partial y}(\ )^n_{(\cdot\cdot)} = -\Big[(\ )^n_T\ (x^n_{i,j} - x^n_{i-1,j}) + (\ )^n_L\ (x^n_{i-1,j} - x^n_{i-1,j-1})$$
$$+ (\ )^n_B\ (x^n_{i-1,j-1} - x^n_{i,j-1}) + (\ )^n_R\ (x^n_{i,j-1} - x^n_{i,j})\Big] / A^n_{(\cdot\cdot)} . \tag{3.31}$$

A further simplification develops in Eq.(3.31) because the quantities $(\ )^n_T$, $(\ )^n_L$, $(\ )^n_B$, and $(\ )^n_R$ are only defined at the four corners of the zone, Thus,

$$(\ )^n_T \equiv \frac{(\ )^n_{TR} + (\ )^n_{TL}}{2} , \qquad (\ )^n_L \equiv \frac{(\ )^n_{TL} + (\ )^n_{BL}}{2} ,$$

$$(\ )^n_B \equiv \frac{(\ )^n_{BL} + (\ )^n_{BR}}{2} , \qquad (\ )^n_R \equiv \frac{(\ )^n_{BR} + (\ )^n_{TR}}{2} . \tag{3.32}$$

Substituting appropriate components of Eq.(3.32) into Eq.(3.31) yields the following formulas for the gradient at the center of the zone $(i-\frac{1}{2},j-\frac{1}{2})$,

$$\begin{aligned}\frac{\partial}{\partial x}(\ )^n_{i-\frac{1}{2},j-\frac{1}{2}} = &\left\{\left[y^n_{i-1,j-1} - y^n_{i,j}\right]\left[(\ )^n_{i-1,j} - (\ )^n_{i,j-1}\right]\right.\\ &\left. - \left[y^n_{i-1,j} - y^n_{i,j-1}\right]\left[(\ )^n_{i-1,j-1} - (\ )^n_{i,j}\right]\right\} / 2A^n_{i-\frac{1}{2},j-\frac{1}{2}} ,\\ \frac{\partial}{\partial y}(\ )^n_{i-\frac{1}{2},j-\frac{1}{2}} = - &\left\{\left[x^n_{i-1,j-1} - x^n_{i,j}\right]\left[(\ )^n_{i-1,j} - (\ )^n_{i,j-1}\right]\right.\\ &\left. - \left[x^n_{i-1,j} - x^n_{i,j-1}\right]\left[(\ )^n_{i-1,j-1} - (\ )^n_{i,j}\right]\right\} / 2A^n_{i-\frac{1}{2},j-\frac{1}{2}} .\end{aligned} \tag{3.33}$$

The area of the zone $(i-\frac{1}{2},j-\frac{1}{2})$ is computed by dividing the zone into two triangles using either diagonal as the separator. Assuming that the line LB in Figure 3.2 divides the zone $(i-\frac{1}{2},j-\frac{1}{2})$, then the previously derived area A^n_{PLBP} in Eq.(3.29a) represents one part of the zone area, $A^n_{\textcircled{1}\,i-\frac{1}{2},j-\frac{1}{2}}$. The other part, $A^n_{\textcircled{2}\,i-\frac{1}{2},j-\frac{1}{2}}$, is derived as follows,

$$\begin{aligned}A^n_{\textcircled{2}\,i-\frac{1}{2},j-\frac{1}{2}} = \frac{1}{2}\Big[&x^n_{i,j-1}(y^n_{i-1,j} - y^n_{i-1,j-1})\\ &+ x^n_{i-1,j}(y^n_{i-1,j-1} - y^n_{i,j-1})\\ &+ x^n_{i-1,j-1}(y^n_{i,j-1} - y^n_{i-1,j})\Big] .\end{aligned} \tag{3.34}$$

The total zone area, $A^n_{i-\frac{1}{2},j-\frac{1}{2}}$, is

$$A^n_{i-\frac{1}{2},j-\frac{1}{2}} = A^n_{\textcircled{1}\,i-\frac{1}{2},j-\frac{1}{2}} + A^n_{\textcircled{2}\,i-\frac{1}{2},j-\frac{1}{2}} . \tag{3.35}$$

Finite-difference formulas for two-dimensional axisymmetric equations may be derived in the same way that Eqs.(3.23) and (3.24) were developed for the nonplanar one-dimensional cases. In Eqs.(2.19a) and (2.19b), terms of the form $\frac{1}{r}\frac{\partial}{\partial r}[r(\;)]$ are all expanded to the form $\frac{\partial}{\partial r}(\;) + \frac{(\;)}{r}$ so that Eqs. (3.28) and (3.33) may be used for both translational and axisymmetric geometries. In the latter case, x represents the radial coordinate and y the axial coordinate.

To derive axisymmetric formulas analogous to Eqs.(3.15) and (3.18) requires that the following substitutions be made in Eq.(3.26). The surface terms are of the form,

$$\begin{aligned} S_{TL_x} &= (y_T - y_L)\, 2\pi \left(\frac{x_T + x_L}{2}\right), \\ S_{TL_y} &= (x_T - y_L)\, 2\pi \left(\frac{x_T + x_L}{2}\right), \end{aligned} \tag{3.36a}$$

where $\frac{x_T + x_L}{2}$ is the average radius to the axisymmetric surface and $x = 0$ is the axis of symmetry. The grid point volume is the sum of the triangular cross-sectional toroidal volumes (rotated about $x = 0$) which make up the quadrilateral cross-sectional (LTRBL) toroidal volume (see Figure 3.2). The formula for a typical triangular cross-section toroid volume is

$$\mathcal{V}_{PLBP} = A_{PLBP}\; 2\pi \left(\frac{x_P + x_L + x_B}{3}\right) \tag{3.36b}$$

where $\left(\frac{x_P + x_L + x_B}{3}\right)$ is the radius of the "center" of the triangle PLBP.

Substituting Eqs.(3.36) into Eq.(3.26) yields a formula of the form

$$\frac{\partial}{\partial x}(\ )^n_P = \frac{3}{2}\,\frac{(\ )^n_{TL}\ \ (y_T - y_L)^n\ \ (x_T + x_L)^n\ +\ \cdots}{A^n_{PLBP}(x_P + x_L + x_B)\ +\ \cdots}\ ,$$

$$\frac{\partial}{\partial y}(\ )^n_P = \frac{3}{2}\,\frac{(\ )^n_{TL}\ \ (x_T - x_L)^n\ \ (x_T + x_L)^n\ +\ \cdots}{A^n_{PLBP}(x_P + x_L + x_B)^n\ +\ \cdots}\ . \qquad (3.37)$$

From Eq.(3.37), equations analogous to Eqs.(3.28) and (3.33) may be derived.

To calculate the two-dimensional zone volume, equations of the form of Eq.(3.36b) are used. Referring to Figure 3.3 and Eqs.(3.29a), (3.34), and (3.35), the true volume of a translational symmetry zone of constant slab depth equal to unity is

$$\mathcal{V}^n_{i-\frac{1}{2},j-\frac{1}{2}} = A^n_{i-\frac{1}{2},j-\frac{1}{2}}\ . \qquad (3.38)$$

The axisymmetric zone volume is

$$\mathcal{V}^n_{i-\frac{1}{2},j-\frac{1}{2}} = A^n_{\textcircled{1}\,i-\frac{1}{2},j-\frac{1}{2}}\ 2\pi\left(\frac{x^n_{i-1,j} + x^n_{i,j} + x^n_{i,j-1}}{3}\right)$$

$$+\ A^n_{\textcircled{2}\,i-\frac{1}{2},j-\frac{1}{2}}\ 2\pi\left(\frac{x^n_{i-1,j} + x^n_{i,j-1} + x^n_{i-1,j-1}}{3}\right)\ ,$$

or, in factored form,

$$\mathcal{V}^n_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{2\pi}{3}\Big[A^n_{\textcircled{1}\,i-\frac{1}{2},j-\frac{1}{2}}\left(x^n_{i-1,j} + x^n_{i,j} + x^n_{i,j-1}\right)$$

$$+\ A^n_{\textcircled{2}\,i-\frac{1}{2},j-\frac{1}{2}}\left(x^n_{i-1,j} + x^n_{i,j-1} + x^n_{i-1,j-1}\right)\Big]\ . \qquad (3.39)$$

A formula for translationally symmetric gradients at the center of a triangle can be derived using a method similar to the one used for gradients at the center of a quadrilateral zone (Eqs. 3.30). Referring to Figure 3.3, consider the triangle formed by the vertices TR-TL-BR-TR, i.e., the BL triangle with respect to grid point (i,j). Eqs.(3.8) become

$$\frac{\partial}{\partial x}(\;)^n_{PLBP} = \frac{(\;)^n_L S^n_{L_x} + (\;)^n_D S^n_{D_x} + (\;)^n_B S^n_{B_x}}{\mathcal{V}^n_{PLBP}} ,$$

$$\frac{\partial}{\partial y}(\;)^n_{PLBP} = - \frac{(\;)^n_L S^n_{L_y} + (\;)^n_D S^n_{D_y} + (\;)^n_B S^n_{B_y}}{\mathcal{V}^n_{PLBP}} . \tag{3.39a}$$

where subscript PLBP refers to the bottom left triangle with respect to grid point P, denoted by (i,j); subscript L refers to the face to the left of grid point (i,j); subscript B refers to the face below grid point (i,j); and subscript D refers to the diagonal face. In index notation, these equations become

$$\frac{\partial}{\partial x}(\;)^n_{PLBP} = \Big[(\;)^n_L (y^n_{i,j} - y^n_{i-1,j}) + (\;)^n_D (y^n_{i-1,j} - y^n_{i,j-1}) + (\;)^n_B (y^n_{i,j-1} - y^n_{i,j})\Big] / A^n_{PLBP} ,$$

$$\frac{\partial}{\partial y}(\;)^n_{PLBP} = - \Big[(\;)^n_L (x^n_{i,j} - x^n_{i-1,j}) + (\;)^n_D (x^n_{i-1,j} - x^n_{i,j-1}) + (\;)^n_B (x^n_{i,j-1} - x^n_{i,j})\Big] / A^n_{PLBP} . \tag{3.39b}$$

The quantities $(\ )^n_L$, $(\ )^n_D$, and $(\ )^n_B$ are defined using the notation of Figure 3.2.

$$(\ )^n_L \equiv \frac{(\ )^n_P + (\ )^n_L}{2} = \frac{(\ )^n_{i,j} + (\ )^n_{i-1,j}}{2} ,$$

$$(\ )^n_D \equiv \frac{(\ )^n_L + (\ )^n_B}{2} = \frac{(\ )^n_{i-1,j} + (\ )^n_{i,j-1}}{2} , \qquad (3.39c)$$

$$(\ )^n_B \equiv \frac{(\ )^n_P + (\ )^n_B}{2} = \frac{(\ )^n_{i,j} + (\ )^n_{i,j-1}}{2} .$$

Substituting Eqs.(3.39c) into (3.39b) yields

$$\frac{\partial}{\partial x}(\ )^n_{PLBP} = \frac{1}{2A^n_{PLBP}} \left\{ y^n_{i,j-1}\left[(\ )^n_{i,j} - (\ )^n_{i-1,j}\right] + y^n_{i,j}\left[(\ )^n_{i-1,j} - (\ )^n_{i,j-1}\right] + y^n_{i-1,j}\left[(\ )^n_{i,j-1} - (\ )^n_{i,j}\right] \right\} ,$$

$$(3.39d)$$

$$\frac{\partial}{\partial y}(\ )^n_{PLBP} = -\frac{1}{2A^n_{PLBP}} \left\{ x^n_{i,j-1}\left[(\ )^n_{i,j} - (\ )^n_{i-1,j}\right] + x^n_{i,j}\left[(\ )^n_{i-1,j} - (\ )^n_{i,j-1}\right] + x^n_{i-1,j}\left[(\ )^n_{i,j-1} - (\ )^n_{i,j}\right] \right\} .$$

The area of the triangle PLBP, A^n_{PLBP}, is computed from Eq.(3.29a).

3.5 THREE-DIMENSIONAL EQUATIONS

The three-dimensional equations are based on the mesh conventions shown in Figure 3.4. The formula to calculate a partial derivative at a point, say at mesh point P, can be derived from the x-, y-, and z-components of Eq.(3.8). The surface integral is defined over the eight triangular surface elements, TLF, TFR, TRA, TAL, BLF, BFR, BRA, and BAL. The volume enclosed by this surface (ALBRTF) is composed of eight tetrahedrons. The vertex of each tetrahedron is at point P, while its base is a surface element.

The area of a typical surface element is given by the formula

$$S = \frac{1}{2} \left| \underline{A} \times \underline{B} \right| \tag{3.40}$$

where $\underline{A}$ and $\underline{B}$ are vectors defining two sides of the surface triangle. Both $\underline{A}$ and $\underline{B}$ are directed from the same vertex. From Figure 3.5, the following more specific formula may be written for triangular element TLF,

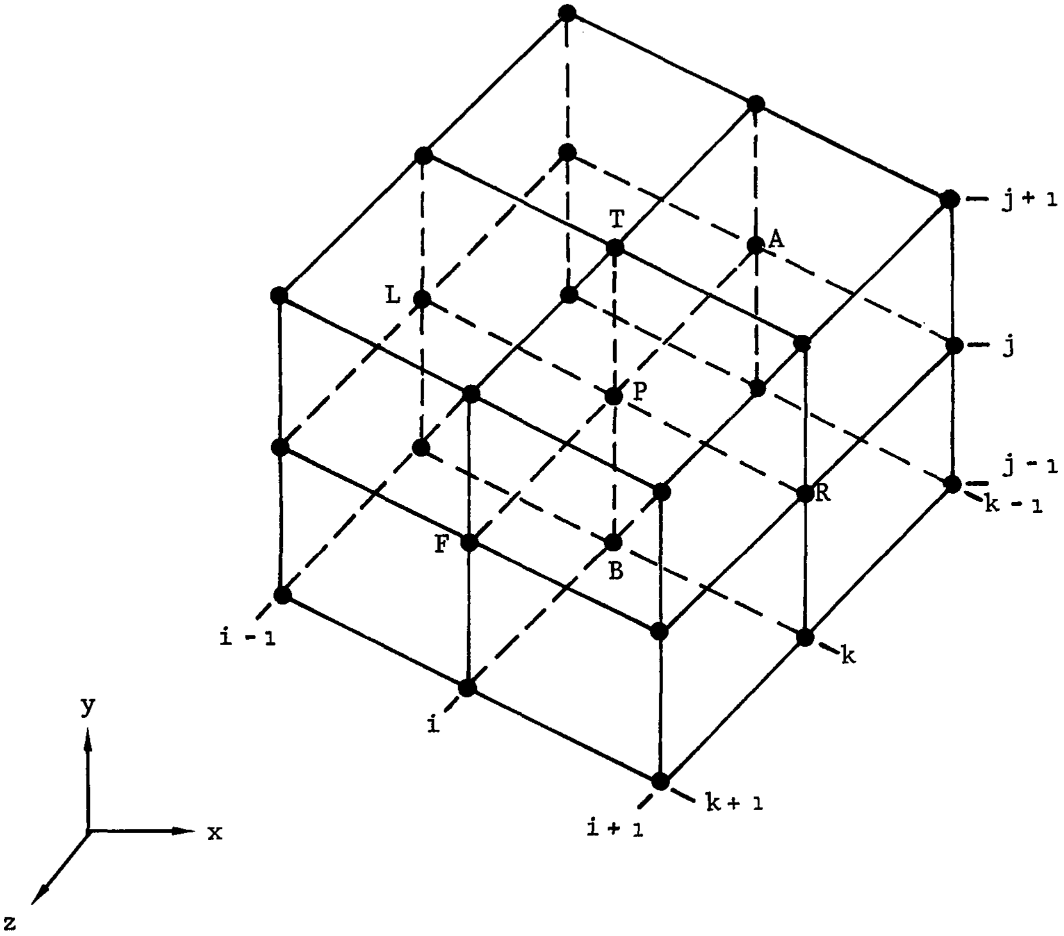
$$S_{TLF} = \frac{1}{2} \begin{vmatrix} i & j & k \\ x_L - x_T & y_L - y_T & z_L - z_T \\ x_F - x_T & y_F - y_T & z_F - z_T \end{vmatrix} \tag{3.41a}$$

Expanding Eq.(3.41a) yields

$$\begin{aligned} S_{TLF} = \frac{1}{2} \Big\{ & \underline{i}\Big[\left(y_L - y_T\right)\left(z_F - z_T\right) - \left(y_F - y_T\right)\left(z_L - z_T\right)\Big] \\ & + \underline{j}\Big[\left(x_F - x_T\right)\left(z_L - z_T\right) - \left(x_L - x_T\right)\left(z_F - z_T\right)\Big] \\ & + \underline{k}\Big[\left(x_L - x_T\right)\left(y_F - y_T\right) - \left(x_F - x_T\right)\left(y_L - y_T\right)\Big] \Big\} \end{aligned} \tag{3.41b}$$

or

$$S_{TLF} = \frac{1}{2}\left[\underline{i}\ S_{TLF_x} + \underline{j}\ S_{TLF_y} + \underline{k}\ S_{TLF_z}\right] . \tag{3.41c}$$



P = Point being calculated, (i,j,k)
L = Left of point P in index space, (i-1,j,k)
B = Bottom of point P in index space, (i,j-1,k)
R = Right of point P in index space, (i+1,j,k)
T = Top of point P in index space, (i,j+1,k)
A = Aft of point P in index space, (i,j,k-1)
F = Front of point P in index space, (i,j,k+1)

Figure 3.4. Three-dimensional Lagrange mesh.

$\underline{A} \equiv \underline{TL}$

$\underline{B} \equiv \underline{TF}$

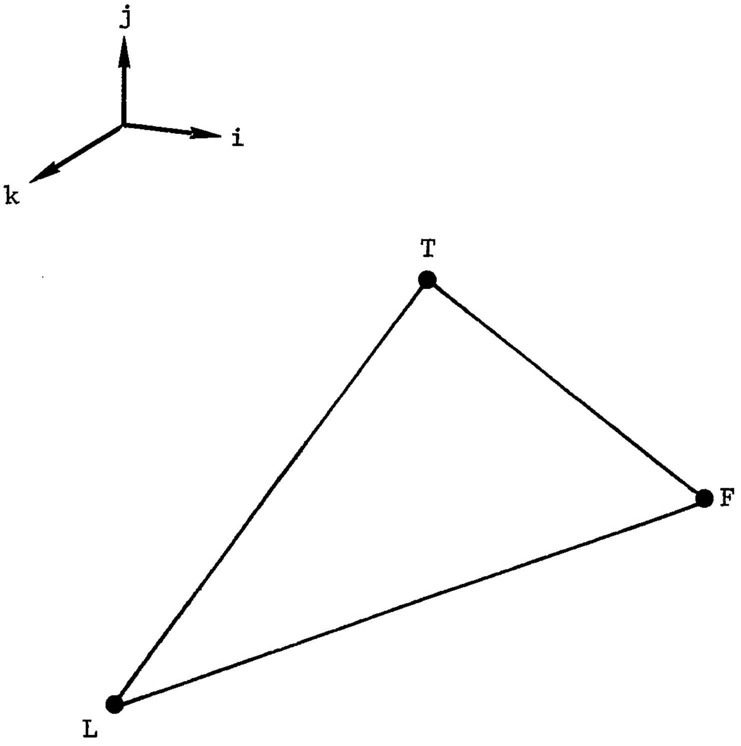


Figure 3.5. Three-dimensional tetrahedron surface area TLF.

Referring to Figure 3.4, the component formulas for defining the surface integral at a mesh point P are

$$\frac{\partial}{\partial x}(\;)^n_P = \Big[(\;)^n_{TLF}\;S^n_{TLF_x} + (\;)^n_{TFR}\;S^n_{TFR_x} + (\;)^n_{TRA}\;S^n_{TRA_x}$$

$$+ (\;)^n_{TAL}\;S^n_{TAL_x} + (\;)^n_{BLF}\;S^n_{BLF_x} + (\;)^n_{BFR}\;S^n_{BFR_x}$$

$$+ (\;)^n_{BRA}\;S^n_{BRA_x} + (\;)^n_{BAL}\;S^n_{BAL_x}\Big] / \;(\text{Volume})^n_{ALBRTF}\;, \tag{3.42a}$$

$$\frac{\partial}{\partial y}(\;)^n_P = \Big[(\;)^n_{TLF}\;S^n_{TLF_y} + (\;)^n_{TFR}\;S^n_{TFR_y} + (\;)^n_{TRA}\;S^n_{TRA_y}$$

$$+ (\;)^n_{TAL}\;S^n_{TAL_y} + (\;)^n_{BLF}\;S^n_{BLF_y} + (\;)^n_{BFR}\;S^n_{BFR_y}$$

$$+ (\;)^n_{BRA}\;S^n_{BRA_y} + (\;)^n_{BAL}\;S^n_{BAL_y}\Big] / \;(\text{Volume})^n_{ALBRTF}\;, \tag{3.42b}$$

$$\frac{\partial}{\partial z}(\;)^n_P = \Big[(\;)^n_{TLF}\;S^n_{TLF_z} + (\;)^n_{TFR}\;S^n_{TFR_z} + (\;)^n_{TRA}\;S^n_{TRA_z}$$

$$+ (\;)^n_{TAL}\;S^n_{TAL_z} + (\;)^n_{BLF}\;S^n_{BLF_z} + (\;)^n_{BFR}\;S^n_{BFR_z}$$

$$+ (\;)^n_{BRA}\;S^n_{BRA_z} + (\;)^n_{BAL}\;S^n_{BAL_z}\Big] / \;(\text{Volume})^n_{ALBRTF} \tag{3.42c}$$

Substituting appropriate index-space forms of Eq.(3.41b) into Eqs.(3.42) yields the following equations,

$$
\begin{aligned}
\frac{\partial}{\partial x}(\ )^n_P = \frac{1}{2}\Bigg\{ (\ )^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} & \Big[\left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right)\left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right) \\
& - \left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right)\left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} & \Big[\left(y^n_{i,j-1,k} - y^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right) \\
& - \left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} & \Big[\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right) \\
& - \left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i+1,j,k}\right)\Big] \\
+ (\ )^n_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} & \Big[\left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right) \\
& - \left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right)\Big] \qquad (3.43a) \\
+ (\ )^n_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} & \Big[\left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right)\left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right) \\
& - \left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right)\left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} & \Big[\left(y^n_{i,j-1,k} - y^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right) \\
& - \left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} & \Big[\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right) \\
& - \left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(y^n_{i,j+1,k} - y^n_{i,j,k+1}\right)\Big] \\
+ (\ )^n_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} & \Big[\left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right) \\
& - \left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right)\Big]\Bigg\} \Big/ \mathcal{V}^n_P ,
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial y}(\ )^n_p = \frac{1}{2} \Bigg\{ (\ )^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} & \Big[\left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right)\left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right) \\
& - \left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right)\left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} & \Big[\left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right) \\
& - \left(x^n_{i,j-1,k} - x^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} & \Big[\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i+1,j,k}\right) \\
& - \left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right)\Big] \\
+ (\ )^n_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} & \Big[\left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right) \\
& - \left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right)\Big] \\
+ (\ )^n_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} & \Big[\left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right)\left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right) \\
& - \left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right)\left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} & \Big[\left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right) \\
& - \left(x^n_{i,j-1,k} - x^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\Big] \\
+ (\ )^n_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} & \Big[\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(x^n_{i,j+1,k} - x^n_{i,j,k+1}\right) \\
& - \left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right)\Big] \\
+ (\ )^n_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} & \Big[\left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right) \\
& - \left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right)\Big] \Bigg\} \Big/ \mathcal{V}^n_p \ ,
\end{aligned}
\tag{3.43b}
$$

$$
\begin{aligned}
\frac{\partial}{\partial z}(\ )^n_P = \frac{1}{2}\Bigg\{ & (\ )^n_{i-\frac12,j-\frac12,k-\frac12}\Big[\left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right)\left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right)\left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right)\Big] \\
& + (\ )^n_{i+\frac12,j-\frac12,k-\frac12}\Big[\left(x^n_{i,j-1,k} - x^n_{i+1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i+1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\Big] \\
& + (\ )^n_{i+\frac12,j+\frac12,k-\frac12}\Big[\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i+1,j,k}\right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i+1,j,k}\right)\Big] \\
& + (\ )^n_{i-\frac12,j+\frac12,k-\frac12}\Big[\left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right)\Big] \\
& + (\ )^n_{i-\frac12,j-\frac12,k+\frac12}\Big[\left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right)\left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right)\left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right)\Big] \\
& + (\ )^n_{i+\frac12,j-\frac12,k+\frac12}\Big[\left(x^n_{i,j-1,k} - x^n_{i,j,k+1}\right)\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i,j,k+1}\right)\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\Big] \\
& + (\ )^n_{i+\frac12,j+\frac12,k+\frac12}\Big[\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\left(y^n_{i,j+1,k} - y^n_{i,j,k+1}\right) \\
& \qquad - \left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\left(x^n_{i,j+1,k} - x^n_{i,j,k+1}\right)\Big] \\
& + (\ )^n_{i-\frac12,j+\frac12,k+\frac12}\Big[\left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right)\Big]\Bigg\} \Big/ \mathcal{V}^n_P \, .
\end{aligned}
\tag{3.43c}
$$

The grid point volume, $\mathcal{V}_p^n$, may be calculated by averaging the zone volumes of the zones surrounding the grid point. An interior grid point will have eight zones to be averaged, a side grid point will have four, an edge will have two, and a corner will have one.

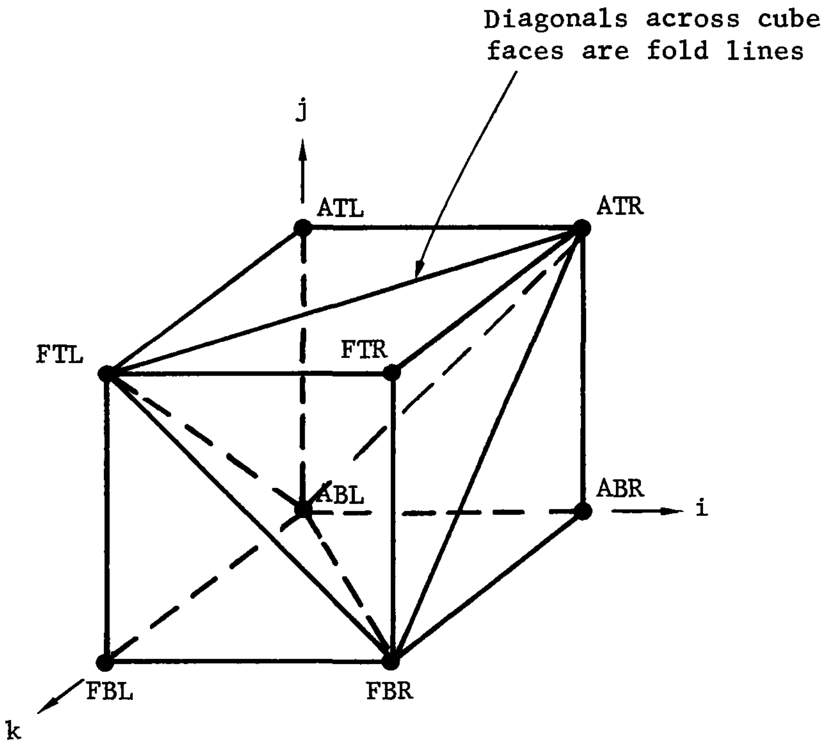
Zones in a three-dimensional mesh are defined by eight mesh points which are allowed to move independently, according to conservation of mass and momentum. These eight mesh points define a hexagon in index space and a duodecahedron in physical space. The duodecahedron (Figure 3.6) is not uniquely defined in that the "fold" in each index space face is arbitrary. Therefore, in order to be properly centered, the volume formula is taken to be the average of the parallelepiped volumes defined at each vertex. A parallelepiped volume is given by

$$\mathcal{V}_{\text{vertex}} = |\underline{A} \cdot (\underline{B} \times \underline{C})| \tag{3.44a}$$

$$= \begin{vmatrix} A_i & A_j & A_k \\ B_i & B_j & B_k \\ C_i & C_j & C_k \end{vmatrix} \tag{3.44b}$$

$$\begin{aligned} &= A_i(B_j C_k - B_k C_j) \\ &\quad + A_j(B_k C_i - B_i C_k) \\ &\quad + A_k(B_i C_j - B_j C_i) \ , \end{aligned} \tag{3.44c}$$

where $\underline{A}$, $\underline{B}$, and $\underline{C}$ are vectors pointing from the vertex. Considering zone $(i-\frac{1}{2}, j-\frac{1}{2}, k-\frac{1}{2})$, which is defined by the eight grid points (i,j,k), $(i,j-1,k)$, $(i,j-1,k-1)$, $(i,j,k-1)$, $(i-1,j,k)$, $(i-1,j-1,k)$, $(i-1,j-1,k-1)$, and $(i-1,j,k-1)$, the volume is



(··) = zone being calculated $(i-\frac{1}{2}, j-\frac{1}{2}, k-\frac{1}{2})$

FTR = front top right grid point (i,j,k)

FTL = front top left grid point (i-1,j,k)

FBL = front bottom left grid point (i-1,j-1,k)

FBR = front bottom right grid point (i,j-1,k)

ATR = aft top right grid point (i,j,k-1)

ATL = aft top left grid point (i-1,j,k-1)

ABL = aft bottom left grid point (i-1,j-1,k-1)

ABR = aft bottom right grid point (i,j-1,k-1)

L = left face (i-1)

R = right face (i)

B = bottom face (j-1)

T = top face (j)

A = aft face (k-1)

F = front face (k)

Figure 3.6. Typical duodecahedron zone.

$$
\begin{aligned}
&\mathcal{V}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \approx \\
&\frac{1}{8}\Bigg\{(x_{i,j,k} - x_{i,j-1,k}) \Big[(y_{i,j-1,k-1} - y_{i,j-1,k})\ (z_{i-1,j-1,k} - z_{i,j-1,k}) \\
&\qquad - (z_{i,j-1,k-1} - z_{i,j-1,k})\ (y_{i-1,j-1,k} - y_{i,j-1,k})\Big] \\
&+ (y_{i,j,k} - y_{i,j-1,k}) \Big[(z_{i,j-1,k-1} - z_{i,j-1,k})\ (x_{i-1,j-1,k} - x_{i,j-1,k}) \\
&\qquad - (x_{i,j-1,k-1} - x_{i,j-1,k})\ (z_{i-1,j-1,k} - z_{i,j-1,k})\Big] \\
&+ (z_{i,j,k} - z_{i,j-1,k}) \Big[(x_{i,j-1,k-1} - x_{i,j-1,k})\ (y_{i-1,j-1,k} - y_{i,j-1,k}) \\
&\qquad - (y_{i,j-1,k-1} - y_{i,j-1,k})\ (x_{i-1,j-1,k} - x_{i,j-1,k})\Big] \\
&+ (x_{i,j,k-1} - x_{i,j-1,k-1}) \Big[(y_{i-1,j-1,k-1} - y_{i,j-1,k-1})(z_{i,j-1,k} - z_{i,j-1,k-1}) \\
&\qquad - (z_{i-1,j-1,k-1} - z_{i,j-1,k-1})(y_{i,j-1,k} - y_{i,j-1,k-1})\Big] \\
&+ (y_{i,j,k-1} - y_{i,j-1,k-1}) \Big[(z_{i-1,j-1,k-1} - z_{i,j-1,k-1})(x_{i,j-1,k} - x_{i,j-1,k-1}) \\
&\qquad - (x_{i-1,j-1,k-1} - x_{i,j-1,k-1})(z_{i,j-1,k} - z_{i,j-1,k-1})\Big] \\
&+ (z_{i,j,k-1} - z_{i,j-1,k-1}) \Big[(x_{i-1,j-1,k-1} - x_{i,j-1,k-1})(y_{i,j-1,k} - y_{i,j-1,k-1}) \\
&\qquad - (y_{i-1,j-1,k-1} - y_{i,j-1,k-1})(x_{i,j-1,k} - x_{i,j-1,k-1})\Big]
\end{aligned}
$$

(This equation is continued on the following page.)

$$
\begin{aligned}
&+ (x_{i-1,j,k-1} - x_{i-1,j-1,k-1}) \Big[(y_{i-1,j-1,k} - y_{i-1,j-1,k-1})(z_{i,j-1,k-1} - z_{i-1,j-1,k-1}) \\
&\qquad - (z_{i-1,j-1,k} - z_{i-1,j-1,k-1})(y_{i,j-1,k-1} - y_{i-1,j-1,k-1})\Big] \\
&+ (y_{i-1,j,k-1} - y_{i-1,j-1,k-1}) \Big[(z_{i-1,j-1,k} - z_{i-1,j-1,k-1})(x_{i,j-1,k-1} - x_{i-1,j-1,k-1}) \\
&\qquad - (x_{i-1,j-1,k} - x_{i-1,j-1,k-1})(z_{i,j-1,k-1} - z_{i-1,j-1,k-1})\Big] \\
&+ (z_{i-1,j,k-1} - z_{i-1,j-1,k-1}) \Big[(x_{i-1,j-1,k} - x_{i-1,j-1,k-1})(y_{i,j-1,k-1} - y_{i-1,j-1,k-1}) \\
&\qquad - (y_{i-1,j-1,k} - y_{i-1,j-1,k-1})(x_{i,j-1,k-1} - x_{i-1,j-1,k-1})\Big] \\
&+ (x_{i-1,j,k} - x_{i-1,j-1,k}) \Big[(y_{i,j-1,k} - y_{i-1,j-1,k})(z_{i-1,j-1,k-1} - z_{i-1,j-1,k}) \\
&\qquad - (z_{i,j-1,k} - z_{i-1,j-1,k}))(y_{i-1,j-1,k-1} - y_{i-1,j-1,k})\Big] \\
&+ (y_{i-1,j,k} - y_{i-1,j-1,k}) \Big[(z_{i,j-1,k} - z_{i-1,j-1,k})(x_{i-1,j-1,k-1} - x_{i-1,j-1,k}) \\
&\qquad - (x_{i,j-1,k} - x_{i-1,j-1,k})(z_{i-1,j-1,k-1} - z_{i-1,j-1,k})\Big] \\
&+ (z_{i-1,j,k} - z_{i-1,j-1,k}) \Big[(x_{i,j-1,k} - x_{i-1,j-1,k})(y_{i-1,j-1,k-1} - y_{i-1,j-1,k}) \\
&\qquad - (y_{i,j-1,k} - y_{i-1,j-1,k})(x_{i-1,j-1,k-1} - x_{i-1,j-1,k})\Big]
\end{aligned}
$$

(This equation is continued on the following page.)

$$
\begin{aligned}
&+ (x_{i,j-1,k} - x_{i,j,k}) \Big[(y_{i-1,j,k} - y_{i,j,k}) (z_{i,j,k-1} - z_{i,j,k}) \\
&\qquad - (z_{i-1,j,k} - z_{i,j,k}) (y_{i,j,k-1} - z_{i,j,k}) \Big] \\
&+ (y_{i,j-1,k} - y_{i,j,k}) \Big[(z_{i-1,j,k} - z_{i,j,k}) (x_{i,j,k-1} - x_{i,j,k}) \\
&\qquad - (x_{i-1,j,k} - x_{i,j,k}) (z_{i,j,k-1} - z_{i,j,k}) \Big] \\
&+ (z_{i,j-1,k} - z_{i,j,k}) \Big[(x_{i-1,j,k} - x_{i,j,k}) (y_{i,j,k-1} - y_{i,j,k}) \\
&\qquad - (y_{i-1,j,k} - y_{i,j,k}) (x_{i,j,k-1} - x_{i,j,k}) \Big] \\
&+ (x_{i,j-1,k-1} - x_{i,j,k-1}) \Big[(y_{i,j,k} - y_{i,j,k-1}) (z_{i-1,j,k-1} - z_{i,j,k-1}) \\
&\qquad - (z_{i,j,k} - z_{i,j,k-1}) (y_{i-1,j,k-1} - y_{i,j,k-1}) \Big] \\
&+ (y_{i,j-1,k-1} - y_{i,j,k-1}) \Big[(z_{i,j,k} - z_{i,j,k-1}) (x_{i-1,j,k-1} - x_{i,j,k-1}) \\
&\qquad - (x_{i,j,k} - x_{i,j,k-1}) (z_{i-1,j,k-1} - z_{i,j,k-1}) \Big] \\
&+ (z_{i,j-1,k-1} - z_{i,j,k-1}) \Big[(x_{i,j,k} - x_{i,j,k-1}) (y_{i-1,j,k-1} - y_{i,j,k-1}) \\
&\qquad - (y_{i,j,k} - y_{i,j,k-1}) (x_{i-1,j,k-1} - x_{i,j,k-1}) \Big]
\end{aligned}
$$

(This equation is continued on the following page.)

$$
\begin{aligned}
&+ (x_{i-1,j-1,k-1} - x_{i-1,j,k-1}) \Big[(y_{i,j,k-1} - y_{i-1,j,k-1})(z_{i-1,j,k} - z_{i-1,j,k-1}) \\
&\qquad - (z_{i,j,k-1} - z_{i-1,j,k-1})(y_{i-1,j,k} - y_{i-1,j,k-1})\Big] \\
&+ (y_{i-1,j-1,k-1} - y_{i-1,j,k-1}) \Big[(z_{i,j,k-1} - z_{i-1,j,k-1})(x_{i-1,j,k} - x_{i-1,j,k-1}) \\
&\qquad - (x_{i,j,k-1} - x_{i-1,j,k-1})(z_{i-1,j,k} - z_{i-1,j,k-1})\Big] \\
&+ (z_{i-1,j-1,k-1} - z_{i-1,j,k-1}) \Big[(x_{i,j,k-1} - x_{i-1,j,k-1})(y_{i-1,j,k} - y_{i-1,j,k-1}) \\
&\qquad - (y_{i,j,k-1} - y_{i-1,j,k-1})(x_{i-1,j,k} - x_{i-1,j,k-1})\Big] \\
&+ (x_{i-1,j-1,k} - x_{i-1,j,k}) \Big[(y_{i-1,j,k-1} - y_{i-1,j,k}) (z_{i,j,k} - z_{i-1,j,k}) \\
&\qquad - (z_{i-1,j,k-1} - z_{i-1,j,k}) (y_{i,j,k} - y_{i-1,j,k})\Big] \\
&+ (y_{i-1,j-1,k} - y_{i-1,j,k}) \Big[(z_{i-1,j,k-1} - z_{i-1,j,k}) (x_{i,j,k} - x_{i-1,j,k}) \\
&\qquad - (x_{i-1,j,k-1} - x_{i-1,j,k}) (z_{i,j,k} - z_{i-1,j,k})\Big] \\
&+ (z_{i-1,j-1,k} - z_{i-1,j,k}) \Big[(x_{i-1,j,k-1} - x_{i-1,j,k}) (y_{i,j,k} - y_{i-1,j,k}) \\
&\qquad - (y_{i-1,j,k-1} - y_{i-1,j,k}) (x_{i,j,k} - x_{i-1,j,k})\Big]\Bigg\} .
\end{aligned}
\tag{3.44d}
$$

Formulas for gradients at the center of a zone $(\cdot\cdot)$ [where $(\cdot\cdot)$ means $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$] can be derived similarly to Eqs.(3.42). Referring to Figure 3.6,

$$\begin{aligned}\frac{\partial}{\partial x}(\ )^n_{(\cdot\cdot)} = \Big[&(\ )^n_L S^n_{L_x} + (\ )^n_R S^n_{R_x} \\ &+ (\ )^n_B S^n_{B_x} + (\ )^n_T S^n_{T_x} \\ &+ (\ )^n_A S^n_{A_x} + (\ )^n_F S^n_{F_x} \Big] / \mathcal{V}^n_{(\cdot\cdot)} \ ,\end{aligned} \tag{3.45a}$$

$$\begin{aligned}\frac{\partial}{\partial y}(\ )^n_{(\cdot\cdot)} = \Big[&(\ )^n_L S^n_{L_y} + (\ )^n_R S^n_{R_y} \\ &+ (\ )^n_B S^n_{B_y} + (\ )^n_T S^n_{T_y} \\ &+ (\ )^n_A S^n_{A_y} + (\ )^n_F S^n_{F_y} \Big] / \mathcal{V}^n_{(\cdot\cdot)} \ ,\end{aligned} \tag{3.45b}$$

$$\begin{aligned}\frac{\partial}{\partial z}(\ )^n_{(\cdot\cdot)} = \Big[&(\ )^n_L S^n_{L_z} + (\ )^n_R S^n_{R_z} \\ &+ (\ )^n_B S^n_{B_z} + (\ )^n_T S^n_{T_z} \\ &+ (\ )^n_A S^n_{A_z} + (\ )^n_F S^n_{F_z} \Big] / \mathcal{V}^n_{(\cdot\cdot)} \ .\end{aligned} \tag{3.45c}$$

A typical term of the form $(\ )^n S^n$ in Eqs.(3.45) is calculated by dividing each face into two triangles twice, evaluating the appropriate factors, and averaging the result. As an example, consider the term $(\ )^n_R S^n_{R_x}$. First, divide the right face into the triangles with a common base formed by the diagonal FBR-ATR. The areas of these triangles are determined from Eqs.(3.41). Denoting the triangles by the vertex opposite the common base, the formula for $(\ )^n_R\, S^n_{R_x}$ based on the diagonal FBR-ATR becomes

$$\begin{aligned}\left[(\ )^n_R\, S^n_{R_x}\right]_{FBR-ATR} = {} & \frac{1}{2}(\ )^n_{\Delta_{FTR}} \Big[(y^n_{FBR} - y^n_{FTR})(z^n_{ATR} - z^n_{FTR}) \\ & - (y^n_{ATR} - y^n_{FTR})(z^n_{FBR} - z^n_{FTR})\Big] \\ & + \frac{1}{2}(\ )^n_{\Delta_{ABR}} \Big[(y^n_{FBR} - y^n_{ATR})(z^n_{ABR} - z^n_{ATR}) \\ & - (y^n_{ABR} - y^n_{ATR})(z^n_{FBR} - z^n_{ATR})\Big] \ . \end{aligned} \tag{3.46a}$$

Changing the diagonal to connect the grid points FTR-ABR yields the formula

$$\begin{aligned}\left[(\ )^n_R\, S^n_{R_x}\right]_{FTR-ABR} = {} & \frac{1}{2}(\ )^n_{\Delta_{FBR}} \Big[(y^n_{FBR} - y^n_{FTR})(z^n_{ABR} - z^n_{FTR}) \\ & - (y^n_{ABR} - y^n_{FTR})(z^n_{FBR} - z^n_{FTR})\Big] \\ & + \frac{1}{2}(\ )^n_{\Delta_{ATR}} \Big[(y^n_{ABR} - y^n_{FTR})(z^n_{ATR} - z^n_{FTR}) \\ & - (y^n_{ATR} - y^n_{FTR})(z^n_{ABR} - z^n_{FTR})\Big] \ . \end{aligned} \tag{3.46b}$$

Averaging Eqs.(3.46a) and (3.46b) yields a formula for $(\ )_R^n\, S_{R_x}^n$ which is independent of the choice of diagonal

$$(\ )_R^n\, S_{R_x}^n = \frac{1}{2}\left\{\left[(\ )_R^n\, S_{R_x}^n\right]_{FBR-ATR} + \left[(\ )_R^n\, S_{R_x}^n\right]_{FTR-ABR}\right\} . \tag{3.46c}$$

The triangle-centered values of the variable for which the gradient is being taken are usually computed as the average of the grid point centered values. Thus,

$$(\ )_{\Delta_{FTR}}^n \equiv \frac{1}{3}\left[(\ )_{FTR}^n + (\ )_{ATR}^n + (\ )_{FBR}^n\right] ,$$

$$(\ )_{\Delta_{ABR}}^n \equiv \frac{1}{3}\left[(\ )_{ABR}^n + (\ )_{FBR}^n + (\ )_{ATR}^n\right] ,$$

$$(\ )_{\Delta_{FBR}}^n \equiv \frac{1}{3}\left[(\ )_{FBR}^n + (\ )_{FTR}^n + (\ )_{ABR}^n\right] ,$$

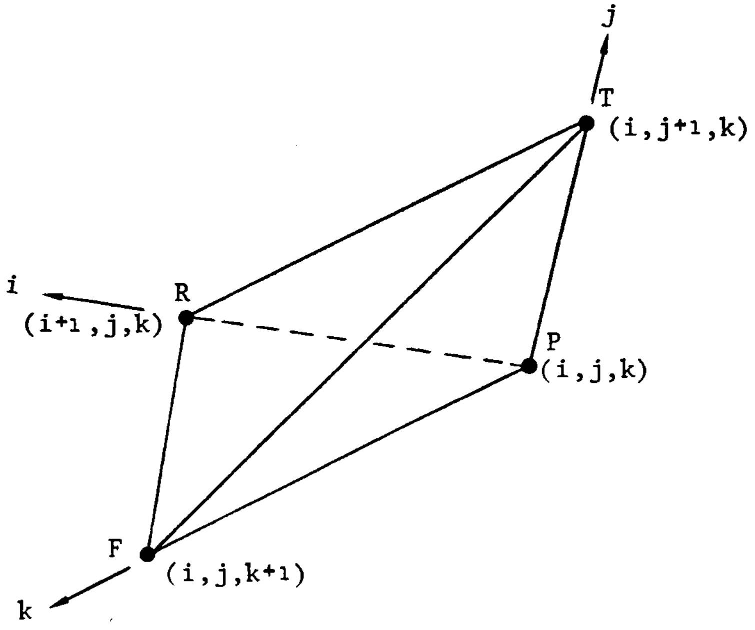
$$(\ )_{\Delta_{ATR}}^n \equiv \frac{1}{3}\left[(\ )_{ATR}^n + (\ )_{ABR}^n + (\ )_{FTR}^n\right] . \tag{3.46d}$$

Formulas for gradients at the center of a tetrahedral volume can be derived using a method similar to the one used for gradients at the center of the duodecahedron zone, Eqs.(3.45). Referring to Figure 3.7, which shows the front-top-left tetrahedron, PRTF, with respect to grid point (i,j,k), Eqs.(3.8) become

$$\frac{\partial}{\partial x}(\ )^n_{PRTF} = \left[(\ )^n_\ell\, S^n_{\ell_x} + (\ )^n_i\, S^n_{i_x} + (\ )^n_j\, S^n_{j_x} + (\ )^n_k\, S^n_{k_x}\right] / \mathcal{V}^n_{PRTF}\,, \qquad (3.47a)$$

$$\frac{\partial}{\partial y}(\ )^n_{PRTF} = \left[(\ )^n_\ell\, S^n_{\ell_y} + (\ )^n_i\, S^n_{i_y} + (\ )^n_j\, S^n_{j_y} + (\ )^n_k\, S^n_{k_y}\right] / \mathcal{V}^n_{PRTF}\,, \qquad (3.47b)$$

$$\frac{\partial}{\partial z}(\ )^n_{PRTF} = \left[(\ )^n_\ell\, S^n_{\ell_z} + (\ )^n_i\, S^n_{i_z} + (\ )^n_j\, S^n_{j_z} + (\ )^n_k\, S^n_{k_z}\right] / \mathcal{V}^n_{PRTF}\,. \qquad (3.47c)$$



tet_1 = front-top-left tetrahedron

PTF = face i   P = grid point (i,j,k)
PFR = face j   R = grid point (i+1,j,k)
PRT = face k   T = grid point (i,j+1,k)
RFT = face ℓ F = grid point (i,j,k+1)

Figure 3.7. Front-top-left tetrahedron.

A typical term of the form $(\ )^n S^n$ in Eqs. (3.47) is evaluated on a tetrahedral face, i.e., a triangle. The four terms in each component equation correspond to the four triangle surfaces that enclose the tetrahedron. The subscript convention denotes the three faces coming together at grid point (i,j,k), as faces i,j,k corresponding to the index space planes to which they are parallel, and the fourth face as ℓ, which has no vertex at grid point (i,j,k). Face ℓ "leans" on the other three faces. The areas of the surface triangles are determined from Eqs.(3.41).

Using the notation of Figure 3.7, the x-gradient terms are

$$\left[(\ )_i^n\ S_{i_x}^n\right]_{PRTF} = \frac{1}{2}(\ )^n_{\Delta_{PTF}}\left[(y_T^n - y_P^n)(z_F^n - z_P^n) - (y_F^n - y_P^n)(z_T^n - z_P^n)\right] , \tag{3.48a}$$

$$\left[(\ )_j^n\ S_{j_x}^n\right]_{PRTF} = \frac{1}{2}(\ )^n_{\Delta_{PRF}}\left[(y_R^n - y_P^n)(z_F^n - z_P^n) - (y_F^n - y_P^n)(z_R^n - z_P^n)\right] , \tag{3.48b}$$

$$\left[(\ )_k^n\ S_{k_x}^n\right]_{PRTF} = \frac{1}{2}(\ )^n_{\Delta_{PRT}}\left[(y_R^n - y_P^n)(z_T^n - z_P^n) - (y_T^n - y_P^n)(z_R^n - z_P^n)\right] , \tag{3.48c}$$

$$\left[(\ )_\ell^n\ S_{\ell_x}^n\right]_{PRTF} = \frac{1}{2}(\ )^n_{\Delta_{RFT}}\left[(y_F^n - y_R^n)(z_T^n - z_R^n) - (y_T^n - y_R^n)(z_F^n - z_R^n)\right] . \tag{3.48d}$$

The triangle-centered values of the variable for which the gradient is being taken are usually computed as the average of the grid-point-centered values. Thus,

$$
\begin{aligned}
(\ )^n_{\Delta_{PTF}} &\equiv \frac{1}{3}\left[(\ )^n_P + (\ )^n_T + (\ )^n_F\right], \\
(\ )^n_{\Delta_{PRF}} &\equiv \frac{1}{3}\left[(\ )^n_P + (\ )^n_R + (\ )^n_F\right], \\
(\ )^n_{\Delta_{PRT}} &\equiv \frac{1}{3}\left[(\ )^n_P + (\ )^n_R + (\ )^n_T\right], \\
(\ )^n_{\Delta_{RFT}} &\equiv \frac{1}{3}\left[(\ )^n_R + (\ )^n_F + (\ )^n_T\right].
\end{aligned}
\tag{3.49}
$$

The tetrahedron volume can be computed from Eq.(3.44a) by taking one quarter of the volume of the parallelepiped that is formed around the tetrahedron PRTF. The parallelepiped volume is computed from the three vectors coming together at P.

Specific numerical representations of the one-, two-, and three-dimensional Lagrange continuum mechanics equations utilizing the surface integral approach are presented in Sections 4, 5, and 6, respectively.

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SECTION 4

ONE-DIMENSIONAL LAGRANGIAN FINITE-DIFFERENCE EQUATIONS

4.1 INTRODUCTION

The Lagrange explicit finite-difference equations which represent the physical equations of a one-dimensional continuum are solved using two overlapping meshes -- a displacement mesh and a stress mesh. The displacement mesh is made up of grid (mesh) points which define geometric quantities such as shapes, interfaces, and boundaries. Conservation of momentum is used in the displacement mesh to solve for the vector variables, acceleration, $\ddot{x}$, velocity, $\dot{x}$, and position, x, at specific points in space. The stress mesh is made up of zones in which scalars and tensors are calculated as averages over zone volumes and surface areas using conservation of internal energy and constitutive equations to solve for scalar and tensor variables such as stress, σ_{xx}, σ_{yy}, etc., internal energy, u, pressure, p, etc.

