SCIENCE
APPLICATIONS
INCORPORATED

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Y/OWI/SUB-78/16549/3

AN OPTIMIZATION STUDY OF THE EXPLICIT FINITE-DIFFERENCE METHOD FOR QUASI-STATIC THERMOMECHANICAL SIMULATIONS

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

SAI-FR-821-3
(Final Report)

Prepared by

Donald E. Maxwell, Ronald Hofmann, and Krishan K. Wahi

Science Applications, Incorporated
8201 Capwell Drive
Oakland, California 94621

March 1978

This report was prepared by Science Applications, Incorporated
under Subcontract 86Y-16549V with
Union Carbide Corporation, Nuclear Division,
under Contract Number W-7405-eng-26 with the
U.S. Department of Energy.
The Subcontract was administered by the Office of Waste Isolation

Y/OWI/SUB-78/16549/3

AN OPTIMIZATION STUDY OF THE EXPLICIT FINITE-DIFFERENCE METHOD FOR QUASI-STATIC THERMOMECHANICAL SIMULATIONS

SAI-FR-821-3
(Final Report)

Prepared by

Donald E. Maxwell, Ronald Hofmann, and Krishan K. Wahi

Science Applications, Incorporated
8201 Capwell Drive
Oakland, California 94621

March 1978

Prepared for

Office of Waste Isolation
Nuclear Division
Union Carbide Corporation
Oak Ridge, Tennessee 37830

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the U.S. Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.

FOREWORD

The developments presented in this work make it economically feasible to use a time-explicit numerical code to perform thermomechanical simulations of quasi-static systems that incorporate physically small source regions (or centers of activity) in a relatively large space. A nuclear waste repository in a geological medium is an example of such a system. In particular, the techniques developed make it possible to eliminate two major restrictions that explicit-finite difference codes generally have that can considerably limit their efficiency. These restrictions being: (1) the zones of the mesh should be of comparable size; and (2) the smallest zone which controls the global time step restricts the speed at which equilibrium can be achieved elsewhere. When applied properly, the techniques developed in this work can provide enormous savings in computational time without affecting the accuracy of the solution in any significant way.

CONTENTS

		Page
SECTION 1	INTRODUCTION	1
SECTION 2	TECHNICAL BACKGROUND	2
SECTION 3	TIME STEP OPTIMIZATION	10
SECTION 4	SUMMARY	16
REFERENCES		17

SECTION 1
INTRODUCTION

The applicability of the explicit finite-difference (EFD) method for analyzing the mechanical and thermal response of a radioactive waste repository was first demonstrated by two-dimensional numerical simulations of Project Salt Vault (PSV) (Reference 1). The PSV analysis was performed using an already-developed computer code, the STEALTH* 2D EFD continuum mechanics computer code (Reference 2), and two proven optimization techniques: (1) dynamic relaxation (Reference 3), and (2) density scaling. Subsequent simulations of PSV, which included the initial excavation sequence (Reference 4), and some spent fuel (SF) and high level waste (HLW) repository scoping calculations (Reference 5), also used the STEALTH 2D code. However, in these cases, a new time-step optimization method called "pseudo-time steps" (PTS) was developed and tested. The need to develop PTS arose because of the mesh (spatial accuracy) requirements of the SF and HLW scoping calculations. However, it has proven to be generally applicable to quasi-static thermomechanical problems.

PTS effectively allows each zone in a quasi-static problem to use an individually optimized, locally stable time step to advance states of stress. The method automatically scales the mechanical time step to a prescribed fraction of the stable thermal time step of each finite-difference zone to optimum values. The technique was used successfully in one PSV simulation which did not require its use and in all three thermomechanical response calculations which did require a time-step optimization procedure in order to be efficient. PTS has been derived so as to be general for one-, two-, and three-dimensional problems and can be used with dynamic relaxation. This report describes the motivation, derivation, and implementation of the PTS method.

---

*"Solids and Thermal hydraulics codes for EPRI Adapted from Lagrange TOODY and HEMP," developed for Electric Power Research Institute by Science Applications, Inc. under Contract RP307.

