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Title:	Exploration of a Cell-Centered Lagrangian Hydrodynamics Method
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Exploration of a Cell-Centered Lagrangian Hydrodynamics Method

D. E. Burton[1], T.C. Carney[1], N.R. Morgan[2], S. Runnels[1], M.J. Shashkov[1]

We present a new cell-centered Lagrange hydro method, discuss some of its aspects that are still being explored, and demonstrate its performance on several test problems. The method is second-order in both space and time, enforcing conservation equations for volume, linear momentum, and total energy on the same control volume, while enforcing angular momentum on a dual control volume. The method employs a compatible decomposition of total energy that enables the computation of specific kinetic and internal energy at the cell's center of mass. Trial values for stress and velocity at cell interfaces are determined using a multi-dimensional, two-shock Riemann-like solution with innovations that increase its effectiveness for skewed cells. These trial values are then combined to compute velocity and stress at the vertices that are then propagated back to the cell interfaces in a way that maintains geometric volume compatibility and angular momentum.

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Abstract

We present a new cell-centered Lagrange hydro method, discuss some of its aspects that are still being explored, and demonstrate its performance on several test problems. The method is second-order in both space and time, enforcing conservation equations for volume, linear momentum, and total energy on the same control volume, while enforcing angular momentum on a dual control volume. The method employs a compatible decomposition of total energy that enables the computation of specific kinetic and internal energy at the cell's center of mass. Trial values for stress and velocity at cell interfaces are determined using a multi-dimensional, two-shock Riemann-like solution with innovations that increase its effectiveness for skewed cells. These trial values are then combined to compute velocity and stress at the vertices that are then propagated back to the cell interfaces in a way that maintains geometric volume compatibility and angular momentum.

We are interested in cell-centered hydro (CCH) as a possible alternative to staggered-grid hydro (SGH)

Background

- Staggered Lagrangian methods (SGH) have been a practical tool for large-scale simulations since before 1950
- Nevertheless, SGH has many known flaws with respect to: mesh imprinting, spurious vorticity, shock capturing, symmetry preservation, and energy conservation

- Cell-centered Eulerian hydro formulations have been around for many years
- Earliest suggestion for cell-centered Lagrangian (CCH) seems to have been by Ruppel & Harlow in 1981, leading to the CAVEAT code
- Recently there has been renewed interest in CCH (Barlow, Burton, Despres, Luttwak, Maire, Shashkov, & others)

To be a viable alternative to SGH, CCH must have comparable capabilities in the areas of:

- Material strength
- Multi-material cells
- Unstructured polytopal grids
- Multi-dimensional formulation with curvilinear geometry
- Advection
- *etc.*

We will demonstrate some of these capabilities, but the presentation will focus on:

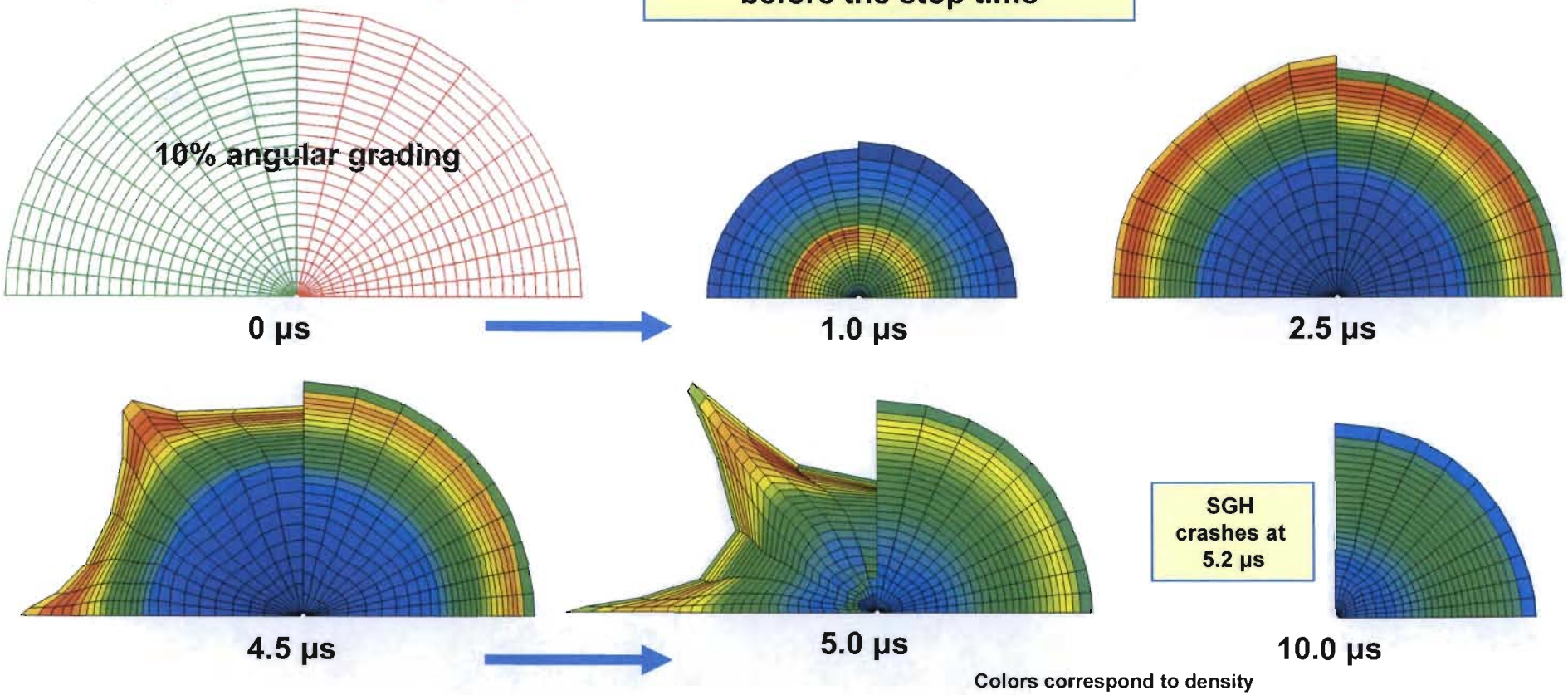
- Mimetic derivation of the difference equations

Interest in alternatives to SGH is motivated by problems like the Pressurized Ball that suggest CCH is more stable

Spherical ball of gas with constant boundary pressure & 10% angular grading

Undergoes several bounces before the stop time

cells: 25 radial x 10 angular
10% angular grading
initial radius 10
stop time 10
ρ=1, e=1, Y=5/3
boundary pressure=200/3
rz geometry



Colors correspond to density

Because we are in relatively unexplored territory, we used a mimetic approach to guide the derivation of the difference scheme

Motivation:

- Areas of interest (strength, multi-material cells, …) have not been widely investigated in a CCH context
- Our preliminary implementations of CCH seemed to be sensitive (or surprisingly insensitive) to algorithmic variations

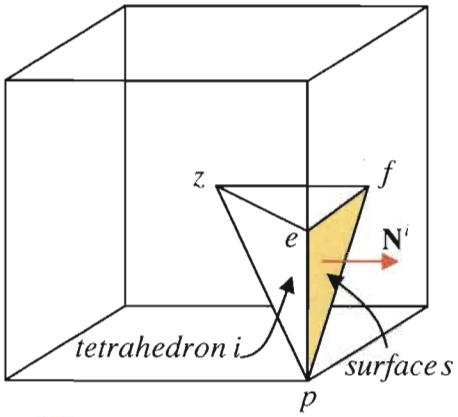
The **mimetic approach** considers not only the finite volume differencing of

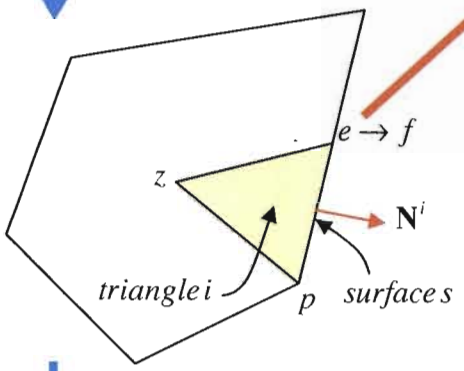
- Evolution equations
- Flux conservation equations

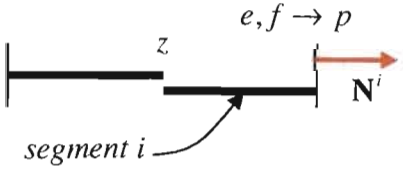
but also ancillary relationships that place constraints on the formulation