Both meshes describe the same region of space and are related through identical satisfaction of conservation of mass; that is, density, ρ, in both meshes describes the existence of material in the same way. Thus the relationship between meshes is that the grid points of the displacement mesh uniquely define the zones of the stress mesh.

4.2 DISPLACEMENT MESH

4.2.1 Calculational Sequence. The one-dimensional Lagrange continuum mechanics equations are solved in three steps. First, the momentum equation is solved to determine mechanical motion from stress, internal energy, and density distributions. Next, conservation of mass is used to calculate new density distribution, and finally, the constitutive relations and conservation of internal energy are solved simultaneously to calculate a new stress and internal energy distribution. This procedure is shown schematically in Figure 4.1.

$$\left. x_i^n,\ \dot{x}_i^{n-\frac{1}{2}},\qquad \rho^n_{i-\frac{1}{2}},\ \sigma^n_{i-\frac{1}{2}} \right\}\ \text{Initial Conditions}$$

$$\left. \ddot{x}_i^n \right\}\ \text{Conservation of Momentum}$$

$$\text{Explicit Integration}\ \left\{ \begin{array}{l} \dot{x}_i^{n+\frac{1}{2}},\ \Delta t^n \\ x_i^{n+1},\ \Delta t^{n+\frac{1}{2}} \end{array} \right.$$

$$\left. \rho^{n+1}_{i-\frac{1}{2}} \right\}\ \text{Conservation of Mass}$$

$$\begin{array}{l}\text{Simultaneous} \\ \text{Solution for} \\ \text{Explicit} \\ \text{Time Step} \\ \Delta t^{n+1/2}\end{array} \left\{ \begin{array}{ll} \left. u^{n+1}_{i-\frac{1}{2}} = u\left(p^{n+1}_{i-\frac{1}{2}},\ \rho^{n+1}_{i-\frac{1}{2}},\ s^{n+1}_{i-\frac{1}{2}}\right) \right\} & \begin{array}{l}\text{Conservation} \\ \text{of Energy}\end{array} \\ \\ \left. \begin{array}{l} p^{n+1}_{i-\frac{1}{2}} = p\left(u^{n+1}_{i-\frac{1}{2}},\ \rho^{n+1}_{i-\frac{1}{2}}\right) \\ s^{n+1}_{i-\frac{1}{2}} = s\left(\rho^{n+1}_{i-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2}},\ u^{n+1}_{i-\frac{1}{2}}\right) \end{array} \right\} & \begin{array}{l}\text{Constitutive} \\ \text{Relations}\end{array} \end{array} \right.$$

$$\left. \sigma^{n+1}_{i-\frac{1}{2}} \right\}\ \begin{array}{l}\text{Initial Conditions} \\ \text{for Next Time Step (cycle)}\end{array}$$

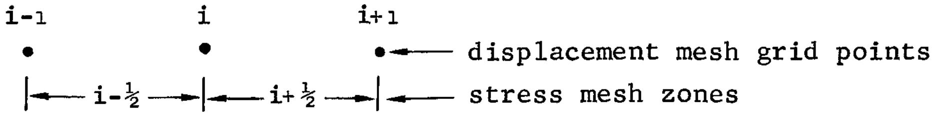
$$\left. \Delta t^{n+1} \right\}\ \begin{array}{l}\text{Time Step} \\ \text{for Next Cycle from} \\ \text{Courant Stability Criterion}\end{array}$$

Figure 4.1. One-dimensional calculational cycle.

4.2.2 Momentum Equation. The general momentum equation for one independent space variable (for slab, cylindrical, and spherical symmetries) is

$$\ddot{x} = \frac{1}{\rho}\frac{\partial\sigma_{xx}}{\partial x} + f\,\frac{1}{\rho}\left[\frac{\sigma_{xx}-\sigma_{yy}}{x}\right] + g_x\,, \qquad (4.1)^*$$

where $f=0$ for plane (slab) symmetry, $f=1$ for cylindrical** symmetry, and $f=2$ for spherical** symmetry. The finite-difference form of this equation can be derived in such a way that it is possible to use the same numerical equation for boundary points as well as interior points. Consider the nonboundary grid point, i, and its immediate neighbors, as shown below.



The grid point neighbors of grid point i are points $i-1$ on the left, and $i+1$ on the right. The volume defined by grid points $i-1$ and i is called zone $i-\frac{1}{2}$. The volume defined by grid points i and $i+1$ is called zone $i+\frac{1}{2}$.

To derive a properly centered finite-difference form of the momentum equation, Eq.(4.1) is rewritten as follows,

$$\ddot{x}_i^n = \frac{1}{\rho_i^n}\left(\frac{\Delta\sigma_{xx}}{\Delta x}\right)_i^n + f\,\frac{1}{\rho_i^n}\left[\frac{\sigma_{xx}-\sigma_{yy}}{x}\right]_i^n + g_x\,, \qquad (4.2a)$$

where superscripts denote the time centering, while subscripts denote space centering; or

$$\ddot{x}_i^n = \frac{V_i^n}{\rho_i^o}\left(\frac{\Delta\sigma_{xx}}{\Delta x}\right)_i^n + f\,\frac{V_i^n}{\rho_i^o}\left[\frac{\sigma_{xx}-\sigma_{yy}}{x}\right]_i^n + g_x\,, \qquad (4.2b)$$

---

[*] In general, gravity (g_x) may only act in slab symmetry.

[**] For divergent symmetries, replace x with r; xx with rr; and yy with $\theta\theta$. See Eqs. (2.15a), (2.16a), and (2.17a).

where V_i^n is the relative volume, defined as

$$V_i^n \equiv \frac{\rho_i^o}{\rho_i^n} ,$$

where ρ_i^o is a reference density usually taken to be the density at zero stress. Equations (4.2a) and (4.2b) represent a time- and space-centered partial differential equation which can be reduced to

$$\ddot{x}_i^n = \frac{\Delta\sigma_{xx_i}^n}{\alpha_i^n} + f\,\beta_i^n + g_x , \tag{4.3}$$

where α_i^n is the areal density,

$$\alpha_i^n \equiv \frac{\alpha_{i-\frac{1}{2}}^n + \alpha_{i+\frac{1}{2}}^n}{2} , \tag{4.3a}$$

and β_i^n is the circumferential stress contribution,

$$\beta_i^n \equiv \beta_{i-\frac{1}{2}}^n + \beta_{i+\frac{1}{2}}^n . \tag{4.3b}$$

Equation (4.3a) is derived using the definition of a first-order spatial average and $\Delta\sigma_{xx_i}^n$ can be derived from the definition of a first-order spatial difference,

$$(\;)_i \equiv \frac{(\;)_{i-\frac{1}{2}} + (\;)_{i+\frac{1}{2}}}{2} , \tag{4.4a}$$

$$\Delta(\;)_i \equiv (\;)_{i+\frac{1}{2}} - (\;)_{i-\frac{1}{2}} . \tag{4.4b}$$

Rewriting Eq.(4.3) in spatially centered difference notation using Eqs.(4.4a) and (4.4b), yields

$$\ddot{x}_i^n = \left(\frac{2}{\alpha^n_{i-\frac{1}{2}} + \alpha^n_{i+\frac{1}{2}}}\right)\left(\sigma^n_{xx_{i+\frac{1}{2}}} - \sigma^n_{xx_{i-\frac{1}{2}}}\right) + f\left(\beta^n_{i-\frac{1}{2}} + \beta^n_{i+\frac{1}{2}}\right) + g_x \ , \quad (4.5)$$

where $\alpha^n_{i-\frac{1}{2}}$, $\alpha^n_{i+\frac{1}{2}}$, $\beta^n_{i-\frac{1}{2}}$, and $\beta^n_{i+\frac{1}{2}}$ are defined as follows,

$$\alpha^n_{i-\frac{1}{2}} = \rho^n_{i-\frac{1}{2}}\left(x^n_i - x^n_{i-1}\right) = \frac{\rho^o_{i-\frac{1}{2}}}{V^n_{i-\frac{1}{2}}}\left(x^n_i - x^n_{i-1}\right) \ ; \quad (4.6a)$$

$$\alpha^n_{i+\frac{1}{2}} = \rho^n_{i+\frac{1}{2}}\left(x^n_{i+1} - x^n_i\right) = \frac{\rho^o_{i+\frac{1}{2}}}{V^n_{i+\frac{1}{2}}}\left(x^n_{i+1} - x^n_i\right) \ ; \quad (4.6b)$$

$$\beta^n_{i-\frac{1}{2}} = \frac{\left(\sigma^n_{xx_{i-\frac{1}{2}}} - \sigma^n_{yy_{i-\frac{1}{2}}}\right)\left(x^n_i - x^n_{i-1}\right)}{\left(\alpha^n_{i-\frac{1}{2}} + \alpha^n_{i+\frac{1}{2}}\right)\left(\frac{x^n_i + x^n_{i-1}}{2}\right)} \ ; \quad (4.6c)$$

$$\beta^n_{i+\frac{1}{2}} = \frac{\left(\sigma^n_{xx_{i+\frac{1}{2}}} - \sigma^n_{yy_{i+\frac{1}{2}}}\right)\left(x^n_{i+1} - x^n_i\right)}{\left(\alpha^n_{i-\frac{1}{2}} + \alpha^n_{i+\frac{1}{2}}\right)\left(\frac{x^n_{i+1} + x^n_i}{2}\right)} \ . \quad (4.6d)$$

Numerical evaluation of Eq.(4.5) yields grid-point acceleration of grid point i at time n. To determine the velocity and position of grid point i requires two time-centered integrations. Figures 4.2 and 4.3 are pictorial representations of these time-centered integrations. Equation (4.7) is a

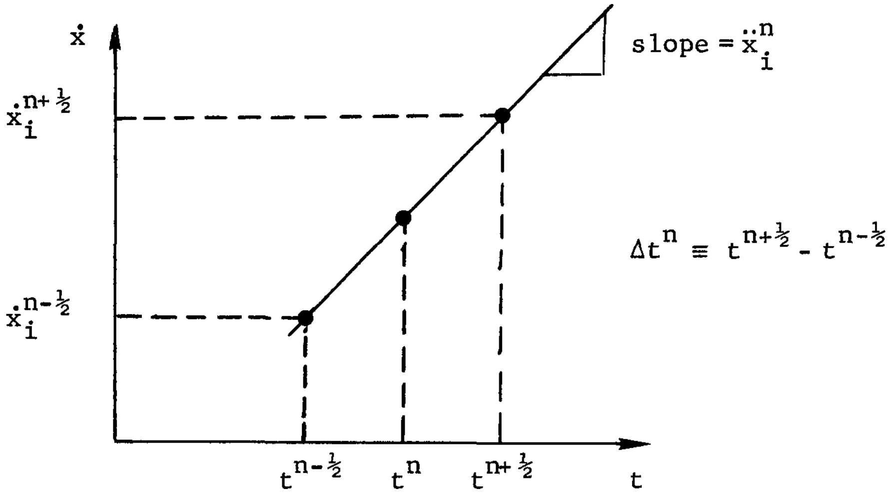


Figure 4.2. Pictorial representation of velocity integration.

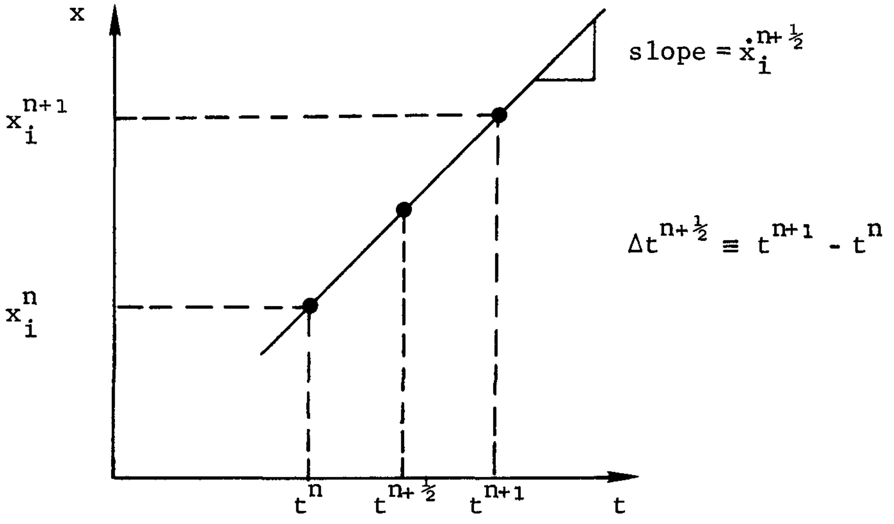


Figure 4.3. Pictorial representation of displacement integration.

time-centered integration of Eq.(4.5) for velocity,

$$\dot{x}_i^{n+\frac{1}{2}} = \dot{x}_i^{n-\frac{1}{2}} + \ddot{x}_i^n \Delta t^n , \tag{4.7}$$

and Eq.(4.8) is a time-centered integration of Eq.(4.7) for position,

$$x_i^{n+1} = x_i^n + \dot{x}_i^{n+\frac{1}{2}} \Delta t^{n+\frac{1}{2}} . \tag{4.8}$$

The time step values Δt^n and $\Delta t^{n+\frac{1}{2}}$ used in Eqs.(4.7) and (4.8) are determined from the stability requirement that a sound signal can only propagate the smallest zone dimension of the entire mesh or less in one time step. Mathematically, this condition, called the Courant stability criterion, is written as follows:

$$\Delta t^n = \text{minimum value of } \Delta t^n_{i-\frac{1}{2}} \text{ for all } i ;$$

$$\Delta t^{n+\frac{1}{2}} = \text{minimum value of } \Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2}} \text{ for all } i ;$$

where, from Eq.(3.1),

$$\Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2}} \le \frac{\Delta \ell^n_{i-\frac{1}{2}}}{c^n_{i-\frac{1}{2}}} , \quad \Delta t^n_{i-\frac{1}{2}} = \frac{\Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2}} + \Delta t^{n-\frac{1}{2}}_{i-\frac{1}{2}}}{2} . \tag{4.9a),(4.9b}$$

$\Delta \ell^n_{i-\frac{1}{2}}$ is the smallest length across zone $i-\frac{1}{2}$ at time n, and $c^n_{i-\frac{1}{2}}$ is the sound speed of zone $i-\frac{1}{2}$ at time n. Values at time n come from initial conditions or a previous cycle.

Equations (4.7) and (4.8) use the definition for a first-order temporal difference analogous to Eq.(4.4b),

$$\Delta(\ )^n \equiv (\ )^{n+\frac{1}{2}} - (\ )^{n-\frac{1}{2}} , \tag{4.10a}$$

and

$$\Delta(\ )^{n+\frac{1}{2}} \equiv (\ )^{n+1} - (\ )^n . \tag{4.10b}$$

Equations (4.5), (4.7), and (4.8) are perfectly centered in space and time. However, a time-centering error can occur in Eq.(4.7) for the initial step because $\dot{x}_i^{n-\frac{1}{2}}$ may not be known at time $n - \frac{1}{2}$. In this case, it is common to let $\dot{x}_i^{n-\frac{1}{2}}$ take on the value of $\dot{x}_i^n$ and to use an initial time step, Δt^o, that is 0.1 of the initial stable value. After the initial time step, Eq.(4.7) is properly centered.*

4.2.3 <u>Momentum Boundary Conditions</u>. Momentum boundary conditions are of two types -- those that use a stress or force and those that use an acceleration, a velocity, or a displacement. The former, known as "stress-type boundaries," affect Eq.(4.5) while the latter, known as "velocity-type boundaries," affect Eqs.(4.7) and (4.8). In addition to the two types of boundary conditions, there are two ways in which boundary values are obtained, i.e., by prescription or by interaction. By prescription means that boundary values are provided as time histories for an entire event; by interaction means that an algorithm for calculating values is provided.

Equation (4.5), which was derived for non-boundary points, is well suited for stress-type boundary conditions. Left boundary conditions affect the $i-\frac{1}{2}$ values in Eq.(4.5), while right boundary conditions affect the $i+\frac{1}{2}$ values. There are four possible boundary orientations in one-dimensional geometry. They are:

(1) outside left,
(2) outside right,
(3) inside left,
(4) inside right.

(The inside left and inside right boundaries are associated with the existence of an interior void located between two independent grids.)

---

*Equation (4.7) may be written in "dynamic relaxation" form so that static and quasi-static calculations are computed more efficiently. A discussion of dynamic relaxation appears in Section 4.5.

An example of a left boundary condition is a free left boundary. Mathematically, the free left boundary is given by

$$\sigma^n_{xx_{i-\frac{1}{2}}} = \sigma^n_{yy_{i-\frac{1}{2}}} = 0 ; \qquad \qquad (4.11)$$

$$\rho^n_{i-\frac{1}{2}} = 0 .$$

Substituting Eq.(4.11) into Eq.(4.5) yields

$$\ddot{x}^n_i = \left(\frac{2}{\alpha^n_{i+\frac{1}{2}}}\right)\left(\sigma^n_{xx_{i+\frac{1}{2}}}\right) + f\beta^n_{i+\frac{1}{2}} \quad . \qquad (4.12)$$

The formula for acceleration of a free right boundary is derived in a similar manner. The condition for a free right boundary is

$$\sigma^n_{xx_{i+\frac{1}{2}}} = \sigma^n_{yy_{i+\frac{1}{2}}} = 0 ; \qquad \qquad (4.13)$$

$$\rho^n_{i+\frac{1}{2}} = 0 .$$

Substituting Eq.(4.13) into Eq.(4.5) yields

$$\ddot{x}^n_i = \left(\frac{2}{\alpha^n_{i-\frac{1}{2}}}\right)\left(-\sigma^n_{xx_{i-\frac{1}{2}}}\right) + f\beta^n_{i-\frac{1}{2}} \quad . \qquad (4.14)$$

Velocity-type boundary conditions eliminate the need for Eq.(4.5). These conditions affect Eqs.(4.7) and/or (4.8) directly.

The simplest way to provide boundary values is by prescription. That is, stress (or velocity) is given at the beginning of a problem for all time at a boundary grid point. The value is a function of time only, since the location of the grid point is always known. If the boundary value is tied to a coordinate which is different from the boundary grid point, then an interaction calculation is required. For example, outside boundaries can interact with geometric constraints (wall segments) and inside boundaries can interact with each other by coming together to close a void. In general, when a boundary grid point engages a constraint or another boundary grid point, a velocity condition is required. When a boundary grid point disengages, a stress-type boundary calculation is required, e.g., it can become free.

Equations of interaction between a grid point and a constraint or between two grid points are governed by the principle of conservation of momentum during the moment of initial contact and during intimate contact. During the time when the points move independently and at the moment of separation, the grid points are separate stress-type boundaries.

In the one-dimensional case, it is possible to close a void (between grid point and constraint or between two grid points) exactly. The procedure requires that the time step be chosen in such a way that it satisfies stability requirements while exactly bringing together grid point and constraint or two grid points. The formula for the time step is derived by inverting the momentum equation as follows:

> Assume that an interior void (defined by two grid points) is closing. Prior to closure, the left side of the void is moving as if it were a free right boundary. Its acceleration, $\ddot{x}_R^n$, is given by Eq.(4.12). The right side of the void is moving as if it were a free left boundary. Its acceleration, $\ddot{x}_L^n$, is given by Eq.(4.14). The condition

for closure is

$$x_L^{n+1} = x_R^{n+1} , \qquad (4.15)$$

where subscripts L and R refer to the grid points (and zones) immediately to the left and right of the void. Equation (4.15) can be rewritten in terms of free left and free right accelerations as follows,

$$x_L^n + \Delta t^{n+\frac{1}{2}} \dot{x}_L^{n+\frac{1}{2}} = x_R^n + \Delta t^{n+\frac{1}{2}} \dot{x}_R^{n+\frac{1}{2}} ,$$

$$x_L^n + \Delta t^{n+\frac{1}{2}}\left(\dot{x}_L^{n-\frac{1}{2}} + \Delta t^n \ddot{x}_L^n\right) = x_R^n + \Delta t^{n+\frac{1}{2}}\left(\dot{x}_R^{n-\frac{1}{2}} + \Delta t^n \ddot{x}_R^n\right) . \qquad (4.16)$$

Combining left and right positions, left and right velocities, and left and right accelerations yields

$$\Delta t^{n+\frac{1}{2}} \Delta t^n\left(\ddot{x}_R^n - \ddot{x}_L^n\right) + \Delta t^{n+\frac{1}{2}}\left(\dot{x}_R^{n-\frac{1}{2}} - \dot{x}_L^{n-\frac{1}{2}}\right) + \left(x_R^n - x_L^n\right) = 0 . \qquad (4.17)$$

Letting

$$A \equiv \ddot{x}_R^n - \ddot{x}_L^n = 2\left(\frac{\sigma_{xx_R}^n}{\alpha_R^n} + \frac{\sigma_{xx_L}^n}{\alpha_L^n}\right) + f\left(\beta_R^n - \beta_L^n\right) ,$$

$$B \equiv \dot{x}_R^{n-\frac{1}{2}} - \dot{x}_L^{n-\frac{1}{2}} ,$$

$$C \equiv x_R^n - x_L^n ,$$

$$\Delta t^n \equiv \frac{\Delta t^{n+\frac{1}{2}} + \Delta t^{n-\frac{1}{2}}}{2} ,$$

Rev. 1
30 SEP 80

Eq.(4.17) can be rewritten as

$$\Delta t^{n+\frac{1}{2}}\left(\frac{\Delta t^{n+\frac{1}{2}}+\Delta t^{n-\frac{1}{2}}}{2}\right) A + \Delta t^{n+\frac{1}{2}}\, B + C = 0 ,$$

$$\left(\Delta t^{n+\frac{1}{2}}\right)^{2} A + \left(\Delta t^{n+\frac{1}{2}}\right)\left(2B+A\Delta t^{n-\frac{1}{2}}\right) + 2C = 0 . \qquad (4.18)$$

Equation (4.18) is a quadratic equation in $\Delta t^{n+\frac{1}{2}}$. The value which corresponds to the correct closure time step is always the more positive of the two roots. The actual value of the closure time step is usually obtained by iteration (e.g., using Newton's method).

Upon closure, the velocity of the interface becomes the constraint velocity or the momentum conserved velocity. In the latter case, the formula is

$$\dot{x}_{i-1}^{n+\frac{1}{2}} = \dot{x}_{i}^{n+\frac{1}{2}} = \frac{m_L\, \dot{x}_L^{n+\frac{1}{2}} + m_R\, \dot{x}_R^{n+\frac{1}{2}}}{m_L + m_R} . \qquad (4.19)$$

4.2.4 Mass Equation. The general continuity or conservation of mass equation for one-dimensional symmetries is

$$\frac{\dot{V}}{V} = \frac{\partial \dot{x}}{\partial x} + f\,\frac{\dot{x}}{x} , \qquad (4.20)$$

where V, $\dot{x}$, x, and f are previously defined. The left side of Eq.(4.20) is called the volumetric strain rate while the right side contains directional (or component) values of strain rate. The first term on the right is the one-dimensional principal strain rate.

A finite-difference analog must be derived separately but consistently for each term in Eq.(4.20). First, consider the volumetric strain rate, written in the following differential form,

$$\left(\frac{\dot{V}}{V}\right)_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}}/\Delta t^{n+\frac{1}{2}}}{V_{i-\frac{1}{2}}^{n+\frac{1}{2}}} \quad . \tag{4.21}$$

where $\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}}$ is the change in relative volume of zone $i-\frac{1}{2}$ at time $n+\frac{1}{2}$ and $\Delta t^{n+\frac{1}{2}}$ is the time increment. Applying Eq.(4.10b) to the definition of relative volume, the change of relative volume is

$$\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} \equiv V_{i-\frac{1}{2}}^{n+1} - V_{i-\frac{1}{2}}^{n} \, , \tag{4.22a}$$

$$\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \rho_{i-\frac{1}{2}}^{o}\left(\frac{1}{\rho_{i-\frac{1}{2}}^{n+1}} - \frac{1}{\rho_{i-\frac{1}{2}}^{n}}\right) . \tag{4.22b}$$

Since the mesh is Lagrangian, Eq.(4.22b) may be written in terms of true volume, $\mathcal{V}$, as follows,

$$\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\rho_{i-\frac{1}{2}}^{o}}{m_{i-\frac{1}{2}}^{o}}\left(\mathcal{V}_{i-\frac{1}{2}}^{n+1} - \mathcal{V}_{i-\frac{1}{2}}^{n}\right) . \tag{4.23}$$

Equation (4.23) is a formula for change of relative volume in terms of change of true volume. The change of true volume is related directly to coordinates and symmetry. Using the mesh notation shown on Page 4.3, the formulas for change of true volume for each of the three natural one-dimensional symmetries are derived as follows:

(1) Zones in slab symmetry are one-dimensional, variable-thickness slabs of specified cross-sectional area. The Lagrange coordinate is perpendicular to the unit cross section. The true volume of a zone is

$$\mathcal{V} = (\text{slab thickness})(\text{cross-section}).$$

When the cross-sectional area is constant for all zones, the slab symmetry is called planar; when the cross-sectional area is variable, it is called "planar-flume" or "planar duct" symmetry or simply one-dimensional pipe flow geometry. The true volume formula for constant cross-sectional area slab symmetry is

$$\mathcal{V}_{i-\frac{1}{2}} = \left(x_i - x_{i-1}\right) \times (1) \,. \tag{4.24a}$$

Equation (4.24a) assumes a unit cross-sectional area; however, any constant may be used, since it will affect all equations in the same way and, in effect, cancel out.

(2) Zones in cylindrical symmetry are concentric cylindrical shells of constant height and finite thickness. The Lagrange coordinate is the radius of the cylindrical shells, always beginning at the point of concentricity (i.e., the center) and directed outward. The true volume at time n comes from the difference in circular cross-sectional areas multiplied by the cylinder height,

$$\mathcal{V}_{i-\frac{1}{2}} = \pi\left[\left(x_i\right)^2 - \left(x_{i-1}\right)^2\right] \times (1) \,. \tag{4.24b}$$

Equation (4.24b) assumes a unit constant height. As in the plane slab geometry, any constant may be used. A geometry analogous to pipe flow geometry will result from variable heights. This symmetry is known as one-dimensional divergent flow between variably separated plates.

(3) Zones in spherical symmetry are finite, concentric spherical shells. The Lagrange coordinate begins at the point of concentricity and is directed outward. The true volume is

$$\mathcal{V}_{i-\frac{1}{2}} = \frac{4}{3}\pi\left[\left(x_i\right)^3 - \left(x_{i-1}\right)^3\right] . \tag{4.24c}$$

The change of relative volume using Eq.(4.23) may be written in terms of coordinates for each symmetry, as follows:

<u>slab</u>

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{\rho^0_{i-\frac{1}{2}}}{m^0_{i-\frac{1}{2}}}\left[\left(x^{n+1}_i - x^{n+1}_{i-1}\right) - \left(x^n_i - x^n_{i-1}\right)\right] ; \tag{4.25a}$$

<u>cylindrical</u>

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{\rho^0_{i-\frac{1}{2}}}{m^0_{i-\frac{1}{2}}}\pi\left\{\left[\left(x^{n+1}_i\right)^2 - \left(x^{n+1}_{i-1}\right)^2\right] - \left[\left(x^n_i\right)^2 - \left(x^n_{i-1}\right)^2\right]\right\} ; \tag{4.25b}$$

<u>spherical</u>

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{\rho^0_{i-\frac{1}{2}}}{m^0_{i-\frac{1}{2}}}\frac{4}{3}\pi\left\{\left[\left(x^{n+1}_i\right)^3 - \left(x^{n+1}_{i-1}\right)^3\right] - \left[\left(x^n_i\right)^3 - \left(x^n_{i-1}\right)^3\right]\right\} . \tag{4.25c}$$

Equations (4.25a), (4.25b), and (4.25c) are exact formulas for change of relative volume independent of the amount of strain in the zone. However, numerically these equations are subject to round-off error when the motion (change in time) of a particular coordinate is small compared to the absolute value of the coordinate. For these cases (and in general), it is desirable to make the formulas independent of the absolute value of the coordinate.

A simple way to do this is to re-derive the change of relative volume formulas in terms of the derivative of the coordinate as a function of the "change" variable, time (i.e., velocity). These formulas are easily derived by using a Taylor's series expansion about the time value, $t^{n+\frac{1}{2}}$, using all non-zero terms in the series.

The formulas for change of relative volume in terms of velocity are:

slab

$$\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\rho_{i-\frac{1}{2}}^{o}}{m_{i-\frac{1}{2}}^{o}} \left(\dot{x}_{i}^{n+\frac{1}{2}} - \dot{x}_{i-1}^{n+\frac{1}{2}} \right) \Delta t^{n+\frac{1}{2}} \; ; \tag{4.26a}$$

cylindrical

$$\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\rho_{i-\frac{1}{2}}^{o}}{m_{i-\frac{1}{2}}^{o}} \, 2\pi \left(x_{i}^{n+\frac{1}{2}} \, \dot{x}_{i}^{n+\frac{1}{2}} - x_{i-1}^{n+\frac{1}{2}} \, \dot{x}_{i-1}^{n+\frac{1}{2}} \right) \Delta t^{n+\frac{1}{2}} \; ; \tag{4.26b}$$

spherical

$$\begin{aligned} \Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\rho_{i-\frac{1}{2}}^{o}}{m_{i-\frac{1}{2}}^{o}} \, 4\pi \Bigg\{ & \left[\left(x_{i}^{n+\frac{1}{2}} \right)^{2} \dot{x}_{i}^{n+\frac{1}{2}} - \left(x_{i-1}^{n+\frac{1}{2}} \right)^{2} \dot{x}_{i-1}^{n+\frac{1}{2}} \right] \Delta t^{n+\frac{1}{2}} \\ & + \left[\left(\dot{x}_{i}^{n+\frac{1}{2}} \right)^{3} - \left(\dot{x}_{i-1}^{n+\frac{1}{2}} \right)^{3} \right] \frac{\left(\Delta t^{n+\frac{1}{2}} \right)^{3}}{12} \Bigg\} \; , \end{aligned} \tag{4.26c}$$

where $x_{i-1}^{n+\frac{1}{2}}$ and $x_i^{n+\frac{1}{2}}$ are computed from the definition of a first-order temporal average analogous to Eq.(4.4a),

$$(\ )^{n+\frac{1}{2}} \equiv \frac{(\ )^{n+1} + (\ )^{n}}{2} \ . \tag{4.27}$$

Equations (4.26a) (4.26b), and (4.26c) are round-off-free formulas for the change of relative volume of zone i-½ at time n+½. To calculate volumetric strain-rate from Eq.(4.21) requires the relative volume of zone i-½ at time n+½. The formula for $V_{i-\frac{1}{2}}^{n+\frac{1}{2}}$ comes from Eq.(4.27),

$$V_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{V_{i-\frac{1}{2}}^{n+1} + V_{i-\frac{1}{2}}^{n}}{2} \ , \tag{4.28}$$

where $V_{i-\frac{1}{2}}^{n}$ is known and $V_{i-\frac{1}{2}}^{n+1}$ can be calculated from Eq.(4.22a). Solving Eq.(4.22a) for $V_{i-\frac{1}{2}}^{n+1}$ yields

$$V_{i-\frac{1}{2}}^{n+1} = V_{i-\frac{1}{2}}^{n} + \Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} \ . \tag{4.29}$$

If $\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}}$ is a number whose order of magnitude is less than the order of magnitude of $V_{i-\frac{1}{2}}^{n}$ by an amount greater than the significant decimal digits of the computer being used, then a round-off error will result. This error can be eliminated by transforming variables by shifting the order of magnitude of $V_{i-\frac{1}{2}}^{n}$ nearer to that of $\Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}}$, computing the transformed variable using an analog of Eq.(4.29), and then transforming the variable back to $V_{i-\frac{1}{2}}^{n+1}$. The transformation is achieved using the following shift definitions:

$$C^{n+1}_{i-\frac{1}{2}} \equiv V^{o}_{i-\frac{1}{2}} - V^{n+1}_{i-\frac{1}{2}} , \tag{4.30a}$$

$$C^{n}_{i-\frac{1}{2}} \equiv V^{o}_{i-\frac{1}{2}} - V^{n}_{i-\frac{1}{2}} , \tag{4.30b}$$

where V^{o} is a reference relative volume and the transformations become

$$\Delta C^{n+\frac{1}{2}}_{i-\frac{1}{2}} \equiv C^{n+1}_{i-\frac{1}{2}} - C^{n}_{i-\frac{1}{2}} , \tag{4.31}$$

$$\Delta C^{n+\frac{1}{2}}_{i-\frac{1}{2}} = -\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2}} . \tag{4.32}$$

It is obvious after a comparison of Eqs.(4.30b) and (4.32) that the variable $C^{n}_{i-\frac{1}{2}}$, which is often called compression,* is on the order of $\Delta C^{n+\frac{1}{2}}_{i-\frac{1}{2}}$, the change of compression. Therefore, $C^{n+1}_{i-\frac{1}{2}}$ calculated from Eq.(4.31) is free of round-off error and $V^{n+1}_{i-\frac{1}{2}}$ can be calculated from Eq.(4.30a) in a round-off-free manner.

The next step in calculating the terms of Eq.(4.20) is the computation of the one-dimensional principal strain rate. By definition, it is

$$\left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{\Delta \dot{x}^{n+\frac{1}{2}}_{i-\frac{1}{2}}}{\Delta x^{n+\frac{1}{2}}_{i-\frac{1}{2}}} , \tag{4.33}$$

which by definition of first-order spatial difference, Eq.(4.4b), yields

$$\left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{\dot{x}^{n+\frac{1}{2}}_{i} - \dot{x}^{n+\frac{1}{2}}_{i-1}}{x^{n+\frac{1}{2}}_{i} - x^{n+\frac{1}{2}}_{i-1}} , \tag{4.34a}$$

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*This definition of compression is different from the variable, μ, used for equation-of-state models defined in Section 2.

where

$$\left(\frac{\partial \dot{x}}{\partial x}\right)_{i-\frac{1}{2}}^{n+\frac{1}{2}} = 0 \tag{4.34b}$$

when $x_{i-\frac{1}{2}}^{n+1} - x_{i-\frac{1}{2}}^{n} = 0$.

The final step in calculating the terms of Eq.(4.20) is the computation of the two other principal strain rates which depend on the symmetry. The simplest way to compute these terms is to first rearrange Eq.(4.20) in the following form,

$$f\,\frac{\dot{x}}{x} = \frac{\dot{V}}{V} - \frac{\partial \dot{x}}{\partial x}\ . \tag{4.35}$$

Since both terms on the right-hand side of Eq.(4.35) are known, it is possible to compute the term on the left-hand side and divide its value into appropriate components of strain.

In slab symmetry, the term on the left is zero, which is consistent with the one-dimensional planar assumption,

$$\frac{\partial \dot{y}}{\partial y} = \frac{\partial \dot{z}}{\partial z} = 0\ , \tag{4.36}$$

where y and z are coordinates perpendicular to x and to each other.

In cylindrical and spherical symmetries, the term on the left is only zero if Eq.(4.34b) is satisfied. When Eq.(4.34a) is non-zero, the term on the left is interpreted as follows:

cylindrical

$$\frac{\partial\dot{y}}{\partial y} = \frac{\dot{V}}{V} - \frac{\partial\dot{x}}{\partial x}\, , \qquad (4.37a)$$

$$\frac{\partial\dot{z}}{\partial z} = 0\ ; \qquad (4.37b)$$

spherical

$$\frac{\partial\dot{y}}{\partial y} = \frac{1}{2}\left(\frac{\dot{V}}{V} - \frac{\partial\dot{x}}{\partial x}\right), \qquad (4.38a)$$

$$\frac{\partial\dot{z}}{\partial z} = \frac{1}{2}\left(\frac{\dot{V}}{V} - \frac{\partial\dot{x}}{\partial x}\right)\ . \qquad (4.38b)$$

4.3 STRESS MESH

4.3.1 Artificial Viscosity. Although the finite-difference momentum equation, Eq.(4.5), is general, it cannot economically handle high frequency mechanical phenomena (such as shocks) because the spatial resolution of a mesh would have to be several times smaller than the thickness of the shock for Eq.(4.5) to be applicable. To calculate the transmission of a shock for a distance of a few centimeters would require tens of millions of zones or a shock-following microzoner and a very small time step if the shock thickness were on the order of angstroms. Clearly, this approach is not economically feasible.

An economical approach with considerable merit was devised by John von Neumann (Reference 4.1). He proposed that the presence of a shock within a zone (where the zone is millions of times larger than the thickness of the shock front) could be detected by the rate of change of volumetric strain and that the stress rise could be simulated by artificially spreading it over several zones. The crux of the idea is to add an artificial viscous stress, q_Q, dependent on the square of the volumetric strain rate, to the mean stress (pressure). The artificial viscous stress (sometimes called the quadratic artificial viscosity) is given by

$$q_Q = C_Q^2 \rho (\Delta x)^2 \left(\frac{\partial \dot{x}}{\partial x}\right)^2 , \tag{4.39}$$

where C_Q is a dimensionless constant dependent on differential stress across the shock front and the number of zones over which the stress is to be artificially spread. A value of 2.0 for C_Q spreads a shock front over three zones and is good for differential stresses up to 1 Mbar.*

Another consequence of applying the momentum equation to a discretized mesh is computational noise, i.e., stable zone-to-zone oscillations of low amplitude. In general, noise does not invalidate a solution and does not have to be eliminated if its effects can be clearly determined. However, it is possible to reduce, and in some cases completely eliminate noise by applying a viscous damping stress, q_L,

$$q_L = -C_L \rho \Delta x \sqrt{\frac{pV}{\rho_o}} \frac{\partial \dot{x}}{\partial x} , \tag{4.40}$$

where C_L is a dimensionless constant dependent on the amount of damping required to eliminate the noise oscillations. A typical value of C_L is 0.8. Equation (4.40) is a simple dashpot (viscous stress is proportional to velocity) and q_L is called a linear artificial viscosity.

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*The value of C_Q for collapsing porous materials (as well as foams and frangible material) should be 4.0 or 6.0, depending on the degree of porosity and the level of loading. Even then, the formulation for quadratic artificial viscosity may not accurately describe the Rayleigh line process for porous matrix collapse.

Equations (4.39) and (4.40) may be written in finite-difference form as follows:

$$q_{Q_{i-\frac{1}{2}}}^{n+\frac{1}{2}} = -\left(C^{o}_{Q_{i-\frac{1}{2}}}\right)^{2} \rho^{n+\frac{1}{2}}_{i-\frac{1}{2}} \left(\Delta x^{n+\frac{1}{2}}_{i-\frac{1}{2}}\right)^{2} \left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2}} \left|\left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2}}\right| , \tag{4.41}$$

and

$$q_{L_{i-\frac{1}{2}}}^{n+\frac{1}{2}} = -C^{o}_{L_{i-\frac{1}{2}}} \rho^{n+\frac{1}{2}}_{i-\frac{1}{2}} \Delta x^{n+\frac{1}{2}}_{i-\frac{1}{2}} \left(\frac{\left| p^{n}_{i-\frac{1}{2}}\right| V^{n+\frac{1}{2}}_{i-\frac{1}{2}}}{\rho^{o}_{i-\frac{1}{2}}}\right)^{\frac{1}{2}} \left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2}} . \tag{4.42}$$

4.3.2 <u>Internal Energy Equation</u>. The conservation of internal energy equation may be written in the following form,

$$\dot{u} = -(p+q)\dot{V} + \dot{Z} + \dot{h} + \dot{U}''' . \tag{4.43}$$

u, p, q, and V have been previously defined. $\dot{Z}$ is the distortional energy rate which, for one independent space variable, is

$$\dot{Z} = V\left(s_{xx}\,\dot{\epsilon}_{xx} + s_{yy}\,\dot{\epsilon}_{yy} + s_{zz}\,\dot{\epsilon}_{zz}\right) . \tag{4.44}$$

s_{xx}, s_{yy}, and s_{zz} are stress deviator components and $\dot{\epsilon}_{xx}$, $\dot{\epsilon}_{yy}$, and $\dot{\epsilon}_{zz}$ are strain rate components. The strain rate components have already been defined as follows:

$$\dot{\epsilon}_{xx} \equiv \frac{\partial \dot{x}}{\partial x} \qquad \text{[see Eq.(4.33)];}$$

slab

$$\dot{\varepsilon}_{yy} = \dot{\varepsilon}_{zz} = 0 \qquad \text{[see Eq.(4.36)];}$$

cylindrical

$$\dot{\varepsilon}_{yy} = \frac{\dot{V}}{V} - \dot{\varepsilon}_{xx} \qquad \text{[see Eq.(4.37a)];}$$

$$\dot{\varepsilon}_{zz} = 0 \qquad \text{[see Eq.(4.37b)];}$$

spherical

$$\dot{\varepsilon}_{yy} = \dot{\varepsilon}_{zz} = \frac{1}{2}\left(\frac{\dot{V}}{V} - \dot{\varepsilon}_{xx}\right) \qquad \text{[see Eq.(4.38)].}$$

$\dot{h}$ is the heat flow and $\dot{U}'''$ is the source or sink energy rate.

Substituting Eq.(4.44) into Eq.(4.43) yields an equation with six unknowns, since V can be determined from Eq.(4.29). To solve for the internal energy rate, $\dot{u}$, requires equations for p, s_{xx}, s_{yy}, s_{zz}, and $\dot{h}$.

4.3.3 Constitutive Equations. The equations that relate p, s_{xx}, s_{yy}, s_{zz}, and $\dot{h}$ to u and V are known as constitutive equations and may be categorized as follows:

equation of state

$$p = p(u,V); \tag{4.45a}$$

strength description

$$s_{xx} = s(u,V), \quad s_{yy} = s(u,V), \quad s_{zz} = s(u,V); \tag{4.45b}$$

Rev. 1
15 NOV 77

heat flow model

$$\dot{h} = h(u,V) \ . \tag{4.45c}$$

Given the functions p(u,V), s(u,V) and h(u,V) and knowing that Eq.(4.29) has been solved to give V, then Eqs.(4.43), (4.45a), (4.45b), and (4.45c) can be solved simultaneously (using the same explicit time step used to solve the momentum equation) by iteration or, in some cases, by substitution. A two-step iteration procedure is described in Section 4.3.4.

Typically, the equation of state, p(u,V), requires material constants (e.g., bulk modulus) that describe compressibility for the mechanical contribution to pressure and a specific heat ratio or a Grüneisen coefficient for the thermal contribution to pressure. The strength description requires a shear modulus, yield stress, flow rule, and yield criterion. The heat flux model needs thermal conductivity. In all cases, these or equivalent material constants may be functions of other thermodynamic variables.

The equation of state is usually simple or complex, depending on the number of phases and components that must be described. A single phase, one-component material is by far the simplest equation of state. A linear elastic solid or an "ideal" gas are examples of simple equations of state.

Strength descriptions are more or less complex, depending on strain-rate dependence during loading, relaxation to or from a failed state, reload characteristics after failure, ductility, brittleness, the existence of microfractures, etc. The simplest strength description is small strain elastic, where no failure is allowed to occur. Elastic-plastic models having a yield criterion based on the second stress invariant are also fairly simple. Plasticity can be handled using an appropriate flow rule. Strain hardening, fracture, dilatational effects, etc., increase the complexity of a strength model.

The heat flux model can be viewed in two separate categories -- conduction modeling and radiation modeling. An adequate model describing conduction is Fourier's Law,

$$\dot{h}'' = -k\nabla T \, . \tag{4.46}$$

Radiation, on the other hand, is more complex and no simple equation such as Eq.(4.46) can be used in a physically correct and economical manner.

Once Eq.(4.43) has been solved in conjunction with appropriate constitutive equations, Eqs.(4.45a), (4.45b), and (4.45c), all remaining thermodynamic state variables can be computed. In particular, stress can be calculated from

$$\begin{aligned} \sigma_{xx} &= s_{xx} - (p+q) \, , \\ \sigma_{yy} &= s_{yy} - (p+q) \, , \\ \sigma_{zz} &= s_{zz} - (p+q) \, , \end{aligned} \tag{4.47}$$

where $q = q_Q + q_L$. Once stress is computed, the computational cycle (Figure 4.1) is complete. All that remains is to determine a stable time step for the next cycle.

Rev. 1
15 NOV 77

4.3.4 Simultaneous Solution of Constitutive Equations and Conservation of Energy by a Two-Step Iteration.

The procedure used to calculate new values of internal energy density, pressure, deviatoric stress components, and heat flow was discussed in Section 4.3.3. For the standard models in STEALTH, a two-step iteration is used to solve simultaneously the coupled constitutive equations and the internal energy conservation equation for u, ρ, s, and h.

The logic, which is located in subroutine ZONMDL, is as follows.

1. Calculate the approximate change in distortional energy density, $\Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2}}$, in zone $i-\frac{1}{2}$,

$$\Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2}} = V^{n+\frac{1}{2}}_{i-\frac{1}{2}}\,\Delta t^{n+\frac{1}{2}}\left(s^{n}_{xx_{i-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2}}} + s^{n}_{yy_{i-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2}}} + s^{n}_{zz_{i-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2}}}\right).$$

2. Calculate the heat transfer energy density, $\Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2}}$, into zone $i-\frac{1}{2}$ at time $n+\frac{1}{2}$,

$$\Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2}} = f_{i-\frac{1}{2}}\,\frac{\rho^{o}_{i-\frac{1}{2}}}{m_{i-\frac{1}{2}}}\left(\dot{h}''^{\,n+\frac{1}{2}}_{i-1} - \dot{h}''^{\,n+\frac{1}{2}}_{i}\right)\Delta t^{n+\frac{1}{2}} ,$$

where, in zone $i-\frac{1}{2}$, f is a geometry factor depending on symmetry,

Symmetry	f
plane 1D	1
cylindrical 1D	2π
spherical 1D	4π
planar flume	1
cylindrical flume	2π

ρ^{o} is the reference density and m is the mass; $\Delta t^{n+\frac{1}{2}}$ is the time step for the entire mesh; and at grid points i-1 and i, $\dot{h}''^{\,n+\frac{1}{2}}$ is the heat flux. The heat flux is calculated from Fourier's heat conduction law,

$$\dot{h}'' = -k(T)\,\nabla T \;,$$

where k is the conductivity and the gradient ∇ affects the conduction formula in the following way for interior points:

Plane symmetry (also planar flume)

$$\dot{h}''^{\,n+\frac{1}{2}}_{i} = \frac{k^{n}_{i-\frac{1}{2}}\, k^{n}_{i+\frac{1}{2}} \left(T^{n}_{i+\frac{1}{2}} - T^{n}_{i-\frac{1}{2}}\right)}{k^{n}_{i-\frac{1}{2}}\, \Delta x^{n}_{i+\frac{1}{2}} + k^{n}_{i+\frac{1}{2}}\, \Delta x^{n}_{i-\frac{1}{2}}} \;,$$

where

$$\Delta x_{i-\frac{1}{2}} \equiv \frac{x_{i} - x_{i-1}}{2} \;,$$

$$\Delta x_{i+\frac{1}{2}} \equiv \frac{x_{i+1} - x_{i}}{2} \;;$$

Cylindrical symmetry (also cylindrical flume)

$$\dot{h}''^{\,n+\frac{1}{2}}_{i} = \frac{-k^{n}_{i-\frac{1}{2}}\, k^{n}_{i+\frac{1}{2}} \left(T^{n}_{i+\frac{1}{2}} - T^{n}_{i-\frac{1}{2}}\right)}{k^{n}_{i-\frac{1}{2}}\, \ln\left(\dfrac{x^{n}_{i}}{x^{n}_{i+\frac{1}{2}}}\right) + k^{n}_{i+\frac{1}{2}}\, \ln\left(\dfrac{x^{n}_{i-\frac{1}{2}}}{x^{n}_{i}}\right)} \;;$$

Spherical symmetry

$$\dot{h}''^{\,n+\frac{1}{2}}_{i} = \frac{-k^{n}_{i-\frac{1}{2}}\, k^{n}_{i+\frac{1}{2}} \left(T^{n}_{i+\frac{1}{2}} - T^{n}_{i-\frac{1}{2}}\right)}{k^{n}_{i-\frac{1}{2}} \left(\frac{1}{x^{n}_{i}} - \frac{1}{x^{n}_{i+\frac{1}{2}}}\right) + k^{n}_{i-\frac{1}{2}} \left(\frac{1}{x^{n}_{i-\frac{1}{2}}} - \frac{1}{x^{n}_{i}}\right)} \;;$$

where for all symmetries

$$x^{n}_{i-\frac{1}{2}} \equiv \frac{x^{n}_{i-1} + x^{n}_{i}}{2}\,, \qquad x^{n}_{i+\frac{1}{2}} \equiv \frac{x^{n}_{i} + x^{n}_{i+1}}{2}\;.$$

For left side boundary points, the heat flux is given by

$$\dot{h}''^{\,n+\frac{1}{2}}_{i} = f_{i}\, \frac{-k^{n}_{i+\frac{1}{2}}\left(T^{n}_{i+\frac{1}{2}} - T^{n}_{BDY}\right)}{\left(\frac{x^{n}_{i} + x^{n}_{i+\frac{1}{2}}}{2}\right)} \quad \text{or} \quad f_{i}\dot{h}''^{\,n+\frac{1}{2}}_{BDY}\,,$$

while for right side boundary points ,

$$\dot{h}''^{\,n+\frac{1}{2}}_{i} = f_{i}\, \frac{-k^{n}_{i-\frac{1}{2}}\left(T^{n}_{BDY} - T^{n}_{i-\frac{1}{2}}\right)}{\left(\frac{x^{n}_{i-\frac{1}{2}} + x^{n}_{i}}{2}\right)} \quad \text{or} \quad f_{i}\dot{h}''^{\,n+\frac{1}{2}}_{BDY}\,,$$

where f_i takes on the following values:

Symmetry	f
plane	1
cylindrical	x^n_i
spherical	$(x^n_i)^2$
planar flume	1
cylindrical flume	x^n_i

3. Calculate source energy density, $U^n_{i-\frac{1}{2}}$, to be deposited in zone i-½ at time n,

$$U^n_{i-\frac{1}{2}} = U_{i-\frac{1}{2}}(t^n) ,$$

where $U_{i-\frac{1}{2}}(t^n)$ is a time-dependent function of energy deposition for zone i-½ evaluated at time t^n.

4. Add approximate reversible work (old pressure multiplied by new change of relative volume), approximate distortional energy density, heat transfer energy density, and source energy density in zone i-½ to internal energy density $(u^n_{i-\frac{1}{2}})$ in zone i-½ to get the approximate internal energy density $(\tilde{u}^{n+1}_{i-\frac{1}{2}})$ in zone i-½,

$$\tilde{u}^{n+1}_{i-\frac{1}{2}} = u^n_{i-\frac{1}{2}} - \left(p^n_{i-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2}}\right)\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2}} + \Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2}} + \Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2}} + U^n_{i-\frac{1}{2}} .$$

5. Calculate an approximate pressure, $\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2}}$, in zone i-½ for time n+½ by first calculating the approximate n+1 pressure, $p^{n+1}_{i-\frac{1}{2}}$, from internal energy density in zone i-½,

$$\tilde{p}^{n+1}_{i-\frac{1}{2}} = p_{i-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2}}, V^{n+1}_{i-\frac{1}{2}}\right) ,$$

where $V^{n+1}_{i-\frac{1}{2}}$ is the relative volume already calculated in zone i-½ for time n+1 [Eq.(4.29)], $p_{i-\frac{1}{2}}$ is the pressure equation of state, and $\tilde{p}^{n+1}_{i-\frac{1}{2}}$ is the approximate pressure for zone i-½ at time n+1 .