SECTION 2
TECHNICAL BACKGROUND

The EFD method was originally developed for the efficient computation of transient mechanical shock problems. The explicit approach insures correct thermodynamic path dependence by limiting the time step to a value that allows grid points to communicate only with their immediate neighbor zones, and zones to communicate only with their immediate neighbor grid points. Mechanical changes are, therefore, communicated through a mesh at a finite rate equal to or less than the value of the local sound speed. When an event has a material velocity on the order of the sound speed (i.e., when the local Mach number approaches unity), the event is communicated at the numerically optimum rate. When, on the other hand, the value of the material velocity is many orders of magnitude below the value of the local sound speed (as it is in a quasi-static event), the spatial communication process is far too slow for efficient computation on a real time scale.

The explicit time-step limit for a mechanical event based on the Courant stability requirement (Reference 6) is

$$\Delta t_i = \frac{\Delta \ell_i}{c_i} \tag{2.1}$$

where Δt_i is the maximum stable time step that can be used at point i, $\Delta \ell_i$ is a characteristic length at point i, and c_i is the local longitudinal sound speed at point i. The characteristic length is the distance across a zone in the direction of maximum acceleration (gradient of stress). The fastest sound speed is the isentropic sound speed usually associated with the direction of the maximum principal stress:

$$c_\ell^2 \equiv \left.\frac{\partial \sigma_\ell}{\partial \rho}\right)_{\text{isentropic}} \tag{2.2}$$

In a uniform mesh made up of square zones (of side length a) in which the sound speed is a constant, the characteristic length is bounded as follows:

$$a \leq \Delta\ell \leq \sqrt{2}\ a\ . \tag{2.3}$$

Thus, the time step for the entire mesh, which is taken to be the smallest value of Δt_i, will depend entirely on the smallest value of $\Delta\ell_i$.

In a non-uniform mesh in which the sound speed is a constant, the characteristic length is not necessarily bounded over such a small range. The smallest zone dimension limits the smallest value that a time step can attain. Larger values of the time step are possible, depending on the gradient of stress (direction of maximum acceleration), but the largest time step is limited by the least largest* dimension. Thus, where both large and small zones exist, the large zones are usually computed at time steps far below their optimum value. In transient problems (expecially nonlinear ones), this constraint is unavoidable (and desirable) in order to preserve the time sequencing of interacting events which are communicating at sound speed. The frequency of time steps is consistent with the response frequency of the transient event. In quasi-static problems in which momentum effects are small, the Courant time-step constraint is too restrictive. The response frequency is many orders below the one implied by the mechanical sound speed and a zone-related characteristic length.

For isotropic, quasi-static simulations in which zone sizes are relatively uniform, satisfaction of Eq.(2.1) requires that the mechanical sound speed be artificially scaled down in order to achieve an increased time step. The magnitude of sound speed scaling must be limited by the need to guarantee a proper description of physical processes. It is useful to view an

*The least largest dimension is determined by the two-step process of first finding the largest dimension of each zone and then taking the minimum value of these largest dimensions.

artificial reduction in sound speed in terms of the effective elastic moduli and mass densities which are used to compute the value of sound speed. One can view a reduction of the sound speed (1) as an artificial reduction in the bulk and shear moduli, (2) as an artificial increase in the density, or (3) as a combined moduli reduction and density increase.

Scaling the moduli down is most applicable when inertial effects are quite important, but compressibility is unimportant. Under modulus scaling, stress is assumed to be a weak function of strain. There are two classes of problems in which modulus scaling is obviously applicable: (1) incompressible flow and (2) rigid body motion. In both cases, the values of the moduli are assumed to be unimportant and can be chosen small enough to improve computational efficiency. To understand the implications of modulus scaling, the logic for the incompressible case is described below.

The physical assumption associated with incompressibility implies that the mechanical sound speed is indeterminant. Often, it is said that 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 $M \leqslant 0.3$. 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 according to $M \leqslant 0.3$. 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. A similar logic may be applied to the rigid case.

When inertial effects are unimportant but where compressibility may be important, density scaling may be used. In these problems, the time scale of the problem must be determined by some other mechanism -- for example, heat transfer. Density scaling allows one to compute the intermediate state points of the process. Density scaling is applicable to repository type of calculations.

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 two-dimensional momentum equations become

$$\Sigma F_x \cong 0, \qquad \Sigma F_y \cong 0,$$

or

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} \cong 0, \qquad \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} \cong 0 , \tag{2.4}$$

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.(2.4), one can write

$$\rho\ddot{x} \cong 0, \qquad \rho\ddot{y} \cong 0 . \tag{2.5}$$

Equation (2.5) is valid because $\ddot{x}$ and $\ddot{y}$ are small. Therefore, ρ can be any value (in units consistent with $\ddot{x}$ and $\ddot{y}$) so long as Eq.(2.5) remains satisfied. Increasing the density has the effect of lowering the sound speed, which, in turn, raises the time step. Since the sound speed is inversely proportional to the square root of density, the time step is directly proportional to the square root of density.