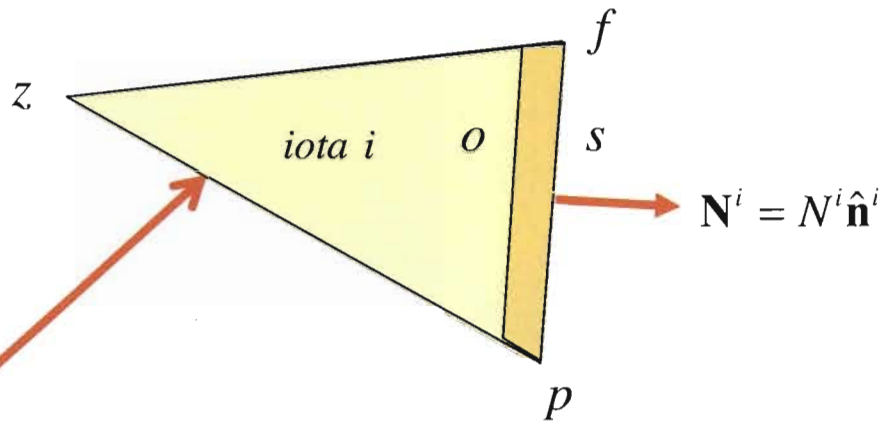
- Geometric volume conservation
- Curl & divergence identities
- Angular momentum
- Entropy production

Polytopal grids are described by connectivity that collapses naturally from 3D to 2D & 1D









The basic connectivity structure is called an "iota"

Variables are located relative to the iota; e.g.,

$\mathbf{u}_z^i$ is the cell center velocity relative to iota i

σ_s^i is the surface stress tensor for iota i

$\mathbf{N}^i = N^i \hat{\mathbf{n}}^i$ is the outward surface normal

Sums are usually over iotas connected to points or cells; e.g.,

The sum of surface vectors about a cell is

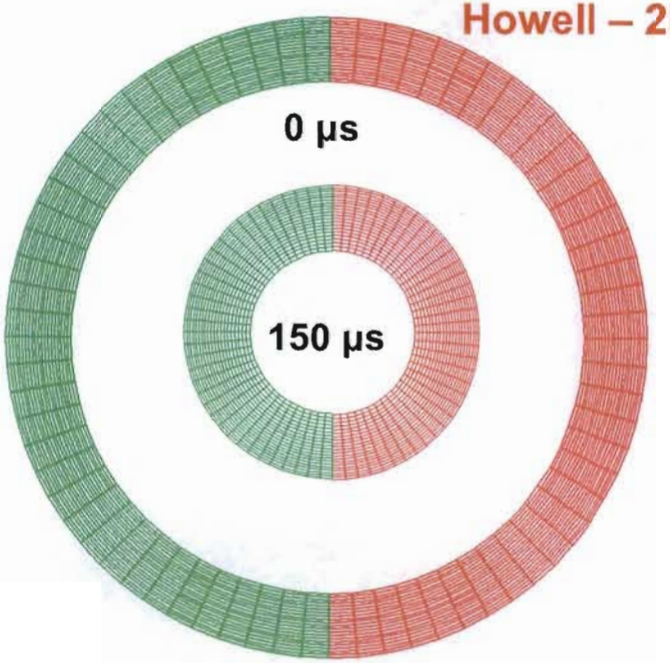
$$\sum_i^z \mathbf{N}^i = 0$$

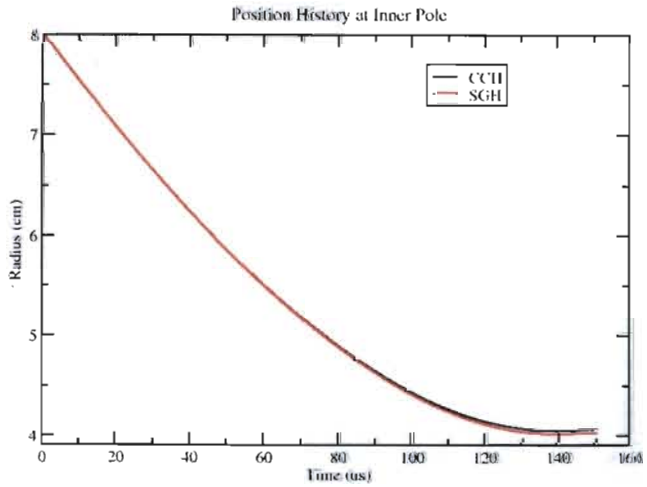
and that about a point is

$$\sum_i^p \mathbf{N}^i = 0$$

The Howell (2Dxy) and Verney (3D) problems demonstrate both multi-dimensional and strength capabilities