Rev. 1
15 NOV 77

Then adjust this pressure, $\tilde{p}^{n+1}_{i-\frac{1}{2}}$, to satisfy explosive or spall criteria. (These criteria are mutually exclusive.) Calculate the approximate spall pressure, $\tilde{p}^{n+1}_{\min_{i-\frac{1}{2}}}$, in zone i-½,

$$\tilde{p}^{n+1}_{\min_{i-\frac{1}{2}}} = p_{\min_{i-\frac{1}{2}}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2}},\ \tilde{Z}^{n+1}_{i-\frac{1}{2}}\right),$$

where $p_{\min_{i-\frac{1}{2}}}$ is a material function for zone i-½. If $\tilde{p}^{n+1}_{i-\frac{1}{2}} \le \tilde{p}^{n+1}_{\min_{i-\frac{1}{2}}}$, adjust $\tilde{p}^{n+1}_{i-\frac{1}{2}}$ to its spalled value. Then calculate $\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2}}$ from

$$\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{\tilde{p}^{n+1}_{i-\frac{1}{2}} + p^{n}_{i-\frac{1}{2}}}{2}\ .$$

6. Calculate shear modulus, $G^{n+\frac{1}{2}}_{i-\frac{1}{2}}$, for zone i-½ at time n+½ by first calculating the shear modulus, $G^{n+1}_{i-\frac{1}{2}}$, for zone i-½ at time n+1,

$$G^{n+1}_{i-\frac{1}{2}} = G_{i-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2}},\ \tilde{p}^{n+1}_{i-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2}}\right),$$

where $G_{i-\frac{1}{2}}$ is the material function for zone i-½, and then using

$$G^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{G^{n+1}_{i-\frac{1}{2}} + G^{n}_{i-\frac{1}{2}}}{2}\ .$$

7. Calculate elastic stress deviators, $s^{e^{n+1}}_{xx_{i-\frac{1}{2}}}$, $s^{e^{n+1}}_{yy_{i-\frac{1}{2}}}$, $s^{e^{n+1}}_{zz_{i-\frac{1}{2}}}$, in zone i-½ at time n+1 as follows.

$$s^{e^{n+1}}_{xx_{i-\frac{1}{2}}} = s^{n}_{xx_{i-\frac{1}{2}}} + 2.0\,G^{n+\frac{1}{2}}_{i-\frac{1}{2}}\left(\dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2}}} - \frac{1}{3}\,\frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2}}}\right)\Delta t^{n+\frac{1}{2}} ,$$

where $s^{n}_{xx_{i-\frac{1}{2}}}$ is the xx-stress deviator in zone i-½ from time n, $\dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2}}}$ is the previously calculated xx-strain rate in zone i-½ at time n (Eq. 4.33), and $\Delta t^{n+\frac{1}{2}}$ is the stable centered time step for this cycle; and from symmetry,

Plane symmetry

$$s^{e^{n+1}}_{yy_{i-\frac{1}{2}}} = -s^{e^{n+1}}_{xx_{i-\frac{1}{2}}}/2 ,$$

$$s^{e^{n+1}}_{zz_{i-\frac{1}{2}}} = -s^{e^{n+1}}_{xx_{i-\frac{1}{2}}}/2 ;$$

Cylindrical symmetry

$$s^{e^{n+1}}_{yy_{i-\frac{1}{2}}} = s^{n}_{yy_{i-\frac{1}{2}}} + 2.0\,G^{n+\frac{1}{2}}_{i-\frac{1}{2}}\left(\dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2}}} - \frac{1}{3}\,\frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2}}}\right)\Delta t^{n+\frac{1}{2}} ,$$

$$s^{e^{n+1}}_{zz_{i-\frac{1}{2}}} = -\left(s^{e^{n+1}}_{xx_{i-\frac{1}{2}}} + s^{e^{n+1}}_{yy_{i-\frac{1}{2}}}\right) ;$$

Spherical symmetry

$$s^{e^{n+1}}_{yy_{i-\frac{1}{2}}} = -s^{e^{n+1}}_{xx_{i-\frac{1}{2}}}/2 ,$$

$$s^{e^{n+1}}_{zz_{i-\frac{1}{2}}} = -s^{e^{n+1}}_{xx_{i-\frac{1}{2}}}/2 .$$

8. Calculate the elastic yield stress squared, $\left(Y^{e^{n+1}}_{i-\frac{1}{2}}\right)^2$, for zone $i-\frac{1}{2}$ at time n+1 from the second stress deviator invariant,

$$\left(Y^{e^{n+1}}_{i-\frac{1}{2}}\right)^2 = \frac{3}{2}\left[\left(s^{e^{n+1}}_{xx_{i-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{yy_{i-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{zz_{i-\frac{1}{2}}}\right)^2\right] .$$

9. Calculate the allowable yield stress, $Y^{n+1}_{i-\frac{1}{2}}$, for zone $i-\frac{1}{2}$ at time n+1,

$$Y^{n+1}_{i-\frac{1}{2}} = Y_{i-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2}},\ \tilde{p}^{n+1}_{i-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2}}\right) ,$$

where $Y_{i-\frac{1}{2}}$ is a material function for zone $i-\frac{1}{2}$.

10. Compare the allowable yield stress, $Y^{n+1}_{i-\frac{1}{2}}$, with the elastic yield stress, $Y^{e^{n+1}}_{i-\frac{1}{2}}$;

if $Y^{n+1}_{i-\frac{1}{2}} > Y^{e^{n+1}}_{i-\frac{1}{2}}$, material is linear elastic;

if $Y^{n+1}_{i-\frac{1}{2}} \leq Y^{e^{n+1}}_{i-\frac{1}{2}}$, material has exceeded allowable yield stress.

Rev. 1
1 DEC 76

11. If the material is linear elastic, the elastic stress deviators already calculated are correct,

$$s_{xx_{i-\frac{1}{2}}}^{n+1} = s_{xx_{i-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{yy_{i-\frac{1}{2}}}^{n+1} = s_{yy_{i-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{zz_{i-\frac{1}{2}}}^{n+1} = s_{zz_{i-\frac{1}{2}}}^{e^{n+1}} .$$

12. When the material has exceeded its allowable yield stress, adjust the stress deviators according to the Prandtl-Reuss flow rule,

$$s_{xx_{i-\frac{1}{2}}}^{n+1} = \left(\frac{Y_{i-\frac{1}{2}}^{n+1}}{Y_{i-\frac{1}{2}}^{e^{n+1}}} \right) s_{xx_{i-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{yy_{i-\frac{1}{2}}}^{n+1} = \left(\frac{Y_{i-\frac{1}{2}}^{n+1}}{Y_{i-\frac{1}{2}}^{e^{n+1}}} \right) s_{yy_{i-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{zz_{i-\frac{1}{2}}}^{n+1} = \left(\frac{Y_{i-\frac{1}{2}}^{n+1}}{Y_{i-\frac{1}{2}}^{e^{n+1}}} \right) s_{zz_{i-\frac{1}{2}}}^{e^{n+1}} .$$

13. Calculate the change in distortional energy density, $\Delta Z_{i-\frac{1}{2}}^{n+\frac{1}{2}}$, in zone $i-\frac{1}{2}$ at time $n+\frac{1}{2}$,

$$\Delta Z_{i-\frac{1}{2}}^{n+\frac{1}{2}} = V_{i-\frac{1}{2}}^{n+\frac{1}{2}} \Delta t^{n+\frac{1}{2}} \left(s_{xx_{i-\frac{1}{2}}}^{n+\frac{1}{2}} \dot{\varepsilon}_{xx_{i-\frac{1}{2}}}^{n+\frac{1}{2}} + s_{yy_{i-\frac{1}{2}}}^{n+\frac{1}{2}} \dot{\varepsilon}_{yy_{i-\frac{1}{2}}}^{n+\frac{1}{2}} + s_{zz_{i-\frac{1}{2}}}^{n+\frac{1}{2}} \dot{\varepsilon}_{zz_{i-\frac{1}{2}}}^{n+\frac{1}{2}} \right),$$

where

$$s_{xx_{i-\frac{1}{2}}}^{n+\frac{1}{2}} = \frac{s_{xx_{i-\frac{1}{2}}}^{n+1} + s_{xx_{i-\frac{1}{2}}}^{n}}{2},$$

$$s_{yy_{i-\frac{1}{2}}}^{n+\frac{1}{2}} = \frac{s_{yy_{i-\frac{1}{2}}}^{n+1} + s_{yy_{i-\frac{1}{2}}}^{n}}{2},$$

$$s_{zz_{i-\frac{1}{2}}}^{n+\frac{1}{2}} = \frac{s_{zz_{i-\frac{1}{2}}}^{n+1} + s_{zz_{i-\frac{1}{2}}}^{n}}{2}.$$

14. Calculate the internal energy density, $u_{i-\frac{1}{2}}^{n+1}$, in zone $i-\frac{1}{2}$ at time n+1,

$$u_{i-\frac{1}{2}}^{n+1} = u_{i-\frac{1}{2}}^{n} - \left(\tilde{p}_{i-\frac{1}{2}}^{n+\frac{1}{2}} + q_{i-\frac{1}{2}}^{n+\frac{1}{2}} \right) \Delta V_{i-\frac{1}{2}}^{n+\frac{1}{2}} + \Delta Z_{i-\frac{1}{2}}^{n+\frac{1}{2}} + \Delta h_{i-\frac{1}{2}}^{n+\frac{1}{2}} + U_{i-\frac{1}{2}}^{n}.$$

15. Calculate the pressure, $p_{i-\frac{1}{2}}^{n+1}$, in zone $i-\frac{1}{2}$ at time n+1,

$$p_{i-\frac{1}{2}}^{n+1} = p_{i-\frac{1}{2}} \left(u_{i-\frac{1}{2}}^{n+1}, V_{i-\frac{1}{2}}^{n+1} \right).$$

16. Calculate the spall pressure, $p_{min_{i-\frac{1}{2}}}^{n+1}$, in zone $i-\frac{1}{2}$ at time $n+1$,

$$p_{min_{i-\frac{1}{2}}}^{n+1} = p_{min_{i-\frac{1}{2}}}\left(u_{i-\frac{1}{2}}^{n+1}, V_{i-\frac{1}{2}}^{n+1}, Z_{i-\frac{1}{2}}^{n+1}\right),$$

where $p_{min_{i-\frac{1}{2}}}$ is a material function for zone $i-\frac{1}{2}$. If $p_{i-\frac{1}{2}}^{n+1} \le p_{min_{i-\frac{1}{2}}}^{n+1}$, adjust $p_{i-\frac{1}{2}}^{n+1}$ to its spalled value.

17. Calculate the total stress, $\sigma_{xx_{i-\frac{1}{2}}}^{n+1}$, $\sigma_{yy_{i-\frac{1}{2}}}^{n+1}$, $\sigma_{zz_{i-\frac{1}{2}}}^{n+1}$, in zone $i-\frac{1}{2}$ at at time $n+1$,

$$\sigma_{xx_{i-\frac{1}{2}}}^{n+1} = s_{xx_{i-\frac{1}{2}}}^{n+1} - \left(p_{i-\frac{1}{2}}^{n+1} + q_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right),$$

$$\sigma_{yy_{i-\frac{1}{2}}}^{n+1} = s_{yy_{i-\frac{1}{2}}}^{n+1} - \left(p_{i-\frac{1}{2}}^{n+1} + q_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right),$$

$$\sigma_{zz_{i-\frac{1}{2}}}^{n+1} = s_{zz_{i-\frac{1}{2}}}^{n+1} - \left(p_{i-\frac{1}{2}}^{n+1} + q_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right).$$

18. Calculate the longitudinal sound speed squared, $\left(c_{\ell_{i-\frac{1}{2}}}^{n+1}\right)^2$, in zone $i-\frac{1}{2}$ at time $n+1$,

$$c_{\ell_{i-\frac{1}{2}}}^{n+1} = c_{\ell_{i-\frac{1}{2}}}\left(u_{i-\frac{1}{2}}^{n+1}, p_{i-\frac{1}{2}}^{n+1}, V_{i-\frac{1}{2}}^{n+1}\right),$$

where $c_{\ell_{i-\frac{1}{2}}}$ is a material function for zone $i-\frac{1}{2}$.

19. Calculate the temperature, $T^{n+1}_{i-\frac{1}{2}}$, in zone i-½ at time n+1 ,

$$T^{n+1}_{i-\frac{1}{2}} = T_{i-\frac{1}{2}} \left(u^{n+1}_{i-\frac{1}{2}} ,\ p^{n+1}_{i-\frac{1}{2}} ,\ V^{n+1}_{i-\frac{1}{2}} \right) ,$$

where $T_{i-\frac{1}{2}}$ is a material function for zone i-½ .

20. Calculate the conductivity, $k^{n+1}_{i-\frac{1}{2}}$, in zone i-½ at time n+1 ,

$$k^{n+1}_{i-\frac{1}{2}} = k_{i-\frac{1}{2}} \left(u^{n+1}_{i-\frac{1}{2}} ,\ p^{n+1}_{i-\frac{1}{2}} ,\ V^{n+1}_{i-\frac{1}{2}} \right) ,$$

where $k_{i-\frac{1}{2}}$ is a material function for zone i-½ .

21. Calculate the specific heat capacity, $C^{n+1}_{i-\frac{1}{2}}$, in zone i-½ at time n+1,

$$C^{n+1}_{i-\frac{1}{2}} = C_{i-\frac{1}{2}} \left(u^{n+1}_{i-\frac{1}{2}} ,\ p^{n+1}_{i-\frac{1}{2}} ,\ V^{n+1}_{i-\frac{1}{2}} \right) ,$$

where $C_{i-\frac{1}{2}}$ is a material function for zone i-½ .

4.4 EXPLICIT TIME STEP

4.4.1 Overview. The explicit calculational scheme has two identifying characteristics:

(1) New values are computed from old values; e.g., values at n+1 are computed from values at n.

(2) Data for computations come only from nearest neighbors; i.e., information can propagate across only one zone in one calculational time step.

These characteristics are the essential elements of the explicit numerical method and are embodied in the criteria required to calculate stable time steps.

4.4.2 Stable Mechanical Time Steps. The physical criterion required for the calculation of a stable time step was described in Section 4.2.2 and is summarized in Eqs.(4.9a) and (4.9b). If artificial viscosity were not present, the most conservative (largest) value of mechanical sound speed would be the isentropic longitudinal sound speed. The general form of the isentropic longitudinal sound speed is

$$c_\ell^2 \equiv \left.\frac{\partial \sigma_\ell}{\partial \rho}\right)_{\text{isentropic}} , \tag{4.48}$$

where the subscript ℓ denotes the longitudinal direction, σ_ℓ is calculated from Eq.(4.47), and ρ is the actual density. Equation (4.48) can also be written in component form,

$$c_\ell^2 = c_s^2 + c_p^2 + c_q^2, \tag{4.49a}$$

$$= \left.\frac{\partial s}{\partial \rho}\right)_{\text{isen}} + \left.\frac{\partial p}{\partial \rho}\right)_{\text{isen}} + \left.\frac{\partial q}{\partial \rho}\right)_{\text{isen}} , \tag{4.49b}$$

where "isen" means isentropic.

c_s is the deviatoric contribution to sound speed and can be calculated conservatively from the formula,

$$c_s^2 = \frac{\frac{4}{3}G}{\rho^o} , \tag{4.50}$$

where G is the shear modulus and ρ^o is the reference density. c_s^2 is 4/3 times the elastic shear velocity squared.

c_p is the pressure (or mean stress) contribution to sound speed and is calculated from the equation of state. When the equation of state is of the form

$$p = A + Bu , \tag{4.51}$$

where $A = A(\eta)$, $B = B(\eta)$, and $\eta \equiv \frac{1}{V}$, then from the isentropic condition that $du = -pdV$, the thermodynamic (hydrostatic) sound speed is

$$c_p^2 = \frac{A' + B'u + BpV^2}{\rho^o} , \tag{4.52}$$

where $A' = \frac{dA}{d\eta}$, $B' = \frac{dB}{d\eta}$. When the equation of state is not in the form of Eq.(4.51) then a more specialized approach must be taken.

c_q is the artificial viscosity contribution to sound speed and is composed of two components, linear and quadratic. The formula is

$$c_q^2 = \left.\frac{\partial q_L}{\partial \rho}\right)_{isen} + \left.\frac{\partial q_Q}{\partial \rho}\right)_{isen} \quad . \tag{4.53}$$

Using Eqs.(4.41) and (4.42), c_q^2 becomes (References 4.2 and 4.1, respectively),

$$c_q^2 = 4C_L^2 \, \frac{|p| \, V}{\rho^o} + \left(2C_Q\right)^4 \, (\Delta x)^2 \, \left(\frac{\partial \dot{x}}{\partial x}\right)^2 \, . \tag{4.54}$$

Combining Eqs.(4.50), (4.52), and (4.54) yields the formula for the maximum stable time step of zone $i - \frac{1}{2}$,

$$\left(\Delta t^{n+1}_{i-\frac{1}{2}}\right)^2 = \frac{\left(\Delta x^{n+1}_{i-\frac{1}{2}}\right)^2}{\left(c^{n+1}_{\ell_{i-\frac{1}{2}}}\right)^2 + 4C^2_{L_{i-\frac{1}{2}}} \dfrac{\left|p^{n+1}_{i-\frac{1}{2}}\right| V^{n+1}_{i-\frac{1}{2}}}{\rho^o_{i-\frac{1}{2}}} + \left(2C_{Q_{i-\frac{1}{2}}}\right)^4 \left(\Delta x^{n+\frac{1}{2}}_{i-\frac{1}{2}}\right)^2 \left[\left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2}}\right]^2} \, . \tag{4.55}$$

In determining a time step for the next cycle, only n+1 data exist in order to predict the n+3/2 time step. This dilemma is not critical provided that one understands the pathological cases which can arise from a poorly estimated time step.

There are two pathological cases that must be considered when calculating the new n+3/2 time step. These cases can be seen from a plot of time step versus time. See Figure 4.4. If the time step is increasing with time (Case 1), predictions of the n+3/2 time step based on n+1 data will be conservative whether constant extrapolation (i.e., setting $\Delta t^{n+3/2} = t^{n+1}$) or linear extrapolation is used. On the other hand, if the time step is decreasing with time (Case 2), the

Rev. 1
30 SEP 80

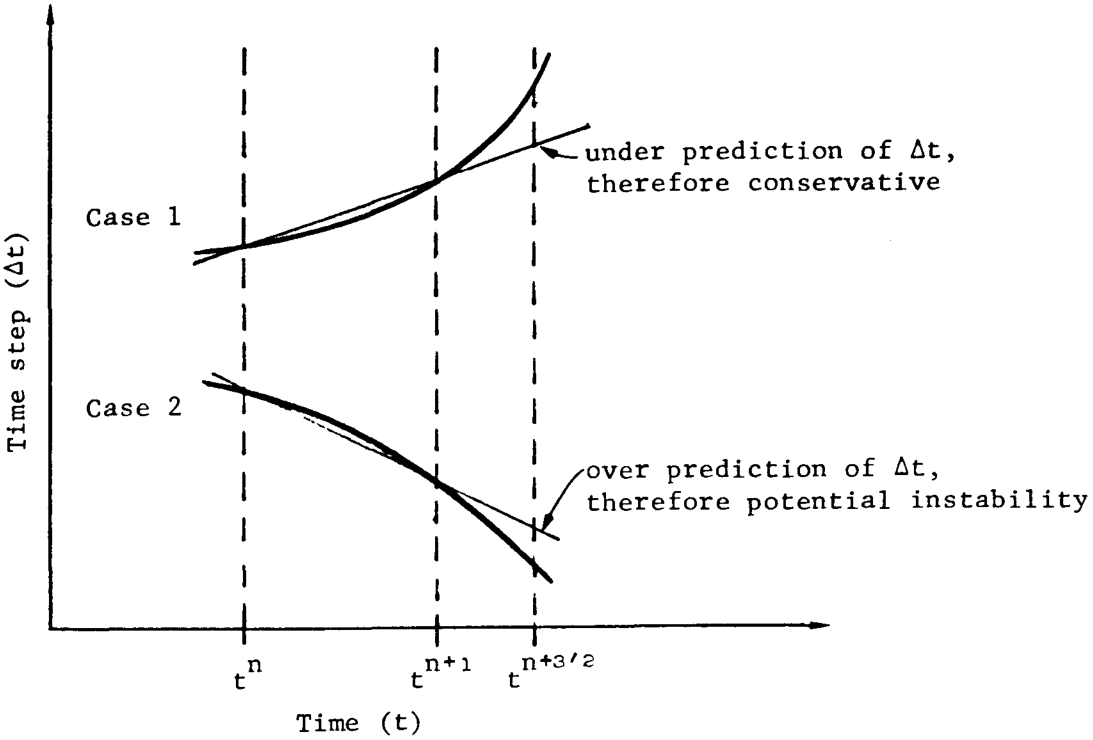

Figure 4.4. Example of need for f_{SFR}.

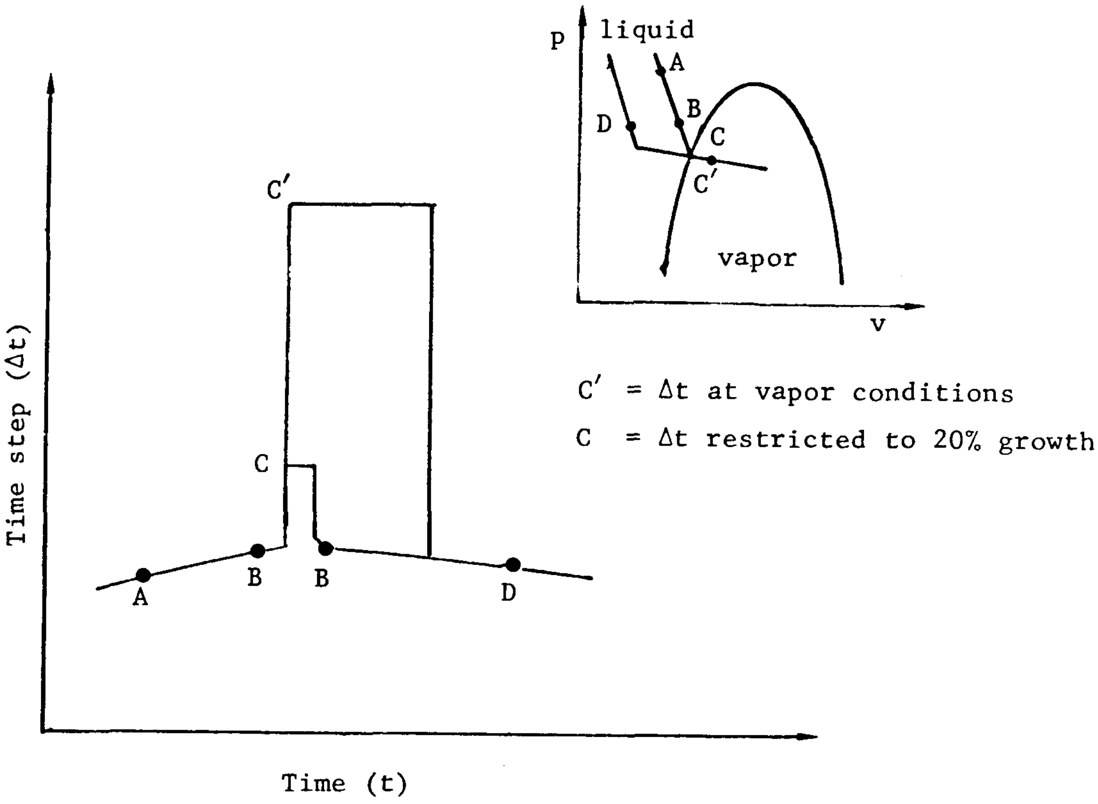

Figure 4.5. Example of need for f_{GRF}.

constant extrapolation procedure will predict a time step that is apt to be too high to maintain stability. The linear extrapolation is much better but can also be inaccurate if the rate of time step decay is large. In problems in which the time step is expected to experience rapid drops in time, it is advisable to use a safety factor multiplier of 2/3. This will add another level of conservatism to the calculation of the n+3/2 time step.

Thus, when the n+1 time step is greater than the n+1/2 time step (Case 1), set the n+3/2 time step equal to the n+1 value and recompute the n+1 time step to be the average of this n+3/2 value and the n+1/2 time step. This will also be conservative. If, on the other hand, the n+1 time step is less than than the n+1/2 time step, calculate an n+3/2 time step based on a linear extrapolation of the n+1/2 and n+1 values. This procedure should lead to a relatively safe value for most calculations. When the n+1 time step equals the n+1/2 value, either approach will work.

There are other time-step constraints which insure the stability of a calculation. First, there is a safety factor multiplier (f_{SFR}), which may be applied when c_p cannot be calculated in a conservative way or when Eq.(4.55) may not be conservative. The value of f_{SFR} may vary from 0.1 to 1.0.

Next, there is a growth factor multiplier (f_{GRF}), which may be applied so that a time step cannot grow faster than a certain rate. The value of f_{GRF} may vary from 1.0 to 1.2 (no growth to 20% growth). The need for a 20% growth factor limitation on a time step is justified as follows: Consider the problem in which a change of material phase is possible. Furthermore, allow for the situation that during the early response periods, the time step is controlled by the higher sound speed phase (i.e., lower time step) but that at some later time during the simulation, all of the material is "flashed" to the lower sound speed phase. Assume that this change of sound speed results in a change of the maximum stable time step of at least a factor of 2. Furthermore, one cycle after the global change of phase has occurred, one of the zones returns to its higher sound speed state. If the time step had been allowed to rise rapidly to its much larger value for the one cycle when all the zones switched phase to the lower sound speed material, it is possible that the instantaneously larger time step could result either in an instablity when the time step drops again to the lower value, or in inaccurate results because of some numerically induced high amplitude wave that resulted in the one cycle in which the time step was large. This scenario is shown schematically in Figure 4.5.

And finally, there are minimum and maximum values of time step. When the stable time step goes below the minimum value, the problem is terminated. When the stable time step has a value above the maximum value, the time step is adjusted to the maximum value exactly.

Thus, stable time steps for the next cycle ($\Delta t^{n+3/2}$ and Δt^{n+1}) are calculated as follows,

$$\Delta t^{n+3/2} = f_{SFR} \left[\text{minimum for all zones of Eq.(4.55)}\right] , \qquad (4.56)$$

subject to the condition that

$$\Delta t_{min} \leq \Delta t^{n+3/2} \leq f_{GRF} \, \Delta t^{n+\frac{1}{2}} \leq \Delta t_{max} \; . \qquad (4.57)$$

Then, by interpolation,

$$\Delta t^{n+1} = \frac{\Delta t^{n+3/2} + \Delta t^{n+\frac{1}{2}}}{2} \; . \qquad (4.58)$$

4.4.3 Stable Thermal Time Steps. When a particular problem is dominated by heat conduction phenomena rather than by mechanical phenomena, the problem time step stability criterion may be controlled by thermal diffusion rather than by mechanical sound speed. Therefore, when heat conduction is present, it is necessary to calculate the minimum stable heat conduction time step as follows,

$$\Delta t^n = \text{minimum value of } \Delta t^n_{i-\frac{1}{2}} \text{ for all } i,$$

where

$$\Delta t^n_{i-\frac{1}{2}} \le \frac{\left(\Delta x^n_{i-\frac{1}{2}}\right)^2}{2\left(k^n_{i-\frac{1}{2}}/C^n_{V_{i-\frac{1}{2}}}\right)} . \tag{4.59}$$

$\Delta x^n_{i-\frac{1}{2}}$ is the smallest length across zone i-½ at time n, $k^n_{i-\frac{1}{2}}$ is the conductivity of zone i-½ at time n, and $C^n_{V_{i-\frac{1}{2}}}$ is the specific heat capacity* of zone i-½ at time n.

As in the case of the mechanical stability criterion, the smallest maximum stable thermal time step in the grid is saved in order to be used for the next cycle of calculations. When thermal and mechanical mechanisms are both present, the smallest of the two stable time steps is chosen to be the time step for both mechanisms in the next cycle.

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*Per reference unit volume.

4.5 USE OF THE DEVELOPED EQUATIONS FOR EFFICIENT SOLUTION OF NON-TRANSIENT CASES

4.5.1 The Problem. Although the explicit finite-difference equations developed in Sections 4.2 and 4.3 can be used to analyze transient, steady-state, static, and quasi-static time-dependent thermomechanical systems, these numerical equations are most efficient for simulating transient behavior because time steps are computed from the minimum of the Courant stability criterion and the diffusion limit. The Courant condition gives the largest possible stable time step for a finite representation of a continuum consistent with the laws of physics for most initial value (transient) problems involving stress. The diffusion limit does the same for transient thermal problems. For mechanical boundary value (non-transient) problems, the Courant condition may needlessly restrict the time step. Two important exceptions to these guidelines are as follows: (1) linear elastic, small-strain, transient mechanical problems can sometimes be more efficiently solved implicitly in the frequency domain than explicitly in the time domain, and (2) nonlinear, non-transient problems often require that time be an independent explicit variable with the resulting equations being solved explicitly so that path-dependent thermodynamics are properly computed. Thermal boundary value problems are still efficiently solved using the diffusion limit time step criterion.

In other words, when time-dependent, nonlinear partial differential equations must be solved, it is usually most efficient to solve the explicit-in-time, physical equations using an explicit numerical scheme. When the equations exhibit weak time dependence but strong nonlinear effects (e.g., large deformation), the physical equations, though not explicitly time-dependent, are still probably most efficiently solved by explicit-in-time equations using a modified explicit numerical method. For the latter case, it is possible to separate the modifications to explicit methods for weakly time-dependent problems into three useful categories: (1) density scaling, (2) velocity damping, and (3) modulus scaling.

Density scaling is consistent with the situation where inertia effects are unimportant, where compressibility may be important, and where the time scale of the problem is determined by some other consideration, for example, heat transfer. Density scaling allows one to compute the intermediate state points of the process. Velocity damping (dynamic relaxation) may be used when inertia is somewhat important, compressibility may also be important, and the time scale is somewhat arbitrary. Velocity damping concerns itself only with the end states of a process. Intermediate states are not guaranteed to be accurate because the process (thermodynamic path dependence) is always assumed to be critically damped. Modulus scaling is at the other end of the spectrum from density scaling. When modulus scaling is most applicable, inertia effects are quite important, but compressibility is unimportant. The problem time scale is determined by an external constraint.

For example, most static problems can be categorized as "problems in which inertial influences are not important". Thus, density scaling can be used to increase the calculational time step in order to improve solution efficiency. Quasi-static problems, by definition, have a "sluggish" response, lending themselves to "dynamic relaxation" critical damping as a means of achieving an efficient solution. Steady-state processes are usually associated with incompressible flow or rigid body motion assumptions, in which case modulus scaling appears to be the most appropriate choice to improve computational efficiency.

4.5.2 Density Scaling. When a problem is static or nearly static, the density (or mass) does not play an important role in the stress equilibrium process. Inertial effects disappear and the momentum equation becomes

$$\Sigma F_x \cong 0 \tag{4.60a}$$

or

$$\nabla \sigma_{xx} \cong 0 \tag{4.60b}$$

where F_x are forces and σ_{xx} are stresses. The zero on the right-hand side of the equal sign indicates that the inertial force is negligible. So, for

Eq.(4.60b), we can write

$$\rho \ddot{x} \cong 0 . \tag{4.61}$$

The reason Eq.(4.61) applies is that $\ddot{x}$ is small. Therefore, ρ can be any value (in units consistent with $\ddot{x}$) so long as Eq.(4.61) is still satisfied.

Referring to Eq.(4.55), it can be shown that the dominant term in the denominator for static and quasi-static problems is c_ℓ^2. Since c_ℓ^2 is a direct function of the bulk and shear moduli and an inverse function of the reference density, it can be seen that in order to increase the time step for a particular zone, it is necessary to lower the sound speed, c_ℓ, which means either lowering the moduli or raising the density (or both). For static problems, Eq.(4.61) indicates that the density may be increased until the product, $\rho\ddot{x}$, produces an anomalous inertial effect.

Employing density scaling to achieve a larger time step for static problems requires only a change of input. The momentum equation and the Courant stability condition are unchanged.

4.5.3 <u>Dynamic Relaxation</u>. Another approach to economical static solutions is achieved by adding a viscous damping term to the momentum equation which acts to critically damp the fundamental response mode. This method reduces the number of time steps (iterations) required to achieve stress equilibrium, instead of increasing the magnitude of individual time steps. Quasi-static solutions can also be found using this approach. This approach is useful only when the integrated value of time is of no consequence, i.e., it doesn't matter what the "real time" is. Density scaling, on the other hand, preserves time as a meaningful variable.

The equations of motion are modified as follows,

$$\Sigma F_x = m\left(\ddot{x} + \frac{\eta}{\tau}\dot{x}\right) \tag{4.62a}$$

where η is a dimensionless damping coefficient, $\ddot{x}$ is the acceleration resulting from the externally applied forces, F_x, $\dot{x}$ is the velocity that results from integrating $\ddot{x}$ with critical damping applied, and τ is the longest fundamental period of the system when the boundary conditions are present. In terms of stress, Eq.(4.62a) becomes

$$\frac{\delta\sigma_{xx}}{\delta x} = \rho\left(\ddot{x} + \frac{\eta'}{\tau}\dot{x}\right) \tag{4.62b}$$

where η' is $\eta/\mathcal{V}$. η (or η') is chosen to critically damp the lowest fundamental frequency of the grid. For linear elastic problems, it is a relatively simple matter to determine the damping (or relaxation) factor from a modal analysis or a dynamic excitation without damping. Even for mildly nonlinear systems, the latter technique can be used. For strongly nonlinear systems, an appropriate relaxation factor is far more difficult to compute and often requires considerable judgment.

The calculational form of the dynamic relaxation equation analogous to Eq.(4.7) comes from solving Eq.(4.62b) for acceleration (including gravitation),

$$\ddot{x}^n = \frac{1}{\rho^n}\left(\frac{\delta\sigma_{xx}}{\delta x}\right)^n - \frac{1}{\rho^n}\frac{\eta'}{\tau}\dot{x}^n + g_x \ . \tag{4.63}$$

Integrating Eq.(4.63) with respect to time and making the following substitutions,

$$\frac{\eta'}{\rho^n} \equiv \frac{\eta}{m}$$

$$\dot{x}^n \equiv \frac{\dot{x}^{n+\frac{1}{2}} + \dot{x}^{n-\frac{1}{2}}}{2}$$

yields

$$\dot{x}^{n+\frac{1}{2}} - \dot{x}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\delta\sigma_{xx}}{\delta x}\right)^n + g_x\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{x}^{n+\frac{1}{2}} + \dot{x}^{n-\frac{1}{2}}\right] \ . \tag{4.64}$$

Solving Eq.(4.64) for new velocity and defining the relaxation factor, ω, to be

$$\omega \equiv \frac{\eta}{2m\tau} ,$$

results in

$$\dot{x}^{n+\frac{1}{2}} = \dot{x}^{n-\frac{1}{2}} \left[\frac{2}{1+\omega\Delta t^{n}} - 1 \right] + \ddot{x}^{n} \left[\frac{\Delta t^{n}}{1+\omega\Delta t^{n}} \right] \qquad (4.65)$$

where

$$\ddot{x}^{n} = \frac{1}{\rho^{n}} \left(\frac{\partial\sigma_{xx}}{\partial x} \right)^{n} + g_{x} .$$

4.5.4 Modulus Scaling. There are several forms of modulus scaling: (1) sound speed scaling for incompressible cases, and (2) elastic constants scaling for rigid body motion. The approach to computational efficiency is similar to density scaling in that the time step improvement comes from reducing the sound speed.

The physical assumption associated with incompressibility implies that the mechanical sound speed is indeterminant. Often it is said the sound speed is infinite (or, similarly, that the Mach number is zero, $M = 0$). However, as a practical matter, a better condition might be that incompressibility for real materials exists when $M \leqslant 0.3$. For many cases, this means that the sound speed can be reduced (scaled) below its actual value provided that $M \leqslant 0.3$.

An example of sound speed scaling is described as follows: Suppose an air bubble is expanding in water at approximately 15 ft/sec and it is necessary to compute the resulting pressure in the water. The sound speed of water is about 5000 ft/sec, which for this problem means that the Mach number is about 3×10^{-3}. The flow is incompressible. Therefore, the sound speed is not important and can be artificially dropped up to two orders of magnitude without exceeding the Mach number criterion for incompressibility. To be conservative, let's drop the sound speed only one order of magnitude to 500 ft/sec. This improves the time step by a factor of 10. To drop the sound speed means that the bulk modulus is effectively reduced by a factor of 100 (i.e., the compressibility is increased by 100). Since the flow at 15 ft/sec is incompressible, the change of modulus will be applied to infinitesimal strains and the pressures will be only slightly affected.

REFERENCES FOR SECTION 4

4.1 J. Von Neumann and R. D. Richtmyer, "A Method for the Numerical Calculation of Hydrodynamic Shocks", J. Appl. Phys., 21, March 1950, pp. 232-237.

4.2 E. D. Giroux, "HEMP User's Manual", UCRL-51079, Rev. 1, Lawrence Livermore National Laboratory, Livermore, California, December 17, 1973.

SECTION 5

TWO-DIMENSIONAL LAGRANGIAN FINITE-DIFFERENCE EQUATIONS[*]

5.1 INTRODUCTION

The Lagrange explicit finite-difference equations which represent the physical equations of a two-dimensional continuum are solved using two overlapping meshes -- a displacement mesh and a stress mesh. The displacement mesh is made up of grid (mesh) points which define geometric quantities such as shapes, interfaces, and boundaries. Conservation of momentum is used in the displacement mesh to solve for the vector variables, acceleration $(\ddot{x},\ddot{y})$, velocity $(\dot{x},\dot{y})$, and position (x,y), at specific points in space. The stress mesh is made up of zones in which scalars and tensors are calculated as averages over zone volumes and surface areas using conservation of internal energy and constitutive equations to solve for scalar and tensor variables such as stress, σ_{xx}, σ_{yy}, etc., internal energy, u, pressure, p, etc.

Both meshes describe the same region of space and are related through identical satisfaction of conservation of mass; that is, density, ρ, in both meshes describes the existence of material in the same way. Thus, the relationship between meshes is that the grid points of the displacement mesh uniquely define the zones of the stress mesh.

5.2 DISPLACEMENT MESH

5.2.1 Calculational Sequence. The two-dimensional Lagrange continuum mechanics equations are solved in three steps. First, the momentum equations are solved to determine mechanical motion from stress, internal energy, and density distributions. Next, conservation of mass is used to calculate new density distribution, and finally, the constitutive relations and conservation of internal energy are solved simultaneously to calculate a new stress and internal energy distribution. This procedure is shown schematically in Figure 5.1.

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[*] Section 5 is identical to Section 4 wherever possible.

$$\left.\begin{array}{ll} x^{n}_{i,j},\ y^{n}_{i,j} & \rho^{n}_{i-\frac{1}{2},j-\frac{1}{2}},\ \sigma^{n}_{i-\frac{1}{2},j-\frac{1}{2}} \\ \dot{x}^{n-\frac{1}{2}}_{i,j},\ \dot{y}^{n-\frac{1}{2}}_{i,j} & \end{array}\right\}\ \text{Initial Conditions}$$

$$\left.\ddot{x}^{n}_{i,j},\ \ddot{y}^{n}_{i,j}\right\}\ \text{Conservation of Momentum}$$

$$\text{Explicit Integration}\ \left\{\begin{array}{l} \dot{x}^{n+\frac{1}{2}}_{i,j},\ \dot{y}^{n+\frac{1}{2}}_{i,j},\ \Delta t^{n} \\ x^{n+1}_{i,j},\ y^{n+1}_{i,j},\ \Delta t^{n+\frac{1}{2}} \end{array}\right.$$

$$\left.\rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right\}\ \text{Conservation of Mass}$$

$$\begin{array}{c}\text{Simultaneous} \\ \text{Solution for} \\ \text{Explicit} \\ \text{Time Step} \\ \Delta t^{n+1/2}\end{array}\left\{\begin{array}{ll} u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = u\left(p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ \rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ s^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right) & \Big\}\ \begin{array}{l}\text{Conservation} \\ \text{of Energy}\end{array} \\ \left.\begin{array}{l} p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = p\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ \rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right) \\ s^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = s\left(\rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right) \end{array}\right\} & \begin{array}{l}\text{Constitutive} \\ \text{Relations}\end{array} \end{array}\right.$$

$$\left.\sigma^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right\}\ \begin{array}{l}\text{Initial Conditions} \\ \text{for Next Time Step (cycle)}\end{array}$$

$$\left.\Delta t^{n+1}\right\}\ \begin{array}{l}\text{Time Step} \\ \text{for Next Cycle from} \\ \text{Courant Stability Criterion}\end{array}$$

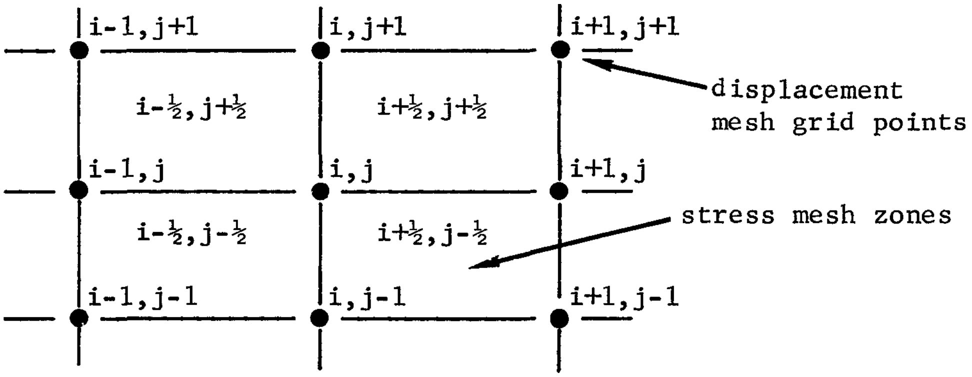
Figure 5.1. Two-dimensional calculational cycle.

5.2.2 Momentum Equations. The general momentum equations for two independent space variables (for translational and axial symmetries) are

$$\ddot{x} = \frac{1}{\rho}\left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y}\right) + f\,\frac{1}{\rho}\left(\frac{\sigma_{xx} - \sigma_{zz}}{x}\right) + (1 - f)g_x \,,$$

$$\ddot{y} = \frac{1}{\rho}\left(\frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{xy}}{\partial x}\right) + f\,\frac{1}{\rho}\left(\frac{\sigma_{xy}}{x}\right) + g_y \,, \tag{5.1}$$

where $f = 0$ for translational symmetry and $f = 1$ for axial* symmetry; and g_x and g_y are gravity acceleration components. The finite-difference form of these equations can be derived in such a way that it is possible to use the same numerical equation for boundary points as well as for interior points. Consider the nonboundary point (i,j) and its immediate neighbors, as shown below.



The grid point neighbors of grid point (i,j) are point (i-1,j) on the left, point (i+1,j) on the right, point (i,j-1) on the bottom, and point (i,j+1) on the top. The volume defined by grid points (i,j), (i-1,j), (i-1,j-1), and (i,j-1) is called zone (i-½,j-½). This zone is the bottom left zone with respect to grid point (i,j). Similar descriptions can be made for the bottom right zone (i+½,j-½), the top right zone (i+½,j+½), and the top left zone (i-½,j+½).

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[*] The axial equations assume that x and y are the radial and axial coordinates, respectively. See Eqs. (2.18a) and (2.19a).

To derive properly centered finite-difference forms of the momentum equations, Eqs.(5.1) are rewritten as follows,

$$\ddot{x}^n_{i,j} = \frac{1}{\rho^n_{i,j}}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n_{i,j} + f\,\frac{1}{\rho^n_{i,j}}\left(\frac{\sigma_{xx} - \sigma_{zz}}{x}\right)^n_{i,j} + (1 - f)g_x \;, \tag{5.2a}$$

$$\ddot{y}^n_{i,j} = \frac{1}{\rho^n_{i,j}}\left(\frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{xy}}{\partial x}\right)^n_{i,j} + f\,\frac{1}{\rho^n_{i,j}}\left(\frac{\sigma_{xy}}{x}\right)^n_{i,j} + g_y \;,$$

where superscripts denote the time centering, while subscripts denote space centering; or

$$\ddot{x}^n_{i,j} = \frac{V^n_{i,j}}{\rho^o_{i,j}}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n_{i,j} + f\,\frac{V^n_{i,j}}{\rho^o_{i,j}}\left(\frac{\sigma_{xx} - \sigma_{zz}}{x}\right)^n_{i,j} + (1 - f)g_x \;, \tag{5.2b}$$

$$\ddot{y}^n_{i,j} = \frac{V^n_{i,j}}{\rho^o_{i,j}}\left(\frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{xy}}{\partial x}\right)^n_{i,j} + f\,\frac{V^n_{i,j}}{\rho^o_{i,j}}\left(\frac{\sigma_{xy}}{x}\right)^n_{i,j} + g_y \;,$$

where $V^n_{i,j}$ is the relative volume, defined as

$$V^n_{i,j} \equiv \frac{\rho^o_{i,j}}{\rho^n_{i,j}} \;,$$

where $\rho^o_{i,j}$ is a reference density usually taken to be the density at zero stress. Equations (5.2a) and (5.2b) represent a time- and space-centered partial differential equation which can be reduced to

Rev. 2
15 NOV 77

$$\ddot{x}^n_{i,j} = \frac{V^n_{i,j}}{\rho^o_{i,j}} \left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} \right)^n_{i,j} + f\,\beta^n_{x_{i,j}} + (1-f)g_x \,,$$

$$\ddot{y}^n_{i,j} = \frac{V^n_{i,j}}{\rho^o_{i,j}} \left(\frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{xy}}{\partial x} \right)^n_{i,j} + f\,\beta^n_{y_{i,j}} + g_y \,, \tag{5.3}$$

where $\beta^n_{x_{i,j}}$ is a hoop stress contribution to the radial motion, x, about the axis of symmetry, y,*

$$\beta^n_{x_{i,j}} = \frac{V^n_{i,j}}{\rho^o_{i,j}} \left(\frac{\sigma_{xx} - \sigma_{zz}}{x} \right)^n_{i,j} \,, \tag{5.3a}$$

and $\beta^n_{y_{i,j}}$ is the shear stress contribution to the axial motion, y, due to radial divergence, x,*

$$\beta^n_{y_{i,j}} = \frac{V^n_{i,j}}{\rho^o_{i,j}} \left(\frac{\sigma_{xy}}{x} \right)^n_{i,j} \,. \tag{5.3b}$$

Using the definition of first-order spatial average of zone quantities,

$$(\ )^n_{i,j} \equiv \frac{1}{4}\left[(\ )^n_{i+\frac{1}{2},j+\frac{1}{2}} + (\ )^n_{i-\frac{1}{2},j+\frac{1}{2}} + (\ )^n_{i-\frac{1}{2},j-\frac{1}{2}} + (\ )^n_{i+\frac{1}{2},j-\frac{1}{2}} \right] \,, \tag{5.4}$$

it is possible to derive formulas for hoop stress, β_x, and shear stress, β_y, contributions in axial symmetry.

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*These comments apply only to axial symmetry since f = 0 for translational symmetry.

Using Eqs.(3.13), Eqs.(5.3) can be rewritten as

$$\ddot{x}^n_{i,j} = \frac{1}{2}\,\frac{V^n_{i,j}}{\rho^o_{i,j}A^n_{i,j}}\Bigg[\sigma^n_{xx_{i+\frac{1}{2},j+\frac{1}{2}}}\left(y^n_{i,j+1} - y^n_{i+1,j}\right)$$

$$+\ \sigma^n_{xx_{i-\frac{1}{2},j+\frac{1}{2}}}\left(y^n_{i-1,j} - y^n_{i,j+1}\right)$$

$$+\ \sigma^n_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}\left(y^n_{i,j-1} - y^n_{i-1,j}\right)$$

$$+\ \sigma^n_{xx_{i+\frac{1}{2},j-\frac{1}{2}}}\left(y^n_{i+1,j} - y^n_{i,j-1}\right)$$

$$-\ \sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2}}}\left(x^n_{i,j+1} - x^n_{i+1,j}\right)$$

$$-\ \sigma^n_{xy_{i-\frac{1}{2},j+\frac{1}{2}}}\left(x^n_{i-1,j} - x^n_{i,j+1}\right)$$

$$-\ \sigma^n_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}\left(x^n_{i,j-1} - x^n_{i-1,j}\right)$$

$$-\ \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2}}}\left(x^n_{i+1,j} - x^n_{i,j-1}\right)\Bigg]$$

$$+\ f\beta^n_{x_{i,j}} + (1 - f)g_x\ ; \qquad (5.5a)$$

$$\ddot{y}^n_{i,j} = \frac{1}{2}\,\frac{V^n_{i,j}}{\rho^o_{i,j}A^n_{i,j}}\Bigg[-\sigma^n_{yy_{i+\frac{1}{2},j+\frac{1}{2}}}\left(x^n_{i,j+1} - x^n_{i+1,j}\right)$$

$$-\sigma^n_{yy_{i-\frac{1}{2},j+\frac{1}{2}}}\left(x^n_{i-1,j} - x^n_{i,j+1}\right)$$

$$-\sigma^n_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}\left(x^n_{i,j-1} - x^n_{i-1,j}\right)$$

$$-\sigma^n_{yy_{i+\frac{1}{2},j-\frac{1}{2}}}\left(x^n_{i+1,j} - x^n_{i,j-1}\right)$$

$$+\sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2}}}\left(y^n_{i,j+1} - y^n_{i+1,j}\right)$$

$$+\sigma^n_{xy_{i-\frac{1}{2},j+\frac{1}{2}}}\left(y^n_{i-1,j} - y^n_{i,j+1}\right)$$

$$+\sigma^n_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}\left(y^n_{i,j-1} - y^n_{i-1,j}\right)$$

$$+\sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2}}}\left(y^n_{i+1,j} - y^n_{i,j-1}\right)\Bigg]$$

$$+ f\beta^n_{y_{i,j}} + g_y \; ; \qquad (5.5b)$$

where $\dfrac{V^n_{i,j}}{\rho^o_{i,j}A^n} = \dfrac{1}{\alpha^n_{i,j}}$. $\alpha^n_{i,j}$ is the mass per unit length at grid point (i,j) defined by

$$\alpha^n_{i,j} \equiv \frac{1}{4}\left[\alpha^n_{i+\frac{1}{2},j+\frac{1}{2}} + \alpha^n_{i-\frac{1}{2},j+\frac{1}{2}} + \alpha^n_{i-\frac{1}{2},j-\frac{1}{2}} + \alpha^n_{i+\frac{1}{2},j-\frac{1}{2}}\right] .$$

The factor of 2 multiplying $\alpha^n_{i,j}$ in Eqs.(5.5) is necessary to make the momentum mass (α^n) consistent with the volume enclosed by the surface integral used to calculate the gradient of stress.