When a mesh is very non-uniform, it is desirable to scale density differently in different zones in order to counteract the characteristic zone length constraint on the time step. The technique of non-uniform density

scaling corresponds to applying a different time step to each mass point in the grid during the same computing cycle. If each of these local time steps has the maximum value allowed by the Courant condition for local stability, then each point of the grid will respond as vigorously as possible to relieve the current unbalanced forces. Though each mass point responds according to a different time step, the resulting stresses will be on the time scale of the applied load to the extent that stress equilibrium is approached.

Non-uniform density scaling is attractive in principle but cumbersome to apply. PTS scaling corresponds to employing the maximum stable time step to each mass point. These so-called "pseudo-time steps" provide the identical features of variable density scaling, including the feature of different time steps for the motion in the orthogonal directions at the same point. This is very useful for hydrodynamic systems (zero shear strength), but requires care when Poisson's ratio is less than 0.5. Instabilities can be generated in this latter case when the orthogonal time steps have different values. The precise conditions for stability when the directional time-step feature is included have not been established at this time.

Using an explicit-in-time code to do static simulations requires that some form of damping be added to the equations of motion which will act to reduce spurious oscillations. A velocity damping method known as dynamic relaxation (DR) has been used successfully by many people. 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 chosen to be critically damped or, at worst, slightly underdamped. DR is quite useful in establishing overburden in complex geologies.

In DR, a viscous damping term is added to the momentum equation. This acts to critically damp the fundamental response mode. In this way, the number of time steps (iterations) required to achieve stress equilibrium is reduced. In scaling methods, the magnitude of individual time steps is

increased to improve efficiency. DR is most useful when the integrated value of time is of little or 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.

In DR, the equations of motion are modified as follows,

$$\Sigma F_x = m\left(\ddot{x} + \frac{\eta}{\tau}\dot{x}\right) , \qquad \Sigma F_y = m\left(\ddot{y} + \frac{\eta}{\tau}\dot{y}\right) , \tag{2.6}$$

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, and $\dot{x}$ and $\dot{y}$ are the components of velocity that result from integrating $\ddot{x}$ and $\ddot{y}$, respectively, with critical damping applied. In terms of stress, Eqs.(2.6) become

$$\frac{\partial\sigma_{xx}}{\partial x} \quad \frac{\partial\sigma_{xy}}{\partial y} = \rho\left(\ddot{x} + \frac{\eta'}{\tau}\dot{x}\right) + \rho g_x ,$$

$$\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} = \rho\left(\ddot{y} + \frac{\eta'}{\tau}\dot{y}\right) + \rho g_y ,$$

where η' is $\eta/\mathcal{V}$. The value of 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 momentum equation comes from solving Eq.(2.7) for acceleration,*

$$\ddot{x}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n - \frac{1}{\rho^n}\frac{\eta'}{\tau}\dot{x}^n + g_x ,$$

$$\ddot{y}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}\right)^n - \frac{1}{\rho^n}\frac{\eta'}{\tau}\dot{y}^n + g_y . \tag{2.8}$$

Integrating Eq.(2.8) 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

$$\dot{x}^{n+\frac{1}{2}} - \dot{x}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n + g_x\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{x}^{n+\frac{1}{2}} + \dot{x}^{n-\frac{1}{2}}\right] ,$$

$$\dot{y}^{n+\frac{1}{2}} - \dot{y}^{n-\frac{1}{2}} = \left[\frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}\right)^n + g_y\right]\Delta t^n - \frac{\eta\Delta t^n}{2m\tau}\left[\dot{y}^{n+\frac{1}{2}} + \dot{y}^{n-\frac{1}{2}}\right] . \tag{2.9}$$

Solving Eq.(2.9) for new velocity and defining the relaxation factor, ω, to be

$$\omega \equiv \frac{\eta}{2m\tau} ,$$

---

*Superscript n denotes time orientation.

results in

$$\dot{x}^{n+\frac{1}{2}} = \dot{x}^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\Delta t^n} - 1\right] + \ddot{x}^n\left[\frac{\Delta t^n}{1+\omega\Delta t^n}\right],$$

$$\dot{y}^{n+\frac{1}{2}} = \dot{y}^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\Delta t^n} - 1\right] + \ddot{y}^n\left[\frac{\Delta t^n}{1+\omega\Delta t^n}\right], \tag{2.10}$$

where

$$\ddot{x}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\right)^n + g_x ,$$

$$\ddot{y}^n = \frac{1}{\rho^n}\left(\frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}\right)^n + g_y .$$

Equations (2.10) are general equations of motion which reduce to the undamped form when $\omega = 0$.