Howell – 2Dxy





Elastic-plastic shell coasts inward until it stops

- 4 cm cylindrical
- 3 cm spherical

Initial velocity field is divergence-free

$$u(r) = u_0 \left(\frac{R_{outer}}{r} \right)^{\alpha - 1}$$

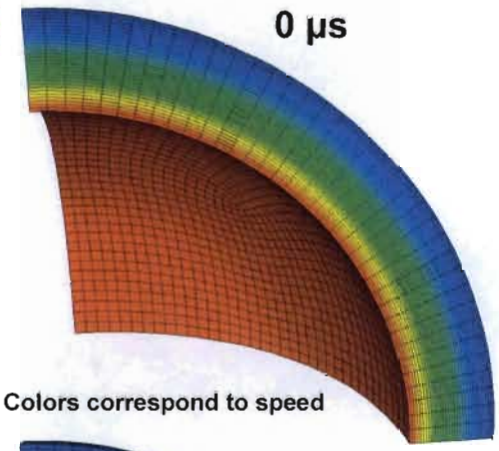
Solid model

- Generic hypo-elastic plastic

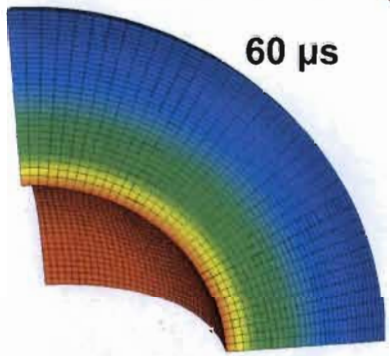
Hugoniot

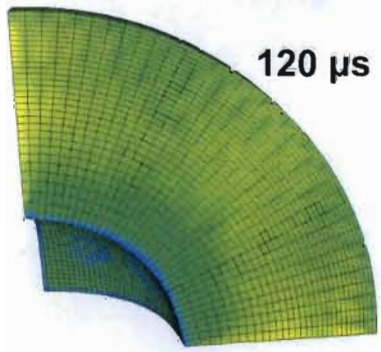
- Approximated by Dukowicz form

Verney – 3D



Colors correspond to speed



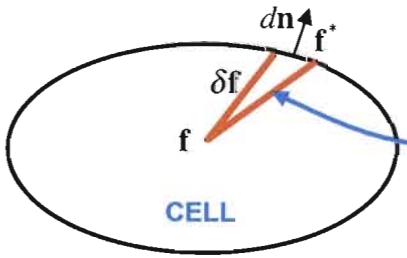


The mimetic approach begins with a conservative finite volume method

Differential $\rho \frac{df}{dt} = \nabla \cdot \mathbf{f}$

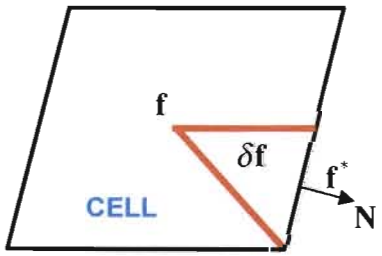
Integral $M\dot{f} = \oint d\mathbf{n} \cdot \mathbf{f}^*$

Cast the evolution equations in integral (not differential) form



Second-order requires in-cell gradients

Finite volume $M\dot{f} = \sum_i \mathbf{N}_i \cdot \mathbf{f}_i^*$



Implement as finite volume integrals

Mass constant $\dot{M} = 0$ ← Lagrange

Strain $M\dot{\gamma} = \oint d\mathbf{n}\,\mathbf{u}^*$ ← Velocity

Momentum $M\dot{\mathbf{u}} = \oint d\mathbf{n} \cdot \sigma^*$ ← Stress

Total energy $M\dot{j} = \oint d\mathbf{n} \cdot \mathbf{j}^*$ ← Total energy flux

Entropy

etc.