Rev. 2
15 NOV 77

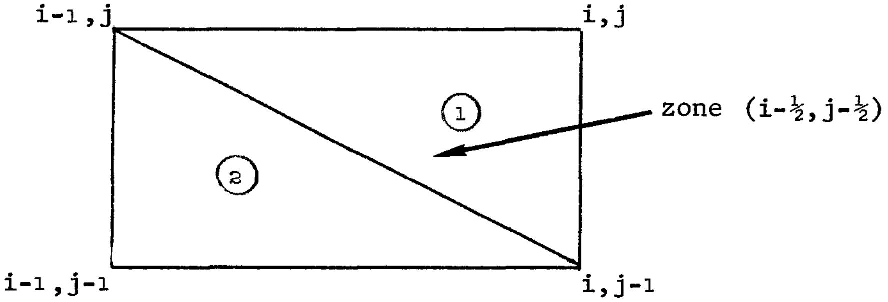
Thus, $\frac{V^n_{i,j}}{\rho^o_{i,j} A^n_{i,j}}$, $\beta^n_{x_{i,j}}$ and $\beta^n_{y_{i,j}}$ are defined as follows,

$$\frac{V^n_{i,j}}{\rho^o_{i,j} A^n_{i,j}} = \frac{1}{4}\left[\frac{V^n_{i+\frac{1}{2},j+\frac{1}{2}}}{\rho^o_{i+\frac{1}{2},j+\frac{1}{2}} A^n_{i+\frac{1}{2},j+\frac{1}{2}}} + \frac{V^n_{i-\frac{1}{2},j+\frac{1}{2}}}{\rho^o_{i-\frac{1}{2},j+\frac{1}{2}} A^n_{i-\frac{1}{2},j+\frac{1}{2}}} + \frac{V^n_{i-\frac{1}{2},j-\frac{1}{2}}}{\rho^o_{i-\frac{1}{2},j-\frac{1}{2}} A^n_{i-\frac{1}{2},j-\frac{1}{2}}} + \frac{V^n_{i+\frac{1}{2},j-\frac{1}{2}}}{\rho^o_{i+\frac{1}{2},j-\frac{1}{2}} A^n_{i+\frac{1}{2},j-\frac{1}{2}}}\right] ; \qquad (5.6a)$$

$$\beta^n_{x_{i,j}} = \frac{2\pi}{4}\left[\left(\sigma_{xx} - \sigma_{zz}\right)^n_{i+\frac{1}{2},j+\frac{1}{2}} \frac{A^n_{i+\frac{1}{2},j+\frac{1}{2}}}{m_{i+\frac{1}{2},j+\frac{1}{2}}} + \left(\sigma_{xx} - \sigma_{zz}\right)^n_{i-\frac{1}{2},j+\frac{1}{2}} \frac{A^n_{i-\frac{1}{2},j+\frac{1}{2}}}{m_{i-\frac{1}{2},j+\frac{1}{2}}} + \left(\sigma_{xx} - \sigma_{zz}\right)^n_{i-\frac{1}{2},j-\frac{1}{2}} \frac{A^n_{i-\frac{1}{2},j-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2}}} + \left(\sigma_{xx} - \sigma_{zz}\right)^n_{i+\frac{1}{2},j-\frac{1}{2}} \frac{A^n_{i+\frac{1}{2},j-\frac{1}{2}}}{m_{i+\frac{1}{2},j-\frac{1}{2}}}\right] ; \qquad (5.6b)$$

$$\beta^n_{y_{i,j}} = \frac{2\pi}{4}\left[\sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2}}} \left(\frac{A^n_{i+\frac{1}{2},j+\frac{1}{2}}}{m_{i+\frac{1}{2},j+\frac{1}{2}}}\right) + \sigma^n_{xy_{i-\frac{1}{2},j+\frac{1}{2}}} \left(\frac{A^n_{i-\frac{1}{2},j+\frac{1}{2}}}{m_{i-\frac{1}{2},j+\frac{1}{2}}}\right) + \sigma^n_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \left(\frac{A^n_{i-\frac{1}{2},j-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2}}}\right) + \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2}}} \left(\frac{A^n_{i+\frac{1}{2},j-\frac{1}{2}}}{m_{i+\frac{1}{2},j-\frac{1}{2}}}\right)\right] ; \qquad (5.6c)$$

where A is the area of the quadrilateral zone and m is the mass of the zone. The equation for area is derived by dividing the zone into two triangles, calculating the area of each triangle, and summing the areas of the two triangles to get the quadrilateral area. For example, consider zone $(i-\frac{1}{2},j-\frac{1}{2})$, which is defined by the four grid points (i,j), $(i-1,j)$, $(i,j-1)$, and $(i-1,j-1)$. The zone area is determined by dividing the zone into two triangles, as follows.



$$A_{\textcircled{1}} = \frac{1}{2}\left[x_{i,j-1}\left(y_{i,j} - y_{i-1,j}\right) + x_{i,j}\left(y_{i-1,j} - y_{i,j-1}\right) + x_{i-1,j}\left(y_{i,j-1} - y_{i,j}\right)\right] ;$$

$$A_{\textcircled{2}} = \frac{1}{2}\left[x_{i,j-1}\left(y_{i-1,j} - y_{i-1,j-1}\right) + x_{i-1,j}\left(y_{i-1,j-1} - y_{i,j-1}\right) + x_{i-1,j-1}\left(y_{i,j-1} - y_{i-1,j}\right)\right] ;$$

and

$$A_{i-\frac{1}{2},j-\frac{1}{2}} = A_{\textcircled{1}} + A_{\textcircled{2}} . \qquad (5.6d)$$

The equation for mass depends on the equation for true volume, $\mathcal{V}$, and the equation for true volume depends on the symmetry condition. In translational symmetry the true volume formula is

$$\mathcal{V} = 1 \times A .$$

In axial symmetry the true volume is

$$\mathcal{V} = 2\pi x A ,$$

where x is the radius to the centroid of the area A. Mass is derived from

$$m = \rho \mathcal{V} ,$$

so that m in Eqs.(5.6b) and (5.6c) is

$$m = \rho \, 2\pi x A .$$

In practice, the formula for mass in axial symmetry becomes

$$m = 2\pi \rho \left[\frac{1}{3}\left(x_{i,j-1} + x_{i,j} + x_{i-1,j}\right) A_{①} + \frac{1}{3}\left(x_{i,j-1} + x_{i-1,j} + x_{i-1,j-1}\right) A_{②} \right] . \tag{5.6e}$$

Numerical evaluation of Eqs.(5.5) yields grid point acceleration of grid point (i,j) at time n. To determine the velocity and position of grid point (i,j) requires time-centered integrations analogous to Eqs.(4.7) and (4.8), pictorially described by Figures 4.2 and 4.3. The two-dimensional versions of these equations are for velocity

$$\dot{x}_{i,j}^{n+\frac{1}{2}} = \dot{x}_{i,j}^{n-\frac{1}{2}} + \ddot{x}_{i,j}^{n} \, \Delta t^{n} ,$$
$$\dot{y}_{i,j}^{n+\frac{1}{2}} = \dot{y}_{i,j}^{n-\frac{1}{2}} + \ddot{y}_{i,j}^{n} \, \Delta t^{n} , \tag{5.7}$$

and for position,

$$x^{n+1}_{i,j} = x^{n}_{i,j} + \dot{x}^{n+\frac{1}{2}}_{i,j} \Delta t^{n+\frac{1}{2}} ,$$

$$y^{n+1}_{i,j} = y^{n}_{i,j} + \dot{y}^{n+\frac{1}{2}}_{i,j} \Delta t^{n+\frac{1}{2}} . \qquad (5.8)$$

The time step values, Δt^{n} and $\Delta t^{n+\frac{1}{2}}$, used in Eqs.(5.7) and (5.8) are determined from the stability requirement that a sound signal can only propagate the smallest zone dimension of the entire mesh or less in one time step. Mathematically, this condition, called the Courant stability criterion, is written as follows:

$$\Delta t^{n} = \text{minimum value of } \Delta t^{n}_{i-\frac{1}{2},j-\frac{1}{2}} \text{ for all } i > 1,\ j > 1,$$

$$\Delta t^{n+\frac{1}{2}} = \text{minimum value of } \Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \text{ for all } i > 1,\ j > 1,$$

where

$$\Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \le \frac{\Delta \ell^{n}_{i-\frac{1}{2},j-\frac{1}{2}}}{c^{n}_{i-\frac{1}{2},j-\frac{1}{2}}} , \quad \Delta t^{n}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{\Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} + \Delta t^{n-\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}}{2} . \qquad \begin{matrix}(5.9a),\\(5.9b)\end{matrix}$$

$\Delta \ell^{n}_{i-\frac{1}{2},j-\frac{1}{2}}$ is the smallest length across zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n, and $c^{n}_{i-\frac{1}{2},j-\frac{1}{2}}$ is the sound speed of zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n. Values at time n come from initial conditions or from a previous cycle.

Equations (5.7) and (5.8) use the definition for a first-order temporal difference analogous to Eqs.(4.10a) and (4.10b),

$$\Delta(\ )^{n}_{i,j} \equiv (\ )^{n+\frac{1}{2}}_{i,j} - (\ )^{n-\frac{1}{2}}_{i,j} , \qquad (5.10a)$$

and

$$\Delta(\ )_{i,j}^{n+\frac{1}{2}} \equiv (\ )_{i,j}^{n+1} - (\ )_{i,j}^{n} . \tag{5.10b}$$

Equations (5.5), (5.7), and (5.8) are perfectly centered in space and time. However, a time-centering error can occur in Eqs.(5.7) for the initial step because $\dot{x}_{i,j}^{n-\frac{1}{2}}$ and $\dot{y}_{i,j}^{n-\frac{1}{2}}$ may not be known at time n-½. In this case, it is customary to let $\dot{x}_{i,j}^{n-\frac{1}{2}}$ and $\dot{y}_{i,j}^{n-\frac{1}{2}}$ take on the value of $\dot{x}_{i,j}^{n}$ and $\dot{y}_{i,j}^{n}$, respectively, and to use an initial time step, Δt^{o}, that is 0.1 of the initial stable value. After the initial time step, Eqs.(5.7) are properly centered.*

5.2.3 Momentum Boundary Conditions. Momentum boundary conditions are of two types -- those that use a stress or force, and those that use an acceleration, a velocity, or a displacement. The former, known as "stress-type boundaries," affect Eqs.(5.5), while the latter, known as "velocity-type boundaries," affect Eqs.(5.7) and (5.8). In addition to the two types of boundary conditions, there are two ways in which boundary values are obtained, i.e., by prescription or by interaction. By prescription means that boundary values are provided as time histories for an entire event; by interaction means that an algorithm for calculating values is provided.

Equations (5.5), which were derived for non-boundary points, are well suited for stress-type boundary conditions. Left boundary conditions affect the i-½ values in Eqs.(5.5), right boundary conditions affect the i+½ values, bottom boundary conditions affect the j-½ values, and top boundary conditions affect the j+½ values. There are eight possible outside boundary

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*Equations (5.7) may be written in "dynamic relaxation" form so that static and quasi-static calculations are computed more efficiently. A discussion of dynamic relaxation appears in Section 5.5.

orientations in two-dimensional geometry. They are:

(1) bottom left corner
(2) bottom
(3) bottom right corner
(4) left
(5) right
(6) top left corner
(7) top
(8) top right corner

An example of a left boundary condition is a free left boundary. Mathematically, the free left boundary condition applied to Eqs.(5.5) is given by

$$
\begin{aligned}
& x^n_{i-1,j} = x^n_{i,j}\,, \qquad y^n_{i-1,j} = y^n_{i,j}\,, \\
& \sigma^n_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} = \sigma^n_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} = \sigma^n_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} = \sigma^n_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} = 0\,, \\
& \sigma^n_{xx_{i-\frac{1}{2},j+\frac{1}{2}}} = \sigma^n_{yy_{i-\frac{1}{2},j+\frac{1}{2}}} = \sigma^n_{zz_{i-\frac{1}{2},j+\frac{1}{2}}} = \sigma^n_{xy_{i-\frac{1}{2},j+\frac{1}{2}}} = 0\,, \qquad (5.11) \\
& \rho^n_{i-\frac{1}{2},j-\frac{1}{2}} = 0\,, \\
& \rho^n_{i-\frac{1}{2},j+\frac{1}{2}} = 0\,.
\end{aligned}
$$

Substituting Eqs.(5.11) into Eqs.(5.5) yields

$$\begin{aligned}\ddot{x}^n_{i,j} = \frac{1}{2}\,\frac{V^n_{i,j}}{\rho^o_{i,j}\,A^n_{i,j}}\Bigg[&\sigma^n_{xx_{i+\frac{1}{2},j+\frac{1}{2}}}\left(y^n_{i,j+1} - y^n_{i+1,j}\right)\\ &+ \sigma^n_{xx_{i+\frac{1}{2},j-\frac{1}{2}}}\left(y^n_{i+1,j} - y^n_{i,j-1}\right)\\ &- \sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2}}}\left(x^n_{i,j+1} - x^n_{i+1,j}\right)\\ &- \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2}}}\left(x^n_{i+1,j} - x^n_{i,j-1}\right)\Bigg] + f\beta^n_{x_{i,j}}\ ;\end{aligned} \tag{5.12a}$$

$$\begin{aligned}\ddot{y}^n_{i,j} = \frac{1}{2}\,\frac{V^n_{i,j}}{\rho^o_{i,j}\,A^n_{i,j}}\Bigg[&- \sigma^n_{yy_{i+\frac{1}{2},j+\frac{1}{2}}}\left(x^n_{i,j+1} - x^n_{i+1,j}\right)\\ &- \sigma^n_{yy_{i+\frac{1}{2},j-\frac{1}{2}}}\left(x^n_{i+1,j} - x^n_{i,j-1}\right)\\ &+ \sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2}}}\left(y^n_{i,j+1} - y^n_{i+1,j}\right)\\ &+ \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2}}}\left(y^n_{i+1,j} - y^n_{i,j-1}\right)\Bigg] + f\beta^n_{y_{i,j}}\ ;\end{aligned} \tag{5.12b}$$

where $\dfrac{V^n_{i,j}}{\rho^o_{i,j}\, A^n_{i,j}}$, $\beta^n_{x_{i,j}}$ and $\beta^n_{y_{i,j}}$ are,

$$\frac{V^n_{i,j}}{\rho^o_{i,j} \quad A^n_{i,j}} = \frac{1}{2}\left[\frac{V^n_{i+\frac{1}{2},j+\frac{1}{2}}}{\rho^o_{i+\frac{1}{2},j+\frac{1}{2}}\; A^n_{i+\frac{1}{2},j+\frac{1}{2}}} + \frac{V^n_{i+\frac{1}{2},j-\frac{1}{2}}}{\rho^o_{i+\frac{1}{2},j-\frac{1}{2}}\; A^n_{i+\frac{1}{2},j-\frac{1}{2}}}\right] \;; \tag{5.12c}$$

$$\beta^n_{x_{i,j}} = \frac{2\pi}{2}\left[\left(\sigma_{xx} - \sigma_{zz}\right)^n_{i+\frac{1}{2},j+\frac{1}{2}} \frac{A^n_{i+\frac{1}{2},j+\frac{1}{2}}}{m_{i+\frac{1}{2},j+\frac{1}{2}}} + \left(\sigma_{xx} - \sigma_{zz}\right)^n_{i+\frac{1}{2},j-\frac{1}{2}} \frac{A^n_{i+\frac{1}{2},j-\frac{1}{2}}}{m_{i+\frac{1}{2},j-\frac{1}{2}}}\right] \;; \tag{5.12d}$$

$$\beta^n_{y_{i,j}} = \frac{2\pi}{2}\left[\sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2}}}\left(\frac{A^n_{i+\frac{1}{2},j+\frac{1}{2}}}{m_{i+\frac{1}{2},j+\frac{1}{2}}}\right) + \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2}}}\left(\frac{A^n_{i+\frac{1}{2},j-\frac{1}{2}}}{m_{i+\frac{1}{2},j-\frac{1}{2}}}\right)\right]. \tag{5.12e}$$

The formulas for acceleration of any "stress" boundary are derived in a similar manner. The general formulas are Eqs.(5.5) using the appropriate boundary stress in place of the zone stress and using i,j coordinate values for x and y whenever a point is not on the boundary. Equations (5.6) become

$$\frac{V^n_{i,j}}{\rho^o_{i,j}\,A^n_{i,j}} = \frac{1}{N}\Bigg[E_{i+\frac{1}{2},j+\frac{1}{2}}\,\frac{V^n_{i+\frac{1}{2},j+\frac{1}{2}}}{\rho^o_{i+\frac{1}{2},j+\frac{1}{2}}\,A^n_{i+\frac{1}{2},j+\frac{1}{2}}} + E_{i-\frac{1}{2},j+\frac{1}{2}}\,\frac{V^n_{i-\frac{1}{2},j+\frac{1}{2}}}{\rho^o_{i-\frac{1}{2},j+\frac{1}{2}}\,A^n_{i-\frac{1}{2},j+\frac{1}{2}}} + E_{i-\frac{1}{2},j-\frac{1}{2}}\,\frac{V^n_{i-\frac{1}{2},j-\frac{1}{2}}}{\rho^o_{i-\frac{1}{2},j-\frac{1}{2}}\,A^n_{i-\frac{1}{2},j-\frac{1}{2}}} + E_{i+\frac{1}{2},j-\frac{1}{2}}\,\frac{V^n_{i+\frac{1}{2},j-\frac{1}{2}}}{\rho^o_{i+\frac{1}{2},j-\frac{1}{2}}\,A^n_{i+\frac{1}{2},j-\frac{1}{2}}}\Bigg], \qquad (5.13)$$

where N is the sum of the existence factors,

$$N \equiv E_{i+\frac{1}{2},j+\frac{1}{2}} + E_{i-\frac{1}{2},j+\frac{1}{2}} + E_{i-\frac{1}{2},j-\frac{1}{2}} + E_{i+\frac{1}{2},j-\frac{1}{2}}, \qquad (5.14)$$

and the existence factors, E, are equal to zero if the zone does not exist and equal to one if it does exist.

$$\beta^n_{x_{i,j}} = \frac{2\pi}{N}\Bigg[E_{i+\frac{1}{2},j+\frac{1}{2}}\left(\sigma_{xx} - \sigma_{zz}\right)^n_{i+\frac{1}{2},j+\frac{1}{2}}\frac{A^n_{i+\frac{1}{2},j+\frac{1}{2}}}{m_{i+\frac{1}{2},j+\frac{1}{2}}} + E_{i-\frac{1}{2},j+\frac{1}{2}}\left(\sigma_{xx} - \sigma_{zz}\right)^n_{i-\frac{1}{2},j+\frac{1}{2}}\frac{A^n_{i-\frac{1}{2},j+\frac{1}{2}}}{m_{i-\frac{1}{2},j+\frac{1}{2}}} + E_{i-\frac{1}{2},j-\frac{1}{2}}\left(\sigma_{xx} - \sigma_{zz}\right)^n_{i-\frac{1}{2},j-\frac{1}{2}}\frac{A^n_{i-\frac{1}{2},j-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2}}} + E_{i+\frac{1}{2},j-\frac{1}{2}}\left(\sigma_{xx} - \sigma_{zz}\right)^n_{i+\frac{1}{2},j-\frac{1}{2}}\frac{A^n_{i+\frac{1}{2},j-\frac{1}{2}}}{m_{i+\frac{1}{2},j-\frac{1}{2}}}\Bigg]. \qquad (5.15)$$

$$\beta^n_{y_{i,j}} = \frac{2\pi}{N}\left[E_{i+\frac{1}{2},j+\frac{1}{2}}\,\sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2}}}\,\frac{A^n_{i+\frac{1}{2},j+\frac{1}{2}}}{m_{i+\frac{1}{2},j+\frac{1}{2}}}\right.$$

$$+ E_{i-\frac{1}{2},j+\frac{1}{2}}\,\sigma^n_{xy_{i-\frac{1}{2},j+\frac{1}{2}}}\,\frac{A^n_{i-\frac{1}{2},j+\frac{1}{2}}}{m_{i-\frac{1}{2},j+\frac{1}{2}}}$$

$$+ E_{i-\frac{1}{2},j-\frac{1}{2}}\,\sigma^n_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}\,\frac{A^n_{i-\frac{1}{2},j-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2}}}$$

$$\left.+ E_{i+\frac{1}{2},j-\frac{1}{2}}\,\sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2}}}\,\frac{A^n_{i+\frac{1}{2},j-\frac{1}{2}}}{m_{i+\frac{1}{2},j-\frac{1}{2}}}\right] . \qquad (5.16)$$

Velocity-type boundary conditions eliminate the need for Eqs.(5.5). These conditions affect Eqs.(5.7) and/or (5.8) directly.

The simplest way to provide boundary values is by prescription. That is, stress (or velocity) is given at the beginning of a problem for all time at a boundary grid point. The value is a function of time only, since the location of the grid point is always known. If the boundary value is tied to a coordinate which is different from the boundary grid point, then an interaction calculation is required. For example, outside boundaries can interact with geometric constraints (wall segments) or they can interact with each other by coming together to close a void. In general, when a boundary grid point engages a constraint or another boundary grid point, a velocity condition is required. When a boundary grid point disengages, a stress-type boundary calculation is required, e.g., it can become free.

Equations of interaction between a grid point and a constraint, or between two grid points, are governed by the principle of conservation of momentum during the moment of initial contact and during intimate contact. During the time when the points move independently and at the moment of separation, the grid points are separate stress-type boundaries.

Rev. 1
15 NOV 77

An example of an interactive boundary condition occurs when a boundary grid point interacts with another grid segment. In this case, the interaction algorithm is as follows:

1. The grid point is calculated as a free boundary point in order to get the free acceleration vector of the grid point; e.g., Eqs.(5.12).

2. A test is made to see if the grid point has "broken away" from the grid segment,

$$d_{\perp} > d_{min} \quad \text{implies break away,} \tag{5.17}$$

where $d_{\perp}$ is perpendicular distance from the boundary grid point to the grid segment. d_{min} is a prescribed minimum perpendicular "capture" distance. If Eq.(5.17) is satisfied, then the free acceleration vector is correct and the new velocity and position of the grid point may be calculated from it using Eqs.(5.7) and (5.8).

3. If the grid point has not broken away, then the acceleration vector is resolved into components along the grid segment and perpendicular to the grid segment. The component parallel to the grid segment is

$$a^n_{\parallel} = \ddot{x}^n w^n_x + \ddot{y}^n w^n_y \tag{5.18a}$$

where w_x and w_y are the direction components of the grid segment. The perpendicular acceleration component is set to zero and the total acceleration of the grid point becomes equal to the acceleration parallel to the grid segment. The components of this acceleration are

$$\ddot{x}^n_w = a^n_{\parallel} w^n_x , \quad \ddot{y}^n_w = a^n_{\parallel} w^n_y . \tag{5.18b}$$

4. New velocity and position of the grid point are calculated using the acceleration along the grid segment, i.e., Eqs. (5.7) and (5.8).

5. The position of the grid point is now adjusted to be the intersection of the grid segment with a perpendicular line constructed through the new position of the boundary grid point. The intersection formula is

$$x_{int} = \left[x_1 m + x_3\left(\frac{1}{m}\right) + y_3 - y_1\right] \Big/ \left(m + \frac{1}{m}\right) \tag{5.19 a}$$

$$y_{int} = m\left(x_{int} - x_1\right) + y_1$$

where x_{int}, y_{int} are the coordinates of intersection and m is the slope of the line segment defined by the end points (x_1, y_1) and (x_2, y_2).

6. The acceleration and velocity of the grid point are adjusted to be consistent with the intersection coordinates;

$$\dot{x}_{int}^{n+\frac{1}{2}} = \left(x_{int} - x^{n}\right) \Big/ \Delta t^{n+\frac{1}{2}} \tag{5.19b}$$

$$\dot{y}_{int}^{n+\frac{1}{2}} = \left(y_{int} - y^{n}\right) \Big/ \Delta t^{n+\frac{1}{2}} ;$$

$$\ddot{x}_{int}^{n} = \left(\dot{x}_{int}^{n\ \frac{1}{2}} - \dot{x}^{n-\frac{1}{2}}\right) \Big/ \Delta t^{n} \tag{5.19c}$$

$$\ddot{y}_{int}^{n} = \left(\dot{y}_{int}^{n\ \frac{1}{2}} - \dot{y}^{n-\frac{1}{2}}\right) \Big/ \Delta t^{n} .$$

A more detailed discussion of grid interaction logic may be found in Appendix BIA (Boundary Interaction Algorithms). Wall interaction logic is also described in Appendix BIA.

5.2.4 Mass Equation. The general continuity or conservation of mass equation for two-dimensional symmetries is

$$\frac{\dot{V}}{V} = \frac{\partial \dot{x}}{\partial x} + \frac{\partial \dot{y}}{\partial y} + f\,\frac{\dot{x}}{x} \tag{5.20}$$

where V, x, y, and f are previously defined. The left side of Eq.(5.20) is called the volumetric strain rate, while the right side contains directional (or component) values of strain rate. The first two terms on the right are the two-dimensional principal strain rates.

A finite-difference analog must be derived separately but consistently for each term in Eq.(5.20). First, consider the volumetric strain rate, written in the following differential form,

$$\left(\frac{\dot{V}}{V}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}/\Delta t^{n+\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \;, \tag{5.21}$$

where $\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$ is the change in relative volume of zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+\frac{1}{2}$ and $\Delta t^{n+\frac{1}{2}}$ is the time increment. Applying Eq.(5.10b) to the definition of relative volume, the change of relative volume is

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \equiv V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} - V^{n}_{i-\frac{1}{2},j-\frac{1}{2}} \;; \tag{5.22a}$$

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \rho^{o}_{i-\frac{1}{2},j-\frac{1}{2}} \left(\frac{1}{\rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}} - \frac{1}{\rho^{n}_{i-\frac{1}{2},j-\frac{1}{2}}} \right) . \tag{5.22b}$$

Since the mesh is Lagrangian, Eq.(5.22b) may be written in terms of true volume, $\mathcal{V}$, as follows,

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2}}}{m^{o}_{i-\frac{1}{2},j-\frac{1}{2}}} \left(\mathcal{V}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} - \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2}} \right) . \tag{5.23}$$

Equation (5.23) is a formula for change of relative volume in terms of change of true volume. The change of true volume is related directly to coordinates and symmetry. Using the mesh notation shown on Page 5.3, the formulas for change of true volume for the two natural two-dimensional symmetries are derived as follows:

(1) Zones is translational symmetry are arbitrary quadrilateral area slabs of specified constant thickness. The Lagrange coordinates are in the plane of the quadrilateral area. The true volume of a zone is

$$\mathcal{V} = (\text{slab thickness})\ (\text{quadrilateral area}).$$

$$\mathcal{V}_{i-\frac{1}{2},j-\frac{1}{2}} = (1) \times A_{i-\frac{1}{2},j-\frac{1}{2}} \, . \tag{5.24a}$$

Equation (5.24a) assumes a unit thickness; however, any constant may be used since it will affect all equations in the same way and will, in effect, cancel out. The area, A, was defined in Eq.(5.6d).

(2) Zones in axial symmetry are toroids of quadrilateral cross-sectional area. The Lagrange coordinates are in the plane of the quadrilateral cross section. The true volume at time n comes from the sum of the two triangular cross-sectional toroids which make up the quadrilateral cross-sectional toroid,

$$\mathcal{V}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{2\pi}{3}\left[\left(x_{i,j-1} + x_{i,j} + x_{i-1,j}\right) A_{①} + \left(x_{i,j-1} + x_{i-1,j} + x_{i-1,j-1}\right) A_{②}\right] . \tag{5.24b}$$

Equation (5.24b) is identical to Eq.(5.6e) except for the factor of density.

The new relative volume is computed from the new zone volume,

$$V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = \mathcal{V}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2}}} , \tag{5.25}$$

and the new density comes from new relative volume,

$$\rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2}}}{V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}} . \tag{5.26}$$

From the definition of a first-order temporal average,

$$(\ )^{n+\frac{1}{2}} \equiv \frac{(\ )^{n+1} + (\ )^{n}}{2} , \tag{5.27}$$

the formula for $V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$ in Eq.(5.21) is

$$V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} + V^{n}_{i-\frac{1}{2},j-\frac{1}{2}}}{2} , \tag{5.28}$$

where $V^{n}_{i-\frac{1}{2},j-\frac{1}{2}}$ is known and $V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$ can be calculated from Eq.(5.25) or by inverting Eq.(5.22a) as follows,

$$V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = V^{n}_{i-\frac{1}{2},j-\frac{1}{2}} + \Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} . \tag{5.29}$$

New compression is

$$C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} \equiv V^{o}_{i-\frac{1}{2},j-\frac{1}{2}} - V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} , \tag{5.30}$$

and change in compression, defined by

$$\Delta C^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \equiv C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} - C^{n}_{i-\frac{1}{2},j-\frac{1}{2}} , \tag{5.31}$$

is

$$\Delta C^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = -\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} . \tag{5.32}$$

The next step in calculating the terms of Eq.(5.20) is the computation of the two-dimensional principal strain rates. From Eqs.(3.13),

$$\left(\frac{\partial\dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{1}{2A^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \left[\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1} - \dot{x}^{n+\frac{1}{2}}_{i-1,j}\right)\left(y^{n+\frac{1}{2}}_{i,j} - y^{n+\frac{1}{2}}_{i-1,j-1}\right) - \left(\dot{x}^{n+\frac{1}{2}}_{i,j} - \dot{x}^{n+\frac{1}{2}}_{i-1,j-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1} - y^{n+\frac{1}{2}}_{i-1,j}\right)\right] ; \tag{5.33a}$$

$$\left(\frac{\partial\dot{y}}{\partial y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = -\frac{1}{2A^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \left[\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1} - \dot{y}^{n+\frac{1}{2}}_{i-1,j}\right)\left(x^{n+\frac{1}{2}}_{i,j} - x^{n+\frac{1}{2}}_{i-1,j-1}\right) - \left(\dot{y}^{n+\frac{1}{2}}_{i,j} - \dot{y}^{n+\frac{1}{2}}_{i-1,j-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1} - x^{n+\frac{1}{2}}_{i-1,j}\right)\right] ; \tag{5.33b}$$

where

$$\begin{aligned} A^{n+\frac{1}{2}} &\equiv \frac{A^{n+1} + A^{n}}{2} , \\ x^{n+\frac{1}{2}} &\equiv \frac{x^{n+1} + x^{n}}{2} , \\ y^{n+\frac{1}{2}} &\equiv \frac{y^{n+1} + y^{n}}{2} . \end{aligned} \tag{5.34}$$

The shear strain rate is given by

$$\left(\frac{\delta \dot{y}}{\delta x} + \frac{\delta \dot{x}}{\delta y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{1}{2A^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \left[\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1} - \dot{y}^{n+\frac{1}{2}}_{i-1,j}\right)\left(y^{n+\frac{1}{2}}_{i,j} - y^{n+\frac{1}{2}}_{i-1,j-1}\right)\right.$$

$$- \left(\dot{y}^{n+\frac{1}{2}}_{i,j} - \dot{y}^{n+\frac{1}{2}}_{i-1,j-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1} - y^{n+\frac{1}{2}}_{i-1,j}\right)$$

$$- \left(\dot{x}^{n+\frac{1}{2}}_{i,j-1} - \dot{x}^{n+\frac{1}{2}}_{i-1,j}\right)\left(x^{n+\frac{1}{2}}_{i,j} - x^{n+\frac{1}{2}}_{i-1,j-1}\right)$$

$$\left. + \left(\dot{x}^{n+\frac{1}{2}}_{i,j} - \dot{x}^{n+\frac{1}{2}}_{i-1,j-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1} - x^{n+\frac{1}{2}}_{i-1,j}\right)\right] . \qquad (5.35)$$

The final step in calculating the terms of Eq.(5.20) is the computation of the other principal strain rate which depends on the symmetry. In translational plane strain symmetry, the dependent strain rate is exactly zero by definition $(f = 0)$. Thus, $f\frac{\dot{x}}{x}$ may be written as

$$\frac{\delta \dot{z}}{\delta z} = 0 , \qquad (5.36)$$

where z is the coordinate perpendicular to the x and y plane.

In translational plane stress, the dependent strain rate is a constant consistent with the plane stress condition

$$\sigma_{zz} = 0 . \qquad (5.37)$$

In axial symmetry, the tangential strain rate $\left(\frac{\delta \dot{z}}{\delta z} = \frac{\dot{x}}{x}\right)$ may be calculated using Eq.(5.20) as follows,

$$\frac{\dot{x}}{x} = \frac{\dot{V}}{V} - \frac{\delta \dot{x}}{\delta x} - \frac{\delta \dot{y}}{\delta y} , \qquad (5.38)$$

where x is the radial coordinate, y is the axial coordinate, $f = 1$, and z is the tangential or angular coordinate.

Strain rates can also be defined using triangular areas. For example, see four triangles surrounding grid point P shown in Figure 3.2. The triangle formulas are derived using the methodology shown in Eqs.(3.39a) for the triangle PLBP. For the bottom left triangle with respect to grid point (i,j), the strain rate formulas come directly from Eqs.(3.39d),

$$\left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{PLBP} = \frac{1}{2A^{n+\frac{1}{2}}_{PLBP}} \Big[y^{n+\frac{1}{2}}_{i,j-1} (\dot{x}^{n+\frac{1}{2}}_{i-1,j} - \dot{x}^{n+\frac{1}{2}}_{i,j}) + y^{n+\frac{1}{2}}_{i,j} (\dot{x}^{n+\frac{1}{2}}_{i,j-1} - \dot{x}^{n+\frac{1}{2}}_{i-1,j}) + y^{n+\frac{1}{2}}_{i-1,j} (\dot{x}^{n+\frac{1}{2}}_{i,j} - \dot{x}^{n+\frac{1}{2}}_{i,j-1}) \Big] ,$$

$$\left(\frac{\partial \dot{y}}{\partial y}\right)^{n+\frac{1}{2}}_{PLBP} = - \frac{1}{2A^{n+\frac{1}{2}}_{PLBP}} \Big[x^{n+\frac{1}{2}}_{i,j-1} (\dot{y}^{n+\frac{1}{2}}_{i-1,j} - \dot{y}^{n+\frac{1}{2}}_{i,j}) + x^{n+\frac{1}{2}}_{i,j} (\dot{y}^{n+\frac{1}{2}}_{i,j-1} - \dot{y}^{n+\frac{1}{2}}_{i-1,j}) + x^{n+\frac{1}{2}}_{i-1,j} (\dot{y}^{n+\frac{1}{2}}_{i,j} - \dot{y}^{n+\frac{1}{2}}_{i,j-1}) \Big] ,$$

$$
\begin{aligned}
\left(\frac{\partial \dot{y}}{\partial x} + \frac{\partial \dot{x}}{\partial y}\right)^{n+\frac{1}{2}}_{PLBP} = \frac{1}{2A^{n+\frac{1}{2}}_{PLBP}} \Big[& y^{n+\frac{1}{2}}_{i,j-1} \left(\dot{y}^{n+\frac{1}{2}}_{i-1,j} - \dot{y}^{n+\frac{1}{2}}_{i,j}\right) \\
& + y^{n+\frac{1}{2}}_{i,j} \left(\dot{y}^{n+\frac{1}{2}}_{i,j-1} - \dot{y}^{n+\frac{1}{2}}_{i-1,j}\right) \\
& + y^{n+\frac{1}{2}}_{i-1,j} \left(\dot{y}^{n+\frac{1}{2}}_{i,j} - \dot{y}^{n+\frac{1}{2}}_{i,j-1}\right) \\
& - x^{n+\frac{1}{2}}_{i,j-1} \left(\dot{x}^{n+\frac{1}{2}}_{i-1,j} - \dot{x}^{n+\frac{1}{2}}_{i,j}\right) \\
& - x^{n+\frac{1}{2}}_{i,j} \left(\dot{x}^{n+\frac{1}{2}}_{i,j-1} - \dot{x}^{n+\frac{1}{2}}_{i-1,j}\right) \\
& - x^{n+\frac{1}{2}}_{i-1,j} \left(\dot{x}^{n+\frac{1}{2}}_{i,j} - \dot{x}^{n+\frac{1}{2}}_{i,j-1}\right) \Big] \; . \qquad (5.38a)
\end{aligned}
$$

Similar formulas can be written for the other three triangles surrounding grid point P in Figure 3.2.

5.3 STRESS MESH

5.3.1 Artificial Viscosity. Although the finite-difference momentum equations, Eqs.(5.5), are general, they cannot economically handle high frequency mechanical phenomena (such as shocks) because the spatial resolution of a mesh would have to be several times smaller than the thickness of the shock for Eqs.(5.5) to be applicable. To calculate the transmission of a shock for a distance of a few centimeters would require tens of millions of zones or a shock-following microzoner and a very small time step if the shock thickness were on the order of angstroms. Clearly, this approach is not economically feasible.

An economical approach with considerable merit was devised by John von Neumann (Reference 5.1). He proposed that the presence of a shock within a zone (where the zone is millions of times larger than the thickness of the shock front) could be detected by the rate of change of volumetric strain and that the stress rise could be simulated by artificially spreading it over several zones. The crux of the idea is to add an artificial viscous stress, q_Q, dependent on the square of the volumetric strain rate, to the mean stress (pressure). The artificial viscous stress (sometimes called the quadratic artificial viscosity) is given by

$$q_Q = C_Q^2 \rho \left(\Delta\ell\right)^2 \left(\frac{\delta\dot{\ell}}{\delta\ell}\right)^2 , \qquad (5.39)$$

where C_Q is a dimensionless constant dependent on differential stress across the shock front and the number of zones over which the stress is to be artificially spread. A value of 2.0 for C_Q spreads a shock front over three zones and is good for differential stresses up to 1 Mbar.*

Another consequence of applying the momentum equation to a discretized mesh is computational noise, i.e., stable zone-to-zone oscillations of low amplitude. In general, noise does not invalidate a solution and

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*The value of C_Q for collapsing porous materials (as well as foams and frangible material) should be 4.0 or 6.0, depending on the degree of porosity and the level of loading. Even then, the formulation for quadratic artificial viscosity may not accurately describe the Rayleigh line process for porous matrix collapse.

does not have to be eliminated if its effects can be clearly determined. However, it is possible to reduce, and in some cases completely eliminate, noise by applying a viscous damping stress, q_L,

$$q_L = - C_L \rho \Delta\ell \sqrt{\frac{pV}{\rho_o}} \frac{\delta\dot{\ell}}{\delta\ell} , \qquad (5.40)$$

where C_L is a dimensionless constant dependent on the amount of damping required to eliminate the noise oscillations. A typical value of C_L is 0.8. Equation (5.40) is a simple dashpot (viscous stress is proportional to velocity) and q_L is called a linear artificial viscosity.

Equations (5.39) and (5.40) may be written in finite-difference form as follows,

$$q_{Q_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+\frac{1}{2}} = - \left(C^o_{Q_{i-\frac{1}{2},j-\frac{1}{2}}}\right)^2 \rho^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \left(\Delta\ell^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}\right)^2 \left(\frac{\delta\dot{\ell}}{\delta\ell}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \left|\left(\frac{\delta\dot{\ell}}{\delta\ell}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}\right| , \qquad (5.41a)$$

and

$$q_{L_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+\frac{1}{2}} = -C^o_{L_{i-\frac{1}{2},j-\frac{1}{2}}} \rho^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \Delta\ell^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \left(\frac{\left|p^n_{i-\frac{1}{2},j-\frac{1}{2}}\right| V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}}{\rho^o_{i-\frac{1}{2},j-\frac{1}{2}}}\right)^{\frac{1}{2}} \left(\frac{\delta\dot{\ell}}{\delta\ell}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} . \qquad (5.41b)$$

The sum of Eqs.(5.39) and (5.40) is called the total scalar artificial viscosity, q, and its value is added to the hydrostatic (thermodynamic) pressure in both the energy and momentum equations. The total scalar artificial viscosity is defined to be positive for compression (i.e., negative values of $\delta\dot{\ell}/\delta\ell$).

Finally, one other numerical problem that arises in discrete calculations can also be handled through the use of artificial viscosity. This is the problem of constant-volume mesh motions that result from numerically generated excitations. In a two-dimensional quadrilateral mesh, the four grid points that describe the stress mesh can oscillate in an "hourglassing" mode in which the volume of the zone remains unchanged and in which zone distortion can grow anomolously after many calculational cycles. This particular type of mesh motion is unopposed by the continuum physics in the zones. Since it is a numerical problem, some sort of artifice is needed to counteract the oscillation.

A simple tensor artificial viscosity proposed by Wilkins (Reference 5.2) is one approach that can be used effectively to damp the hourglass degree of freedom. Other approaches include a velocity subtraction method developed by Hancock (Reference 5.3).

The artificial viscosity concept is based on the fact that the hourglass mode exists only for quadrilateral zones and does not exist for triangular zones. Therefore, a grid-point dashpot is derived, based on the strain rates (velocity field) for the point being calculated and each of its two closest neighbor pairs (i.e., four triangles). See Figure 3.2. The finite-difference formulas for the strain rates in each of the four triangles surrounding an interior grid point are derived similarly to the bottom-left triangle strain-rate formulas shown in Eqs.(5.38a).

The tensor viscosity (mesh dashpot) for each triangle is then formulated as follows:

$$q_{xx} = \frac{2}{3} C_T \rho \sqrt{A} \, (2\dot{\epsilon}_{xx} - \dot{\epsilon}_{yy})$$

$$q_{yy} = \frac{2}{3} C_T \rho \sqrt{A} \, (2\dot{\epsilon}_{yy} - \dot{\epsilon}_{xx}) \tag{5.42}$$

$$q_{xy} = C_T \rho \sqrt{A} \, \dot{\epsilon}_{xy}$$

where

$$\dot{\epsilon}_{xx} = \frac{\partial \dot{x}}{\partial x}, \quad \dot{\epsilon}_{yy} = \frac{\partial \dot{y}}{\partial y}, \quad \dot{\epsilon}_{xy} = \frac{\partial \dot{y}}{\partial x} + \frac{\partial \dot{x}}{\partial y},$$

and C_T is a dimensionless constant dependent on the amount of damping required to eliminate the mesh oscillations. A typical value of C_T is 1.0. The difference equations for Eqs.(5.42) depend on the chosen triangle; for example, triangle PLBP, shown in Figure 3.2, could be derived from Eqs.(5.38a).

5.3.2 Internal Energy Equation. The conservation of internal energy equation may be written in the following form,

$$\dot{u} = -(p+q)\dot{V} + \dot{Z} + \dot{h} + \dot{U}''' . \tag{5.43}$$

u, p, q, and V have been previously defined. $\dot{Z}$ is the distortional energy rate which, for two independent space variables, is

$$\dot{Z} = V\left(s_{xx}\,\dot{\epsilon}_{xx} + s_{yy}\,\dot{\epsilon}_{yy} + s_{zz}\,\dot{\epsilon}_{zz} + s_{xy}\,\dot{\epsilon}_{xy}\right) . \qquad (5.44)$$

s_{xx}, s_{yy}, s_{zz}, and s_{xy} are stress deviator components and $\dot{\epsilon}_{xx}$, $\dot{\epsilon}_{yy}$, $\dot{\epsilon}_{zz}$, and $\dot{\epsilon}_{xy}$ are strain rate components. The strain rate components have already been defined as follows,

$$\dot{\epsilon}_{xx} \equiv \frac{\partial\dot{x}}{\partial x} \qquad \text{[see Eq.(5.33a)];}$$

$$\dot{\epsilon}_{yy} \equiv \frac{\partial\dot{y}}{\partial y} \qquad \text{[see Eq.(5.33b)];}$$

$$\dot{\epsilon}_{xy} \equiv \frac{\partial\dot{y}}{\partial x} + \frac{\partial\dot{x}}{\partial y} \qquad \text{[see Eq.(5.35)] ;}$$

Translational (plane strain)

$$\dot{\epsilon}_{zz} = 0 \qquad \text{[see Eq.(5.36)] ;}$$

Translational (plane stress)

$$\dot{\epsilon}_{zz} \neq 0 \qquad \text{[see Eq.(5.37)] ;}$$

Axial

$$\dot{\epsilon}_{zz} = \frac{\dot{V}}{V} - \dot{\epsilon}_{xx} - \dot{\epsilon}_{yy} \qquad \text{[see Eq.(5.38)].}$$

$\dot{h}$ is the heat flow and $\dot{U}'''$ is the source or sink energy rate.

Substituting Eq.(5.44) into Eq.(5.43) yields an equation with seven unknowns, since V can be determined from Eq.(5.29). To solve for the internal energy rate, u, requires equations for p, s_{xx}, s_{yy}, s_{zz}, s_{xy}, and $\dot{h}$.

5.3.3 Constitutive Equations. The equations that relate p, s_{xx}, s_{yy}, s_{zz}, s_{xy}, and $\dot{h}$ to u and V are known as constitutive equations and may be categorized as follows,

Equation of State

$$p = p(u, V) ; \tag{5.45a}$$

Strength Description

$$s_{xx} = s(u,V), \quad s_{yy} = s(u,V), \quad s_{zz} = s(u,V), \quad s_{xy} = s(u,V) ; \tag{5.45b}$$

Heat Flow Model

$$\dot{h} = h(u,V) . \tag{5.45c}$$

Given the functions p(u,V), s(u,V), and h(u,V), and knowing that Eq.(5.29) has been solved to give V, then Eqs.(5.43), (5.45a), (5.45b), and (5.45c) can be solved simultaneously (using the same explicit time step used to solve the momentum equation) by iteration or, in some cases, by substitution. A two-step iteration procedure is described in Section 5.3.4.

Typically, the equation of state, p(u,V), requires material constants (e.g., bulk modulus) that describe compressibility for the mechanical contribution to pressure and a specific heat ratio or a Grüneisen coefficient for the thermal contribution to pressure. The strength description requires a shear modulus, yield stress, flow rule, and yield criterion. The heat flux model needs thermal conductivity. In all cases, these or equivalent material constants may be functions of other thermodynamic variables.

The equation of state is usually simple or complex, depending on the number of phases and components that must be described. A single phase, one-component material is by far the simplest equation of state. A linear elastic solid or an "ideal" gas are examples of simple equations of state.

Strength descriptions are more or less complex, depending on strain-rate dependence during loading, relaxation to or from a failed state, reload characteristics after failure, ductility, brittleness, the existence of microfractures, etc. The simplest strength description is small strain elastic, where no failure is allowed to occur. Elastic-plastic models having a yield criterion based on the second stress invariant are also fairly simple. Plasticity can be handled using an appropriate flow rule. Strain hardening, fracture, dilatational effects, etc., increase the complexity of a strength model.

The heat flux model can be viewed in two separate categories -- conduction modeling and radiation modeling. An adequate model describing conduction is Fourier's Law,

$$\dot{h}'' = -k \nabla T . \tag{5.46}$$

Radiation, on the other hand, is more complex and no simple equation such as Eq.(5.46) can be used in a physically correct and economical manner.

Once Eq.(5.43) has been solved in conjunction with appropriate constitutive equations, Eqs.(5.45a), (5.45b), and (5.45c), all remaining thermodynamic state variables can be computed. In particular, stress can be calculated from

$$\begin{aligned}
\sigma_{xx} &= s_{xx} + q_{xx} - (p + q) , \\
\sigma_{yy} &= s_{yy} + q_{yy} - (p + q) , \\
\sigma_{zz} &= s_{zz} - (p + q) , \\
\sigma_{xy} &= s_{xy} + q_{xy} ,
\end{aligned} \tag{5.47}$$

where $q = q_Q + q_L$, and q_{xx}, q_{yy}, q_{xy} are tensor viscosities to inhibit mesh hourglassing instability. Once stress is computed, the computational cycle (Figure 5.1) is complete. All that remains is to determine a stable time step for the next cycle.

5.3.4 Simultaneous Solution of Constitutive Equations and Conservation of Energy by a Two-Step Iteration.

The procedure used to calculate new values of internal energy density, pressure, deviatoric stress components, and heat flow was discussed in Section 5.3.3. For the standard models in STEALTH, a two-step iteration is used to solve simultaneously the coupled constitutive equations and the internal energy conservation equation for u, ρ, s, and h.

The logic, which is located in subroutine ZONMDL, is as follows.