SECTION 3
TIME STEP OPTIMIZATION

A primary optimization requirement for a quasi-static thermomechanical problem is that the mechanical and thermal time steps be brought into order-of magnitude proximity for efficient computation. Unscaled, Courant-stable, mechanical time steps are usually three orders of magnitude smaller than diffusion-limited, stable thermal time steps. In the absence of inertial effects, thermal transport (diffusion) limits the mechanical response so that the mechanical time step may be increased to the thermally stable value without violating thermodynamic consistency. The simplest way to achieve time-step parity between mechanical and thermal mechanisms without violating the Courant stability criterion is to scale up the mass density. The scaled value is limited such that no artificial inertial effects are created. The arbitrarily increased density lowers the sound speed, which, in turn, creates larger stable mechanical time steps. However, the characteristic zone length will become an overriding factor in problems in which the zone size exhibits aspect ratios in excess of 2 to 1, and in which very small zones co-exist with very large zones. In these cases, the Courant characteristic length becomes the dominant impediment to efficient computation in the same way that the mechanical sound speed does when inertial effects are low.

All repository calculations exhibit negligible inertia, which means that density scaling is applicable, but stress is a sensitive function of strain, so that modulus scaling is not valid. Mesh requirements vary from problem to problem. The meshes used for all the PSV calculations are extremely regular. Most of the zones are squares and those that are not, are rectangles which never exceed a 2 to 1 aspect ratio. The SF and HLW scoping calculations, on the other hand, required initial meshes that had rectangular zones of varying size and shape. Zones near the repository were long and thin, with aspect ratios as high as 50 to 1. Away from the repository, zones became more square-like.

In order to overcome the limitations due to zone length, it is desirable to employ a non-uniform density scale. However, prescribing density as a function of space and time, in order to optimize time steps, is cumbersome to implement and not amenable to stability analysis. For these reasons, an alternative approach (PTS) was developed which would provide the features of (1) scaling the mass densities throughout the entire grid by a constant factor to increase the stable mechanical time step to be more compatible with the real time scale of the driving forces (e.g., thermal) and (2) adjusting the global density scale to a value that effectively matches the sound transit times in unequal size zones.

Before deriving the formulas for PTS optimization, it is useful to see the effect of global density scaling on the standard DR equations of motion. The velocity and coordinate update equations for grid point i of a one-dimensional system are written as follows,

$$\dot{x}_{i_s}^{n+\frac{1}{2}} = \dot{x}_{i_s}^{n-\frac{1}{2}} \left[\frac{2}{1+\omega_s \Delta t_s^n} - 1 \right] + \ddot{x}_{i_s}^{n} \left[\frac{\Delta t_s^n}{1+\omega_s \Delta t_s^n} \right] \tag{3.1}$$

$$x_i^{n+1} = x_i^n + \dot{x}_{i_s}^{n+\frac{1}{2}} \Delta t_s^{n+\frac{1}{2}} \tag{3.2}$$

where

x_i = coordinate

$\dot{x}_i$ = velocity

$\ddot{x}_i$ = acceleration (including body forces)

ω_s = damping frequency for dynamic relaxation

Δt_s = time step in real time controlled by mechanical, thermal, or other constraints.

The subscript s denotes a scaled value. Density scaling is defined as

$$\rho_s \equiv \rho s_o , \quad s_o > 1 , \tag{3.3}$$

where s_o is a global scaling factor and ρ is the unscaled mass density. As a result, one can write

$$\ddot{x}_s = \ddot{x} \frac{1}{s_o} \tag{3.4a}$$

because, from conservation of momentum, $\ddot{x}$ is inversely proportional to density. Similarly, one can write

$$\dot{x}_s = \dot{x} \frac{1}{\sqrt{s_o}} , \tag{3.4b}$$

and

$$\omega_s = \omega \frac{1}{\sqrt{s_o}} ,$$

because each is inversely proportional to Δt^n, and Δt^n is proportional to the square root of density through the Courant condition. Thus, Eq.(3.2) is invariant with respect to scale, and displacement (and stress-strain response) is the same in either the scaled or unscaled time domain. A single scale factor, c_o, applied globally to an entire mesh allows one to scale the grid's mechanical time step to any convenient size consistent with the initial and boundary conditions.

To optimize the relaxation rate of each individual grid point on a cycle basis, one can provide a point-dependent scale factor so that each grid point in each cycle moves the maximum distance allowed by the Courant condition at its safety factor, F. For an unscaled problem, the global time-step is

chosen as the minimum stable time step for the entire mesh, i.e.,

$$\Delta t = \text{minimum}(\delta t_i)$$

where δt_i are the mechanical time steps of the zones surrounding grid point i. The formula for a particular zone's time step is

$$\delta t = F \cdot \frac{\Delta x}{c} \tag{3.5}$$

where F is a time step safety factor, usually less than, but never greater than 1. F is used to compensate for uncertainties with respect to a precise stability limit for an arbitrary material. Δx is the distance across a zone, and c is the local sound speed of the zone. Therefore, the point-dependent scale factor would be

$$s_i \propto \left(\frac{\delta t_i}{\Delta t}\right)^2 . \tag{3.6}$$

Combining Eq.(2.6) with the global scale, s_o, yields

$$s_i = s_o\left(\frac{\delta t_i}{\Delta t}\right)^2 . \tag{3.7}$$

Equation (3.7) results in a time-dependent mass when zones distort and δt_i changes in time.

Density scaling can be eliminated by defining a "pseudo-velocity update" equation as follows,

$$v_i^{n+\frac{1}{2}} = v_i^{n-\frac{1}{2}}\left[\frac{2}{1+\omega\delta t_i^n} - 1\right] + \ddot{x}_i^n\left[\frac{\Delta t_s^n}{1+\omega\delta t_i^n}\right] , \tag{3.8}$$

where v is the pseudo-velocity and

$$\delta t_i^n \equiv \frac{1}{2}\left[\delta t_i^{n+\frac{1}{2}} + \delta t_i^{n-\frac{1}{2}}\right] .$$

Equation (3.8) provides the largest stable displacement allowed by the stability fraction, F. The resulting coordinate update is

$$x_i^{n+1} = x_i^n + v_i^{n+\frac{1}{2}}\, \delta t_i^{n+\frac{1}{2}} . \tag{3.9}$$

Equations (3.8) and (3.9) can be used directly or, if the form is inconvenient, can be expressed in alternate forms. For example, it is customary to update coordinates with the global time step, Δt_s, associated with the driving forces in the real time scale, i.e., Eq.(3.2). The real velocity, $\dot{x}_i^{n+\frac{1}{2}}$, determined from the pseudo-velocity uses the identity

$$v_i^{n+\frac{1}{2}}\, \delta t_i^{n+\frac{1}{2}} = \dot{x}_i^{n+\frac{1}{2}}\, \Delta t_s^{n+\frac{1}{2}} , \tag{3.10}$$

to obtain

$$\dot{x}_i^{n+\frac{1}{2}} = \frac{v_i^{n+\frac{1}{2}}\, \delta t_i^{n+\frac{1}{2}}}{\Delta t_s^{n+\frac{1}{2}}} . \tag{3.11}$$

Substituting Eq.(3.8) into Eq.(3.11) yields

$$\dot{x}_i^{n+\frac{1}{2}} = \frac{\delta t_i^{n+\frac{1}{2}}}{\delta t_i^{n-\frac{1}{2}}}\, \frac{\Delta t_s^{n-\frac{1}{2}}}{\Delta t_s^{n+\frac{1}{2}}}\, \dot{x}_i^{n-\frac{1}{2}} \left[\frac{2}{1+\omega\delta t_i^n} - 1\right] + \frac{\delta t_i^n\, \delta t_i^{n+\frac{1}{2}}}{\Delta t_s^{n+\frac{1}{2}}} \left[\frac{\ddot{x}_i^n}{1+\omega\delta t_i^n}\right] . \tag{3.12}$$

When the imposed value, $\Delta t_s^{n+\frac{1}{2}}$ is not constrained by mechanical stability and, in certain cases, when it varies substantially from cycle to cycle, Eq.(3.12) must be used.