1. Calculate the approximate change in distortional energy density, $\Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$,

$$\Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \Delta t^{n+\frac{1}{2}} \left(s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \right).$$

2. Calculate the heat transfer energy density, $\Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$ into zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+\frac{1}{2}$,

$$\Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2}}} \left(\dot{h}^{n+\frac{1}{2}}_{i-1} + \dot{h}^{n+\frac{1}{2}}_{i} + \dot{h}^{n+\frac{1}{2}}_{j-1} + \dot{h}^{n+\frac{1}{2}}_{j} \right) \Delta t^{n+\frac{1}{2}} ,$$

where ρ^{o} is the reference density and m is the mass; $\Delta t^{n+\frac{1}{2}}$ is the time step for the entire mesh; $\dot{h}_{i-1}$ is the heat flow into zone $(i-\frac{1}{2},j-\frac{1}{2})$

through the left face, $\dot{h}_i$ is the heat flow through the right face, $\dot{h}_{j-1}$ is the heat flow through the bottom face, and $\dot{h}_j$ is the heat flow through the top face. The heat flow is calculated from Fourier's heat conduction law,

$$\dot{h} = -k(T)\,\underline{\nabla T} \cdot \underline{S}$$

where k is the conductivity, $\underline{S}$ is the area through which heat flows, and the gradient ∇ affects the conduction formula in the following way for interior points:

Translational symmetry

$$\dot{h}_{i-1}^{n+\frac{1}{2}} = -\frac{k_{i-1}^{n}}{2}\left\{\left[\left(\frac{\partial T}{\partial x}\right)_{i-1,j}^{n} + \left(\frac{\partial T}{\partial x}\right)_{i-1,j-1}^{n}\right]\left(y_{i-1,j}^{n+\frac{1}{2}} - y_{i-1,j-1}^{n+\frac{1}{2}}\right) - \left[\left(\frac{\partial T}{\partial y}\right)_{i-1,j}^{n} + \left(\frac{\partial T}{\partial y}\right)_{i-1,j-1}^{n}\right]\left(x_{i-1,j}^{n+\frac{1}{2}} - x_{i-1,j-1}^{n+\frac{1}{2}}\right)\right\};$$

$$\dot{h}_{i}^{n+\frac{1}{2}} = -\frac{k_{i}^{n}}{2}\left\{\left[\left(\frac{\partial T}{\partial x}\right)_{i,j-1}^{n} + \left(\frac{\partial T}{\partial x}\right)_{i,j}^{n}\right]\left(y_{i,j-1}^{n+\frac{1}{2}} - y_{i,j}^{n+\frac{1}{2}}\right) - \left[\left(\frac{\partial T}{\partial y}\right)_{i,j-1}^{n} + \left(\frac{\partial T}{\partial y}\right)_{i,j}^{n}\right]\left(x_{i,j-1}^{n+\frac{1}{2}} - x_{i,j}^{n+\frac{1}{2}}\right)\right\};$$

$$\dot{h}_{j-1}^{n+\frac{1}{2}} = -\frac{k_{j-1}^{n}}{2}\left\{\left[\left(\frac{\partial T}{\partial x}\right)_{i-1,j-1}^{n} + \left(\frac{\partial T}{\partial x}\right)_{i,j-1}^{n}\right]\left(y_{i-1,j-1}^{n+\frac{1}{2}} - y_{i,j-1}^{n+\frac{1}{2}}\right) - \left[\left(\frac{\partial T}{\partial y}\right)_{i-1,j-1}^{n} + \left(\frac{\partial T}{\partial y}\right)_{i,j-1}^{n}\right]\left(x_{i-1,j-1}^{n+\frac{1}{2}} - x_{i,j-1}^{n+\frac{1}{2}}\right)\right\};$$

$$\begin{aligned}\dot{h}_j^{n+\frac{1}{2}} = -\frac{k_j^n}{2}\Bigg\{&\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j}\right]\left(y^{n+\frac{1}{2}}_{i,j} - y^{n+\frac{1}{2}}_{i-1,j}\right)\\ &- \left[\left(\frac{\partial T}{\partial y}\right)^n_{i,j} + \left(\frac{\partial T}{\partial y}\right)^n_{i-1,j}\right]\left(x^{n+\frac{1}{2}}_{i,j} - x^{n+\frac{1}{2}}_{i-1,j}\right)\Bigg\};\end{aligned}$$

Axial symmetry

$$\begin{aligned}\dot{h}_{i-1}^{n+\frac{1}{2}} = -\frac{2\pi}{3}\,k^n_{i-1}\Bigg\{&\Bigg[\left(\frac{\partial T}{\partial x}\right)^n_{i-1,j-1}\left(y^{n+\frac{1}{2}}_{i-1,j} - y^{n+\frac{1}{2}}_{i-1,j-1}\right)\\ &- \left(\frac{\partial T}{\partial y}\right)^n_{i-1,j-1}\left(x^{n+\frac{1}{2}}_{i-1,j} - x^{n+\frac{1}{2}}_{i-1,j-1}\right)\Bigg]\left(x^{n+\frac{1}{2}}_{i-1,j-1} + \frac{1}{2}\,x^{n+\frac{1}{2}}_{i-1,j}\right)\\ &+ \Bigg[\left(\frac{\partial T}{\partial x}\right)^n_{i-1,j}\left(y^{n+\frac{1}{2}}_{i-1,j} - y^{n+\frac{1}{2}}_{i-1,j-1}\right)\\ &- \left(\frac{\partial T}{\partial y}\right)^n_{i-1,j}\left(x^{n+\frac{1}{2}}_{i-1,j} - x^{n+\frac{1}{2}}_{i-1,j-1}\right)\Bigg]\left(\frac{1}{2}\,x^{n+\frac{1}{2}}_{i-1,j-1} + x^{n+\frac{1}{2}}_{i-1,j}\right)\Bigg\};\end{aligned}$$

$$\begin{aligned}\dot{h}_{i}^{n+\frac{1}{2}} = -\frac{2\pi}{3}\,k^n_{i}\Bigg\{&\Bigg[\left(\frac{\partial T}{\partial x}\right)^n_{i,j}\left(y^{n+\frac{1}{2}}_{i,j-1} - y^{n+\frac{1}{2}}_{i,j}\right)\\ &- \left(\frac{\partial T}{\partial y}\right)^n_{i,j}\left(x^{n+\frac{1}{2}}_{i,j-1} - x^{n+\frac{1}{2}}_{i,j}\right)\Bigg]\left(x^{n+\frac{1}{2}}_{i,j} + \frac{1}{2}\,x^{n+\frac{1}{2}}_{i,j-1}\right)\\ &+ \Bigg[\left(\frac{\partial T}{\partial x}\right)^n_{i,j-1}\left(y^{n+\frac{1}{2}}_{i,j-1} - y^{n+\frac{1}{2}}_{i,j}\right)\\ &- \left(\frac{\partial T}{\partial y}\right)^n_{i,j-1}\left(x^{n+\frac{1}{2}}_{i,j-1} - x^{n+\frac{1}{2}}_{i,j}\right)\Bigg]\left(\frac{1}{2}\,x^{n+\frac{1}{2}}_{i,j} + x^{n+\frac{1}{2}}_{i,j-1}\right)\Bigg\};\end{aligned}$$

$$\begin{aligned}\dot{h}^{n+\frac{1}{2}}_{j-1} = -\frac{2\pi}{3}\, k^{n}_{j-1} \Bigg\{ & \Bigg[\left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1} \left(y^{n+\frac{1}{2}}_{i-1,j-1} - y^{n+\frac{1}{2}}_{i,j-1}\right) \\ & - \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1} \left(x^{n+\frac{1}{2}}_{i-1,j-1} - x^{n+\frac{1}{2}}_{i,j-1}\right)\Bigg] \left(x^{n+\frac{1}{2}}_{i,j-1} + \frac{1}{2}\, x^{n+\frac{1}{2}}_{i-1,j-1}\right) \\ & + \Bigg[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1} \left(y^{n+\frac{1}{2}}_{i-1,j-1} - y^{n+\frac{1}{2}}_{i,j-1}\right) \\ & - \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1} \left(x^{n+\frac{1}{2}}_{i-1,j-1} - x^{n+\frac{1}{2}}_{i,j-1}\right)\Bigg] \left(\frac{1}{2}\, x^{n+\frac{1}{2}}_{i,j-1} + x^{n+\frac{1}{2}}_{i-1,j-1}\right)\Bigg\} ;\end{aligned}$$

$$\begin{aligned}h^{n+\frac{1}{2}}_{j} = -\frac{2\pi}{3}\, k^{n}_{j} \Bigg\{ & \Bigg[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j} \left(y^{n+\frac{1}{2}}_{i,j} - y^{n+\frac{1}{2}}_{i-1,j}\right) \\ & - \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j} \left(x^{n+\frac{1}{2}}_{i,j} - x^{n+\frac{1}{2}}_{i-1,j}\right)\Bigg] \left(x^{n+\frac{1}{2}}_{i-1,j} + \frac{1}{2}\, x^{n+\frac{1}{2}}_{i,j}\right) \\ & + \Bigg[\left(\frac{\partial T}{\partial x}\right)^{n}_{i,j} \left(y^{n+\frac{1}{2}}_{i,j} - y^{n+\frac{1}{2}}_{i-1,j}\right) \\ & - \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j} \left(x^{n+\frac{1}{2}}_{i,j} - x^{n+\frac{1}{2}}_{i-1,j}\right)\Bigg] \left(\frac{1}{2}\, x^{n+\frac{1}{2}}_{i-1,j} + x^{n+\frac{1}{2}}_{i,j}\right)\Bigg\} ;\end{aligned}$$

where for all symmetries

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2}\,, \qquad y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2}\,,$$

the conductivities are

$$k^n_{i-1} = \frac{A^n_{i-3/2,j-1/2} + A^n_{i-1/2,j-1/2}}{\left(\frac{A}{k}\right)^n_{i-3/2,j-1/2} + \left(\frac{A}{k}\right)^n_{i-1/2,j-1/2}} \quad ;$$

$$k^n_{i} = \frac{A^n_{i+\frac{1}{2},j-\frac{1}{2}} + A^n_{i-\frac{1}{2},j-\frac{1}{2}}}{\left(\frac{A}{k}\right)^n_{i+\frac{1}{2},j-\frac{1}{2}} + \left(\frac{A}{k}\right)^n_{i-\frac{1}{2},j-\frac{1}{2}}} \quad ;$$

$$k^n_{j-1} = \frac{A^n_{i-1/2,j-3/2} + A^n_{i-1/2,j-1/2}}{\left(\frac{A}{k}\right)^n_{i-1/2,j-3/2} + \left(\frac{A}{k}\right)^n_{i-1/2,j-1/2}} \quad ;$$

$$k^n_{j} = \frac{A^n_{i-\frac{1}{2},j+\frac{1}{2}} + A^n_{i-\frac{1}{2},j-\frac{1}{2}}}{\left(\frac{A}{k}\right)^n_{i-\frac{1}{2},j+\frac{1}{2}} + \left(\frac{A}{k}\right)^n_{i-\frac{1}{2},j-\frac{1}{2}}} \quad ;$$

and a typical temperature gradient, e.g., at grid point (i,j), is given by its components as follows,

$$\begin{aligned}\left(\frac{\partial T}{\partial x}\right)^n_{i,j} = \frac{1}{A^n_{i,j}} \Big[& T^n_{i-\frac{1}{2},j-\frac{1}{2}} \left(y^n_{i,j-1} - y^n_{i-1,j}\right) \\ & + T^n_{i+\frac{1}{2},j-\frac{1}{2}} \left(y^n_{i+1,j} - y^n_{i,j-1}\right) \\ & + T^n_{i+\frac{1}{2},j+\frac{1}{2}} \left(y^n_{i,j+1} - y^n_{i+1,j}\right) \\ & + T^n_{i-\frac{1}{2},j+\frac{1}{2}} \left(y^n_{i-1,j} - y^n_{i,j+1}\right) \Big] \quad ;\end{aligned}$$

$$\left(\frac{\partial T}{\partial y}\right)^n_{i,j} = -\frac{1}{A^n_{i,j}}\left[T^n_{i-\frac{1}{2},j-\frac{1}{2}}\left(x^n_{i,j-1} - x^n_{i-1,j}\right)\right.$$

$$+ T^n_{i+\frac{1}{2},j-\frac{1}{2}}\left(x^n_{i+1,j} - x^n_{i,j-1}\right)$$

$$+ T^n_{i+\frac{1}{2},j+\frac{1}{2}}\left(x^n_{i,j+1} - x^n_{i+1,j}\right)$$

$$\left. + T^n_{i-\frac{1}{2},j+\frac{1}{2}}\left(x^n_{i-1,j} - x^n_{i,j+1}\right)\right] ;$$

where

$$A^n_{i,j} \equiv \frac{1}{2}\left(A^n_{i-\frac{1}{2},j-\frac{1}{2}} + A^n_{i+\frac{1}{2},j-\frac{1}{2}} + A^n_{i+\frac{1}{2},j+\frac{1}{2}} + A^n_{i-\frac{1}{2},j+\frac{1}{2}}\right) .$$

Temperature and heat flow boundary conditions use the same equations for a boundary point or zone as are used for an interior. When a temperature history is prescribed, it is used in the interior gradient calculation as if a phantom zone existed with the temperature equal to boundary temperature. The conductivity and area of the phantom zone are zero and the integration for partial derivatives is taken along the boundary surface where no zone exists.

Heat flow boundary conditions are activated by assuming that the boundary is adiabatic for the temperature gradient calculation, then by adding or subtracting the boundary heat through appropriate boundary faces. The adiabatic boundary, temperature gradient calculation is performed in two steps:

- The temperature gradient calculation is made assuming that the phantom zones have the same temperature as their nearest interior neighbor.

- Then the dot product of the temperature gradient and the line segment perpendicular to the direction of no heat flow is calculated in order to eliminate temperature gradients perpendicular to the line segment.

3. Calculate source energy density, $U^n_{i-\frac{1}{2},j-\frac{1}{2}}$, to be deposited in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n,

$$U^n_{i-\frac{1}{2},j-\frac{1}{2}} = U_{i-\frac{1}{2},j-\frac{1}{2}}\left(t^n\right) ,$$

where $U_{i-\frac{1}{2},j-\frac{1}{2}}(t^n)$ is a time-dependent function of energy deposition for zone $(i-\frac{1}{2},j-\frac{1}{2})$ evaluated at time t^n.

4. Add approximate reversible work (old pressure multiplied by new change of relative volume), approximate distortional energy density, heat transfer energy density, and source energy density in zone $(i-\frac{1}{2},j-\frac{1}{2})$ to internal energy density $\left(u^n_{i-\frac{1}{2},j-\frac{1}{2}}\right)$ in zone $(i-\frac{1}{2},j-\frac{1}{2})$ to get the approximate internal energy density $\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right)$ in zone $(i-\frac{1}{2},j-\frac{1}{2})$,

$$\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = u^n_{i-\frac{1}{2},j-\frac{1}{2}} - \left(p^n_{i-\frac{1}{2},j-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}\right) \Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$$

$$+ \Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} + \Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} + U^n_{i-\frac{1}{2},j-\frac{1}{2}} .$$

5. Calculate an approximate pressure, $\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$ in zone $(i-\frac{1}{2},j-\frac{1}{2})$ for time $n+\frac{1}{2}$ by first calculating the approximate $n+1$ pressure, $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, from internal energy density in zone $(i-\frac{1}{2},j-\frac{1}{2})$,

$$\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = p_{i-\frac{1}{2},j-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} ,\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right) ,$$

where $V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$ is the relative volume already calculated in zone $(i-\frac{1}{2},j-\frac{1}{2})$ for time $n+1$ [Eq.(5.29)], $p_{i-\frac{1}{2},j-\frac{1}{2}}$ is the pressure equation of state, and $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$ is the approximate pressure for zone

$(i-\frac{1}{2}, j-\frac{1}{2})$ at time $n+1$. Then adjust this pressure, $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, to satisfy explosive or spall criteria. (These criteria are mutually exclusive.) Calculate the approximate spall pressure, $\tilde{p}^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}$, in zone $(i-\frac{1}{2}, j-\frac{1}{2})$,

$$\tilde{p}^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2}}} = p_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ \tilde{Z}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right),$$

where $p_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}$ is a material function for zone $(i-\frac{1}{2}, j-\frac{1}{2})$. If $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} \leq \tilde{p}^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}$, adjust $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$ to its spalled value. Then calculate $\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$ from

$$\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} + p^{n}_{i-\frac{1}{2},j-\frac{1}{2}}}{2}.$$

6. Calculate shear modulus, $G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$, for zone $(i-\frac{1}{2}, j-\frac{1}{2})$ at time $n+\frac{1}{2}$ by first calculating the shear modulus, $G^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, for zone $(i-\frac{1}{2}, j-\frac{1}{2})$ at time $n+1$,

$$G^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = G_{i-\frac{1}{2},j-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ \tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right),$$

where $G_{i-\frac{1}{2},j-\frac{1}{2}}$ is the material function for zone $(i-\frac{1}{2}, j-\frac{1}{2})$, and then using

$$G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{G^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} + G^{n}_{i-\frac{1}{2},j-\frac{1}{2}}}{2}.$$

7. Calculate elastic stress deviators, $s^{e^{n+1}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}$, $s^{e^{n+1}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}$, $s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$ as follows.

$$s^{e^{n+1}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} + 2.0\ G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \left(\dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} - \frac{1}{3} \frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \right) \Delta t^{n+\frac{1}{2}}$$

$$+\ \delta^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} \quad ;$$

$$s^{e^{n+1}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} + 2.0\ G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \left(\dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} - \frac{1}{3} \frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \right) \Delta t^{n+\frac{1}{2}}$$

$$+\ \delta^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} \quad ;$$

$$s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} + G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}\ \dot{\epsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}\ \Delta t^{n+\frac{1}{2}} + \delta^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \quad ;$$

where $s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}$, $s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}$, and $s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}$ are the xx-, yy-, and xy-stress deviators in zone $(i-\frac{1}{2},j-\frac{1}{2})$ from time n, $\dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}$, $\dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}$, and $\dot{\epsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}$ are the previously calculated xx-, yy-, and xy-strain rates in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n [Eq.(5.33)], $\delta^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}$, $\delta^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}$, and $\delta^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}$ are the xx-, yy-, and xy-stress rotation corrections in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+\frac{1}{2}$,

$$\delta^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} = \left(\frac{s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} - s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}}{2} \right) \left[\cos\left(2\alpha^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \right) - 1.0 \right]$$

$$- s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \sin\left(2\alpha^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \right) ,$$

$$\delta^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} = - \delta^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} ,$$

$$\delta^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} = \left(\frac{s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} - s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}}{2} \right) \sin\left(2\alpha^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \right)$$

$$+ s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \left[\cos\left(2\alpha^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \right) - 1.0 \right] ,$$

where

$$\alpha^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \equiv \frac{\Delta t^{n+\frac{1}{2}}}{4A^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \left[\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1} - \dot{y}^{n+\frac{1}{2}}_{i-1,j} \right) \left(y^{n+\frac{1}{2}}_{i,j} \quad y^{n+\frac{1}{2}}_{i-1,j-1} \right) \right.$$

$$- \left(\dot{y}^{n+\frac{1}{2}}_{i,j} - \dot{y}^{n+\frac{1}{2}}_{i-1,j-1} \right) \left(y^{n+\frac{1}{2}}_{i,j-1} - y^{n+\frac{1}{2}}_{i-1,j} \right)$$

$$+ \left(\dot{x}^{n+\frac{1}{2}}_{i,j-1} - \dot{x}^{n+\frac{1}{2}}_{i-1,j} \right) \left(x^{n+\frac{1}{2}}_{i,j} - x^{n+\frac{1}{2}}_{i-1,j-1} \right)$$

$$\left. - \left(\dot{x}^{n+\frac{1}{2}}_{i,j} - \dot{x}^{n+\frac{1}{2}}_{i-1,j-1} \right) \left(x^{n+\frac{1}{2}}_{i,j-1} - x^{n+\frac{1}{2}}_{i-1,j} \right) \right] ,$$

and $\Delta t^{n+\frac{1}{2}}$ is the stable centered time step for this cycle; and from symmetry the zz-elastic stress deviator, $s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}}$, is

Rev. 1
15 NOV 77

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Translational symmetry

$$s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} - \frac{2}{3} G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \Delta t^{n+\frac{1}{2}};$$

Axial symmetry

$$s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} + 2.0\, G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \left(\dot{\varepsilon}^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} - \frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}} \right) \Delta t^{n+\frac{1}{2}} .$$

8. Calculate the elastic yield stress squared, $\left(Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}\right)^2$, for zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n+1 from the second stress deviator invariant,

$$\left(Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}\right)^2 = \frac{3}{2} \left[\left(s^{e^{n+1}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}}\right)^2 \right]$$

$$+ 3 \left(s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}\right)^2 .$$

9. Calculate the allowable yield stress, $Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$ for zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n+1,

$$Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = Y_{i-\frac{1}{2},j-\frac{1}{2}} \left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ \tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} \right),$$

where $Y_{i-\frac{1}{2},j-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2})$.

10. Compare the allowable yield stress, $Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, with the elastic yield stress, $Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}$,

if $Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} > Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}$, material is linear elastic;

if $Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} \leq Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}$, material has exceeded allowable yield stress.

11. If the material is linear elastic, the elastic stress deviators already calculated are correct,

$$s^{n+1}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{e^{n+1}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} ,$$

$$s^{n+1}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{e^{n+1}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} ,$$

$$s^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} ,$$

$$s^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} = s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} .$$

12. When the material has exceeded its allowable yield stress, adjust the stress deviators according to the Prandtl-Reuss flow rule,

$$s^{n+1}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}}\right) s^{e^{n+1}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} ,$$

$$s^{n+1}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}}\right) s^{e^{n+1}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} ,$$

$$s^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}}\right) s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} ,$$

$$s^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2}}}\right) s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} .$$

13. Calculate the change in distortional energy density, $\Delta Z^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+\frac{1}{2}$,

$$\Delta Z^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} = V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} \Delta t^{n+\frac{1}{2}} \Bigg(s^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}$$

$$+ s^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}}$$

$$+ s^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \dot{\epsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} \Bigg) ,$$

where

$$s^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} = \frac{s^{n+1}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} = \frac{s^{n+1}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} = \frac{s^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} = \frac{s^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}} + s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}}{2} .$$

14. Calculate the internal energy density, $u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = u^{n}_{i-\frac{1}{2},j-\frac{1}{2}} - \left(\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}\right) \Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}}$$

$$+ \Delta Z^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} + \Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2}} + U^{n}_{i-\frac{1}{2},j-\frac{1}{2}} .$$

15. Calculate the pressure, $p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = p_{i-\frac{1}{2},j-\frac{1}{2}} \left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right) .$$

16. Calculate the spall pressure, $p_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$p_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} = p_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}\left(u_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1},\ V_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1},\ Z_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1}\right),$$

where $p_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2})$. If $p_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1} \leq p_{\min_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1}$, adjust $p_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1}$ to its spalled value.

17. Calculate the total stress, $\sigma_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1}$, $\sigma_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1}$, $\sigma_{zz_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1}$, $\sigma_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$\sigma_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} = s_{xx_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} - \left(p_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1} + q_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}}\right);$$

$$\sigma_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} = s_{yy_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} - \left(p_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1} + q_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}}\right);$$

$$\sigma_{zz_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} = s_{zz_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} - \left(p_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1} + q_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}}\right);$$

$$\sigma_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1} = s_{xy_{i-\frac{1}{2},j-\frac{1}{2}}}^{n+1}\ .$$

18. Calculate the longitudinal sound speed squared, $\left(c^{n+1}_{\ell_{i-\frac{1}{2},j-\frac{1}{2}}}\right)^2$ in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$c^{n+1}_{\ell_{i-\frac{1}{2},j-\frac{1}{2}}} = c_{\ell_{i-\frac{1}{2},j-\frac{1}{2}}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right),$$

where $c_{\ell_{i-\frac{1}{2},j-\frac{1}{2}}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2})$.

19. Calculate the temperature, $T^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$T^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = T_{i-\frac{1}{2},j-\frac{1}{2}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right),$$

where $T_{i-\frac{1}{2},j-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2})$.

20. Calculate the conductivity, $k^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$k^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = k_{i-\frac{1}{2},j-\frac{1}{2}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right),$$

where $k_{i-\frac{1}{2},j-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2})$.

21. Calculate the specific heat capacity, $C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time $n+1$,

$$C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}} = C_{i-\frac{1}{2},j-\frac{1}{2}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2}}\right),$$

where $C_{i-\frac{1}{2},j-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2})$.

5.4 EXPLICIT TIME STEP

5.4.1 Overview. The explicit calculational scheme has two identifying characteristics:

(1) New values are computed from old values; e.g., values at $n+1$ are computed from values at n.

(2) Data for computations come only from nearest neighbors; i.e., information can propagate only across one zone in one calculational time step.

These characteristics are the essential elements of the explicit numerical method and are embodied in the criteria required to calculate stable time steps.

5.4.2 Stable Mechanical Time Steps. The physical criterion required for the calculation of a stable time step was described in Section 5.2.2 and is summarized in Eqs.(5.9a) and (5.9b). If artificial viscosity were not present, the most conservative (largest) value of mechanical sound speed would be the isentropic longitudinal sound speed. The general form of the isentropic longitudinal sound speed is

$$c_\ell^2 \equiv \left.\frac{\partial \sigma_\ell}{\partial \rho}\right)_{\text{isentropic}} , \tag{5.48}$$

where the subscript ℓ denotes the longitudinal direction, σ_ℓ is calculated from Eq.(5.47), and ρ is the actual density. Equation (5.48) can also be written in component form,

$$c_\ell^2 = c_s^2 + c_p^2 + c_q^2 \ , \tag{5.49a}$$

$$= \left.\frac{\partial s}{\partial \rho}\right)_{isen} + \left.\frac{\partial p}{\partial \rho}\right)_{isen} + \left.\frac{\partial q}{\partial \rho}\right)_{isen} \ , \tag{5.49b}$$

where "isen" means isentropic.

c_s is the deviatoric contribution to sound speed and can be calculated conservatively from the formula,

$$c_s^2 = \frac{\frac{4}{3}G}{\rho^o} \ , \tag{5.50}$$

where G is the shear modulus and ρ^o is the reference density. c_s^2 is 4/3 times the elastic shear velocity squared.

c_p is the pressure (or mean stress) contribution to sound speed and is calculated from the equation of state. When the equation of state is of the form

$$p = A + Bu \ , \tag{5.51}$$

where $A = A(\eta)$, $B = B(\eta)$, and $\eta \equiv \frac{1}{V}$, then from the isentropic condition that $du = -pdV$, the thermodynamic (hydrostatic) sound speed is

$$c_p^2 = \frac{A' + B'u + BpV^2}{\rho^o} \ , \tag{5.52}$$

where $A' = \frac{dA}{d\eta}$, $B' = \frac{dB}{d\eta}$. When the equation of state is not in the form of Eq.(5.51) then a more specialized approach must be taken.

c_q is the artificial viscosity contribution to sound speed and is composed of two components, linear and quadratic. The formula is

$$c_q^2 = \left.\frac{\partial q_L}{\partial \rho}\right)_{isen} + \left.\frac{\partial q_Q}{\partial \rho}\right)_{isen} . \tag{5.53}$$

Using Eqs.(5.41) and (5.42), c_q^2 becomes (References 5.2 and 5.1, respectively),

$$c_q^2 = 4C_L^2 \frac{|p|\ V}{\rho^o} + \left(2C_Q\right)^4 (\Delta \ell)^2 \left(\frac{\partial \dot{\ell}}{\partial \ell}\right)^2 . \tag{5.54}$$

Combining Eqs.(5.50), (5.52), and (5.54) yields the formula for the maximum stable time step of zone (i-½,j-½).*

$$\left(\Delta t^{n+1}_{(\cdot\cdot)}\right)^2 = \frac{\left(\Delta \ell^{n+1}_{(\cdot\cdot)}\right)^2}{\left(c^{n+1}_{\ell\,(\cdot\cdot)}\right)^2 + 4C^2_{L\,(\cdot\cdot)} \dfrac{\left|p^{n+1}_{(\cdot\cdot)}\right| V^{n+1}_{(\cdot\cdot)}}{\rho^o_{(\cdot\cdot)}} + \left(2C_{Q\,(\cdot\cdot)}\right)^4 \left(\Delta \ell^{n+\frac{1}{2}}_{(\cdot\cdot)}\right)^2 \left[\left(\dfrac{\partial \dot{\ell}}{\partial \ell}\right)^{n+\frac{1}{2}}_{(\cdot\cdot)}\right]^2} . \tag{5.55}$$

In determining a time step for the next cycle, only n+1 data exist in order to predict the n+3/2 time step. This dilemma is not critical provided that one understands the pathological cases which can arise from a poorly estimated time step.

There are two pathological cases that must be considered when calculating the new n+3/2 time step. These cases can be seen from a plot of time step versus time. See Figure 5.2. If the time step is increasing with time (Case 1), predictions of the n+3/2 time step based on n+1 data will be conservative whether constant extrapolation (i.e., setting $\Delta t^{n+3/2} = t^{n+1}$) or linear extrapolation is used. On the other hand, if the time step is decreasing with time (Case 2), the

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*In Eq.(5.55), subscripts i-½,j-½ are denoted by (··).

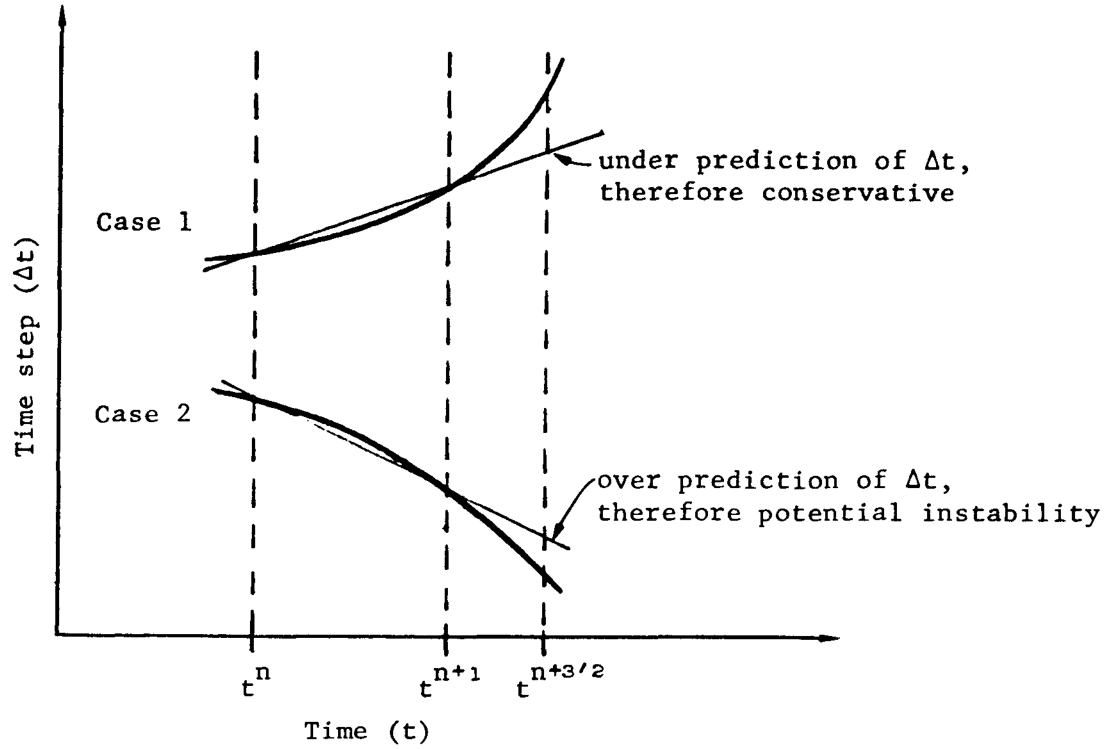

Figure 5.2 Example of need for f_{SFR}.

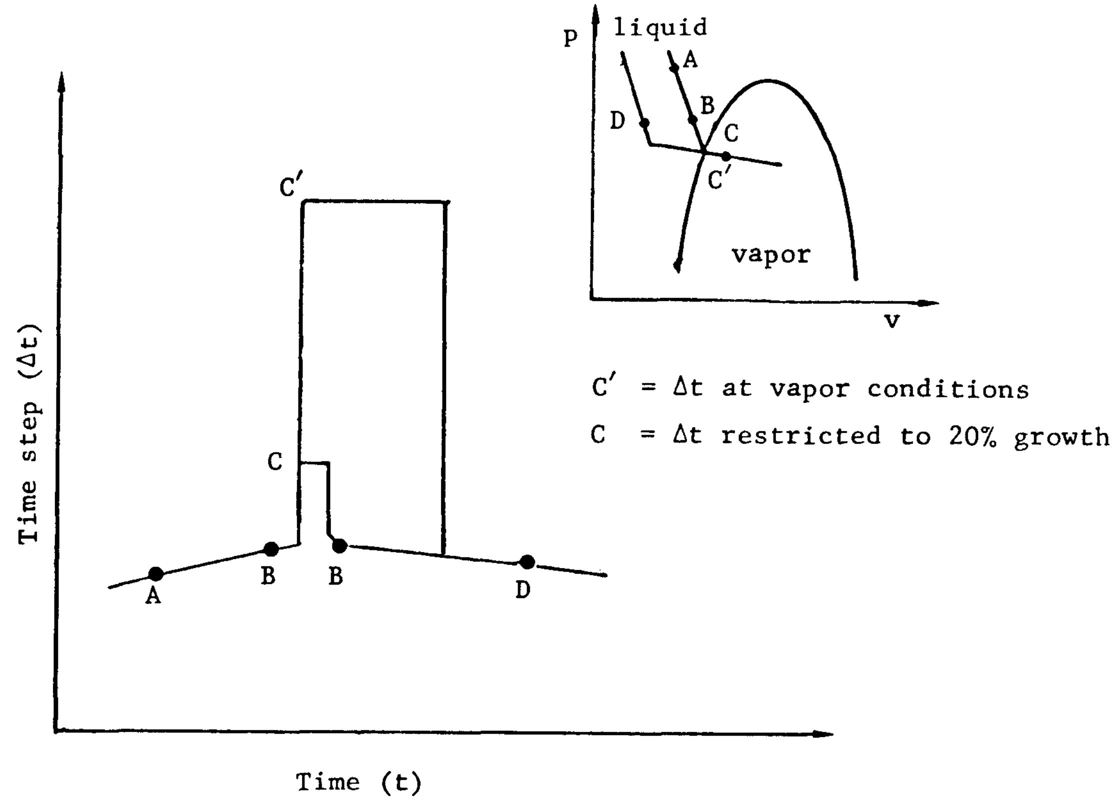

Figure 5.3. Example of need for f_{GRF}.

constant extrapolation procedure will predict a time step that is apt to be too high to maintain stability. The linear extrapolation is much better but can also be inaccurate if the rate of time step decay is large. In problems in which the time step is expected to experience rapid drops in time, it is advisable to use a safety factor multiplier of 2/3. This will add another level of conservatism to the calculation of the n+3/2 time step.

Thus, when the n+1 time step is greater than the n+1/2 time step (Case 1), set the n+3/2 time step equal to the n+1 value and recompute the n+1 time step to be the average of this n+3/2 value and the n+1/2 time step. This will also be conservative. If, on the other hand, the n+1 time step is less than than the n+1/2 time step, calculate an n+3/2 time step based on a linear extrapolation of the n+1/2 and n+1 values. This procedure should lead to a relatively safe value for most calculations. When the n+1 time step equals the n+1/2 value, either approach will work.

There are other time-step constraints which insure the stability of a calculation. First, there is a safety factor multiplier (f_{SFR}), which may be applied when c_p cannot be calculated in a conservative way or when Eq.(5.55) may not be conservative. The value of f_{SFR} may vary from 0.1 to 1.0.

Next, there is a growth factor multiplier (f_{GRF}), which may be applied so that a time step cannot grow faster than a certain rate. The value of f_{GRF} may vary from 1.0 to 1.2 (no growth to 20% growth). The need for a 20% growth factor limitation on a time step is justified as follows: Consider the problem in which a change of material phase is possible. Furthermore, allow for the situation that during the early response periods, the time step is controlled by the higher sound speed phase (i.e., lower time step) but that at some later time during the simulation, all of the material is "flashed" to the lower sound speed phase. Assume that this change of sound speed results in a change of the maximum stable time step of at least a factor of 2. Furthermore, one cycle after the global change of phase has occurred, one of the zones returns to its higher sound speed state. If the time step had been allowed to rise rapidly to its much larger value for the one cycle when all the zones switched phase to the lower sound speed material, it is possible that the instantaneously larger time step could result either in an instablity when the time step drops again to the lower value, or in inaccurate results because of some numerically induced high amplitude wave that resulted in the one cycle in which the time step was large. This scenario is shown schematically in Figure 5.3.

And finally, there are minimum and maximum values of time step. When the stable time step goes below the minimum value, the problem is terminated. When the stable time step has a value above the maximum value, the time step is adjusted to the maximum value exactly.

Thus, stable time steps for the next cycle ($\Delta t^{n+3/2}$ and Δt^{n+1}) are calculated as follows,

$$\Delta t^{n+3/2} = f_{SFR} \left[\text{minimum for all zones of Eq.(5.55)}\right] , \tag{5.56}$$

subject to the condition that

$$\Delta t_{min} \le \Delta t^{n+3/2} \le f_{GRF}\, \Delta t^{n+\frac{1}{2}} \le \Delta t_{max} . \tag{5.57}$$

Then, by interpolation,

$$\Delta t^{n+1} = \frac{\Delta t^{n+3/2} + \Delta t^{n+\frac{1}{2}}}{2} . \tag{5.58}$$

5.4.3 Stable Thermal Time Steps. When a particular problem is dominated by heat conduction phenomena rather than by mechanical phenomena, the problem time step stability criterion may be controlled by thermal diffusion rather than by mechanical sound speed. Therefore, when heat conduction is present, it is necessary to calculate the minimum stable heat conduction time step as follows,

$$\Delta t^n = \text{minimum value of } \Delta t^n_{i-\frac{1}{2},j-\frac{1}{2}} \text{ for all } i > 1,\ j > 1,$$

where

$$\Delta t^n_{i-\frac{1}{2},j-\frac{1}{2}} \leq \frac{\left(\Delta \ell^n_{i-\frac{1}{2},j-\frac{1}{2}}\right)^2}{2\left(k^n_{i-\frac{1}{2},j-\frac{1}{2}}/C^n_{V_{i-\frac{1}{2},j-\frac{1}{2}}}\right)} . \qquad (5.59)$$

$\Delta \ell^n_{i-\frac{1}{2},j-\frac{1}{2}}$ is the smallest length across zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n, $k^n_{i-\frac{1}{2},j-\frac{1}{2}}$ is the conductivity of zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n, and $C^n_{V_{i-\frac{1}{2},j-\frac{1}{2}}}$ is the specific heat capacity* of zone $(i-\frac{1}{2},j-\frac{1}{2})$ at time n.

As in the case of the mechanical stability criterion, the smallest maximum stable thermal time step in the grid is saved in order to be used for the next cycle of calculations. When thermal and mechanical mechanisms are both present, the smallest of the two stable time steps is chosen to be the time step for both mechanisms in the next cycle.

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*Per reference unit volume.

5.5 USE OF THE DEVELOPED EQUATIONS FOR EFFICIENT SOLUTION OF NON-TRANSIENT CASES

5.5.1 The Problem. Although the explicit finite-difference equations developed in Sections 5.2 and 5.3 can be used to analyze transient, steady-state, static, and quasi-static time-dependent thermomechanical systems, these numerical equations are most efficient for simulating transient behavior because time steps are computed from the minimum of the Courant stability criterion and the diffusion limit. The Courant condition gives the largest possible stable time step for a finite representation of a continuum consistent with the laws of physics for most initial value (transient) problems involving stress. The diffusion limit does the same for transient thermal problems. For mechanical boundary value (non-transient) problems, the Courant condition may needlessly restrict the time step. Two important exceptions to these guidelines are as follows: (1) linear elastic, small-strain, transient mechanical problems can sometimes be more efficiently solved implicitly in the frequency domain than explicitly in the time domain, and (2) nonlinear, non-transient problems often require that time be an independent explicit variable with the resulting equations being solved explicitly so that path-dependent thermodynamics are properly computed. Thermal boundary value problems are still efficiently solved using the diffusion limit time step criterion.

In other words, when time-dependent, nonlinear partial differential equations must be solved, it is usually most efficient to solve the explicit-in-time, physical equations using an explicit numerical scheme. When the equations exhibit weak time dependence but strong nonlinear effects (e.g., large deformation), the physical equations, though not explicitly time-dependent, are still probably most efficiently solved by explicit-in-time equations using a modified explicit numerical method. For the latter case, it is possible to separate the modifications to explicit methods for weakly time-dependent problems into three useful categories: (1) density scaling, (2) velocity damping, and (3) modulus scaling.

Density scaling is consistent with the situation where inertia effects are unimportant, where compressibility may be important, and where the time scale of the problem is determined by some other consideration, for example, heat transfer. Density scaling allows one to compute the intermediate state points of the process. Velocity damping (dynamic relaxation) may be used when inertia is somewhat important, compressibility may also be important, and the time scale is somewhat arbitrary. Velocity damping concerns itself only with the end states of a process. Intermediate states are not guaranteed to be accurate because the process (thermodynamic path dependence) is always assumed to be critically damped. Modulus scaling is at the other end of the spectrum from density scaling. When modulus scaling is most applicable, inertia effects are quite important, but compressibility is unimportant. The problem time scale is determined by an external constraint.

For example, most static problems can be categorized as "problems in which inertial influences are not important". Thus, density scaling can be used to increase the calculational time step in order to improve solution efficiency. Quasi-static problems, by definition, have a "sluggish" response, lending themselves to "dynamic relaxation" critical damping as a means of achieving an efficient solution. Steady-state processes are usually associated with incompressible flow or rigid body motion assumptions, in which case, modulus scaling appears to be the most appropriate choice to improve computational efficiency.

5.5.2 Density Scaling. When a problem is static or nearly static, the density (or mass) does not play an important role in the stress equilibrium process. Inertial effects disappear and the momentum equation becomes

$$\Sigma F_x \cong 0 \ , \quad \Sigma F_y \cong 0 \tag{5.60a}$$

or

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} \cong 0 \ , \qquad \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} \cong 0 \tag{5.60b}$$

where F_x and F_y are forces and σ_{xx}, σ_{yy}, and σ_{xy} are stresses. The zero on the right-hand side of the equal sign indicates that the inertial force is negligible. So, for Eq.(5.60b), we can write

$$\rho \ddot{x} \cong 0 , \quad \rho \ddot{y} \cong 0 . \tag{5.61}$$

The reason Eq.(5.61) applies is that $\ddot{x}$ and $\ddot{y}$ are small. Therefore, ρ can be any value (in units consistent with $\ddot{x}$ and $\ddot{y}$) so long as Eq.(5.61) is still satisfied.

Referring to Eq.(5.55), it can be shown that the dominant term in the denominator for static and quasi-static problems is c_ℓ^2. Since c_ℓ^2 is a direct function of the bulk and shear moduli and an inverse function of the reference density, it can be seen that in order to increase the time step for a particular zone, it is necessary to lower the sound speed, c_ℓ, which means either lowering the moduli or raising the density (or both). For static problems, Eq.(5.61) indicates that the density may be increased until the products, $\rho\ddot{x}$ and $\rho\ddot{y}$, produce an anomalous inertial effect.

Employing density scaling to achieve a larger time step for static problems requires only a change of input. The momentum equation and the Courant stability condition are unchanged.

5.5.3 Dynamic Relaxation. Another approach to economical static solutions is achieved by adding a viscous damping term to the momentum equation which acts to critically damp the fundamental response mode. This method reduces the number of time steps (iterations) required to achieve stress equilibrium, instead of increasing the magnitude of individual time steps. Quasi-static solutions can also be found using this approach. This approach is useful only when the integrated value of time is of no consequence, i.e., it doesn't matter what the "real time" is. Density scaling, on the other hand, preserves time as a meaningful variable.

The equations of motion are modified as follows,

$$\Sigma F_x = m\left(\ddot{x} + \frac{\eta}{\tau}\dot{x}\right) \quad , \qquad \Sigma F_y = m\left(\ddot{y} + \frac{\eta}{\tau}\dot{y}\right) \tag{5.62a}$$

where η is a dimensionless damping coefficient, $\ddot{x}$ and $\ddot{y}$ are the components of acceleration resulting from the externally applied forces, F_x and F_y, $\dot{x}$ and $\dot{y}$ are the components of velocity that result from integrating $\ddot{x}$ and $\ddot{y}$, respectively, with critical damping applied, and τ is the longest fundamental period of the system when the boundary conditions are present. In terms of stress, Eqs.(5.62a) become

$$\begin{aligned} \frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} &= \rho\left(\ddot{x} + \frac{\eta'}{\tau}\dot{x}\right) \\ \frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} &= \rho\left(\ddot{y} + \frac{\eta'}{\tau}\dot{y}\right) \end{aligned} \tag{5.62b}$$

where η' is $\eta/\mathcal{V}$. η (or η') is chosen to critically damp the lowest fundamental frequency of the grid. For linear elastic problems, it is a relatively simple matter to determine the damping (or relaxation) factor from a modal analysis or a dynamic excitation without damping. Even for mildly nonlinear systems, the latter technique can be used. For strongly nonlinear systems, an appropriate relaxation factor is far more difficult to compute and often requires considerable judgment.

The calculational form of the dynamic relaxation equation analogous to Eq.(5.7) comes from solving Eq.(5.62b) for acceleration (including gravitation),

$$\begin{aligned} \ddot{x}^n &= \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n - \frac{1}{\rho^n}\frac{\eta'}{\tau}\dot{x}^n + g_x \ , \\ \ddot{y}^n &= \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}\right)^n - \frac{1}{\rho^n}\frac{\eta'}{\tau}\dot{y}^n + g_y \ . \end{aligned} \tag{5.63}$$

Integrating Eq.(5.63) with respect to time and making the following substitutions,

$$\frac{\eta'}{\rho^n} \equiv \frac{\eta}{m}$$

$$\dot{x}^n \equiv \frac{\dot{x}^{n+\frac{1}{2}} + \dot{x}^{n-\frac{1}{2}}}{2} , \qquad \dot{y}^n \equiv \frac{\dot{y}^{n+\frac{1}{2}} + \dot{y}^{n-\frac{1}{2}}}{2}$$

yields

$$\dot{x}^{n+\frac{1}{2}} - \dot{x}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n + g_x\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{x}^{n+\frac{1}{2}} + \dot{x}^{n-\frac{1}{2}}\right]$$

$$\dot{y}^{n+\frac{1}{2}} - \dot{y}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}\right)^n + g_y\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{y}^{n+\frac{1}{2}} + \dot{y}^{n-\frac{1}{2}}\right] . \tag{5.64}$$

Solving Eq.(5.64) for new velocity and defining the relaxation factor, ω, to be

$$\omega \equiv \frac{\eta}{2m\tau} ,$$

results in

$$\dot{x}^{n+\frac{1}{2}} = \dot{x}^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\Delta t^n} - 1\right] + \ddot{x}^n\left[\frac{\Delta t^n}{1+\omega\Delta t^n}\right]$$

$$\dot{y}^{n+\frac{1}{2}} = \dot{y}^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\Delta t^n} - 1\right] + \ddot{y}^n\left[\frac{\Delta t^n}{1+\omega\Delta t^n}\right] \tag{5.65}$$

where

$$\ddot{x}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n + g_x ,$$

$$\ddot{y}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}\right)^n + g_y .$$

5.5.4 Modulus Scaling. There are several forms of modulus scaling: (1) sound speed scaling for incompressible cases, and (2) elastic constants scaling for rigid body motion. The approach to computational efficiency is similar to density scaling in that the time step improvement comes from reducing the sound speed.

The physical assumption associated with incompressibility implies that the mechanical sound speed is indeterminant. Often it is said the sound speed is infinite (or, similarly, that the Mach number is zero, $M = 0$). However, as a practical matter, a better condition might be that incompressibility for real materials exists when $M \leqslant 0.3$. For many cases, this means that the sound speed can be reduced (scaled) below its actual value provided that $M \leqslant 0.3$.

An example of sound speed scaling is described as follows: Suppose an air bubble is expanding in water at approximately 15 ft/sec and it is necessary to compute the resulting pressure in the water. The sound speed of water is about 5000 ft/sec, which for this problem means that the Mach number is about 3×10^{-3}. The flow is incompressible. Therefore, the sound speed is not important and can be artificially dropped up to two orders of magnitude without exceeding the Mach number criterion for incompressibility. To be conservative, let's drop the sound speed only one order of magnitude to 500 ft/sec. This improves the time step by a factor of 10. To drop the sound speed means that the bulk modulus is effectively reduced by a factor of 100 (i.e., the compressibility is increased by 100). Since the flow at 15 ft/sec is incompressible, the change of modulus will be applied to infinitesimal strains and the pressures will be only slightly affected.

REFERENCES FOR SECTION 5

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SECTION 6

THREE-DIMENSIONAL LAGRANGIAN FINITE-DIFFERENCE EQUATIONS*

6.1 INTRODUCTION

The Lagrange explicit finite-difference equations which represent the physical equations of a three-dimensional continuum are solved using two overlapping meshes -- a displacement mesh and a stress mesh. The displacement mesh is made up of grid (mesh) points which define geometric quantities such as shapes, interfaces, and boundaries. Conservation of momentum is used in the displacement mesh to solve for the vector variables, acceleration $(\ddot{x},\ddot{y},\ddot{z})$, velocity $(\dot{x},\dot{y},\dot{z})$, and position (x,y,z), at specific points in space. The stress mesh is made up of zones in which scalars and tensors are calculated as averages over zone volumes and surface areas, using conservation of internal energy and constitutive equations to solve for scalar and tensor variables such as stress, σ_{xx}, σ_{yy}, etc., internal energy, u, pressure, p, etc.

Both meshes describe the same region of space and are related through identical satisfaction of conservation of mass; that is, density, ρ, in both meshes describes the existence of material in the same way. Thus, the relationship between meshes is that the grid points of the displacement mesh uniquely define the zones of the stress mesh.

6.2 DISPLACEMENT MESH

6.2.1 Calculational Sequence. The three-dimensional Lagrange continuum mechanics equations are solved in three steps. First, the momentum equations are solved to determine mechanical motion from stress, internal energy, and density distributions. Next, conservation of mass is used to calculate new density distribution, and finally, the constitutive relations and conservation of internal energy are solved simultaneously to calculate a new stress and internal energy distribution. This procedure is shown schematically in Figure 6.1.

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*Section 6 is identical to Sections 4 and 5 wherever possible.

$$\left.\begin{array}{l} x^{n}_{i,j,k},\ y^{n}_{i,j,k},\ z^{n}_{i,j,k} \\[1ex] \dot{x}^{n-\frac{1}{2}}_{i,j,k},\ \dot{y}^{n-\frac{1}{2}}_{i,j,k},\ \dot{z}^{n-\frac{1}{2}}_{i,j,k} \\[1ex] \rho^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ \sigma^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \end{array}\right\} \text{Initial Conditions}$$

$$\left.\ddot{x}^{n}_{i,j,k},\ \ddot{y}^{n}_{i,j,k},\ \ddot{z}^{n}_{i,j,k}\right\} \text{Conservation of Momentum}$$

$$\begin{array}{c}\text{Explicit}\\ \text{Integration}\end{array} \left\{\begin{array}{l} \dot{x}^{n+\frac{1}{2}}_{i,j,k},\ \dot{y}^{n+\frac{1}{2}}_{i,j,k},\ \dot{z}^{n+\frac{1}{2}}_{i,j,k},\ \Delta t^{n} \\[1ex] x^{n+1}_{i,j,k},\ y^{n+1}_{i,j,k},\ z^{n+1}_{i,j,k},\ \Delta t^{n+\frac{1}{2}} \end{array}\right.$$

$$\left.\rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right\} \text{Conservation of Mass}$$

$$\begin{array}{l}\text{Simultaneous}\\ \text{Solution for}\\ \text{Explicit}\\ \text{Time Step}\\ \Delta t^{n+1/2}\end{array} \left\{\begin{array}{l} \left. u^{n+1}_{*} = u\left(p^{n+1}_{*},\ \rho^{n+1}_{*},\ s^{n+1}_{*}\right)\right\} \begin{array}{l}\text{Conservation}\\ \text{of Energy}\end{array} \\[2ex] \left.\begin{array}{l} p^{n+1}_{*} = p\left(u^{n+1}_{*},\ \rho^{n+1}_{*}\right) \\[2ex] s^{n+1}_{*} = s\left(\rho^{n+1}_{*},\ p^{n+1}_{*},\ u^{n+1}_{*}\right) \end{array}\right\} \begin{array}{l}\text{Constitutive}\\ \text{Relations}\end{array} \end{array}\right.$$

$$* \equiv i-\tfrac{1}{2},j-\tfrac{1}{2},k-\tfrac{1}{2}$$

$$\left.\sigma^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right\} \begin{array}{l}\text{Initial Conditions}\\ \text{for Next Time Step (cycle)}\end{array}$$

$$\left.\Delta t^{n+1}\right\} \begin{array}{l}\text{Time Step}\\ \text{for Next Cycle from}\\ \text{Courant Stability Criterion}\end{array}$$

Figure 6.1. Three-dimensional calculational cycle.