Equation (3.12) can be approximated when the fractional change of Δt and δt are both less than $1 - F$, since the lack of centering will not induce mechanical instability. Using this approximation, Eq.(3.12) becomes

$$\dot{x}_i^{n+\frac{1}{2}} = \dot{x}_i^{n-\frac{1}{2}} \left[\frac{2}{1+\omega\delta t_i^n} - 1 \right] + \frac{\delta t_i^n \; \delta t_i^{n+\frac{1}{2}}}{\Delta t_s^{n+\frac{1}{2}}} \left[\frac{\ddot{x}_i^n}{1+\omega\delta t_i^n} \right], \tag{3.13}$$

or, more simply,

$$\dot{x}_i^{n+\frac{1}{2}} = \dot{x}_i^{n-\frac{1}{2}} \left[\frac{2}{1+\omega\delta t_i^n} - 1 \right] + \frac{\left[\delta t_i^{n+\frac{1}{2}}\right]^2}{\Delta t_s^{n+\frac{1}{2}}} \left[\frac{\ddot{x}_i^n}{1+\omega\delta t_i^n} \right] . \tag{3.14}$$

Equations (3.12), (3.13), and (3.14) yield no significant difference in velocity when they all converge toward stress equilibrium.

The above equations provide a vigorous and stable response driving toward local stress equilibrium at every point. However, the damping term, $\omega\delta t_i^n$, varies from point to point in contrast to the verified method of dynamic relaxation which employs a uniform global damping term, $\omega_s \Delta t_s^n$. There may be advantages in using $\omega\delta t_i^n$. This has not been explored. Instead, the verified method of dynamic relaxation was employed to obtain the verified equation,

$$\dot{x}_i^{n+\frac{1}{2}} = \dot{x}_i^{n-\frac{1}{2}} \left[\frac{2}{1+\omega_s \Delta t_s^n} - 1 \right] + \frac{\left[\delta t_i^{n+\frac{1}{2}}\right]^2}{\Delta t_s^{n+\frac{1}{2}}} \left[\frac{\ddot{x}_i^n}{1+\omega_s \Delta t_s^n} \right] \tag{3.15}$$

SECTION 4

SUMMARY

PTS scaling is a technique to optimize the time step of each grid point so that the zone length and zone sound speed needed to satisfy the Courant condition do not arbitrarily limit computing efficiency. Past notions of computing inefficiency with respect to solving non-transient problems using the EFD method are no longer valid because PTS eliminates the transient mechanical constraint on the global time step. In fact, where nonlinear rate-sensitive constitutive equations are required, it may be that the EFD approach, using PTS scaling, is more efficient than implicit-in-time approaches because time still remains an independent variable.

REFERENCES

1. Wahi, K. K., Maxwell, D. E., and Hofmann, R.; A Simulation of the Thermomechanical Response of Project Salt Vault; Final Report (SAI-FR-702) prepared by Science Applications, Inc. for Union Carbide Corporation, Nuclear Division, Office of Waste Isolation, Y/OWI/SUB-77/16519/1 (February 1977)

2. Hofmann, R.; STEALTH, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis; EPRI NP-260, Vol. 1, User's Manual, prepared by Science Applications, Inc. for Electric Power Research Institute, Palo Alto, California (August 1976)

3. Otter, J. R. H., Cassell, A. C., and Hobbs, R. E.; "Dynamic Relaxation," Proc. Inst. Civ. Engineers 1966 35 (Dec.), pp.633-656, 37 (Aug.), pp.723-750

4. Wahi, K. K., Maxwell, D. E., and Hofmann, R.; A Two-Dimensional Simulation of the Thermomechanical Response of Project Salt Vault Including the Excavation Sequence; Final Report (SAI-FR-821-2) prepared by Science Applications, Inc. for Union Carbide Corporation, Nuclear Division, Office of Waste Isolation, Y/OWI/SUB-78/16549/2 (March 1978)

5. Wahi, K. K., Maxwell, D. E., and Hofmann, R.; The Thermomechanical Response of a One-Level Spent Fuel Nuclear Waste Repository; Final Report (SAI-FR-821-1) prepared by Science Applications, Inc. for Union Carbide Corporation, Nuclear Division, Office of Waste Isolation, Y/OWI/SUB-78/16549/1 (March 1978)

6. Richtmyer, R. D. and Morton, K. W.; Difference Methods for Initial-Value Problems, John Wiley & Sons, New York (1967)