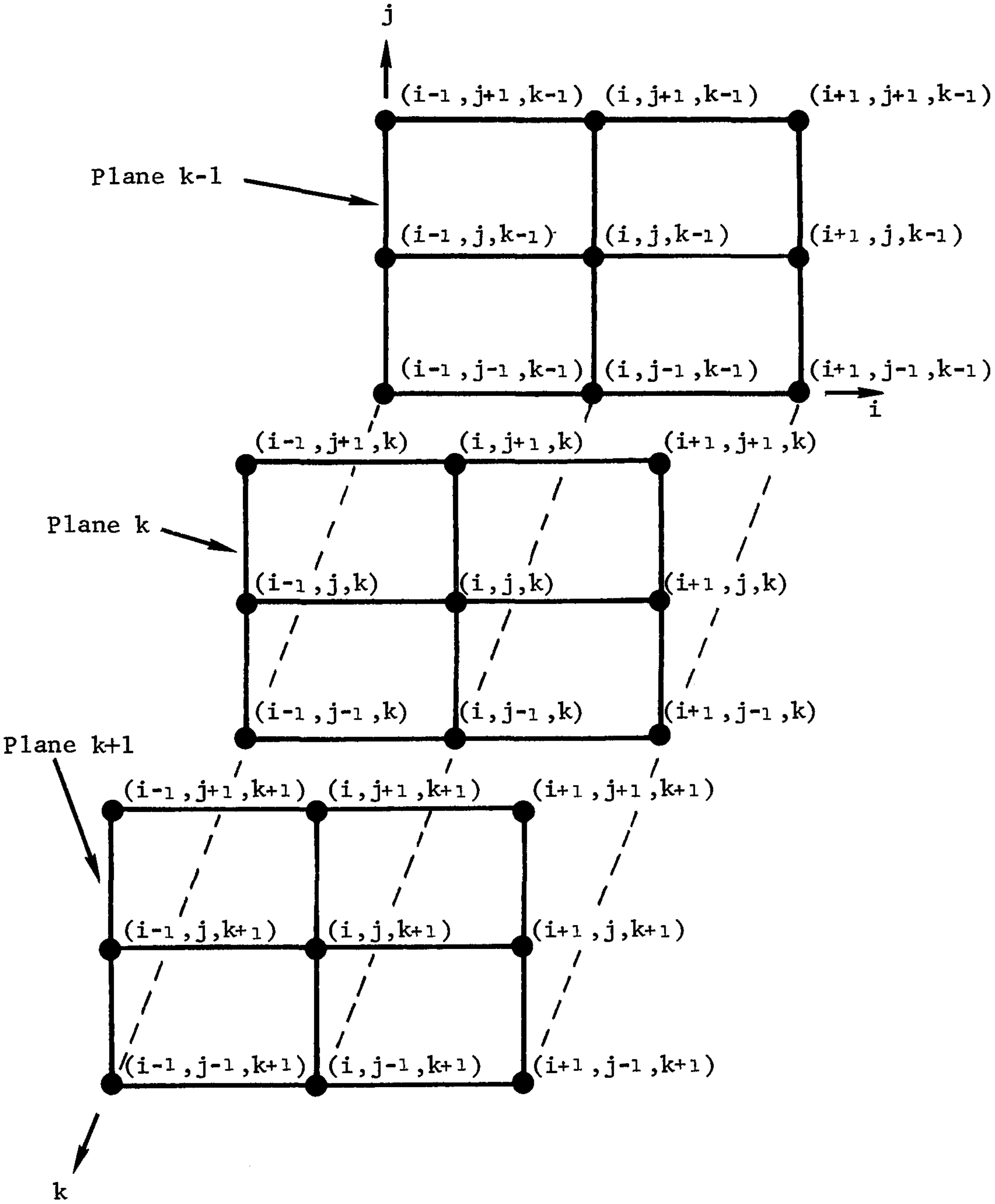
6.2.2 Momentum Equations. The general momentum equations for three independent space variables are

$$\ddot{x} = \frac{1}{\rho}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{zx}}{\partial z}\right),$$

$$\ddot{y} = \frac{1}{\rho}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z}\right), \qquad (6.1)$$

$$\ddot{z} = \frac{1}{\rho}\left(\frac{\partial\sigma_{zx}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z}\right).$$

The finite difference form of these equations can be derived in such a way that it is possible to use the same numerical equation for boundary points as well as for interior points. Consider the non-boundary point (i, j, k) and its immediate neighbors, as shown on Page 6.4. The grid point neighbors of grid point (i,j,k) are point (i-1,j,k) on the left, point (i+1,j,k) on the right, point (i,j-1,k) on the bottom, point (i,j+1,k) on the top, point (i,j,k-1) aft, and point (i,j,k+1) in front. The volume defined by grid points (i,j,k), (i-1,j,k), (i-1,j-1,k) and (i,j-1,k) in plane k and grid points (i,j,k-1), (i-1,j,k-1), (i-1,j-1,k-1), and (i,j-1,k-1) in plane k-1 is called zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$. This zone is the aft bottom left zone with respect to grid point (i,j,k). Similar descriptions can be made for the aft bottom right zone $(i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$, the aft top right zone $(i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2})$, and the aft top left zone $(i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2})$. The four front zones are the front bottom left zone $(i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2})$, the front bottom right zone $(i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2})$, the front top right zone $(i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2})$, and the front top left zone $(i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2})$.


j
(i-1,j+1,k-1)
(i,j+1,k-1)
(i+1,j+1,k-1)
Plane k-1
(i-1,j,k-1)
(i,j,k-1)
(i+1,j,k-1)
(i-1,j-1,k-1)
(i,j-1,k-1)
(i+1,j-1,k-1)
i
(i-1,j+1,k)
(i,j+1,k)
(i+1,j+1,k)
Plane k
(i-1,j,k)
(i,j,k)
(i+1,j,k)
(i-1,j-1,k)
(i,j-1,k)
(i+1,j-1,k)
Plane k+1
(i-1,j+1,k+1)
(i,j+1,k+1)
(i+1,j+1,k+1)
(i-1,j,k+1)
(i,j,k+1)
(i+1,j,k+1)
(i-1,j-1,k+1)
(i,j-1,k+1)
(i+1,j-1,k+1)
k

To derive properly centered finite-difference forms of the momentum equations, Eqs.(6.1) are rewritten as follows,

$$\ddot{x}^n_{i,j,k} = \frac{1}{\rho^n_{i,j,k}}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{zx}}{\partial z}\right)^n_{i,j,k} ,$$

$$\ddot{y}^n_{i,j,k} = \frac{1}{\rho^n_{i,j,k}}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z}\right)^n_{i,j,k} , \tag{6.2}$$

$$\ddot{z}^n_{i,j,k} = \frac{1}{\rho^n_{i,j,k}}\left(\frac{\partial\sigma_{zx}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z}\right)^n_{i,j,k} ,$$

where superscripts denote the time centering, while subscripts denote space centering; or substituting $m/\mathcal{V}$ for ρ,

$$\ddot{x}^n_{i,j,k} = \frac{\mathcal{V}^n_{i,j,k}}{m_{i,j,k}}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{zx}}{\partial z}\right)^n_{i,j,k} ,$$

$$\ddot{y}^n_{i,j,k} = \frac{\mathcal{V}^n_{i,j,k}}{m_{i,j,k}}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z}\right)^n_{i,j,k} , \tag{6.3}$$

$$\ddot{z}^n_{i,j,k} = \frac{\mathcal{V}^n_{i,j,k}}{m_{i,j,k}}\left(\frac{\partial\sigma_{zx}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z}\right)^n_{i,j,k} .$$

The finite-difference equations for the gradients of stress are shown on the next nine pages. The form of these equations was derived in Section 3, Eqs. (3.17).

$$
\begin{aligned}
\frac{\partial \sigma^n_{xx}}{\partial x_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^n_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^n_{i,j,k-1} - y^n_{i-1,j,k}\Big)\Big(z^n_{i,j-1,k} - z^n_{i-1,j,k}\Big) \\
& \qquad - \Big(z^n_{i,j,k-1} - z^n_{i-1,j,k}\Big)\Big(y^n_{i,j-1,k} - y^n_{i-1,j,k}\Big)\Big] \\
& + \sigma^n_{xx_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^n_{i,j-1,k} - y^n_{i+1,j,k}\Big)\Big(z^n_{i,j,k-1} - z^n_{i+1,j,k}\Big) \\
& \qquad - \Big(z^n_{i,j-1,k} - z^n_{i+1,j,k}\Big)\Big(y^n_{i,j,k-1} - y^n_{i+1,j,k}\Big)\Big] \\
& + \sigma^n_{xx_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^n_{i,j,k-1} - y^n_{i+1,j,k}\Big)\Big(z^n_{i,j+1,k} - z^n_{i+1,j,k}\Big) \\
& \qquad - \Big(z^n_{i,j,k-1} - z^n_{i+1,j,k}\Big)\Big(y^n_{i,j+1,k} - y^n_{i+1,j,k}\Big)\Big] \\
& + \sigma^n_{xx_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^n_{i,j+1,k} - y^n_{i-1,j,k}\Big)\Big(z^n_{i,j,k-1} - z^n_{i-1,j,k}\Big) \\
& \qquad - \Big(z^n_{i,j+1,k} - z^n_{i-1,j,k}\Big)\Big(y^n_{i,j,k-1} - y^n_{i-1,j,k}\Big)\Big] \\
& + \sigma^n_{xx_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^n_{i,j-1,k} - y^n_{i-1,j,k}\Big)\Big(z^n_{i,j,k+1} - z^n_{i-1,j,k}\Big) \\
& \qquad - \Big(z^n_{i,j-1,k} - z^n_{i-1,j,k}\Big)\Big(y^n_{i,j,k+1} - y^n_{i-1,j,k}\Big)\Big] \\
& + \sigma^n_{xx_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^n_{i,j-1,k} - y^n_{i,j,k+1}\Big)\Big(z^n_{i+1,j,k} - z^n_{i,j,k+1}\Big) \\
& \qquad - \Big(z^n_{i,j-1,k} - z^n_{i,j,k+1}\Big)\Big(y^n_{i+1,j,k} - y^n_{i,j,k+1}\Big)\Big] \\
& + \sigma^n_{xx_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^n_{i+1,j,k} - y^n_{i,j,k+1}\Big)\Big(z^n_{i,j+1,k} - z^n_{i,j,k+1}\Big) \\
& \qquad - \Big(z^n_{i+1,j,k} - z^n_{i,j,k+1}\Big)\Big(y^n_{i,j+1,k} - y^n_{i,j,k+1}\Big)\Big] \\
& + \sigma^n_{xx_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^n_{i,j,k+1} - y^n_{i-1,j,k}\Big)\Big(z^n_{i,j+1,k} - z^n_{i-1,j,k}\Big) \\
& \qquad - \Big(z^n_{i,j,k+1} - z^n_{i-1,j,k}\Big)\Big(y^n_{i,j+1,k} - y^n_{i-1,j,k}\Big)\Big] \Bigg\} \mathcal{V}^n_{i,j,k}
\end{aligned}
\tag{6.4a}
$$

$$
\begin{aligned}
\frac{\partial \sigma^{n}_{xy}}{\partial y_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j,k-1} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j-1,k} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j,k-1} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j-1,k} - z^{n}_{i-1,j,k} \right) \Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j-1,k} - z^{n}_{i+1,j,k} \right) \left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i+1,j,k} \right) \left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k} \right) \Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i+1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k} \right) \left(z^{n}_{i,j+1,k} - z^{n}_{i+1,j,k} \right) \Big] \\
& + \sigma^{n}_{xy_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j+1,k} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j,k-1} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j+1,k} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j,k-1} - z^{n}_{i-1,j,k} \right) \Big] \\
& + \sigma^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i,j-1,k} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j,k+1} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j,k+1} - z^{n}_{i-1,j,k} \right) \Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i,j-1,k} - z^{n}_{i,j,k+1} \right) \left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1} \right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i,j,k+1} \right) \left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1} \right) \Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i,j,k+1} \right) \\
& \qquad - \left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1} \right) \left(z^{n}_{i,j+1,k} - z^{n}_{i,j,k+1} \right) \Big] \\
& + \sigma^{n}_{xy_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i,j,k+1} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j,k+1} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j+1,k} - z^{n}_{i-1,j,k} \right) \Big] \Bigg\} \Big/ \mathcal{V}^{n}_{i,j,k}
\end{aligned}
\tag{6.4b}
$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
\frac{\partial \sigma^n_{zx}}{\partial z_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^n_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j,k-1} - x^n_{i-1,j,k} \right) \left(y^n_{i,j-1,k} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i-1,j,k} \right) \left(x^n_{i,j-1,k} - x^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j-1,k} - x^n_{i+1,j,k} \right) \left(y^n_{i,j,k-1} - y^n_{i+1,j,k} \right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i+1,j,k} \right) \left(x^n_{i,j,k-1} - x^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j,k-1} - x^n_{i+1,j,k} \right) \left(y^n_{i,j+1,k} - y^n_{i+1,j,k} \right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i+1,j,k} \right) \left(x^n_{i,j+1,k} - x^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j+1,k} - x^n_{i-1,j,k} \right) \left(y^n_{i,j,k-1} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j+1,k} - y^n_{i-1,j,k} \right) \left(x^n_{i,j,k-1} - x^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i,j-1,k} - x^n_{i-1,j,k} \right) \left(y^n_{i,j,k+1} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i-1,j,k} \right) \left(x^n_{i,j,k+1} - x^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i,j-1,k} - x^n_{i,j,k+1} \right) \left(y^n_{i+1,j,k} - y^n_{i,j,k+1} \right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i,j,k+1} \right) \left(x^n_{i+1,j,k} - x^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i+1,j,k} - x^n_{i,j,k+1} \right) \left(y^n_{i,j+1,k} - y^n_{i,j,k+1} \right) \\
& \qquad - \left(y^n_{i+1,j,k} - y^n_{i,j,k+1} \right) \left(x^n_{i,j+1,k} - x^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{zx_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i,j,k+1} - x^n_{i-1,j,k} \right) \left(y^n_{i,j+1,k} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j,k+1} - y^n_{i-1,j,k} \right) \left(x^n_{i,j+1,k} - x^n_{i-1,j,k} \right) \Big] \Bigg\} \Big/ \mathcal{V}^n_{i,j,k}
\end{aligned}
\tag{6.4c}
$$

$$
\begin{aligned}
\frac{\partial\sigma^{n}_{xy}}{\partial x_{i,j,k}} = \frac{1}{2}\Bigg\{ & \sigma^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^{n}_{i,j,k-1} - y^{n}_{i-1,j,k}\Big)\Big(z^{n}_{i,j-1,k} - z^{n}_{i-1,j,k}\Big) \\
& \qquad - \Big(z^{n}_{i,j,k-1} - z^{n}_{i-1,j,k}\Big)\Big(y^{n}_{i,j-1,k} - y^{n}_{i-1,j,k}\Big)\Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^{n}_{i,j-1,k} - y^{n}_{i+1,j,k}\Big)\Big(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k}\Big) \\
& \qquad - \Big(z^{n}_{i,j-1,k} - z^{n}_{i+1,j,k}\Big)\Big(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\Big)\Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\Big)\Big(z^{n}_{i,j+1,k} - z^{n}_{i+1,j,k}\Big) \\
& \qquad - \Big(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k}\Big)\Big(y^{n}_{i,j+1,k} - y^{n}_{i+1,j,k}\Big)\Big] \\
& + \sigma^{n}_{xy_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\Big(y^{n}_{i,j+1,k} - y^{n}_{i-1,j,k}\Big)\Big(z^{n}_{i,j,k-1} - z^{n}_{i-1,j,k}\Big) \\
& \qquad - \Big(z^{n}_{i,j+1,k} - z^{n}_{i-1,j,k}\Big)\Big(y^{n}_{i,j,k-1} - y^{n}_{i-1,j,k}\Big)\Big] \\
& + \sigma^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^{n}_{i,j-1,k} - y^{n}_{i-1,j,k}\Big)\Big(z^{n}_{i,j,k+1} - z^{n}_{i-1,j,k}\Big) \\
& \qquad - \Big(z^{n}_{i,j-1,k} - z^{n}_{i-1,j,k}\Big)\Big(y^{n}_{i,j,k+1} - y^{n}_{i-1,j,k}\Big)\Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^{n}_{i,j-1,k} - y^{n}_{i,j,k+1}\Big)\Big(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1}\Big) \\
& \qquad - \Big(z^{n}_{i,j-1,k} - z^{n}_{i,j,k+1}\Big)\Big(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\Big)\Big] \\
& + \sigma^{n}_{xy_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\Big)\Big(z^{n}_{i,j+1,k} - z^{n}_{i,j,k+1}\Big) \\
& \qquad - \Big(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1}\Big)\Big(y^{n}_{i,j+1,k} - y^{n}_{i,j,k+1}\Big)\Big] \\
& + \sigma^{n}_{xy_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\Big(y^{n}_{i,j,k+1} - y^{n}_{i-1,j,k}\Big)\Big(z^{n}_{i,j+1,k} - z^{n}_{i-1,j,k}\Big) \\
& \qquad - \Big(z^{n}_{i,j,k+1} - z^{n}_{i-1,j,k}\Big)\Big(y^{n}_{i,j+1,k} - y^{n}_{i-1,j,k}\Big)\Big]\Bigg\} \Big/ \mathcal{V}^{n}_{i,j,k}
\end{aligned}
\tag{6.4d}
$$

$$
\begin{aligned}
\frac{\partial \sigma^{n}_{yy}}{\partial y_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j,k-1} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j-1,k} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j,k-1} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j-1,k} - z^{n}_{i-1,j,k} \right) \Big] \\
& + \sigma^{n}_{yy_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j-1,k} - z^{n}_{i+1,j,k} \right) \left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i+1,j,k} \right) \left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k} \right) \Big] \\
& + \sigma^{n}_{yy_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i+1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k} \right) \left(z^{n}_{i,j+1,k} - z^{n}_{i+1,j,k} \right) \Big] \\
& + \sigma^{n}_{yy_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^{n}_{i,j+1,k} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j,k-1} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j+1,k} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j,k-1} - z^{n}_{i-1,j,k} \right) \Big] \\
& + \sigma^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i,j-1,k} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j,k+1} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j,k+1} - z^{n}_{i-1,j,k} \right) \Big] \\
& + \sigma^{n}_{yy_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i,j-1,k} - z^{n}_{i,j,k+1} \right) \left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1} \right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i,j,k+1} \right) \left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1} \right) \Big] \\
& + \sigma^{n}_{yy_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i,j,k+1} \right) \\
& \qquad - \left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1} \right) \left(z^{n}_{i,j+1,k} - z^{n}_{i,j,k+1} \right) \Big] \\
& + \sigma^{n}_{yy_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^{n}_{i,j,k+1} - z^{n}_{i-1,j,k} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i-1,j,k} \right) \\
& \qquad - \left(x^{n}_{i,j,k+1} - x^{n}_{i-1,j,k} \right) \left(z^{n}_{i,j+1,k} - z^{n}_{i-1,j,k} \right) \Big] \Bigg\} \Big/ \mathcal{V}^{n}_{i,j,k}
\end{aligned}
\tag{6.4e}
$$

$$
\begin{aligned}
\frac{\partial \sigma^n_{yz}}{\partial z_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^n_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j,k-1} - x^n_{i-1,j,k} \right) \left(y^n_{i,j-1,k} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i-1,j,k} \right) \left(x^n_{i,j-1,k} - x^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j-1,k} - x^n_{i+1,j,k} \right) \left(y^n_{i,j,k-1} - y^n_{i+1,j,k} \right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i+1,j,k} \right) \left(x^n_{i,j,k-1} - x^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j,k-1} - x^n_{i+1,j,k} \right) \left(y^n_{i,j+1,k} - y^n_{i+1,j,k} \right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i+1,j,k} \right) \left(x^n_{i,j+1,k} - x^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^n_{i,j+1,k} - x^n_{i-1,j,k} \right) \left(y^n_{i,j,k-1} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j+1,k} - y^n_{i-1,j,k} \right) \left(x^n_{i,j,k-1} - x^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i,j-1,k} - x^n_{i-1,j,k} \right) \left(y^n_{i,j,k+1} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i-1,j,k} \right) \left(x^n_{i,j,k+1} - x^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i,j-1,k} - x^n_{i,j,k+1} \right) \left(y^n_{i+1,j,k} - y^n_{i,j,k+1} \right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i,j,k+1} \right) \left(x^n_{i+1,j,k} - x^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i+1,j,k} - x^n_{i,j,k+1} \right) \left(y^n_{i,j+1,k} - y^n_{i,j,k+1} \right) \\
& \qquad - \left(y^n_{i+1,j,k} - y^n_{i,j,k+1} \right) \left(x^n_{i,j+1,k} - x^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{yz_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^n_{i,j,k+1} - x^n_{i-1,j,k} \right) \left(y^n_{i,j+1,k} - y^n_{i-1,j,k} \right) \\
& \qquad - \left(y^n_{i,j,k+1} - y^n_{i-1,j,k} \right) \left(x^n_{i,j+1,k} - x^n_{i-1,j,k} \right) \Big] \Bigg\} \Big/ \mathcal{V}^n_{i,j,k}
\end{aligned}
\tag{6.4f}
$$

$$
\begin{aligned}
\frac{\partial \sigma^n_{zx}}{\partial x_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^n_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(y^n_{i,j,k-1} - y^n_{i-1,j,k} \right) \left(z^n_{i,j-1,k} - z^n_{i-1,j,k} \right) \\
& \qquad - \left(z^n_{i,j,k-1} - z^n_{i-1,j,k} \right) \left(y^n_{i,j-1,k} - y^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(y^n_{i,j-1,k} - y^n_{i+1,j,k} \right) \left(z^n_{i,j,k-1} - z^n_{i+1,j,k} \right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i+1,j,k} \right) \left(y^n_{i,j,k-1} - y^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(y^n_{i,j,k-1} - y^n_{i+1,j,k} \right) \left(z^n_{i,j+1,k} - z^n_{i+1,j,k} \right) \\
& \qquad - \left(z^n_{i,j,k-1} - z^n_{i+1,j,k} \right) \left(y^n_{i,j+1,k} - y^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(y^n_{i,j+1,k} - y^n_{i-1,j,k} \right) \left(z^n_{i,j,k-1} - z^n_{i-1,j,k} \right) \\
& \qquad - \left(z^n_{i,j+1,k} - z^n_{i-1,j,k} \right) \left(y^n_{i,j,k-1} - y^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(y^n_{i,j-1,k} - y^n_{i-1,j,k} \right) \left(z^n_{i,j,k+1} - z^n_{i-1,j,k} \right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i-1,j,k} \right) \left(y^n_{i,j,k+1} - y^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(y^n_{i,j-1,k} - y^n_{i,j,k+1} \right) \left(z^n_{i+1,j,k} - z^n_{i,j,k+1} \right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i,j,k+1} \right) \left(y^n_{i+1,j,k} - y^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{zx_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(y^n_{i+1,j,k} - y^n_{i,j,k+1} \right) \left(z^n_{i,j+1,k} - z^n_{i,j,k+1} \right) \\
& \qquad - \left(z^n_{i+1,j,k} - z^n_{i,j,k+1} \right) \left(y^n_{i,j+1,k} - y^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{zx_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(y^n_{i,j,k+1} - y^n_{i-1,j,k} \right) \left(z^n_{i,j+1,k} - z^n_{i-1,j,k} \right) \\
& \qquad - \left(z^n_{i,j,k+1} - z^n_{i-1,j,k} \right) \left(y^n_{i,j+1,k} - y^n_{i-1,j,k} \right) \Big] \Bigg\} \Big/ \mathcal{V}^n_{i,j,k}
\end{aligned}
\tag{6.4g}
$$

$$
\begin{aligned}
\frac{\partial \sigma^n_{yz}}{\partial y_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^n_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^n_{i,j,k-1} - z^n_{i-1,j,k} \right) \left(x^n_{i,j-1,k} - x^n_{i-1,j,k} \right) \\
& \qquad - \left(x^n_{i,j,k-1} - x^n_{i-1,j,k} \right) \left(z^n_{i,j-1,k} - z^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^n_{i,j-1,k} - z^n_{i+1,j,k} \right) \left(x^n_{i,j,k-1} - x^n_{i+1,j,k} \right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i+1,j,k} \right) \left(z^n_{i,j,k-1} - z^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^n_{i,j,k-1} - z^n_{i+1,j,k} \right) \left(x^n_{i,j+1,k} - x^n_{i+1,j,k} \right) \\
& \qquad - \left(x^n_{i,j,k-1} - x^n_{i+1,j,k} \right) \left(z^n_{i,j+1,k} - z^n_{i+1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^n_{i,j+1,k} - z^n_{i-1,j,k} \right) \left(x^n_{i,j,k-1} - x^n_{i-1,j,k} \right) \\
& \qquad - \left(x^n_{i,j+1,k} - x^n_{i-1,j,k} \right) \left(z^n_{i,j,k-1} - z^n_{i-1,j,k} \right) \Big] \qquad (6.4h) \\
& + \sigma^n_{yz_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^n_{i,j-1,k} - z^n_{i-1,j,k} \right) \left(x^n_{i,j,k+1} - x^n_{i-1,j,k} \right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i-1,j,k} \right) \left(z^n_{i,j,k+1} - z^n_{i-1,j,k} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^n_{i,j-1,k} - z^n_{i,j,k+1} \right) \left(x^n_{i+1,j,k} - x^n_{i,j,k+1} \right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i,j,k+1} \right) \left(z^n_{i+1,j,k} - z^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{yz_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^n_{i+1,j,k} - z^n_{i,j,k+1} \right) \left(x^n_{i,j+1,k} - x^n_{i,j,k+1} \right) \\
& \qquad - \left(x^n_{i+1,j,k} - x^n_{i,j,k+1} \right) \left(z^n_{i,j+1,k} - z^n_{i,j,k+1} \right) \Big] \\
& + \sigma^n_{yz_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^n_{i,j,k+1} - z^n_{i-1,j,k} \right) \left(x^n_{i,j+1,k} - x^n_{i-1,j,k} \right) \\
& \qquad - \left(x^n_{i,j,k+1} - x^n_{i-1,j,k} \right) \left(z^n_{i,j+1,k} - z^n_{i-1,j,k} \right) \Big] \Bigg\} \Big/ \mathcal{V}^n_{i,j,k}
\end{aligned}
$$

$$
\begin{aligned}
\frac{\delta \sigma^{n}_{zz}}{\delta z_{i,j,k}} = \frac{1}{2} \Bigg\{ & \sigma^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^{n}_{i,j,k-1} - x^{n}_{i-1,j,k}\right)\left(y^{n}_{i,j-1,k} - y^{n}_{i-1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j,k-1} - y^{n}_{i-1,j,k}\right)\left(x^{n}_{i,j-1,k} - x^{n}_{i-1,j,k}\right)\Big] \\
& + \sigma^{n}_{zz_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^{n}_{i,j-1,k} - x^{n}_{i+1,j,k}\right)\left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j-1,k} - y^{n}_{i+1,j,k}\right)\left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k}\right)\Big] \\
& + \sigma^{n}_{zz_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k}\right)\left(y^{n}_{i,j+1,k} - y^{n}_{i+1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\right)\left(x^{n}_{i,j+1,k} - x^{n}_{i+1,j,k}\right)\Big] \\
& + \sigma^{n}_{zz_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(x^{n}_{i,j+1,k} - x^{n}_{i-1,j,k}\right)\left(y^{n}_{i,j,k-1} - y^{n}_{i-1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j+1,k} - y^{n}_{i-1,j,k}\right)\left(x^{n}_{i,j,k-1} - x^{n}_{i-1,j,k}\right)\Big] \\
& + \sigma^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^{n}_{i,j-1,k} - x^{n}_{i-1,j,k}\right)\left(y^{n}_{i,j,k+1} - y^{n}_{i-1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j-1,k} - y^{n}_{i-1,j,k}\right)\left(x^{n}_{i,j,k+1} - x^{n}_{i-1,j,k}\right)\Big] \\
& + \sigma^{n}_{zz_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^{n}_{i,j-1,k} - x^{n}_{i,j,k+1}\right)\left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\right) \\
& \qquad - \left(y^{n}_{i,j-1,k} - y^{n}_{i,j,k+1}\right)\left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1}\right)\Big] \\
& + \sigma^{n}_{zz_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1}\right)\left(y^{n}_{i,j+1,k} - y^{n}_{i,j,k+1}\right) \\
& \qquad - \left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\right)\left(x^{n}_{i,j+1,k} - x^{n}_{i,j,k+1}\right)\Big] \\
& + \sigma^{n}_{zz_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(x^{n}_{i,j,k+1} - x^{n}_{i-1,j,k}\right)\left(y^{n}_{i,j+1,k} - y^{n}_{i-1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j,k+1} - y^{n}_{i-1,j,k}\right)\left(x^{n}_{i,j+1,k} - x^{n}_{i-1,j,k}\right)\Big] \Bigg\} \Big/ \mathcal{V}^{n}_{i,j,k}
\end{aligned}
\tag{6.4i}
$$

Multiplying Eqs.(6.4) by $\mathcal{V}^n_{i,j,k}$ yields terms of the form

$$a^n_{11} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{xx}}{\partial x_{i,j,k}} \qquad \text{from Eq.(6.4a)} ,$$

$$a^n_{12} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{xy}}{\partial y_{i,j,k}} \qquad \text{from Eq.(6.4b)} ,$$

$$a^n_{13} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{zx}}{\partial z_{i,j,k}} \qquad \text{from Eq.(6.4c)} ,$$

$$a^n_{21} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{xy}}{\partial x_{i,j,k}} \qquad \text{from Eq.(6.4d)} ,$$

$$a^n_{22} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{yy}}{\partial y_{i,j,k}} \qquad \text{from Eq.(6.4e)} ,$$

$$a^n_{23} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{yz}}{\partial z_{i,j,k}} \qquad \text{from Eq.(6.4f)} ,$$

$$a^n_{31} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{zx}}{\partial x_{i,j,k}} \qquad \text{from Eq.(6.4g)} ,$$

$$a^n_{32} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{yz}}{\partial y_{i,j,k}} \qquad \text{from Eq.(6.4h)} ,$$

$$a^n_{33} = \mathcal{V}^n_{i,j,k} \frac{\partial \sigma^n_{zz}}{\partial z_{i,j,k}} \qquad \text{from Eq.(6.4i)} ,$$

and Eqs.(6.3) become

$$\ddot{x}^{n}_{i,j,k} = \frac{1}{2}\,\frac{1}{m_{i,j,k}}\left(a^{n}_{11} + a^{n}_{12} + a^{n}_{13}\right) ,$$

$$\ddot{y}^{n}_{i,j,k} = \frac{1}{2}\,\frac{1}{m_{i,j,k}}\left(a^{n}_{21} + a^{n}_{22} + a^{n}_{23}\right) , \qquad (6.5)^{*}$$

$$\ddot{z}^{n}_{i,j,k} = \frac{1}{2}\,\frac{1}{m_{i,j,k}}\left(a^{n}_{31} + a^{n}_{32} + a^{n}_{33}\right) .$$

The mass of the momentum cell, $m_{i,j,k}$, is defined as

$$m_{i,j,k} \equiv \frac{1}{8}\left(m_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + m_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + m_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} + m_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}\right.$$
$$\left. + m_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + m_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + m_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} + m_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}\right) .$$

(6.6)

Numerical evaluation of Eqs.(6.5) yields grid point acceleration of grid point (i,j,k) at time n. To determine the velocity and position of grid point (i,j,k) requires time-centered integrations analogous to Eqs.(4.7) and (4.8), pictorially described by Figures 4.2 and 4.3. The three-dimensional versions of these equations are for velocity,

$$\dot{x}^{n+\frac{1}{2}}_{i,j,k} = \dot{x}^{n-\frac{1}{2}}_{i,j,k} + \ddot{x}^{n}_{i,j,k}\,\Delta t^{n} ,$$

$$\dot{y}^{n+\frac{1}{2}}_{i,j,k} = \dot{y}^{n-\frac{1}{2}}_{i,j,k} + \ddot{y}^{n}_{i,j,k}\,\Delta t^{n} , \qquad (6.7)$$

$$\dot{z}^{n+\frac{1}{2}}_{i,j,k} = \dot{z}^{n-\frac{1}{2}}_{i,j,k} + \ddot{z}^{n}_{i,j,k}\,\Delta t^{n} ,$$

---

*The factor of 2 multiplying $m_{i,j,k}$ is necessary so that the amount of mass is consistent with the volume used in the surface integral formula for the gradient of stress.

and for position,

$$x^{n+1}_{i,j,k} = x^{n}_{i,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k} \, \Delta t^{n+\frac{1}{2}} ,$$

$$y^{n+1}_{i,j,k} = y^{n}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k} \, \Delta t^{n+\frac{1}{2}} , \tag{6.8}$$

$$z^{n+1}_{i,j,k} = z^{n}_{i,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k} \, \Delta t^{n+\frac{1}{2}} .$$

The time step values, Δt^n and $\Delta t^{n+\frac{1}{2}}$, used in Eqs.(6.7) and (6.8) are determined from the stability requirement that a sound signal can only propagate the smallest zone dimension of the entire mesh or less in one time step. Mathematically, this condition, called the Courant stability criterion, is written as follows:

$$\Delta t^n = \text{minimum value of } \Delta t^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \text{ for all } i > 1,\ j > 1,\ k > 1,$$

$$\Delta t^{n+\frac{1}{2}} = \text{minimum value of } \Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \text{ for all } i > 1,\ j > 1,\ k > 1,$$

where

$$\Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \le \frac{\Delta \ell^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{c^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} ; \tag{6.9a}$$

$$\Delta t^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{\Delta t^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + \Delta t^{n-\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{2} . \tag{6.9b}$$

$\Delta \ell^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the smallest length across zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n, and $c^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the sound speed of zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n. Values at time n come from initial conditions or from a previous cycle.

Equations (6.7) and (6.8) use the definition for a first-order temporal difference analogous to Eqs.(4.10a) and (4.10b),

$$\Delta(\ )_{i,j,k}^{n} \equiv (\ )_{i,j,k}^{n+\frac{1}{2}} - (\ )_{i,j,k}^{n-\frac{1}{2}} , \tag{6.10a}$$

and

$$\Delta(\ )_{i,j,k}^{n+\frac{1}{2}} \equiv (\ )_{i,j,k}^{n+1} - (\ )_{i,j,k}^{n} . \tag{6.10b}$$

Equations (6.5), (6.7), and (6.8) are perfectly centered in space and time. However, a time-centering error can occur in Eqs.(6.7) for the initial step because $\dot{x}_{i,j,k}^{n-\frac{1}{2}}$, $\dot{y}_{i,j,k}^{n-\frac{1}{2}}$, and $\dot{z}_{i,j,k}^{n-\frac{1}{2}}$ may not be known at time $n-\frac{1}{2}$. In this case, it is customary to let $\dot{x}_{i,j,k}^{n-\frac{1}{2}}$, $\dot{y}_{i,j,k}^{n-\frac{1}{2}}$, and $\dot{z}_{i,j,k}^{n-\frac{1}{2}}$ take on the value of $\dot{x}_{i,j,k}^{n}$, $\dot{y}_{i,j,k}^{n}$, and $\dot{z}_{i,j,k}^{n}$, respectively, and to use an initial time step, Δt^{0}, that is 0.1 of the initial stable value. After the initial time step, Eqs.(6.7) are properly centered.*

6.2.3 Momentum Boundary Conditions. Momentum boundary conditions are of two types -- those that use a stress or force, and those that use an acceleration, a velocity, or a displacement. The former, known as "stress-type boundaries," affect Eqs.(6.5), while the latter, knows as "velocity-type boundaries," affect Eqs.(6.7) and (6.8). In addition to the two types of boundary conditions, there are two ways in which boundary values are obtained, i.e., by prescription or by interaction. By prescription means that boundary values are provided as time histories for an entire event; by interaction means that an algorithm for calculating values is provided.

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*Equations (6.7) may be written in "dynamic relaxation" form so that static and quasi-static calculations are computed more efficiently. A discussion of dynamic relaxation appears in Section 6.5.

Equations (6.5), which were derived for non-boundary points, are well suited for stress-type boundary conditions. Left boundary conditions affect the i-$\frac{1}{2}$ values in Eqs.(6.5), right boundary conditions affect the i+$\frac{1}{2}$ values, bottom boundary conditions affect the j-$\frac{1}{2}$ values, top boundary conditions affect the j+$\frac{1}{2}$ values, aft boundary conditions affect the k-$\frac{1}{2}$ values, and front boundary conditions affect the k+$\frac{1}{2}$ values. There are twenty-six possible outside boundary orientations in three-dimensional geometry. They are:

(1) aft bottom left corner
(2) aft bottom edge
(3) aft bottom right corner
(4) aft left edge
(5) aft face
(6) aft right edge
(7) aft top left corner
(8) aft top edge
(9) aft top right corner
(10) center bottom left edge
(11) center bottom face
(12) center bottom right edge
(13) center left face
(14) center right face
(15) center top left edge
(16) center top face
(17) center top right edge
(18) front bottom left corner
(19) front bottom edge
(20) front bottom right corner
(21) front left edge
(22) front face
(23) front right edge
(24) front top left corner
(25) front top edge
(26) front top right corner

An example of a left boundary condition is a free left face boundary. Mathematically, the free left boundary condition applied to Eqs.(6.5) is given by

$$x^n_{i-1,j,k} = x^n_{i,j,k}, \qquad y^n_{i-1,j,k} = y^n_{i,j,k}, \qquad z^n_{i-1,j,k} = z^n_{i,j,k},$$

$$\sigma^n_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = 0,$$

$$\sigma^n_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = 0,$$

$$\sigma^n_{xx_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{yy_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{zz_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} = 0, \qquad (6.11)$$

$$\sigma^n_{xy_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{yz_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} = \sigma^n_{zx_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} = 0,$$

$$\sigma^n_{xx_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{yy_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{zz_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} = 0,$$

$$\sigma^n_{xy_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{yz_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{zx_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} = 0,$$

$$\sigma^n_{xx_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{yy_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{zz_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} = 0,$$

$$\sigma^n_{xy_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{yz_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} = \sigma^n_{zx_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} = 0,$$

$$m_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = 0, \quad m_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} = 0, \quad m_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} = 0, \quad m_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = 0.$$

Substituting Eqs.(6.11) into Eqs.(6.5) for the momentum mass yields

$$m_{i,j,k} \equiv \frac{1}{N}\left(m_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + m_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} + m_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + m_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}\right) , \qquad (6.12)$$

where N is the sum of the existence factors,

$$\begin{aligned} N \equiv\ & E_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + E_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + E_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} + E_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \\ & + E_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + E_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + E_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} + E_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} , \end{aligned} \qquad (6.13)$$

and the existence factors, E, are equal to zero if the zone does not exist and equal to one if it does exist. Substituting Eqs.(6.11) into Eqs.(6.5) for the terms a_{ij} yields

$$\begin{aligned}
a_{11} = \frac{1}{2}\Bigg\{ \sigma^n_{xx_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(y^n_{i,j-1,k} - y^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right) \\
& - \left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\Big] \\
+ \sigma^n_{xx_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right) \\
& - \left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i+1,j,k}\right)\Big] \\
+ \sigma^n_{xx_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(y^n_{i,j-1,k} - y^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right) \\
& - \left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\Big] \\
+ \sigma^n_{xx_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right) \\
& - \left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(y^n_{i,j+1,k} - y^n_{i,j,k+1}\right)\Big]\Bigg\}
\end{aligned} \tag{6.14a}$$

$$\begin{aligned}
a_{12} = \frac{1}{2}\Bigg\{ \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right) \\
& - \left(x^n_{i,j-1,k} - x^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\Big] \\
+ \sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i+1,j,k}\right) \\
& - \left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right)\Big] \\
+ \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right) \\
& - \left(x^n_{i,j-1,k} - x^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\Big] \\
+ \sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(x^n_{i,j+1,k} - x^n_{i,j,k+1}\right) \\
& - \left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right)\Big]\Bigg\}
\end{aligned} \tag{6.14b}$$

$$
\begin{aligned}
a_{13} = \frac{1}{2}\Biggl\{ & \sigma^{n}_{zx_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Bigl[\left(x^{n}_{i,j-1,k} - x^{n}_{i+1,j,k}\right)\left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j-1,k} - y^{n}_{i+1,j,k}\right)\left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k}\right)\Bigr] \\
& + \sigma^{n}_{zx_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Bigl[\left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k}\right)\left(y^{n}_{i,j+1,k} - y^{n}_{i+1,j,k}\right) \\
& \qquad - \left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\right)\left(x^{n}_{i,j+1,k} - x^{n}_{i+1,j,k}\right)\Bigr] \\
& + \sigma^{n}_{zx_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Bigl[\left(x^{n}_{i,j-1,k} - x^{n}_{i,j,k+1}\right)\left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\right) \\
& \qquad - \left(y^{n}_{i,j-1,k} - y^{n}_{i,j,k+1}\right)\left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1}\right)\Bigr] \\
& + \sigma^{n}_{zx_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Bigl[\left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1}\right)\left(y^{n}_{i,j+1,k} - y^{n}_{i,j,k+1}\right) \\
& \qquad - \left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\right)\left(x^{n}_{i,j+1,k} - x^{n}_{i,j,k+1}\right)\Bigr]\Biggr\}
\end{aligned}
\tag{6.14c}
$$

$$\begin{aligned}
a_{21} = \frac{1}{2}\Bigg\{ & \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(y^n_{i,j-1,k} - y^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\Big] \\
& + \sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right) \\
& \qquad - \left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i+1,j,k}\right)\Big] \\
& + \sigma^n_{xy_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(y^n_{i,j-1,k} - y^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\Big] \\
& + \sigma^n_{xy_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right) \\
& \qquad - \left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(y^n_{i,j+1,k} - y^n_{i,j,k+1}\right)\Big]\Bigg\} \qquad (6.15a)
\end{aligned}$$

$$\begin{aligned}
a_{22} = \frac{1}{2}\Bigg\{ & \sigma^n_{yy_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\Big] \\
& + \sigma^n_{yy_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Big[\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i+1,j,k}\right) \\
& \qquad - \left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right)\Big] \\
& + \sigma^n_{yy_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\Big] \\
& + \sigma^n_{yy_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Big[\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(x^n_{i,j+1,k} - x^n_{i,j,k+1}\right) \\
& \qquad - \left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right)\Big]\Bigg\} \qquad (6.15b)
\end{aligned}$$

$$
\begin{aligned}
a_{23} = \frac{1}{2} \Bigg\{ \sigma^n_{yz_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(x^n_{i,j-1,k} - x^n_{i+1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right) \\
& - \left(y^n_{i,j-1,k} - y^n_{i+1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right) \Big] \\
+ \sigma^n_{yz_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i+1,j,k}\right) \\
& - \left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i+1,j,k}\right) \Big] \\
+ \sigma^n_{yz_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(x^n_{i,j-1,k} - x^n_{i,j,k+1}\right)\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right) \\
& - \left(y^n_{i,j-1,k} - y^n_{i,j,k+1}\right)\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right) \Big] \\
+ \sigma^n_{yz_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\left(y^n_{i,j+1,k} - y^n_{i,j,k+1}\right) \\
& - \left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\left(x^n_{i,j+1,k} - x^n_{i,j,k+1}\right) \Big] \Bigg\} \qquad (6.15c)
\end{aligned}
$$

$$
\begin{aligned}
a_{31} = \frac{1}{2}\Bigg\{ & \sigma^{n}_{zx_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Bigg[\left(y^{n}_{i,j-1,k} - y^{n}_{i+1,j,k}\right)\left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k}\right) \\
& \qquad - \left(z^{n}_{i,j-1,k} - z^{n}_{i+1,j,k}\right)\left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\right)\Bigg] \\
& + \sigma^{n}_{zx_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Bigg[\left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k}\right)\left(z^{n}_{i,j+1,k} - z^{n}_{i+1,j,k}\right) \\
& \qquad - \left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k}\right)\left(y^{n}_{i,j+1,k} - y^{n}_{i+1,j,k}\right)\Bigg] \\
& + \sigma^{n}_{zx_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Bigg[\left(y^{n}_{i,j-1,k} - y^{n}_{i,j,k+1}\right)\left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1}\right) \\
& \qquad - \left(z^{n}_{i,j-1,k} - z^{n}_{i,j,k+1}\right)\left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\right)\Bigg] \\
& + \sigma^{n}_{zx_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Bigg[\left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1}\right)\left(z^{n}_{i,j+1,k} - z^{n}_{i,j,k+1}\right) \\
& \qquad - \left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1}\right)\left(y^{n}_{i,j+1,k} - y^{n}_{i,j,k+1}\right)\Bigg]\Bigg\} \qquad (6.16a)
\end{aligned}
$$

$$
\begin{aligned}
a_{32} = \frac{1}{2}\Bigg\{ & \sigma^{n}_{yz_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Bigg[\left(z^{n}_{i,j-1,k} - z^{n}_{i+1,j,k}\right)\left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k}\right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i+1,j,k}\right)\left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k}\right)\Bigg] \\
& + \sigma^{n}_{yz_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} \Bigg[\left(z^{n}_{i,j,k-1} - z^{n}_{i+1,j,k}\right)\left(x^{n}_{i,j+1,k} - x^{n}_{i+1,j,k}\right) \\
& \qquad - \left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k}\right)\left(z^{n}_{i,j+1,k} - z^{n}_{i+1,j,k}\right)\Bigg] \\
& + \sigma^{n}_{yz_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} \Bigg[\left(z^{n}_{i,j-1,k} - z^{n}_{i,j,k+1}\right)\left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1}\right) \\
& \qquad - \left(x^{n}_{i,j-1,k} - x^{n}_{i,j,k+1}\right)\left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1}\right)\Bigg] \\
& + \sigma^{n}_{yz_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \Bigg[\left(z^{n}_{i+1,j,k} - z^{n}_{i,j,k+1}\right)\left(x^{n}_{i,j+1,k} - x^{n}_{i,j,k+1}\right) \\
& \qquad - \left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1}\right)\left(z^{n}_{i,j+1,k} - z^{n}_{i,j,k+1}\right)\Bigg]\Bigg\} \qquad (6.16b)
\end{aligned}
$$

$$
\begin{aligned}
a_{33} = \frac{1}{2} \Bigg\{ \sigma^{n}_{zz_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(x^{n}_{i,j-1,k} - x^{n}_{i+1,j,k} \right) \left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k} \right) \\
& - \left(y^{n}_{i,j-1,k} - y^{n}_{i+1,j,k} \right) \left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k} \right) \Big] \\
+ \sigma^{n}_{zz_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}} & \Big[\left(x^{n}_{i,j,k-1} - x^{n}_{i+1,j,k} \right) \left(y^{n}_{i,j+1,k} - y^{n}_{i+1,j,k} \right) \\
& - \left(y^{n}_{i,j,k-1} - y^{n}_{i+1,j,k} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i+1,j,k} \right) \Big] \\
+ \sigma^{n}_{zz_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(x^{n}_{i,j-1,k} - x^{n}_{i,j,k+1} \right) \left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1} \right) \\
& - \left(y^{n}_{i,j-1,k} - y^{n}_{i,j,k+1} \right) \left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1} \right) \Big] \\
+ \sigma^{n}_{zz_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} & \Big[\left(x^{n}_{i+1,j,k} - x^{n}_{i,j,k+1} \right) \left(y^{n}_{i,j+1,k} - y^{n}_{i,j,k+1} \right) \\
& - \left(y^{n}_{i+1,j,k} - y^{n}_{i,j,k+1} \right) \left(x^{n}_{i,j+1,k} - x^{n}_{i,j,k+1} \right) \Big] \Bigg\} \qquad (6.16c)
\end{aligned}
$$

Velocity-type boundary conditions eliminate the need for Eqs.(6.5). These conditions affect Eqs.(6.7) and/or (6.8) directly.

The simplest way to provide boundary values is by prescription. That is, stress (or velocity) is given at the beginning of a problem for all time at a boundary grid point. The value is a function of time only, since the location of the grid point is always known. If the boundary value is tied to a coordinate which is different from the boundary grid point, then an interaction calculation is required. For example, outside boundaries can interact with geometric constraints (wall segments) or they can interact with each other by coming together to close a void. In general, when a boundary grid point engages a constraint or another boundary grid point, a velocity condition is required. When a boundary grid point disengages, a stress-type boundary calculation is required, e.g., it can become free.

Equations of interaction between a grid point and a constraint, or between two grid points, are governed by the principle of conservation of momentum during the moment of initial contact and during intimate contact. During the time when the points move independently and at the moment of separation, the grid points are separate stress-type boundaries.

6.2.4 Mass Equation. The general continuity or conservation of mass equation is

$$\frac{\dot{V}}{V} = \frac{\partial \dot{x}}{\partial x} + \frac{\partial \dot{y}}{\partial y} + \frac{\partial \dot{z}}{\partial z} , \tag{6.20}$$

where V, x, y, and z are previously defined. The left side of Eq.(6.20) is called the volumetric strain rate, while the right side contains directional (or component) values of strain rate.

A finite-difference analog must be derived separately but consistently for each term in Eq.(6.20). First, consider the volumetric strain rate of zone ($i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}$), written in the following differential form,

$$\left(\frac{\dot{V}}{V}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} / \Delta t^{n+\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} , \tag{6.21}$$

where $\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the change in relative volume of zone ($i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}$) at time $n+\frac{1}{2}$ and $\Delta t^{n+\frac{1}{2}}$ is the time increment. Applying Eq.(6.10b) to the definition of relative volume, the change of relative volume is

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \equiv V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - V^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} ; \tag{6.22a}$$

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \rho^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \left(\frac{1}{\rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \frac{1}{\rho^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \right) . \tag{6.22b}$$

Since the mesh is Lagrangian, Eq.(6.22b) may be written in terms of true volume, $\mathcal{V}$, as follows,

$$\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{m^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left(\mathcal{V}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right) . \tag{6.23}$$

Equation (6.23) is a formula for change of relative volume in terms of change of true volume. The change of true volume is related directly to the coordinates of the zone. Using the mesh notation shown on Page 6.4, the formula for change of true volume is derived as follows:

> Zones in a three-dimensional mesh are defined by eight mesh points which are allowed to move independently, according to conservation of mass and momentum. These eight mesh points define a hexagon in index space and a duodecahedron in physical space. The duodecahedron is not uniquely defined in that the "fold" in each index space face is arbitrary.* Therefore, in order to be properly centered, the volume formula is taken to be the average of the parallelepiped volumes defined at each vertex. A parallelepiped volume is given by

$$\mathcal{V}_{\text{vertex}} = |\underline{A} \cdot (\underline{B} \times \underline{C})| \tag{6.24a}$$

$$= \begin{vmatrix} A_i & A_j & A_k \\ B_i & B_j & B_k \\ C_i & C_j & C_k \end{vmatrix} \tag{6.24b}$$

$$\begin{aligned} &= A_i(B_j C_k - B_k C_j) \\ &+ A_j(B_k C_i - B_i C_k) \\ &+ A_k(B_i C_j - B_j C_i), \end{aligned} \tag{6.24c}$$

> where $\underline{A}$, $\underline{B}$, and $\underline{C}$ are vectors pointing from the vertex. Considering zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ on Page 6.4, which is defined by the eight grid points (i,j,k), $(i,j-1,k)$, $(i,j-1,k-1)$, $(i,j,k-1)$, $(i-1,j,k)$, $(i-1,j-1,k)$, $(i-1,j-1,k-1)$, and $(i-1,j,k-1)$, the volume is

---

*See Figure 6.2.

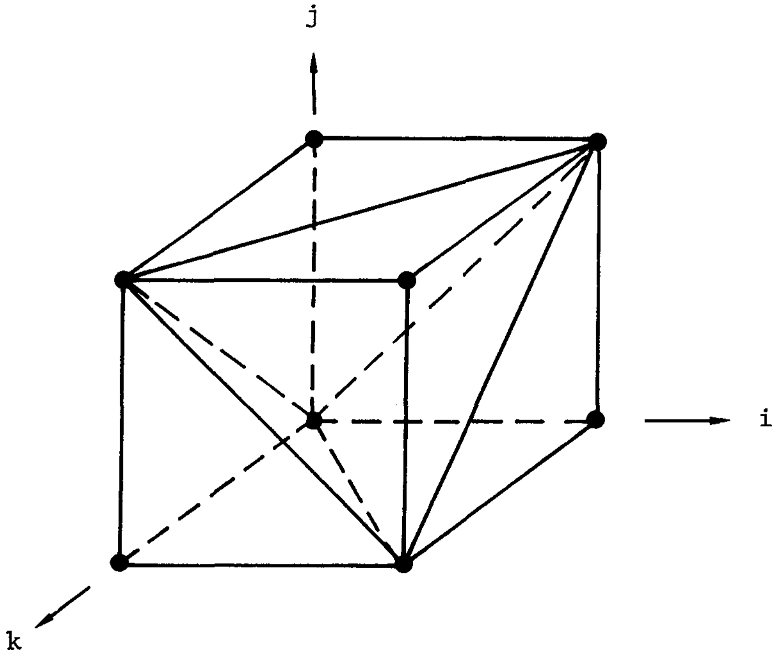

Figure 6.2. Typical duodecahedron zone.

$$\mathcal{V}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \approx$$

$$\begin{aligned}
\frac{1}{8}\Bigg\{ &(x_{i,j,k} - x_{i,j-1,k}) \Big[(y_{i,j-1,k-1} - y_{i,j-1,k})(z_{i-1,j-1,k} - z_{i,j-1,k}) \\
&\qquad - (z_{i,j-1,k-1} - z_{i,j-1,k})(y_{i-1,j-1,k} - y_{i,j-1,k})\Big] \\
&+ (y_{i,j,k} - y_{i,j-1,k}) \Big[(z_{i,j-1,k-1} - z_{i,j-1,k})(x_{i-1,j-1,k} - x_{i,j-1,k}) \\
&\qquad - (x_{i,j-1,k-1} - x_{i,j-1,k})(z_{i-1,j-1,k} - z_{i,j-1,k})\Big] \\
&+ (z_{i,j,k} - z_{i,j-1,k}) \Big[(x_{i,j-1,k-1} - x_{i,j-1,k})(y_{i-1,j-1,k} - y_{i,j-1,k}) \\
&\qquad - (y_{i,j-1,k-1} - y_{i,j-1,k})(x_{i-1,j-1,k} - x_{i,j-1,k})\Big] \\
&+ (x_{i,j,k-1} - x_{i,j-1,k-1}) \Big[(y_{i-1,j-1,k-1} - y_{i,j-1,k-1})(z_{i,j-1,k} - z_{i,j-1,k-1}) \\
&\qquad - (z_{i-1,j-1,k-1} - z_{i,j-1,k-1})(y_{i,j-1,k} - y_{i,j-1,k-1})\Big] \\
&+ (y_{i,j,k-1} - y_{i,j-1,k-1}) \Big[(z_{i-1,j-1,k-1} - z_{i,j-1,k-1})(x_{i,j-1,k} - x_{i,j-1,k-1}) \\
&\qquad - (x_{i-1,j-1,k-1} - x_{i,j-1,k-1})(z_{i,j-1,k} - z_{i,j-1,k-1})\Big] \\
&+ (z_{i,j,k-1} - z_{i,j-1,k-1}) \Big[(x_{i-1,j-1,k-1} - x_{i,j-1,k-1})(y_{i,j-1,k} - y_{i,j-1,k-1}) \\
&\qquad - (y_{i-1,j-1,k-1} - y_{i,j-1,k-1})(x_{i,j-1,k} - x_{i,j-1,k-1})\Big]
\end{aligned}$$

(This equation is continued on the following page.)

$$
\begin{aligned}
&+ (x_{i-1,j,k-1} - x_{i-1,j-1,k-1}) \Big[(y_{i-1,j-1,k} - y_{i-1,j-1,k-1})(z_{i,j-1,k-1} - z_{i-1,j-1,k-1}) \\
&\qquad - (z_{i-1,j-1,k} - z_{i-1,j-1,k-1})(y_{i,j-1,k-1} - y_{i-1,j-1,k-1})\Big] \\
&+ (y_{i-1,j,k-1} - y_{i-1,j-1,k-1}) \Big[(z_{i-1,j-1,k} - z_{i-1,j-1,k-1})(x_{i,j-1,k-1} - x_{i-1,j-1,k-1}) \\
&\qquad - (x_{i-1,j-1,k} - x_{i-1,j-1,k-1})(z_{i,j-1,k-1} - z_{i-1,j-1,k-1})\Big] \\
&+ (z_{i-1,j,k-1} - z_{i-1,j-1,k-1}) \Big[(x_{i-1,j-1,k} - x_{i-1,j-1,k-1})(y_{i,j-1,k-1} - y_{i-1,j-1,k-1}) \\
&\qquad - (y_{i-1,j-1,k} - y_{i-1,j-1,k-1})(x_{i,j-1,k-1} - x_{i-1,j-1,k-1})\Big] \\
&+ (x_{i-1,j,k} - x_{i-1,j-1,k}) \Big[(y_{i,j-1,k} - y_{i-1,j-1,k})(z_{i-1,j-1,k-1} - z_{i-1,j-1,k}) \\
&\qquad - (z_{i,j-1,k} - z_{i-1,j-1,k}))(y_{i-1,j-1,k-1} - y_{i-1,j-1,k})\Big] \\
&+ (y_{i-1,j,k} - y_{i-1,j-1,k}) \Big[(z_{i,j-1,k} - z_{i-1,j-1,k}) (x_{i-1,j-1,k-1} - x_{i-1,j-1,k}) \\
&\qquad - (x_{i,j-1,k} - x_{i-1,j-1,k}) (z_{i-1,j-1,k-1} - z_{i-1,j-1,k})\Big] \\
&+ (z_{i-1,j,k} - z_{i-1,j-1,k}) \Big[(x_{i,j-1,k} - x_{i-1,j-1,k}) (y_{i-1,j-1,k-1} - y_{i-1,j-1,k}) \\
&\qquad - (y_{i,j-1,k} - y_{i-1,j-1,k}) (x_{i-1,j-1,k-1} - x_{i-1,j-1,k})\Big]
\end{aligned}
$$

(This equation is continued on the following page.)

$$
\begin{aligned}
&+ (x_{i,j-1,k} - x_{i,j,k}) \Big[(y_{i-1,j,k} - y_{i,j,k}) (z_{i,j,k-1} - z_{i,j,k}) \\
&\qquad - (z_{i-1,j,k} - z_{i,j,k}) (y_{i,j,k-1} - z_{i,j,k}) \Big] \\
&+ (y_{i,j-1,k} - y_{i,j,k}) \Big[(z_{i-1,j,k} - z_{i,j,k}) (x_{i,j,k-1} - x_{i,j,k}) \\
&\qquad - (x_{i-1,j,k} - x_{i,j,k}) (z_{i,j,k-1} - z_{i,j,k}) \Big] \\
&+ (z_{i,j-1,k} - z_{i,j,k}) \Big[(x_{i-1,j,k} - x_{i,j,k}) (y_{i,j,k-1} - y_{i,j,k}) \\
&\qquad - (y_{i-1,j,k} - y_{i,j,k}) (x_{i,j,k-1} - x_{i,j,k}) \Big] \\
&+ (x_{i,j-1,k-1} - x_{i,j,k-1}) \Big[(y_{i,j,k} - y_{i,j,k-1}) (z_{i-1,j,k-1} - z_{i,j,k-1}) \\
&\qquad - (z_{i,j,k} - z_{i,j,k-1}) (y_{i-1,j,k-1} - y_{i,j,k-1}) \Big] \\
&+ (y_{i,j-1,k-1} - y_{i,j,k-1}) \Big[(z_{i,j,k} - z_{i,j,k-1}) (x_{i-1,j,k-1} - x_{i,j,k-1}) \\
&\qquad - (x_{i,j,k} - x_{i,j,k-1}) (z_{i-1,j,k-1} - z_{i,j,k-1}) \Big] \\
&+ (z_{i,j-1,k-1} - z_{i,j,k-1}) \Big[(x_{i,j,k} - x_{i,j,k-1}) (y_{i-1,j,k-1} - y_{i,j,k-1}) \\
&\qquad - (y_{i,j,k} - y_{i,j,k-1}) (x_{i-1,j,k-1} - x_{i,j,k-1}) \Big]
\end{aligned}
$$

(This equation is continued on the following page.)

$$
\begin{aligned}
&+ (x_{i-1,j-1,k-1} - x_{i-1,j,k-1}) \Big[(y_{i,j,k-1} - y_{i-1,j,k-1})(z_{i-1,j,k} - z_{i-1,j,k-1}) \\
&\qquad - (z_{i,j,k-1} - z_{i-1,j,k-1})(y_{i-1,j,k} - y_{i-1,j,k-1})\Big] \\
&+ (y_{i-1,j-1,k-1} - y_{i-1,j,k-1}) \Big[(z_{i,j,k-1} - z_{i-1,j,k-1})(x_{i-1,j,k} - x_{i-1,j,k-1}) \\
&\qquad - (x_{i,j,k-1} - x_{i-1,j,k-1})(z_{i-1,j,k} - z_{i-1,j,k-1})\Big] \\
&+ (z_{i-1,j-1,k-1} - z_{i-1,j,k-1}) \Big[(x_{i,j,k-1} - x_{i-1,j,k-1})(y_{i-1,j,k} - y_{i-1,j,k-1}) \\
&\qquad - (y_{i,j,k-1} - y_{i-1,j,k-1})(x_{i-1,j,k} - x_{i-1,j,k-1})\Big] \\
&+ (x_{i-1,j-1,k} - x_{i-1,j,k}) \Big[(y_{i-1,j,k-1} - y_{i-1,j,k}) (z_{i,j,k} - z_{i-1,j,k}) \\
&\qquad - (z_{i-1,j,k-1} - z_{i-1,j,k}) (y_{i,j,k} - y_{i-1,j,k})\Big] \\
&+ (y_{i-1,j-1,k} - y_{i-1,j,k}) \Big[(z_{i-1,j,k-1} - z_{i-1,j,k}) (x_{i,j,k} - x_{i-1,j,k}) \\
&\qquad - (x_{i-1,j,k-1} - x_{i-1,j,k}) (z_{i,j,k} - z_{i-1,j,k})\Big] \\
&+ (z_{i-1,j-1,k} - z_{i-1,j,k}) \Big[(x_{i-1,j,k-1} - x_{i-1,j,k}) (y_{i,j,k} - y_{i-1,j,k}) \\
&\qquad - (y_{i-1,j,k-1} - y_{i-1,j,k}) (x_{i,j,k} - x_{i-1,j,k})\Big]\Bigg\} .
\end{aligned}
\tag{6.24d}
$$

The new relative volume is computed from the new zone volume,

$$V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \mathcal{V}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} , \tag{6.25}$$

and the new density comes from new relative volume,

$$\rho^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} . \tag{6.26}$$

From the definition of a first-order temporal average,

$$(\ )^{n+\frac{1}{2}} \equiv \frac{(\ )^{n+1} + (\ )^{n}}{2} , \tag{6.27}$$

the formula for $V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ in Eq.(6.21) is

$$V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + V^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{2} , \tag{6.28}$$

where $V^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is known and $V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ can be calculated from Eq.(6.25) or by inverting Eq.(6.22a) as follows,

$$V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = V^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + \Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} . \tag{6.29}$$

New compression is

$$C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \equiv V^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} , \tag{6.30}$$

and change in compression, defined by

$$\Delta C^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \equiv C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - C^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}, \tag{6.31}$$

is

$$\Delta C^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = -\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}. \tag{6.32}$$

The next step in calculating the terms of Eq.(6.20) is the computation of the velocity gradients (xx-, yy-, and zz-strain rates). From Eqs.(3.45),

$$\left(\frac{\partial \dot{x}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left[b^{n+\frac{1}{2}}_{xx_{i-1,j,k}} + b^{n+\frac{1}{2}}_{xx_{i,j,k}} + b^{n+\frac{1}{2}}_{xx_{i,j-1,k}} + b^{n+\frac{1}{2}}_{xx_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{xx_{i-1,j,k-1}} + b^{n+\frac{1}{2}}_{xx_{i,j,k-1}} + b^{n+\frac{1}{2}}_{xx_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{xx_{i-1,j-1,k-1}} \right]; \tag{6.33}$$

$$\left(\frac{\partial \dot{y}}{\partial y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left[b^{n+\frac{1}{2}}_{yy_{i-1,j,k}} + b^{n+\frac{1}{2}}_{yy_{i,j,k}} + b^{n+\frac{1}{2}}_{yy_{i,j-1,k}} + b^{n+\frac{1}{2}}_{yy_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{yy_{i-1,j,k-1}} + b^{n+\frac{1}{2}}_{yy_{i,j,k-1}} + b^{n+\frac{1}{2}}_{yy_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{yy_{i-1,j-1,k-1}} \right]; \tag{6.34}$$

$$\left(\frac{\partial \dot{z}}{\partial z}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Bigg[b^{n+\frac{1}{2}}_{zz_{i-1,j,k}} + b^{n+\frac{1}{2}}_{zz_{i,j,k}}$$

$$+ b^{n+\frac{1}{2}}_{zz_{i,j-1,k}} + b^{n+\frac{1}{2}}_{zz_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{zz_{i-1,j,k-1}}$$

$$+ b^{n+\frac{1}{2}}_{zz_{i,j,k-1}} + b^{n+\frac{1}{2}}_{zz_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{zz_{i-1,j-1,k-1}} \Bigg] ; \quad (6.35)$$

where

$$\mathcal{V}^{n+\frac{1}{2}} \equiv \frac{\mathcal{V}^{n+1} + \mathcal{V}^{n}}{2} ,$$

and $b^{n+\frac{1}{2}}_{xx}$, $b^{n+\frac{1}{2}}_{yy}$, and $b^{n+\frac{1}{2}}_{zz}$ are defined on the next 24 pages. The factor of 2 in the denominators of Eqs.(6.33), (6.34), and (6.35) compensates for the fact that the surface integration terms, b, actually cover the surface area of the zone twice.

$$\begin{aligned}
b_{xx\,i-1,j,k}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\Bigg[\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right) \\
& \quad -\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\Bigg] \\
& + \frac{1}{3}\left(\dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\Bigg[\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right) \\
& \quad -\left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\Bigg] \\
& - \frac{1}{3}\left(\dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\Bigg[\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right) \\
& \quad -\left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\Bigg],
\end{aligned}$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{xx_{i,j,k}} = &- \frac{1}{3} \left(\dot{x}^{n+\frac{1}{2}}_{i,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
&\frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \right. \\
&\left. - \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k} \right) \left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \right] \\
&+ \frac{1}{3} \left(\dot{x}^{n+\frac{1}{2}}_{i,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
&\frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \right. \\
&\left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \right] \\
&- \frac{1}{3} \left(\dot{x}^{n+\frac{1}{2}}_{i,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1} \right) \times \\
&\frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k} \right) \right. \\
&\left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k} \right) \right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b_{xx_{i,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{x}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b_{xx_{i-1,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{xx\,i-1,j,k-1}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] ,
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{xx_{i,j,k-1}} = & -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{xx_{i,j-1,k-1}} = & -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(z^{n\ \frac{1}{2}}_{i-1,j-1,k-1} - z^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n\ \frac{1}{2}}_{i,j-1,k} - y^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{xx_{i-1,j-1,k-1}} = {} & + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] ,
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yy_{i-1,j,k}} = {} & + \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] \\
& - \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] \\
& + \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{yy\,i,j,k}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right) \left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \right] \\
& - \frac{1}{3}\left(\dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right) \left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \right] \\
& + \frac{1}{3}\left(\dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right) \left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yy_{i,j-1,k}} = &+ \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
&\frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k}\right) \\
&\quad - \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\Big] \\
&- \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
&\frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k}\right) \\
&\quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\Big] \\
&+ \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
&\frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right) \\
&\quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\Big] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{yy\,i-1,j-1,k}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yy_{i-1,j,k-1}} = {} & -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b_{yy_{i,j,k-1}}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{y}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{y}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{y}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$b^{n+\frac{1}{2}}_{yy_{i,j-1,k-1}} = +\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times$$

$$\frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)$$

$$-\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Big]$$

$$-\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times$$

$$\frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)$$

$$-\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Big]$$

$$+\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times$$

$$\frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)$$

$$-\left(z^{n\ \frac{1}{2}}_{i-1,j-1,k-1} - z^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n\ \frac{1}{2}}_{i,j-1,k} - x^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\Big],$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b_{yy_{i-1,j-1,k-1}}^{n+\frac{1}{2}} = & - \frac{1}{3} \left(\dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \Bigg[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \\
& \quad - \left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \Bigg] \\
& + \frac{1}{3} \left(\dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \Bigg[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \\
& \quad - \left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \Bigg] \\
& - \frac{1}{3} \left(\dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \Bigg[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \\
& \quad - \left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \Bigg],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{zz_{i-1,j,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \quad \left.-\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j,k}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \quad \left.-\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j,k}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \quad \left.-\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

$$
\begin{aligned}
b_{zz_{i,j,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{zz_{i,j-1,k}} = {} & -\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right. \\
& \quad \left.-\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\right] \\
& +\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right. \\
& \quad \left.-\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\right] \\
& -\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right. \\
& \quad \left.-\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

$$
\begin{aligned}
b_{zz_{i-1,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{zz_{i-1,j,k-1}} = {} & + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;$$

$$
\begin{aligned}
b_{zz_{i,j,k-1}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

$$\begin{aligned}
b^{n+\frac{1}{2}}_{zz_{i,j-1,k-1}} \equiv {} & -\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right] \\
& +\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right] \\
& -\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(y^{n\ \frac{1}{2}}_{i-1,j-1,k-1} - y^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n\ \frac{1}{2}}_{i,j-1,k} - x^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\right],
\end{aligned}$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
b_{zz}{}^{n+\frac{1}{2}}_{i-1,j-1,k-1} = {} & + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \\
& \quad - \left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\Bigg] \\
& - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \\
& \quad - \left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\Bigg] \\
& + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1}\right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \\
& \quad - \left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\Bigg],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

The velocity gradients that contribute to rotation are also calculated from Eq.(3.17).

$$\left(\frac{\partial\dot{y}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left[b^{n+\frac{1}{2}}_{yx_{i-1,j,k}} + b^{n+\frac{1}{2}}_{yx_{i,j,k}} \right.$$

$$+ b^{n+\frac{1}{2}}_{yx_{i,j-1,k}} + b^{n+\frac{1}{2}}_{yx_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{yx_{i-1,j,k-1}}$$

$$\left. + b^{n+\frac{1}{2}}_{yx_{i,j,k-1}} + b^{n+\frac{1}{2}}_{yx_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{yx_{i-1,j-1,k-1}} \right]; \quad (6.36a)$$

$$\left(\frac{\partial\dot{x}}{\partial y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left[b^{n+\frac{1}{2}}_{xy_{i-1,j,k}} + b^{n+\frac{1}{2}}_{xy_{i,j,k}} \right.$$

$$+ b^{n+\frac{1}{2}}_{xy_{i,j-1,k}} + b^{n+\frac{1}{2}}_{xy_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{xy_{i-1,j,k-1}}$$

$$\left. + b^{n+\frac{1}{2}}_{xy_{i,j,k-1}} + b^{n+\frac{1}{2}}_{xy_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{xy_{i-1,j-1,k-1}} \right]; \quad (6.36b)$$

$$\left(\frac{\partial\dot{z}}{\partial y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left[b^{n+\frac{1}{2}}_{zy_{i-1,j,k}} + b^{n+\frac{1}{2}}_{zy_{i,j,k}} \right.$$

$$+ b^{n+\frac{1}{2}}_{zy_{i,j-1,k}} + b^{n+\frac{1}{2}}_{zy_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{zy_{i-1,j,k-1}}$$

$$\left. + b^{n+\frac{1}{2}}_{zy_{i,j,k-1}} + b^{n+\frac{1}{2}}_{zy_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{zy_{i-1,j-1,k-1}} \right]; \quad (6.37a)$$

$$\left(\frac{\partial\dot{y}}{\partial z}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\left[b^{n+\frac{1}{2}}_{yz_{i-1,j,k}} + b^{n+\frac{1}{2}}_{yz_{i,j,k}} + b^{n+\frac{1}{2}}_{yz_{i,j-1,k}} + b^{n+\frac{1}{2}}_{yz_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{yz_{i-1,j,k-1}} + b^{n+\frac{1}{2}}_{yz_{i,j,k-1}} + b^{n+\frac{1}{2}}_{yz_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{yz_{i-1,j-1,k-1}}\right]; \quad (6.37b)$$

$$\left(\frac{\partial\dot{x}}{\partial z}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\left[b^{n+\frac{1}{2}}_{xz_{i-1,j,k}} + b^{n+\frac{1}{2}}_{xz_{i,j,k}} + b^{n+\frac{1}{2}}_{xz_{i,j-1,k}} + b^{n+\frac{1}{2}}_{xz_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{xz_{i-1,j,k-1}} + b^{n+\frac{1}{2}}_{xz_{i,j,k-1}} + b^{n+\frac{1}{2}}_{xz_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{xz_{i-1,j-1,k-1}}\right]; \quad (6.38a)$$

$$\left(\frac{\partial\dot{z}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{1}{2\mathcal{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\left[b^{n+\frac{1}{2}}_{zx_{i-1,j,k}} + b^{n+\frac{1}{2}}_{zx_{i,j,k}} + b^{n+\frac{1}{2}}_{zx_{i,j-1,k}} + b^{n+\frac{1}{2}}_{zx_{i-1,j-1,k}} + b^{n+\frac{1}{2}}_{zx_{i-1,j,k-1}} + b^{n+\frac{1}{2}}_{zx_{i,j,k-1}} + b^{n+\frac{1}{2}}_{zx_{i,j-1,k-1}} + b^{n+\frac{1}{2}}_{zx_{i-1,j-1,k-1}}\right]; \quad (6.38b)$$

where $b^{n+\frac{1}{2}}_{yx}$, $b^{n+\frac{1}{2}}_{xy}$, $b^{n+\frac{1}{2}}_{zy}$, $b^{n+\frac{1}{2}}_{yz}$, $b^{n+\frac{1}{2}}_{xz}$, and $b^{n+\frac{1}{2}}_{zx}$ are defined on the next 48 pages. The factor of 2 in the denominators of Eqs.(6.36), (6.37), and (6.38) compensates for the fact that the surface integration terms, b, actually cover the surface area of the zone twice.

$$
\begin{aligned}
b_{yx_{i-1,j,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2},
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yx_{i,j,k}} = - \; & \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k} \right) \left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \Bigg] \\
+ \; & \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \Bigg] \\
- \; & \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1} \right) \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k} \right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k} \right) \Bigg] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yx_{i,j-1,k}} = & -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$\begin{aligned}
b_{yx_{i-1,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b_{yx\,i-1,j,k-1}^{n+\frac{1}{2}} = \; & + \frac{1}{3}\left(\dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yx_{i,j,k-1}} = & -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\Big[\Big(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\Big) \\
& \quad -\Big(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big] \\
& + \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\Big[\Big(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\Big) \\
& \quad -\Big(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big] \\
& - \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\Big[\Big(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\Big) \\
& \quad -\Big(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\Big)\Big] ,
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{yx_{i,j-1,k-1}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n\ \frac{1}{2}} - z_{i,j-1,k-1}^{n\ \frac{1}{2}}\right)\left(y_{i,j-1,k}^{n\ \frac{1}{2}} - y_{i,j-1,k-1}^{n\ \frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b_{yx\,i-1,j-1,k-1}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\Big[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\Big] \\
& - \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\Big[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\Big] \\
& + \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1}\right) \times \\
& \frac{1}{2}\Big[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\Big] ,
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{xy\,i-1,j,k}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] \\
& - \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] ,
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b_{xy\,i,j,k}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right)\right. \\
& \left. -\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\right] \\
& - \frac{1}{3}\left(\dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\right] \\
& + \frac{1}{3}\left(\dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}} \right)\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\right],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$\begin{aligned}
b_{xy_{i,j-1,k}}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{x}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{x}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{xy_{i-1,j-1,k}} = {} & + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right] \\
& - \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};
$$

$$\begin{aligned}
b_{xy_{i-1,j,k-1}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left.-\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left.-\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left.-\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right],
\end{aligned}$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b_{xy\,i,j,k-1}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{x}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j,k-1}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{xy_{i,j-1,k-1}} = {} & + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Bigg] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Bigg] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n\ \frac{1}{2}}_{i-1,j-1,k-1} - z^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n\ \frac{1}{2}}_{i,j-1,k} - x^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\Bigg],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
b_{xy_{i-1,j-1,k-1}}^{n+\frac{1}{2}} = {} & -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left.-\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left.-\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left.-\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{zy_{i-1,j,k}} = {} & + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] \\
& - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] \\
& + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k} \right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \right] ,
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b_{zy_{i,j,k}}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k} \right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \\
& \quad -\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k} \right)\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j,k} \right)\Bigg] \\
& - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i,j,k} \right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k} \right) \\
& \quad -\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k} \right)\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j,k} \right)\Bigg] \\
& + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1} \right) \times \\
& \frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i,j,k} \right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k} \right) \\
& \quad -\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k} \right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k} \right)\Bigg],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b_{zy\,i,j-1,k}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{z}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \quad \left. - \left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \quad \left. - \left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \quad \left. - \left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{zy\,i-1,j-1,k}^{n+\frac{1}{2}} = {} & + \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
& \frac{1}{2} \left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \right] \\
& - \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k} \right) \times \\
& \frac{1}{2} \left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \right] \\
& + \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} \right) \times \\
& \frac{1}{2} \left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \right] ,
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b_{zy_{i-1,j,k-1}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{zy_{i,j,k-1}} = {} & + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{zy_{i,j-1,k-1}}^{n+\frac{1}{2}} = {} & + \frac{1}{3} \left(\dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \left[\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \right] \\
& + \frac{1}{3} \left(\dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \right] \\
& + \frac{1}{3} \left(\dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k-1}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(z_{i-1,j-1,k-1}^{n\ \frac{1}{2}} - z_{i,j-1,k-1}^{n\ \frac{1}{2}} \right) \left(x_{i,j-1,k}^{n\ \frac{1}{2}} - x_{i,j-1,k-1}^{n\ \frac{1}{2}} \right) \right] ,
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{zy_{i-1,j-1,k-1}} = & - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yz_{i-1,j,k}} = & -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\right] \\
& + \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\right] \\
& - \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;$$

$$
\begin{aligned}
b_{yz\,i,j,k}^{n+\frac{1}{2}} = & - \frac{1}{3}\left(\dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right)\right. \\
& \left. -\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\right] \\
& + \frac{1}{3}\left(\dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right)\right. \\
& \left. -\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\right] \\
& - \frac{1}{3}\left(\dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right)\right. \\
& \left. -\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right)\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right)\right] ,
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;$$

$$
\begin{aligned}
b_{yz_{i,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{y}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j,k}^{n+\frac{1}{2}} - x_{i,j-1,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};
$$

$$
\begin{aligned}
b_{yz\,i-1,j-1,k}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left.-\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left.-\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left.-\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};
$$

$$\begin{aligned}
b_{yz_{i-1,j,k-1}}^{n+\frac{1}{2}} = {} & + \frac{1}{3} \left(\dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \right] \\
& - \frac{1}{3} \left(\dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \right] \\
& + \frac{1}{3} \left(\dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{y}_{i,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2} \left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j,k-1}^{n+\frac{1}{2}} \right) \right] ,
\end{aligned}$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{yz_{i,j,k-1}} = & -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

$$
\begin{aligned}
b_{yz\,i,j-1,k-1}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right] \\
& +\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right] \\
& -\frac{1}{3}\left(\dot{y}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{y}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. -\left(y^{n\ \frac{1}{2}}_{i-1,j-1,k-1} - y^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n\ \frac{1}{2}}_{i,j-1,k} - x^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
b_{yz_{i-1,j-1,k-1}}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{y}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{y}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{y}_{i-1,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{xz_{i-1,j,k}} = & -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j,k} \right) \\
& \quad - \left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \Big] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} \right) \times \\
& \frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j,k} \right) \\
& \quad - \left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \Big] \\
& - \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k} \right) \times \\
& \frac{1}{2}\Big[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k} \right) \\
& \quad - \left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k} \right) \left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k} \right) \Big],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;
$$

$$
\begin{aligned}
b_{xz_{i,j,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right) \left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \right] \\
& + \frac{1}{3}\left(\dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right) \left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \right] \\
& - \frac{1}{3}\left(\dot{x}_{i,j,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}} \right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right) \right. \\
& \left. - \left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}} \right) \left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j,k}^{n+\frac{1}{2}} \right) \right] ,
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;
$$

$$b_{xz_{i,j-1,k}}^{n+\frac{1}{2}} = -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\Bigg]$$

$$+\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\Bigg]$$

$$-\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k}\right) \times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\Bigg],$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

Rev. 0
15 NOV 77

$$\begin{aligned}
b_{xz_{i-1,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(x_{i-1,j,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

$$
\begin{aligned}
b_{xz_{i-1,j,k-1}}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& - \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{x}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right],
\end{aligned}
$$

$$
x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;
$$

$$
\begin{aligned}
b_{xz}{}^{n+\frac{1}{2}}_{i,j,k-1} = & -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{x}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

$$
\begin{aligned}
b_{xz_{i,j-1,k-1}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i,j-1,k}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k-1}^{n+\frac{1}{2}} - x_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(y_{i-1,j-1,k-1}^{n\ \frac{1}{2}} - y_{i,j-1,k-1}^{n\ \frac{1}{2}}\right)\left(x_{i,j-1,k}^{n\ \frac{1}{2}} - x_{i,j-1,k-1}^{n\ \frac{1}{2}}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2},$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2};$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
b_{xz_{i-1,j-1,k-1}}^{n+\frac{1}{2}} = {} & + \frac{1}{3}\left(\dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i,j-1,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{x}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{x}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{x}_{i-1,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(x_{i-1,j-1,k}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right. \\
& \left. - \left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\left(x_{i-1,j,k-1}^{n+\frac{1}{2}} - x_{i-1,j-1,k-1}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2} ,$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ;$$

$$b_{zx_{i-1,j,k}}^{n+\frac{1}{2}} = -\frac{1}{3}\left(\dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times$$

$$\frac{1}{2}\left[\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\right.$$

$$\left. -\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right]$$

$$+\frac{1}{3}\left(\dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}}\right) \times$$

$$\frac{1}{2}\left[\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\right.$$

$$\left. -\left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right]$$

$$-\frac{1}{3}\left(\dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}}\right) \times$$

$$\frac{1}{2}\left[\left(y_{i-1,j,k-1}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\right.$$

$$\left. -\left(z_{i-1,j,k-1}^{n+\frac{1}{2}} - z_{i-1,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i-1,j,k}^{n+\frac{1}{2}}\right)\right],$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$
\begin{aligned}
b_{zx_{i,j,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k-1}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i,j,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k-1}^{n+\frac{1}{2}} - y_{i,j,k}^{n+\frac{1}{2}}\right)\right],
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2},$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2};$$

$$\begin{aligned}
b_{zx_{i,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& + \frac{1}{3}\left(\dot{z}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k-1}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k-1}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k-1}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& - \frac{1}{3}\left(\dot{z}_{i,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k}^{n+\frac{1}{2}} - z_{i,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j,k}^{n+\frac{1}{2}} - y_{i,j-1,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b_{zx_{i-1,j-1,k}}^{n+\frac{1}{2}} = & -\frac{1}{3}\left(\dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& +\frac{1}{3}\left(\dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i,j-1,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i,j-1,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i,j-1,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] \\
& -\frac{1}{3}\left(\dot{z}_{i-1,j-1,k}^{n+\frac{1}{2}} + \dot{z}_{i-1,j-1,k-1}^{n+\frac{1}{2}} + \dot{z}_{i-1,j,k}^{n+\frac{1}{2}}\right) \times \\
& \frac{1}{2}\left[\left(y_{i-1,j-1,k-1}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(z_{i-1,j,k}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right. \\
& \left. -\left(z_{i-1,j-1,k-1}^{n+\frac{1}{2}} - z_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\left(y_{i-1,j,k}^{n+\frac{1}{2}} - y_{i-1,j-1,k}^{n+\frac{1}{2}}\right)\right] ,
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$\begin{aligned}
b^{n+\frac{1}{2}}_{zx_{i-1,j,k-1}} = & + \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \times \\
& \frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \right] \\
& - \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \times \\
& \frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \right] \\
& + \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1} \right) \times \\
& \frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \right] ,
\end{aligned}$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{zx_{i,j,k-1}} = & -\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& +\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& -\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. -\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

$$
\begin{aligned}
b^{n+\frac{1}{2}}_{zx_{i,j-1,k-1}} = & -\frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\Big[\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Big] \\
& + \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j,k-1}\right) \times \\
& \frac{1}{2}\Big[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Big] \\
& - \frac{1}{3}\left(\dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k}\right) \times \\
& \frac{1}{2}\Big[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n\ \frac{1}{2}}_{i-1,j-1,k-1} - z^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n\ \frac{1}{2}}_{i,j-1,k} - y^{n\ \frac{1}{2}}_{i,j-1,k-1}\right)\Big] ,
\end{aligned}
$$

$$
y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,
$$

$$
z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;
$$

Rev. 0
15 NOV 77

$$
\begin{aligned}
b_{zx}{}^{n+\frac{1}{2}}_{i-1,j-1,k-1} = {} & + \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} \right) \times \\
& \frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \right] \\
& - \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i,j-1,k-1} \right) \times \\
& \frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \right] \\
& + \frac{1}{3} \left(\dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k-1} + \dot{z}^{n+\frac{1}{2}}_{i-1,j-1,k} + \dot{z}^{n+\frac{1}{2}}_{i-1,j,k-1} \right) \times \\
& \frac{1}{2} \left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1} \right) \right] ,
\end{aligned}
$$

$$y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2} ,$$

$$z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2} ;$$

Strain rates can also be defined using tetrahedron volumes. For example, eight tetrahedrons surround an interior grid point. The tetrahedron strain-rate formulas are derived using the methodology shown in Eqs.(3.47) for the front-top-left tetrahedron. In addition to the x-component terms shown in Eqs.(3.48) for Eq.(3.47a), there are similar y-component and z-component relationships for Eqs.(3.47b) and (3.47c), respectively. Analogous sets of formulas can be written for the other seven tetrahedrons surrounding an interior grid point.

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6.3 STRESS MESH

6.3.1 Artificial Viscosity. Although the finite-difference momentum equations, Eqs.(6.5), are general, they cannot economically handle high frequency mechanical phenomena (such as shocks) because the spatial resolution of a mesh would have to be several times smaller than the thickness of the shock for Eqs.(6.5) to be applicable. To calculate the transmission of a shock for a distance of a few centimeters would require tens of millions of zones or a shock-following microzoner and a very small time step if the shock thickness were on the order of angstroms. Clearly, this approach is not economically feasible.

An economical approach with considerable merit was devised by John von Neumann (Reference 6.1). He proposed that the presence of a shock within a zone (where the zone is millions of times larger than the thickness of the shock front) could be detected by the rate of change of volumetric strain and that the stress rise could be simulated by artificially spreading it over several zones. The crux of the idea is to add an artificial viscous stress, q_Q, dependent on the square of the volumetric strain rate, to the mean stress (pressure). The artificial viscous stress (sometimes called the quadratic artificial viscosity) is given by

$$q_Q = C_Q^2 \rho \, (\Delta \ell)^2 \left(\frac{\partial \dot{\ell}}{\partial \ell}\right)^2 , \tag{6.39}$$

where C_Q is a dimensionless constant dependent on differential stress across the shock front and the number of zones over which the stress is to be artificially spread. A value of 2.0 for C_Q spreads a shock front over three zones and is good for differential stresses up to 1 Mbar.*

Another consequence of applying the momentum equation to a discretized mesh is computational noise, i.e., stable zone-to-zone oscillations of low amplitude. In general, noise does not invalidate a solution and

---

*The value of C_Q for collapsing porous materials (as well as foams and frangible material) should be 4.0 or 6.0, depending on the degree of porosity and the level of loading. Even then, the formulation for quadratic artificial viscosity may not accurately describe the Rayleigh line process for porous matrix collapse.

does not have to be eliminated if its effects can be clearly determined. However, it is possible to reduce, and in some cases completely eliminate, noise by applying a viscous damping stress, q_L,

$$q_L = - C_L \, \rho \, \Delta\ell \sqrt{\frac{pV}{\rho_o}} \; \frac{\partial\dot{\ell}}{\partial\ell} \; , \tag{6.40}$$

where C_L is a dimensionless constant dependent on the amount of damping required to eliminate the noise oscillations. A typical value of C_L is 0.8. Equation (6.40) is a simple dashpot (viscous stress is proportional to velocity) and q_L is called a linear artificial viscosity.

Equations (6.39) and (6.40) may be written in finite-difference form as follows,

$$q_{Q\,i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}^{\,n+\frac{1}{2}} =$$

$$- \left(C^{o}_{Q\,i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right)^{2} \rho^{\,n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \left(\Delta\ell^{\,n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right)^{2} \left(\frac{\partial\dot{\ell}}{\partial\ell} \right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \left| \left(\frac{\partial\dot{\ell}}{\partial\ell} \right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right| , \tag{6.41a}$$

and

$$q_{L\,i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}^{\,n+\frac{1}{2}} =$$

$$-C^{o}_{L\,i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \; \rho^{\,n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \; \Delta\ell^{\,n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \left(\frac{\left| p^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right| \; V^{\,n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \right)^{\frac{1}{2}} \times$$

$$\left(\frac{\partial\dot{\ell}}{\partial\ell} \right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} . \tag{6.41b}$$

The sum of Eqs.(6.39) and (6.40) is called the total scalar artificial viscosity, q, and its value is added to the hydrostatic (thermodynamic) pressure in both the energy and momentum equations. The total scalar artificial viscosity is defined to be positive for compression (i.e., negative values of $\partial\dot{\ell}/\partial\ell$).

Finally, one other numerical problem that arises in discrete calculations can also be handled through the use of artificial viscosity. This is the problem of constant-volume mesh motions that result from numerically generated excitations. In a three-dimensional cubical mesh, the eight grid points that describe the stress mesh can oscillate in an "hourglassing" mode in which the volume of the zone remains unchanged and in which zone distortion can grow anomolously after many calculational cycles. This particular type of mesh motion is unopposed by the continuum physics in the zones. Since it is a numerical problem, some sort of artifice is needed to counteract the oscillation.

A simple tensor artificial viscosity proposed by Wilkins (Reference 6.2) is one approach that can be used effectively to damp the hourglass degree of freedom. Other approaches include a velocity subtraction method developed by Hancock (Reference 6.3).

The artificial viscosity concept is based on the fact that the hourglass mode exists only for cubical zones and does not exist for tetrahedron zones. Therefore, a grid-point dashpot is derived, based on the strain rates (velocity field) for the point being calculated and each of its three closest neighbor groups (i.e., eight tetrahedrons). The finite-difference formulas for the strain rates in each of the eight tetrahedrons surrounding an interior grid point are derived similarly to the front-top-left tetrahedron strain-rate formulas shown in Eqs.(3.47), (3.48), and (3.49).

The tensor viscosity (mesh dashpot) for each tetrahedron is then formulated as follows:

$$
\begin{aligned}
q_{xx} &= C_T\, \rho \left(\mathcal{V}_T\right)^{1/3} \left(\dot{\epsilon}_{xx} - \frac{\dot{\Delta}}{3}\right) , \\
q_{yy} &= C_T\, \rho \left(\mathcal{V}_T\right)^{1/3} \left(\dot{\epsilon}_{yy} - \frac{\dot{\Delta}}{3}\right) , \\
q_{zz} &= C_T\, \rho \left(\mathcal{V}_T\right)^{1/3} \left(\dot{\epsilon}_{zz} - \frac{\dot{\Delta}}{3}\right) , \\
q_{xy} &= C_T\, \rho \left(\mathcal{V}_T\right)^{1/3} \dot{\epsilon}_{xy} , \\
q_{yz} &= C_T\, \rho \left(\mathcal{V}_T\right)^{1/3} \dot{\epsilon}_{yz} , \\
q_{xz} &= C_T\, \rho \left(\mathcal{V}_T\right)^{1/3} \dot{\epsilon}_{xz} ,
\end{aligned}
\qquad (6.42)
$$

where

$\mathcal{V}_T$ = tetrahedron volume,

$\dot{\Delta} = \dot{\epsilon}_{xx} + \dot{\epsilon}_{yy} + \dot{\epsilon}_{zz}$,

$$\dot{\epsilon}_{xx} = \frac{\partial \dot{x}}{\partial x} , \qquad \dot{\epsilon}_{yy} = \frac{\partial \dot{y}}{\partial y} , \qquad \dot{\epsilon}_{zz} = \frac{\partial \dot{z}}{\partial z}$$

$$\dot{\epsilon}_{xy} = \frac{1}{2}\left(\frac{\partial \dot{y}}{\partial x} + \frac{\partial \dot{x}}{\partial y}\right) , \qquad \dot{\epsilon}_{yz} = \frac{1}{2}\left(\frac{\partial \dot{z}}{\partial y} + \frac{\partial \dot{y}}{\partial z}\right) , \qquad \dot{\epsilon}_{xz} = \frac{1}{2}\left(\frac{\partial \dot{z}}{\partial x} + \frac{\partial \dot{x}}{\partial z}\right) ,$$

and C_T is a dimensionless constant dependent on the amount of damping required to eliminate the mesh oscillations. A typical value of C_T is 1.0. The difference equations for Eqs.(6.42) depend on the chosen tetrahedron; for example, the front-top-left tetrahedron is derived from Eqs.(3.47), (3.48), and (3.49).

6.3.2 Internal Energy Equation. The conservation of internal energy equation may be written in the following form,

$$\dot{u} = -(p+q)\dot{V} + \dot{Z} + \dot{h} + \dot{U}''' \ . \qquad (6.43)$$

u, p, q, and V have been previously defined. $\dot{Z}$ is the distortional energy rate,

$$\dot{Z} = V\left(s_{xx}\,\dot{\epsilon}_{xx} + s_{yy}\,\dot{\epsilon}_{yy} + s_{zz}\,\dot{\epsilon}_{zz} + s_{xy}\,\dot{\epsilon}_{xy} + s_{yz}\,\dot{\epsilon}_{yz} + s_{zx}\,\dot{\epsilon}_{zx}\right) . \qquad (6.44)$$

s_{xx}, s_{yy}, s_{zz}, s_{xy}, s_{yz}, and s_{zx} are stress deviator components and $\dot{\epsilon}_{xx}$, $\dot{\epsilon}_{yy}$, $\dot{\epsilon}_{zz}$, $\dot{\epsilon}_{xy}$, $\dot{\epsilon}_{yz}$, and $\dot{\epsilon}_{zx}$ are strain rate components. The strain rate components have already been defined as follows,

$$\dot{\epsilon}_{xx} \equiv \frac{\partial \dot{x}}{\partial x} \qquad \text{[see Eq.(6.33)]} \ ;$$

$$\dot{\epsilon}_{yy} \equiv \frac{\partial \dot{y}}{\partial y} \qquad \text{[see Eq.(6.34)]} \ ;$$

$$\dot{\epsilon}_{zz} \equiv \frac{\partial \dot{z}}{\partial z} \qquad \text{[see Eq.(6.35)]} \ ;$$

$$\dot{\epsilon}_{xy} \equiv \frac{\partial \dot{y}}{\partial x} + \frac{\partial \dot{x}}{\partial y} \qquad \text{[see Eq.(6.36)]} \ ;$$

$$\dot{\epsilon}_{yz} \equiv \frac{\partial \dot{z}}{\partial y} \quad \frac{\partial \dot{y}}{\partial z} \qquad \text{[see Eq.(6.37)]} \ ;$$

$$\dot{\epsilon}_{zx} \equiv \frac{\partial \dot{x}}{\partial z} + \frac{\partial \dot{z}}{\partial x} \qquad \text{[see Eq.(6.38)]} \ .$$

$\dot{h}$ is the heat flow and $\dot{U}'''$ is the source or sink energy rate.

Substituting Eq.(6.44) into Eq.(6.43) yields an equation with nine unknowns, since V can be determined from Eq.(6.29). To solve for the internal energy rate, u, requires equations for p, s_{xx}, s_{yy}, s_{zz}, s_{xy}, s_{yz}, s_{zx}, and $\dot{h}$.

6.3.3 Constitutive Equations. The equations that relate p, s_{xx}, s_{yy}, s_{zz}, s_{xy}, s_{yz}, s_{zx}, and $\dot{h}$ to u and V are known as constitutive equations and may be categorized as follows,

Equation of State

$$p = p(u,V); \tag{6.45a}$$

Strength Description

$$\begin{aligned} s_{xx} &= s(u,V), & s_{yy} &= s(u,V), & s_{zz} &= s(u,V), \\ s_{xy} &= s(u,V), & s_{yz} &= s(u,V), & s_{zx} &= s(u,V); \end{aligned} \tag{6.45b}$$

Heat Flow Model

$$\dot{h} = h(u,V). \tag{6.45c}$$

Given the functions p(u,V), s(u,V), and h(u,V), and knowing that Eq.(6.29) has been solved to give V, then Eqs.(6.43), (6.45a), (6.45b), and (6.45c) can be solved simultaneously (using the same explicit time step used to solve the momentum equation) by iteration, or in some cases, by substitution. A two-step iteration procedure is described in Section 6.3.4.

Typically, the equation of state, p(u,V), requires material constants (e.g., bulk modulus) that describe compressibility for the mechanical contribution to pressure and a specific heat ratio or a Grüneisen coefficient for the thermal contribution to pressure. The strength description requires a shear modulus, yield stress, flow rule, and yield criterion. The heat flux model needs thermal conductivity. In all cases, these or equivalent material constants may be functions of other thermodynamic variables.

The equation of state is usually simple or complex, depending on the number of phases and components that must be described. A single-phase, one-component material is, by far, the simplest equation of state. A linear elastic solid or an "ideal" gas are examples of simple equations of state.

Strength descriptions are more or less complex, depending on strain-rate dependence during loading, relaxation to or from a failed state, reload characteristics after failure, ductility, brittleness, the existence of microfractures, etc. The simplest strength description is small strain elastic, where no failure is allowed to occur. Elastic-plastic models having a yield criterion based on the second stress invariant are also fairly simple. Plasticity can be handled using an appropriate flow rule. Strain hardening, fracture, dilatational effects, etc., increase the complexity of a strength model.

The heat flux model can be viewed in two separate categories -- conduction modeling and radiation modeling. An adequate model describing conduction is Fourier's Law,

$$\dot{h}'' = -k \nabla T \, . \tag{6.46}$$

Radiation, on the other hand, is more complex and no simple equation such as Eq.(6.46) can be used in a physically correct and economical manner.

Once Eq.(6.43) has been solved in conjunction with appropriate constitutive equations, Eqs.(6.45a), (6.45b), and (6.45c), all remaining thermodynamic state variables can be computed. In particular, stress can be calculated from

$$
\begin{aligned}
\sigma_{xx} &= s_{xx} + q_{xx} - (p+q) , \\
\sigma_{yy} &= s_{yy} + q_{yy} - (p+q) , \\
\sigma_{zz} &= s_{zz} + q_{zz} - (p+q) , \\
\sigma_{xy} &= s_{xy} + q_{xy} , \\
\sigma_{yz} &= s_{yz} + q_{yz} , \\
\sigma_{zx} &= s_{zx} + q_{zx} ,
\end{aligned}
\tag{6.47}
$$

where $q = q_Q + q_L$ and q_{xx}, q_{yy}, q_{zz}, q_{xy}, q_{yz}, q_{zx} are tensor viscosities to inhibit mesh hourglassing instability. Once stress is computed, the computational cycle (Figure 6.1) is complete. All that remains is to determine a stable time step for the next cycle.

6.3.4 Simultaneous Solution of Constitutive Equations and Conservation of Energy by a Two-Step Iteration. The procedure used to calculate new values of internal energy density, pressure, deviatoric stress components, and heat flow was discussed in Section 6.3.3. For the standard models in STEALTH, a two-step iteration is used to solve simultaneously the coupled constitutive equations and the internal energy conservation equation for u, ρ, s, and h.

The logic, which is located in subroutine ZONMDL, is as follows.

1. Calculate the approximate change in distortional energy density, $\Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$,

$$\begin{aligned}\Delta\tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\,\Delta t^{n+\frac{1}{2}}\Big(& s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\\
&+ s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\\
&+ s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\\
&+ s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\\
&+ s^{n}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\\
&+ s^{n}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\,\dot{\epsilon}^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\Big).\end{aligned}$$

2. Calculate the heat transfer energy density, $\Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, into zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+\frac{1}{2}$,

$$\Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{\rho^{o}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{m_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left(\dot{h}^{n+\frac{1}{2}}_{i-1} + \dot{h}^{n+\frac{1}{2}}_{i} + \dot{h}^{n+\frac{1}{2}}_{j-1} + \dot{h}^{n+\frac{1}{2}}_{j} + \dot{h}^{n+\frac{1}{2}}_{k-1} + \dot{h}^{n+\frac{1}{2}}_{k} \right) \Delta t^{n+\frac{1}{2}} ,$$

where ρ^{o} is the reference density and m is the mass; $\Delta t^{n+\frac{1}{2}}$ is the time step for the entire mesh; $\dot{h}_{i-1}$ is the heat flow into zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ through the left face, $\dot{h}_{i}$ is the heat flow through the right face, $\dot{h}_{j-1}$ is the heat flow through the bottom face, $\dot{h}_{j}$ is the heat flow through the top face, $\dot{h}_{k-1}$ is the heat flow through the aft face, and $\dot{h}_{k}$ is the heat flow through the front face. The heat flow is calculated from Fourier's heat conduction law,

$$\dot{h} = -k(T)\, \underline{\nabla T} \cdot \underline{S} ,$$

where k is the conductivity, $\underline{S}$ is the area through which heat flows, and the gradient, ∇, affects the conduction formula in the following way for interior points,

$$
\begin{aligned}
\dot{h}^{n+\frac{1}{2}}_{i-1} = \frac{k^{n}_{i-1}}{2} \Bigg\{ & \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k}\right)\right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \quad \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right]
\end{aligned}
$$

(This equation is continued on the following page.)

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1}-z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1}-x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k}-z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j,k-1}-z^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i-1,j,k-1}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k}-z^{n+\frac{1}{2}}_{i-1,j,k}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j,k}-z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1}-z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j-1,k}-z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1}-x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1}-z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right]$$

(This equation is continued on the following page.)

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^n_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j,k-1} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j,k}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right.$$

$$\left. - \left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^n_{i-1,j,k-1} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j,k} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j-1,k}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\right.$$

$$\left. - \left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^n_{i-1,j,k} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j-1,k} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j-1,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right.$$

$$\left. - \left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^n_{i-1,j-1,k} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial z}\right)^n_{i-1,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right.$$

$$\left.\left. - \left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right]\right\}$$

$$
\begin{aligned}
\dot{h}_i^{n+\frac{1}{2}} = \frac{k_i^n}{2} \Bigg\{ & \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k-1}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k-1}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\Bigg]
\end{aligned}
$$

(This equation is continued on the following page.)

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k}\right) - \left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right) - \left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right) - \left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j-1,k}\right) - \left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\right]$$

(This equation is continued on the following page.)

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i,j,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1}-y^{n+\frac{1}{2}}_{i,j,k}\right)\right.$$

$$\left.-\left(y^{n+\frac{1}{2}}_{i,j-1,k}-y^{n+\frac{1}{2}}_{i,j,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1}-x^{n+\frac{1}{2}}_{i,j,k}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1}-y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right.$$

$$\left.-\left(y^{n+\frac{1}{2}}_{i,j,k}-y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1}-x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k-1}-x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k}-y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right.$$

$$\left.-\left(y^{n+\frac{1}{2}}_{i,j,k-1}-y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k-1}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k}-y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right.$$

$$\left.\left.-\left(y^{n+\frac{1}{2}}_{i,j-1,k-1}-y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\right]\right]\right\}$$

$$
\begin{aligned}
\dot{h}^{n+\frac{1}{2}}_{j-1} = \frac{k^{n}_{j-1}}{2} \Bigg\{ & \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k-1}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\Bigg]
\end{aligned}
$$

(This equation is continued on the following page.)

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1}-z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k}-z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j-1,k}-z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1}-z^{n+\frac{1}{2}}_{i,j-1,k}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j-1,k}-z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1}-x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1}-z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}\right]\times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j-1,k-1}-z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right.$$

$$\left.-\left(x^{n+\frac{1}{2}}_{i,j-1,k-1}-x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k}-z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right]$$

(This equation is continued on the following page.)

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k}-y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right.$$

$$\left.-\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1}-y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1}-y^{n+\frac{1}{2}}_{i,j-1,k}\right)\right.$$

$$\left.-\left(y^{n+\frac{1}{2}}_{i-1,j-1,k}-y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k-1}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1}-y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right.$$

$$\left.-\left(y^{n+\frac{1}{2}}_{i,j-1,k}-y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1}-x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k}\right]\times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k-1}-x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k}-y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right.$$

$$\left.-\left(y^{n+\frac{1}{2}}_{i,j-1,k-1}-y^{n+\frac{1}{2}}_{i-1,j-\ ,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right]\Bigg\}$$

$$
\begin{aligned}
\dot{h}_j^{n+\frac{1}{2}} = \frac{k_j^n}{2} \Bigg\{ & \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i,j,k}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right]
\end{aligned}
$$

(This equation is continued on the following page.)

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i,j,k}\right)\right.$$

$$\left. - \left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\right.$$

$$\left. - \left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right.$$

$$\left. - \left(x^{n+\frac{1}{2}}_{i-1,j,k} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right.$$

$$\left. - \left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right]$$

(This equation is continued on the following page.)

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i,j,k-1}-x^{n+\frac{1}{2}}_{i,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k}-y^{n+\frac{1}{2}}_{i,j,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i,j,k-1}-y^{n+\frac{1}{2}}_{i,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i,j,k}\right)\Bigg]$$

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k-1}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1}-y^{n+\frac{1}{2}}_{i-1,j,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i,j,k}-y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\Bigg]$$

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1}-y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i-1,j,k}-y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1}-x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\Bigg]$$

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1}-x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k}-y^{n+\frac{1}{2}}_{i,j,k-1}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i-1,j,k-1}-y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i,j,k-1}\right)\Bigg]\Bigg\}$$

$$
\begin{aligned}
\dot{h}^{n+\frac{1}{2}}_{k-1} = \frac{k^{n}_{k-1}}{2} \Bigg\{ & \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial x}\right)^{n}_{i,j,k-1}\right] \times \\
& \frac{1}{2}\left[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right. \\
& \left. - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right]
\end{aligned}
$$

(This equation is continued on the following page.)

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right) - \left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i,j,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right) - \left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right) - \left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k-1} - z^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right]$$

$$+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j-1,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right) - \left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(z^{n+\frac{1}{2}}_{i,j,k-1} - z^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right]$$

(This equation is continued on the following page.)

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\right.$$

$$\left. - \left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i,j,k-1}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right.$$

$$\left. - \left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j,k-1}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right.$$

$$\left. - \left(y^{n+\frac{1}{2}}_{i-1,j,k-1} - y^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k-1} - x^{n+\frac{1}{2}}_{i-1,j-1,k-1}\right)\right]$$

$$+ \frac{1}{3}\left[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k-1} + \left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k-1}\right] \times$$

$$\frac{1}{2}\left[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(y^{n+\frac{1}{2}}_{i,j,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right.$$

$$\left. - \left(y^{n+\frac{1}{2}}_{i-1,j-1,k-1} - y^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\left(x^{n+\frac{1}{2}}_{i,j,k-1} - x^{n+\frac{1}{2}}_{i,j-1,k-1}\right)\right]\Bigg]\Bigg\}$$

$$
\begin{aligned}
\dot{h}_k^{n+\frac{1}{2}} = \frac{k_k^n}{2} \Bigg\{ & \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i-1,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i-1,j,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i-1,j,k}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i,j,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i,j,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i,j,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i,j,k}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j-1,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j,k} - z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k} - y^{n+\frac{1}{2}}_{i,j-1,k}\right)\Bigg] \\
& + \frac{1}{3}\left[\left(\frac{\partial T}{\partial x}\right)^n_{i,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j-1,k} + \left(\frac{\partial T}{\partial x}\right)^n_{i-1,j,k}\right] \times \\
& \frac{1}{2}\Bigg[\left(y^{n+\frac{1}{2}}_{i,j-1,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right) \\
& \quad - \left(z^{n+\frac{1}{2}}_{i,j-1,k} - z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k} - y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\Bigg]
\end{aligned}
$$

(This equation is continued on the following page.)

$$\begin{aligned}
&+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k}\right]\times\\
&\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j-1,k}-z^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\right.\\
&\quad\left.-\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(z^{n+\frac{1}{2}}_{i,j,k}-z^{n+\frac{1}{2}}_{i-1,j,k}\right)\right]
\end{aligned}$$

$$\begin{aligned}
&+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k}\right]\times\\
&\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i-1,j,k}-z^{n+\frac{1}{2}}_{i,j,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i,j,k}\right)\right.\\
&\quad\left.-\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i,j,k}\right)\left(z^{n+\frac{1}{2}}_{i,j-1,k}-z^{n+\frac{1}{2}}_{i,j,k}\right)\right]
\end{aligned}$$

$$\begin{aligned}
&+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}\right]\times\\
&\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j,k}-z^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\right.\\
&\quad\left.-\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j-1,k}-z^{n+\frac{1}{2}}_{i,j-1,k}\right)\right]
\end{aligned}$$

$$\begin{aligned}
&+\frac{1}{3}\left[\left(\frac{\partial T}{\partial y}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial y}\right)^{n}_{i-1,j,k}\right]\times\\
&\frac{1}{2}\left[\left(z^{n+\frac{1}{2}}_{i,j-1,k}-z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right.\\
&\quad\left.-\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(z^{n+\frac{1}{2}}_{i-1,j,k}-z^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\right]
\end{aligned}$$

(This equation is continued on the following page.)

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(y^{n+\frac{1}{2}}_{i,j,k}-y^{n+\frac{1}{2}}_{i-1,j,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i-1,j-1,k}-y^{n+\frac{1}{2}}_{i-1,j,k}\right)\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i-1,j,k}\right)\Bigg]$$

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i,j,k}\right)\left(y^{n+\frac{1}{2}}_{i,j-1,k}-y^{n+\frac{1}{2}}_{i,j,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i-1,j,k}-y^{n+\frac{1}{2}}_{i,j,k}\right)\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i,j,k}\right)\Bigg]$$

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i,j,k}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j-1,k}-y^{n+\frac{1}{2}}_{i,j-1,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i,j,k}-y^{n+\frac{1}{2}}_{i,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j-1,k}-x^{n+\frac{1}{2}}_{i,j-1,k}\right)\Bigg]$$

$$+\frac{1}{3}\Bigg[\left(\frac{\partial T}{\partial z}\right)^{n}_{i,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j-1,k}+\left(\frac{\partial T}{\partial z}\right)^{n}_{i-1,j,k}\Bigg]\times$$

$$\frac{1}{2}\Bigg[\left(x^{n+\frac{1}{2}}_{i,j-1,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(y^{n+\frac{1}{2}}_{i-1,j,k}-y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)$$

$$-\left(y^{n+\frac{1}{2}}_{i,j-1,k}-y^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\left(x^{n+\frac{1}{2}}_{i-1,j,k}-x^{n+\frac{1}{2}}_{i-1,j-1,k}\right)\Bigg]\Bigg]\Bigg\}$$

where for all index points,

$$x^{n+\frac{1}{2}} \equiv \frac{x^{n+1} + x^{n}}{2}\,, \qquad y^{n+\frac{1}{2}} \equiv \frac{y^{n+1} + y^{n}}{2}\,, \qquad z^{n+\frac{1}{2}} \equiv \frac{z^{n+1} + z^{n}}{2}\,,$$

the conductivities are

$$k^{n}_{i-1} = \frac{\mathcal{V}^{n}_{i-3/2,\,j-\frac{1}{2},k-\frac{1}{2}} + \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{\left(\frac{\mathcal{V}}{k}\right)^{n}_{i-3/2,\,j-\frac{1}{2},k-\frac{1}{2}} + \left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ ;$$

$$k^{n}_{i} = \frac{\mathcal{V}^{n}_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{\left(\frac{\mathcal{V}}{k}\right)^{n}_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + \left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ ;$$

$$k^{n}_{j-1} = \frac{\mathcal{V}^{n}_{i-\frac{1}{2},j-3/2,\,k-\frac{1}{2}} + \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{\left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-3/2,\,k-\frac{1}{2}} + \left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ ;$$

$$k^{n}_{j} = \frac{\mathcal{V}^{n}_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} + \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{\left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} + \left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ ;$$

$$k^{n}_{k-1} = \frac{\mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-3/2} + \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{\left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-3/2} + \left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ ;$$

$$k^{n}_{k} = \frac{\mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + \mathcal{V}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{\left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} + \left(\frac{\mathcal{V}}{k}\right)^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ ;$$

and a typical temperature gradient, e.g., at grid point (i,j,k) is given by its components as follows,

$$
\begin{aligned}
\left(\frac{\partial T}{\partial x}\right)^n_{i,j,k} = \frac{1}{2} \Bigg\{ \quad & T^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \Big[\left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right)\left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right) \\
& \qquad - \left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right)\left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \Big[\left(y^n_{i,j-1,k} - y^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \Big[\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right) \\
& \qquad - \left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i+1,j,k}\right)\Big] \\
+ \quad & T^n_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \Big[\left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right) \\
& \qquad - \left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right)\Big] \\
+ \quad & T^n_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} \Big[\left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right)\left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right)\left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} \Big[\left(y^n_{i,j-1,k} - y^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right) \\
& \qquad - \left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \Big[\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right) \\
& \qquad - \left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(y^n_{i,j+1,k} - y^n_{i,j,k+1}\right)\Big] \\
+ \quad & T^n_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \Big[\left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right) \\
& \qquad - \left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right)\Big] \Bigg\} / \mathcal{V}^n_{i,j,}
\end{aligned}
$$

$$
\begin{aligned}
\left(\frac{\partial T}{\partial y}\right)^n_{i,j,k} = \frac{1}{2}\Bigg\{ \; & T^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \Big[\left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right)\left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right) \\
& \qquad - \left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right)\left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right)\Big] \\
+ \; & T^n_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \Big[\left(z^n_{i,j-1,k} - z^n_{i+1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i+1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\Big] \\
+ \; & T^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \Big[\left(z^n_{i,j,k-1} - z^n_{i+1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i+1,j,k}\right) \\
& \qquad - \left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i+1,j,k}\right)\Big] \\
+ \; & T^n_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \Big[\left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right) \\
& \qquad - \left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right)\left(z^n_{i,j,k-1} - z^n_{i-1,j,k}\right)\Big] \\
+ \; & T^n_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} \Big[\left(z^n_{i,j-1,k} - z^n_{i-1,j,k}\right)\left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right)\left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right)\Big] \\
+ \; & T^n_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} \Big[\left(z^n_{i,j-1,k} - z^n_{i,j,k+1}\right)\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right) \\
& \qquad - \left(x^n_{i,j-1,k} - x^n_{i,j,k+1}\right)\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\Big] \\
+ \; & T^n_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \Big[\left(z^n_{i+1,j,k} - z^n_{i,j,k+1}\right)\left(x^n_{i,j+1,k} - x^n_{i,j,k+1}\right) \\
& \qquad - \left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\left(z^n_{i,j+1,k} - z^n_{i,j,k+1}\right)\Big] \\
+ \; & T^n_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \Big[\left(z^n_{i,j,k+1} - z^n_{i-1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right) \\
& \qquad - \left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right)\left(z^n_{i,j+1,k} - z^n_{i-1,j,k}\right)\Big]\Bigg\} \Big/ \mathcal{V}^n_{i,j,k}
\end{aligned}
$$

$$
\begin{aligned}
\left(\frac{\partial T}{\partial z}\right)^n_{i,j,k} = \frac{1}{2}\Bigg\{ \quad & T^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \Big[\left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right)\left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right)\left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \Big[\left(x^n_{i,j-1,k} - x^n_{i+1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i+1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \Big[\left(x^n_{i,j,k-1} - x^n_{i+1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i+1,j,k}\right) \\
& \qquad - \left(y^n_{i,j,k-1} - y^n_{i+1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i+1,j,k}\right)\Big] \\
+ \quad & T^n_{i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}} \Big[\left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right)\left(y^n_{i,j,k-1} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right)\left(x^n_{i,j,k-1} - x^n_{i-1,j,k}\right)\Big] \\
+ \quad & T^n_{i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} \Big[\left(x^n_{i,j-1,k} - x^n_{i-1,j,k}\right)\left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i-1,j,k}\right)\left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}} \Big[\left(x^n_{i,j-1,k} - x^n_{i,j,k+1}\right)\left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right) \\
& \qquad - \left(y^n_{i,j-1,k} - y^n_{i,j,k+1}\right)\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\Big] \\
+ \quad & T^n_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \Big[\left(x^n_{i+1,j,k} - x^n_{i,j,k+1}\right)\left(y^n_{i,j+1,k} - y^n_{i,j,k+1}\right) \\
& \qquad - \left(y^n_{i+1,j,k} - y^n_{i,j,k+1}\right)\left(x^n_{i,j+1,k} - x^n_{i,j,k+1}\right)\Big] \\
+ \quad & T^n_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \Big[\left(x^n_{i,j,k+1} - x^n_{i-1,j,k}\right)\left(y^n_{i,j+1,k} - y^n_{i-1,j,k}\right) \\
& \qquad - \left(y^n_{i,j,k+1} - y^n_{i-1,j,k}\right)\left(x^n_{i,j+1,k} - x^n_{i-1,j,k}\right)\Big]\Big]\Bigg\} / \mathcal{V}^n_{i,j,k}
\end{aligned}
$$

Temperature and heat flow boundary conditions use the same equations for a boundary point or zone as are used for an interior. When a temperature history is prescribed, it is used in the interior gradient calculation as if a phantom zone existed with the temperature equal to boundary temperature. The conductivity and volume of the phantom zone are zero and the integration for partial derivatives is taken along the boundary surface where no zone exists.

Heat flow boundary conditions are activated by assuming that the boundary is adiabatic for the temperature gradient calculation, then by adding or subtracting the boundary heat through appropriate boundary faces. The adiabatic boundary, temperature gradient calculation is performed in two steps:

- The temperature gradient calculation is made assuming that the phantom zones have the same temperature as their nearest interior neighbor.
- Then the dot product of the temperature gradient and the line segment perpendicular to the direction of no heat flow is calculated in order to eliminate temperature gradients perpendicular to the line segment.

3. Calculate source energy density, $U^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, to be deposited in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n,

$$U^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = U_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}(t^{n}) ,$$

where $U_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}(t^{n})$ is a time-dependent function of energy deposition for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ evaluated at time t^{n}.

4. Add approximate reversible work (old pressure multiplied by new change of relative volume), approximate distortional energy density, heat transfer energy density, and source energy density in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ to internal energy density $(u^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}})$ in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ to get the approximate internal energy density $(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}})$ in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$,

$$\begin{aligned}\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = u^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \\ - \left(p^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right)\Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \\ + \Delta \tilde{Z}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + \Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + U^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} .\end{aligned}$$

5. Calculate an approximate pressure, $\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ for time $n+\frac{1}{2}$ by first calculating the approximate $n+1$ pressure, $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, from internal energy density in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$,

$$\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = p_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}, V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right) ,$$

where $V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the relative volume already calculated in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ for time $n+1$ [Eq.(6.29)], $p_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the pressure equation of state, and $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the approximate pressure for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+1$. Then adjust this pressure, $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, to satisfy explosive or spall criteria. (These criteria are mutually exclusive.) Calculate the approximate spall pressure, $\tilde{p}^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$,

$$\tilde{p}^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = p_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ \tilde{Z}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right),$$

where $p_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$.

If $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \leq \tilde{p}^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, adjust $\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ to its spalled value. Then calculate $\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ from

$$\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{\tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + p^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{2}\ .$$

6. Calculate shear modulus, $G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+\frac{1}{2}$ by first calculating the shear modulus, $G^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+1$,

$$G^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = G_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ \tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right),$$

where $G_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$, and then using

$$G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = \frac{G^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + G^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{2}\ .$$

7. Calculate elastic stress deviators, ${s^e_{xx}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, ${s^e_{yy}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, ${s^e_{zz}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, ${s^e_{xy}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, ${s^e_{yz}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, and ${s^e_{zx}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n+1 as follows,

$$
\begin{aligned}
{s^e_{xx}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} &= {s_{xx}}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + {\delta_{xx}}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \\
&\quad + 2.0\, G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \left({\dot{\epsilon}_{xx}}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \frac{1}{3} \frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \right) \Delta t^{n+\frac{1}{2}} \; ;
\end{aligned}
$$

$$
\begin{aligned}
{s^e_{yy}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} &= {s_{yy}}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + {\delta_{yy}}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \\
&\quad + 2.0\, G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \left({\dot{\epsilon}_{yy}}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \frac{1}{3} \frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \right) \Delta t^{n+\frac{1}{2}} \; ;
\end{aligned}
$$

$$
\begin{aligned}
{s^e_{zz}}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} &= {s_{zz}}^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + {\delta_{zz}}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \\
&\quad + 2.0\, G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \left({\dot{\epsilon}_{zz}}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \frac{1}{3} \frac{\dot{V}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \right) \Delta t^{n+\frac{1}{2}} \; ;
\end{aligned}
$$

$$s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + \delta^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$$

$$+ G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \dot{\epsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Delta t^{n+\frac{1}{2}} ;$$

$$s^{e^{n+1}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + \delta^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$$

$$+ G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \dot{\epsilon}^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Delta t^{n+\frac{1}{2}} ;$$

$$s^{e^{n+1}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + \delta^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$$

$$+ G^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \dot{\epsilon}^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Delta t^{n+\frac{1}{2}} ;$$

where $s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $s^{n}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, and $s^{n}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ are the xx-, yy-, zz-, xy-, yz-, and zx-stress deviators in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ from time n; $\dot{\epsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\dot{\epsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\dot{\epsilon}^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\dot{\epsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\dot{\epsilon}^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\dot{\epsilon}^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ are the previously calculated xx-, yy-, zz-, xy-, yz-, and zx-strain rates in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n [Eq.(6.33)]; $\delta^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\delta^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\delta^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\delta^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\delta^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ and $\delta^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ are the xx-, yy-, zz-, xy-, yz-, and zx-stress rotation corrections in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+\frac{1}{2}$,

$$\delta^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = -2\left(\alpha^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \alpha^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) \;;$$

$$\delta^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = +2\left(\alpha^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \alpha^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) \;;$$

$$\delta^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = -\delta^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \delta^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \;;$$

$$\delta^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \alpha^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left(s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) + \alpha^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \alpha^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \;;$$

$$\delta^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \alpha^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left(s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) + \alpha^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \alpha^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \;;$$

$$\delta^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \alpha^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \left(s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \right)$$

$$+ \alpha^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \; s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$$

$$- \alpha^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \; s^{n}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \; ;$$

where

$$\alpha^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{1}{2}\left[\left(\frac{\partial \dot{y}}{\partial x}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \left(\frac{\partial \dot{x}}{\partial y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right] \Delta t^{n+\frac{1}{2}} \quad ,$$

$$\alpha^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{1}{2}\left[\left(\frac{\partial \dot{z}}{\partial y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \left(\frac{\partial \dot{y}}{\partial z}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right] \Delta t^{n+\frac{1}{2}} \quad ,$$

$$\alpha^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{1}{2}\left[\left(\frac{\partial \dot{x}}{\partial z}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \left(\frac{\partial \dot{z}}{\partial y}\right)^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right] \Delta t^{n+\frac{1}{2}} \quad ,$$

and $\Delta t^{n+\frac{1}{2}}$ is the stable time step for this cycle. The velocity gradients have already been defined by Eqs.(6.36), (6.37), and (6.38).

8. Calculate the elastic yield stress squared, $\left(Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right)^2$, for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+1$ from the second stress deviator invariant,

$$\left(Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right)^2 = \frac{3}{2}\left[\left(s^{e^{n+1}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)^2\right]$$

$$+ 3\left[\left(s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)^2 + \left(s^{e^{n+1}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)^2\right] .$$

9. Calculate the allowable yield stress, $Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+1$,

$$Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = Y_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\left(\tilde{u}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}, \tilde{p}^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}, V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right) ,$$

where $Y_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$.

10. Compare the allowable yield stress, $Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, with the elastic yield stress, $Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$,

if $Y^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} > Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, material is linear elastic;

if $Y^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \leq Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, material has exceeded allowable yield stress.

11. If the material is linear elastic, the elastic stress deviators already calculated are correct,

$$s_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = s_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = s_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = s_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = s_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = s_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = s_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} .$$

12. When the material has exceeded its allowable yield stress, adjust the stress deviators according to the Prandtl-Reuss flow rule,

$$s_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = \left(\frac{Y_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}^{n+1}}{Y_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}^{e^{n+1}}} \right) s_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{n+1} = \left(\frac{Y_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}^{n+1}}{Y_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}^{e^{n+1}}} \right) s_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}^{e^{n+1}} ,$$

$$s^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) s^{e^{n+1}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} ,$$

$$s^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) s^{e^{n+1}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} ,$$

$$s^{n+1}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) s^{e^{n+1}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} ,$$

$$s^{n+1}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \left(\frac{Y^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}{Y^{e^{n+1}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right) s^{e^{n+1}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} .$$

13. Calculate the change in distortional energy density, $\Delta Z^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+\frac{1}{2}$,

$$\begin{aligned}\Delta Z^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\, \Delta t^{n+\frac{1}{2}} \Big(& s^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ \dot{\varepsilon}^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \\ & + s^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ \dot{\varepsilon}^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ \dot{\varepsilon}^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \\ & + s^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ \dot{\varepsilon}^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ \dot{\varepsilon}^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \\ & + s^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\ \dot{\varepsilon}^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \Big) ,\end{aligned}$$

where

$$s^{n+\frac{1}{2}}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{s^{n+1}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{s^{n+1}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{s^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{s^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{s^{n+1}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}}{2} ,$$

$$s^{n+\frac{1}{2}}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = \frac{s^{n+1}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} + s^{n}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}}{2} .$$

14. Calculate the internal energy density, $u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+1$,

$$u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = u^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} - \left(\tilde{p}^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right) \Delta V^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$$

$$+ \Delta Z^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + \Delta h^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + U^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} .$$

15. Calculate the pressure, $p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n+1,

$$p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = p_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}, V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right).$$

16. Calculate the spall pressure, $p^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n+1,

$$p^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = p_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}, V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}, Z^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right),$$

where $p_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$. If $p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \le p^{n+1}_{\min_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, adjust $p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ to its spalled value.

17. Calculate the total stress, $\sigma^{n+1}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\sigma^{n+1}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\sigma^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\sigma^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\sigma^{n+1}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$, $\sigma^{n+1}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n+1,

$$\sigma^{n+1}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n+1}_{xx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \left(p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right);$$

$$\sigma^{n+1}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n+1}_{yy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \left(p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right);$$

$$\sigma^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n+1}_{zz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} - \left(p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} + q^{n+\frac{1}{2}}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \right);$$

$$\sigma^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n+1}_{xy_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \;;$$

$$\sigma^{n+1}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n+1}_{yz_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \;;$$

$$\sigma^{n+1}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = s^{n+1}_{zx_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} \;.$$

18. Calculate the longitudinal sound speed squared, $\left(c^{n+1}_{\ell_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)^2$ in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+1$,

$$c^{n+1}_{\ell_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}} = c_{\ell_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right),$$

where $c_{\ell_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$.

19. Calculate the temperature, $T^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time $n+1$,

$$T^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = T_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ p^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right),$$

where $T_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$.

20. Calculate the conductivity, $k^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n+1,

$$k^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = k^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ P^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right),$$

where $k_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$.

21. Calculate the specific heat capacity, $C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$, in zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n+1,

$$C^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} = C_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\left(u^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ P^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}},\ V^{n+1}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right),$$

where $C_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is a material function for zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$.

6.4 EXPLICIT TIME STEP

6.4.1 Overview. The explicit calculational scheme has two identifying characteristics:

(1) New values are computed from old values; e.g., values at n+1 are computed from values at n.

(2) Data for computations come only from nearest neighbors; i.e., information can propagate only across one zone in one calculational time step.

These characteristics are the essential elements of the explicit numerical method and are embodied in the criteria required to calculate stable time steps.

6.4.2 Stable Mechanical Time Steps. The physical criterion required for the calculation of a stable time step was described in Section 6.2.2 and is summarized in Eqs.(6.9a) and (6.9b). If artificial viscosity were not present, the most conservative (largest) value of mechanical sound speed would be the isentropic longitudinal sound speed. The general form of the isentropic longitudinal sound speed is

$$c_\ell^2 \equiv \left.\frac{\partial \sigma_\ell}{\partial \rho}\right)_{\text{isentropic}} , \tag{6.48}$$

where the subscript ℓ denotes the longitudinal direction, σ_ℓ is calculated from Eq.(6.47), and ρ is the actual density. Equation (6.48) can also be written in component form,

$$c_\ell^2 = c_s^2 + c_p^2 + c_q^2 , \tag{6.49a}$$

$$= \left.\frac{\partial s}{\partial \rho}\right)_{\text{isen}} + \left.\frac{\partial p}{\partial \rho}\right)_{\text{isen}} + \left.\frac{\partial q}{\partial \rho}\right)_{\text{isen}} , \tag{6.49b}$$

where "isen" means isentropic.

c_s is the deviatoric contribution to sound speed and can be calculated conservatively from the formula,

$$c_s^2 = \frac{\frac{4}{3}G}{\rho^o} , \qquad (6.50)$$

where G is the shear modulus and ρ^o is the reference density. c_s is the elastic shear velocity.

c_p is the pressure (or mean stress) contribution to sound speed and is calculated from the equation of state. When the equation of state is of the form

$$p = A + Bu , \qquad (6.51)$$

where $A = A(\eta)$, $B = B(\eta)$, and $\eta \equiv \frac{1}{V}$, then from the isentropic condition that $du = -pdV$, the thermodynamic (hydrostatic) sound speed is

$$c_p^2 = \frac{A' + B'u + BpV^2}{\rho^o} , \qquad (6.52)$$

where $A' = \frac{dA}{d\eta}$, $B' = \frac{dB}{d\eta}$. When the equation of state is not in the form of Eq.(6.51), then a more specialized approach must be taken.

c_q is the artificial viscosity contribution to sound speed and is composed of two components, linear and quadratic. The formula is

$$c_q^2 = \left.\frac{\partial q_L}{\partial \rho}\right)_{isen} + \left.\frac{\partial q_Q}{\partial \rho}\right)_{isen} . \qquad (6.53)$$

Using Eqs.(6.41) and (6.42), c_q^2 becomes (References 6.2 and 6.1, respectively),

$$c_q^2 = 4C_L^2 \frac{|p|\, V}{\rho^o} + \left(2C_Q\right)^4 (\Delta \ell)^2 \left(\frac{\delta \dot{\ell}}{\delta \ell}\right)^2 . \tag{6.54}$$

Combining Eqs.(6.50), (6.52), and (6.54) yields the formula for the maximum stable time step of zone (i-½,j-½,k-½),*

$$\left(\Delta t^{n+1}_{(\cdot\cdot)}\right)^2 = \frac{\left(\Delta \ell^{n+1}_{(\cdot\cdot)}\right)^2}{\left(c^{n+1}_{\ell\,(\cdot\cdot)}\right)^2 + 4C^2_{L_{(\cdot\cdot)}} \dfrac{\left|p^{n+1}_{(\cdot\cdot)}\right| V^{n+1}_{(\cdot\cdot)}}{\rho^o_{(\cdot\cdot)}} + \left(2C_{Q_{(\cdot\cdot)}}\right)^4 \left(\Delta \ell^{n+\frac{1}{2}}_{(\cdot\cdot)}\right)^2 \left[\left(\dfrac{\delta \dot{\ell}}{\delta \ell}\right)^{n+\frac{1}{2}}_{(\cdot\cdot)}\right]^2} . \tag{6.55}$$

In determining a time step for the next cycle, only n+1 data exist in order to predict the n+3/2 time step. This dilemma is not critical provided that one understands the pathological cases which can arise from a poorly estimated time step.

There are two pathological cases that must be considered when calculating the new n+3/2 time step. These cases can be seen from a plot of time step versus time. See Figure 6.3. If the time step is increasing with time (Case 1), predictions of the n+3/2 time step based on n+1 data will be conservative whether constant extrapolation (i.e., setting $\Delta t^{n+3/2} = \Delta t^{n+1}$) or linear extrapolation is used. On the other hand, if the time step is decreasing with time (Case 2), the constant extrapolation procedure will predict a time step that is apt to be too high to maintain stability. The linear extrapolation is much better but can also be inaccurate if the rate of time step decay is large. In problems in which the time step is expected to experience rapid drops in time, it is advisable to use a safety factor multiplier of 2/3. This will add another level of conservatism to the calculation of the n+3/2 time step.

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*In Eq.(6.55), subscripts i-½,j-½,k-½ are denoted by (··).

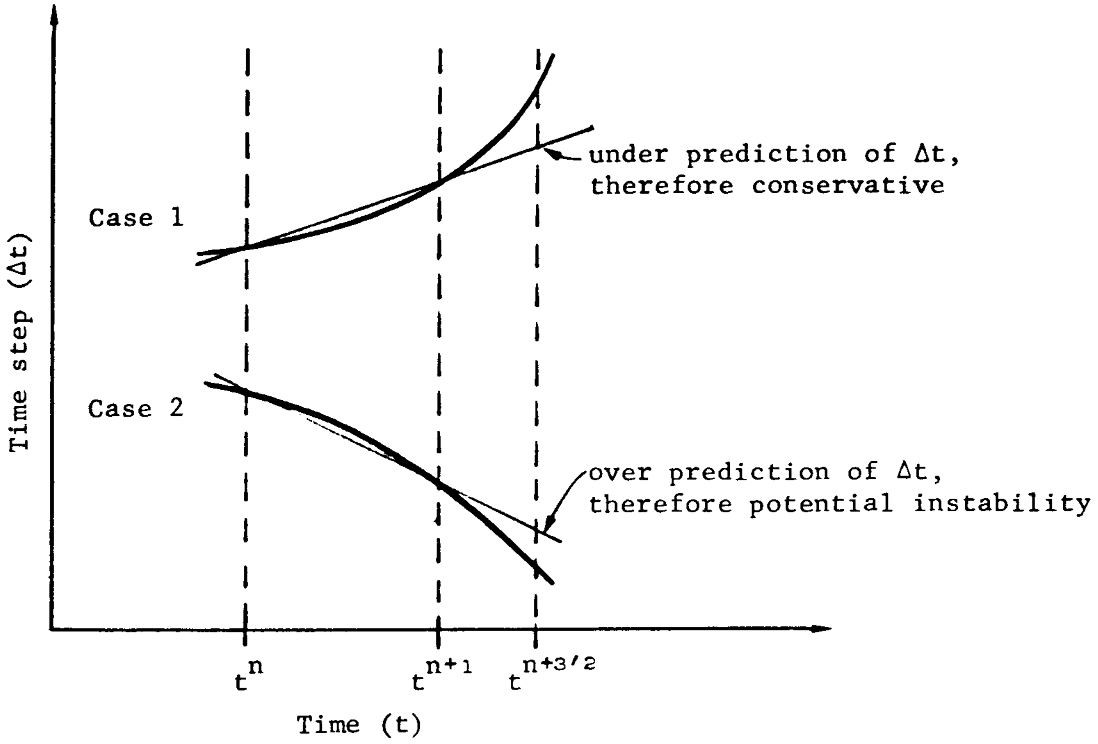
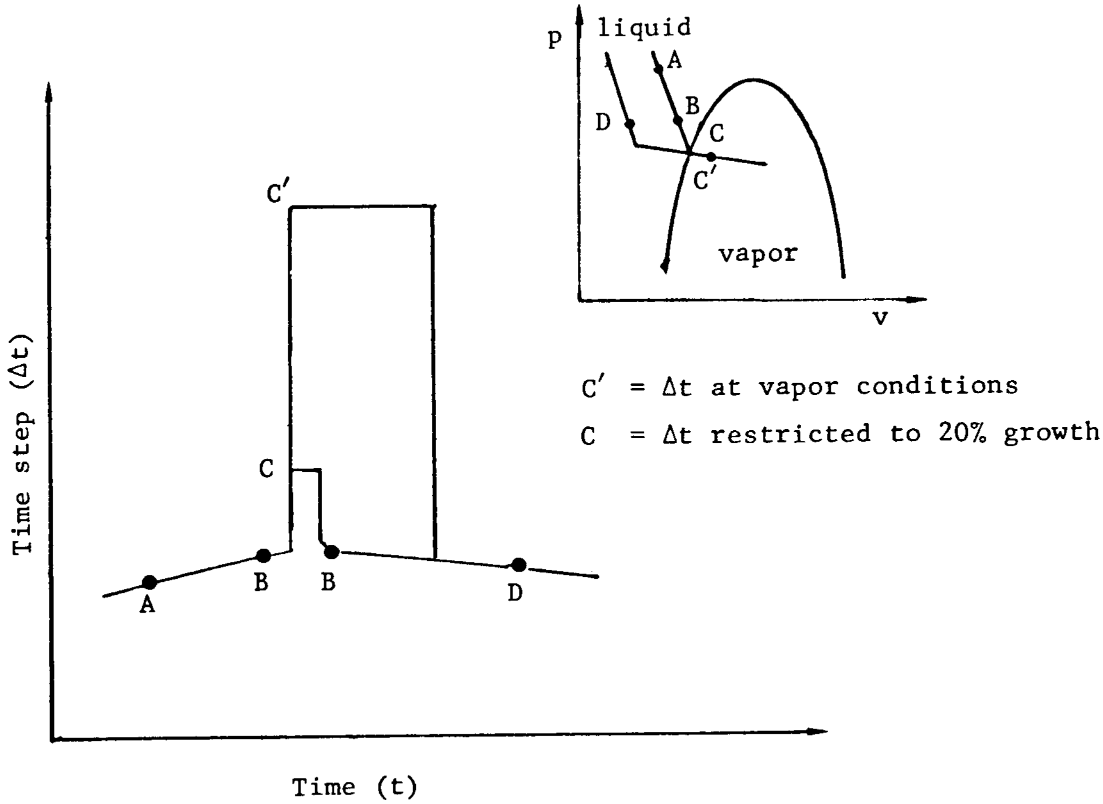


Figure 6.3. Example of need for f_{SFR}.



$C' = \Delta t$ at vapor conditions

$C = \Delta t$ restricted to 20% growth

Figure 6.4. Example of need for f_{GRF}.

Thus, when the n+1 time step is greater than the n+1/2 time step (Case 1), set the n+3/2 time step equal to the n+1 value and recompute the n+1 time step to be the average of this n+3/2 value and the n+1/2 time step. This will also be conservative. If, on the other hand, the n+1 time step is less than than the n+1/2 time step, calculate an n+3/2 time step based on a linear extrapolation of the n+1/2 and n+1 values. This procedure should lead to a relatively safe value for most calculations. When the n+1 time step equals the n+1/2 value, either approach will work.

There are other time-step constraints which insure the stability of a calculation. First, there is a safety factor multiplier (f_{SFR}), which may be applied when c_p cannot be calculated in a conservative way or when Eq.(6.55) may not be conservative. The value of f_{SFR} may vary from 0.1 to 1.0.

Next, there is a growth factor multiplier (f_{GRF}), which may be applied so that a time step cannot grow faster than a certain rate. The value of f_{GRF} may vary from 1.0 to 1.2 (no growth to 20% growth). The need for a 20% growth factor limitation on a time step is justified as follows: Consider the problem in which a change of material phase is possible. Furthermore, allow for the situation that during the early response periods, the time step is controlled by the higher sound speed phase (i.e., lower time step) but that at some later time during the simulation, all of the material is "flashed" to the lower sound speed phase. Assume that this change of sound speed results in a change of the maximum stable time step of at least a factor of 2. Furthermore, one cycle after the global change of phase has occurred, one of the zones returns to its higher sound speed state. If the time step had been allowed to rise rapidly to its much larger value for the one cycle when all the zones switched phase to the lower sound speed material, it is possible that the instantaneously larger time step could result either in an instablity when the time step drops again to the lower value, or in inaccurate results because of some numerically induced high amplitude wave that resulted in the one cycle in which the time step was large. This scenario is shown schematically in Figure 6.4.

And finally, there are minimum and maximum values of time step. When the stable time step goes below the minimum value, the problem is terminated. When the stable time step has a value above the maximum value, the time step is adjusted to the maximum value exactly.

Thus, stable time steps for the next cycle ($\Delta t^{n+3/2}$ and Δt^{n+1}) are calculated as follows,

$$\Delta t^{n+3/2} = f_{SFR} \left[\text{minimum for all zones of Eq.(6.55)}\right] , \tag{6.56}$$

subject to the condition that

$$\Delta t_{min} \leq \Delta t^{n+3/2} \leq f_{GRF} \, \Delta t^{n+\frac{1}{2}} \leq \Delta t_{max} . \tag{6.57}$$

Then, by interpolation,

$$\Delta t^{n+1} = \frac{\Delta t^{n+3/2} + \Delta t^{n+\frac{1}{2}}}{2} . \tag{6.58}$$

6.4.3 Stable Thermal Time Steps. When a particular problem is dominated by heat conduction phenomena rather than by mechanical phenomena, the problem time step stability criterion may be controlled by thermal diffusion rather than by mechanical sound speed. Therefore, when heat conduction is present, it is necessary to calculate the minimum stable heat conduction time step as follows,

$$\Delta t^{n} = \text{minimum value of } \Delta t^{n}_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \text{ for all } i > 1,\ j > 1,\ k > 1,$$

where

$$\Delta t^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}} \le \frac{\left(\Delta\ell^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}\right)^2}{2\left(k^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}/C^n_{V_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}\right)} . \tag{6.59}$$

$\Delta\ell^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the smallest length across zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n;
$k^n_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}$ is the conductivity of zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n; and
$C^n_{V_{i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}}$ is the specific heat capacity* of zone $(i-\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2})$ at time n.

As in the case of the mechanical stability criterion, the smallest maximum stable thermal time step in the grid is saved in order to be used for the next cycle of calculations. When thermal and mechanical mechanisms are both present, the smallest of the two stable time steps is chosen to be the time step for both mechanisms in the next cycle.

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*Per reference unit volume.

6.5 USE OF THE DEVELOPED EQUATIONS FOR EFFICIENT SOLUTION OF NON-TRANSIENT CASES

6.5 1 The Problem. Although the explicit finite-difference equations developed in Sections 6.2 and 6.3 can be used to analyze transient, steady-state, static, and quasi-static time-dependent thermomechanical systems, these numerical equations are most efficient for simulating transient behavior because time steps are computed from the minimum of the Courant stability criterion and the diffusion limit. The Courant condition gives the largest possible stable time step for a finite representation of a continuum consistent with the laws of physics for most initial value (transient) problems involving stress. The diffusion limit does the same for transient thermal problems. For mechanical boundary value (non-transient) problems, the Courant condition may needlessly restrict the time step. Two important exceptions to these guidelines are as follows: (1) linear elastic, small-strain, transient mechanical problems can sometimes be more efficiently solved implicitly in the frequency domain than explcitly in the time domain, and (2) nonlinear, non-transient problems often require that time be an independent explicit variable with the resulting equations being solved explicitly so that path-dependent thermodynamics are properly computed. Thermal boundary value problems are still efficiently solved using the diffusion limit time step criterion.

In other words, when time-dependent, nonlinear partial differential equations must be solved, it is usually most efficient to solve the explicit-in-time, physical equations using an explicit numerical scheme. When the equations exhibit weak time dependence but strong nonlinear effects (e.g., large deformation), the physical equations, though not explicitly time-dependent, are still probably most efficiently solved by explicit-in-time equations using a modified explicit numerical method. For the latter case, it is possible to separate the modifications to explicit methods for weakly time-dependent problems into three useful categories: (1) density scaling, (2) velocity damping, and (3) modulus scaling.

Density scaling is consistent with the situation where inertia effects are unimportant, where compressibility may be important, and where the time scale of the problem is determined by some other consideration (for example, heat transfer). Density scaling allows one to compute the intermediate state points of the process. Velocity damping (dynamic relaxation) may be used when inertia is somewhat important, compressibility may also be important, and the time scale is somewhat arbitrary. Velocity damping concerns itself only with the end states of a process. Intermediate states are not guaranteed to be accurate because the process (thermodynamic path dependence) is always assumed to be critically damped. Modulus scaling is at the other end of the spectrum from density scaling. When modulus scaling is most applicable, inertia effects are quite important, but compressibility is unimportant. The problem time scale is determined by an external constraint.

For example, most static problems can be categorized as "problems in which inertial influences are not important". Thus, density scaling can be used to increase the calculational time step in order to improve solution efficiency. Quasi-static problems, by definition, have a "sluggish" response, lending themselves to "dynamic relaxation" critical damping as a means of achieving an efficient solution. Steady-state processes are usually associated with incompressible flow or rigid body motion assumptions, in which case, modulus scaling appears to be the most appropriate choice to improve computational efficiency.

6.5.2 Density Scaling. When a problem is static or nearly static, the density (or mass) does not play an important role in the stress equilibrium process. Inertial effects disappear and the momentum equation becomes

$$\Sigma F_x \cong 0 , \qquad \Sigma F_y \cong 0 , \qquad \Sigma F_z \cong 0 \qquad (6.60a)$$

or

$$\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{xz}}{\partial z} \cong 0 ,$$

$$\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z} \cong 0 , \qquad (6.60b)$$

$$\frac{\partial\sigma_{xz}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z} \cong 0 ,$$

where F_x, F_y, and F_z are forces and σ_{xx}, σ_{yy}, σ_{zz}, σ_{xy}, σ_{yz}, and σ_{xz} are stresses. The zero on the right-hand side of the equal sign indicates that the inertial force is negligible. So, for Eq.(6.60b), we can write

$$\rho\ddot{x} \cong 0 , \qquad \rho\ddot{y} \cong 0 , \qquad \rho\ddot{z} \cong 0 . \qquad (6.61)$$

The reason Eq.(6.61) applies is that $\ddot{x}$, $\ddot{y}$, and $\ddot{z}$ are small. Therefore, ρ can be any value (in units consistent with $\ddot{x}$, $\ddot{y}$, and $\ddot{z}$) so long as Eq.(6.61) is still satisfied.

Referring to Eq.(6.55), it can be shown that the dominant term in the denominator for static and quasi-static problems is c_ℓ^2. Since c_ℓ^2 is a direct function of the bulk and shear moduli and an inverse function of the reference density, it can be seen that in order to increase the time step for a particular zone, it is necessary to lower the sound speed, c_ℓ, which means either lowering the moduli or raising the density (or both). For static problems, Eq.(6.61) indicates that the density may be increased until the products, $\rho\ddot{x}$, $\rho\ddot{y}$, and $\rho\ddot{z}$ produce an anomalous inertial effect.

Employing density scaling to achieve a larger time step for static problems requires only a change of input. The momentum equation and the Courant stability condition are unchanged.

6.5.3 Dynamic Relaxation. Another approach to economical static solutions is achieved by adding a viscous damping term to the momentum equation which acts to critically damp the fundamental response mode. This method reduces the number of time steps (iterations) required to achieve stress equilibrium, instead of increasing the magnitude of individual time steps. Quasi-static solutions can also be found using this approach. This approach is useful only when the integrated value of time is of no consequence, i.e., it doesn't matter what the "real time" is. Density scaling, on the other hand, preserves time as a meaningful variable.

The equations of motion are modified as follows,

$$\Sigma F_x = m\left(\ddot{x} + \frac{\eta}{\tau}\,\dot{x}\right)\ , \qquad \Sigma F_y = m\left(\ddot{y} + \frac{\eta}{\tau}\,\dot{y}\right)\ , \qquad \Sigma F_z = m\left(\ddot{z} + \frac{\eta}{\tau}\,\dot{z}\right)\ . \qquad (6.62a)$$

where η is a dimensionless damping coefficient, $\ddot{x}$, $\ddot{y}$, and $\ddot{z}$ are the components of acceleration resulting from the externally applied forces, F_x, F_y, and F_z, $\dot{x}$, $\dot{y}$, and $\dot{z}$ are the components of velocity that result from integrating $\ddot{x}$, $\ddot{y}$, and $\ddot{z}$, respectively, with critical damping applied, and τ is the longest fundamental period of the system when the boundary conditions are present. In terms of stress, Eqs.(6.62a) become

$$\begin{aligned}
\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{xz}}{\partial z} &= \rho\left(\ddot{x} + \frac{\eta'}{\tau}\,\dot{x}\right) \\
\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z} &= \rho\left(\ddot{y} + \frac{\eta'}{\tau}\,\dot{y}\right) \qquad (6.62b) \\
\frac{\partial\sigma_{xz}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z} &= \rho\left(\ddot{z} + \frac{\eta'}{\tau}\,\dot{z}\right)
\end{aligned}$$

where η' is $\eta/\mathcal{V}$. η (or η') is chosen to critically damp the lowest fundamental frequency of the grid. For linear elastic problems, it is a relatively simple matter to determine the damping (or relaxation) factor from a modal analysis or a dynamic excitation without damping. Even for mildly nonlinear systems, the latter technique can be used. For strongly nonlinear systems, an appropriate relaxation factor is far more difficult to compute and often requires considerable judgment.

The calculational form of the dynamic relaxation equation analogous to Eq.(6.7) comes from solving Eq(6.62b) for acceleration (including gravitation),

$$
\begin{aligned}
\ddot{x}^n &= \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x}+\frac{\partial\sigma_{xy}}{\partial y}+\frac{\partial\sigma_{xz}}{\partial z}\right)^n - \frac{1}{\rho^n}\,\frac{\eta'}{\tau}\,\dot{x}^n + g_x\,, \\
\ddot{y}^n &= \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x}+\frac{\partial\sigma_{yy}}{\partial y}+\frac{\partial\sigma_{yz}}{\partial z}\right)^n - \frac{1}{\rho^n}\,\frac{\eta'}{\tau}\,\dot{y}^n + g_y\,, \qquad (6.63) \\
\ddot{z}^n &= \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xz}}{\partial x}+\frac{\partial\sigma_{yz}}{\partial y}+\frac{\partial\sigma_{zz}}{\partial z}\right)^n - \frac{1}{\rho^n}\,\frac{\eta'}{\tau}\,\dot{z}^n + g_z\,.
\end{aligned}
$$

Integrating Eq.(6.63) with respect to time and making the following substitutions,

$$\frac{\eta'}{\rho^n} \equiv \frac{\eta}{m}$$

$$\dot{x}^n \equiv \frac{\dot{x}^{n+\frac{1}{2}}+\dot{x}^{n-\frac{1}{2}}}{2}\,, \quad \dot{y}^n \equiv \frac{\dot{y}^{n+\frac{1}{2}}+\dot{y}^{n-\frac{1}{2}}}{2}\,, \quad \dot{z}^n \equiv \frac{\dot{z}^{n+\frac{1}{2}}+\dot{z}^{n-\frac{1}{2}}}{2}$$

yields

$$\dot{x}^{n+\frac{1}{2}} - \dot{x}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{xz}}{\partial z}\right)^n + g_x\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{x}^{n+\frac{1}{2}} + \dot{x}^{n-\frac{1}{2}}\right] ,$$

$$\dot{y}^{n+\frac{1}{2}} - \dot{y}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z}\right)^n + g_y\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{y}^{n+\frac{1}{2}} + \dot{y}^{n-\frac{1}{2}}\right] , \qquad (6.64)$$

$$\dot{z}^{n+\frac{1}{2}} - \dot{z}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\partial\sigma_{xz}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z}\right)^n + g_z\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{z}^{n+\frac{1}{2}} + \dot{z}^{n-\frac{1}{2}}\right] .$$

Solving Eq.(6.64) for new velocity and defining the relaxation factor, ω, to be

$$\omega \equiv \frac{\eta}{2m\tau} ,$$

results in

$$\dot{x}^{n+\frac{1}{2}} = \dot{x}^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\Delta t^n} - 1\right] + \ddot{x}^n\left[\frac{\Delta t^n}{1+\omega\Delta t^n}\right] ,$$

$$\dot{y}^{n+\frac{1}{2}} = \dot{y}^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\Delta t^n} - 1\right] + \ddot{y}^n\left[\frac{\Delta t^n}{1+\omega\Delta t^n}\right] , \qquad (6.65)$$

$$\dot{z}^{n+\frac{1}{2}} = \dot{z}^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\Delta t^n} - 1\right] + \ddot{z}^n\left[\frac{\Delta t^n}{1+\omega\Delta t^n}\right] ,$$

where

$$\ddot{x}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{xz}}{\partial z}\right)^n + g_x \ ,$$

$$\ddot{y}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z}\right)^n + g_y \ ,$$

$$\ddot{z}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xz}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z}\right)^n + g_z \ .$$

6.5.4 Modulus Scaling. There are several forms of modulus scaling: (1) sound speed scaling for incompressible cases, and (2) elastic constants scaling for rigid body motion. The approach to computational efficiency is similar to density scaling in that the time step improvement comes from reducing the sound speed.

The physical assumption associated with incompressibility implies that the mechanical sound speed is indeterminant. Often it is said the sound speed is infinite (or, similarly, that the Mach number is zero, $M = 0$). However, as a practical matter, a better condition might be that incompressibility for real materials exists when $M \leqslant 0.3$. For many cases, this means that the sound speed can be reduced (scaled) below its actual value provided that $M \leqslant 0.3$.

An example of sound speed scaling is described as follows: Suppose an air bubble is expanding in water at approximtely 15 ft/sec and it is necessary to compute the resulting pressure in the water. The sound speed of water is about 5000 ft/sec, which, for this problem, means that the Mach number is about 3×10^{-3}. The flow is incompressible. Therefore, the sound speed is not important and can be artificially dropped up to two orders of magnitude without exceeding the Mach number criterion for incompressibility.

To be conservative, let's drop the sound speed only one order of magnitude to 500 ft/sec. This improves the time step by a factor of 10. To drop the sound speed means that the bulk modulus is effectively reduced by a factor of 100 (i.e., the compressibility is increased by 100). Since the flow at 15 ft/sec is incompressible, the change of modulus will be applied to infinitesimal strains and the pressures will be only slightly affected.

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