Main CCH challenge is the determination of the * surface fluxes

To determine the surface fluxes, we must consider more than the evolution equations

Finite volume

Mass

$$\rho\dot{\gamma} = \nabla\mathbf{u}$$

Strain

Momentum

$$\rho\dot{\mathbf{u}} = \nabla\cdot\sigma$$

Total energy

$$\rho\dot{j} = \nabla\cdot\left(\sigma\cdot\mathbf{u}\right)$$

$$\dot{M}_z = 0$$

$$M_z\dot{\gamma}_z = \sum_i^z \mathbf{N}^i\,\mathbf{u}_s^i$$

$$0 = \sum_i^p \mathbf{N}^i\,\mathbf{u}_s^i$$

Evolution

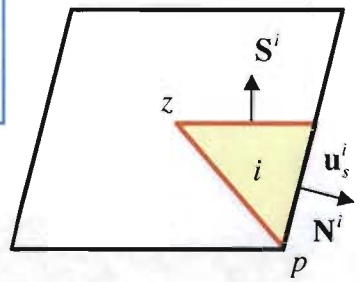
$$M_z\dot{\mathbf{u}}_z = \sum_i^z \mathbf{N}^i\cdot\sigma_s^i$$

Conservation

$$0 = \sum_i^p \mathbf{N}^i\cdot\sigma_s^i$$

$$M_z\dot{j} = \sum_i^z \mathbf{N}^i\cdot\sigma_s^i\cdot\mathbf{u}_s^i$$

$$0 = \sum_i^p \mathbf{N}^i\cdot\sigma_s^i\cdot\mathbf{u}_s^i$$



Ancillary equations

Curl & divergence identities

$$\nabla\times\left(\nabla\mathbf{u}\right) = 0$$
$$\nabla\cdot\left(\nabla\times\mathbf{u}\right) = 0$$
$$\nabla\times\left(\nabla\cdot\sigma\right) = 0$$
$$\nabla\cdot\left(\nabla\times\sigma\right) = 0$$

$$\nabla_p\times\sum_i^z \mathbf{N}^i\,\mathbf{u}_s^i = 0$$

$$\nabla_p\cdot\sum_i^z \mathbf{N}^i\times\mathbf{u}_s^i = 0$$

$$\nabla_p\times\sum_i^z \mathbf{N}^i\cdot\sigma_s^i = 0$$

$$\nabla_p\cdot\sum_i^z \mathbf{N}^i\times\sigma_s^i = 0$$

etc.

Geometric volume compatibility

$$\rho\dot{v} = \nabla\cdot\mathbf{u}$$

$$M_z\dot{v}_z = \sum_i^z \mathbf{N}^i\cdot\mathbf{u}_s^i = geo.vol.chg.$$

Angular momentum

$$\dot{\mathbf{L}}_z = \sum_i^z \mathbf{r}_s^i\times\left(\mathbf{N}^i\cdot\sigma_s^i\right)$$

$$0 = \sum_i^p \mathbf{r}_s^i\times\left(\mathbf{N}^i\cdot\sigma_s^i\right)$$

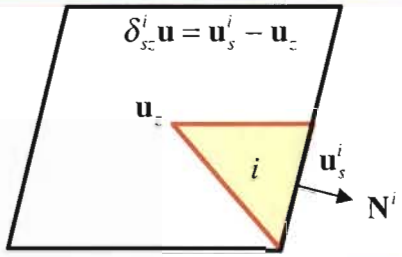
Second law of thermodynamics

To incorporate the Second Law into the discretization, we must first decompose the energy equation

Alternative variable (not a linearization)

$$\sigma_s = \sigma_z + \delta_{sz}\sigma$$

$$\mathbf{u}_s = \mathbf{u}_z + \delta_{sz}\mathbf{u}$$



$$M_z \dot{j}_z = \sum_i^z \mathbf{N}^i \cdot \left(\sigma^i_s \cdot \mathbf{u}^i_s\right)$$
$$= \left[\sum_i^z \mathbf{N}^i \cdot \sigma^i_s\right] \cdot \mathbf{u}_z + \sigma_z : \left[\sum_i^z \mathbf{N}^i \mathbf{u}^i_s\right] + \left[\sum_i^z \mathbf{N}^i \cdot \left(\delta^i_{sz}\sigma \cdot \delta^i_{sz}\mathbf{u}\right)\right]$$
$$= M_z\left[\dot{k}_z + \dot{w}_z + \dot{d}_z\right]$$

Total energy

Kinetic energy

Internal energy

$$\dot{e}_z = \begin{cases} \dot{j}_z - \dot{k}_z \\ \dot{w}_z + \dot{d} \end{cases}$$

$$\dot{k}_z = \frac{1}{M_z}\left[\sum_i^z \mathbf{N}^i \cdot \sigma^i_s\right] \cdot \mathbf{u}_z$$
$$= \dot{\mathbf{u}}_z \cdot \mathbf{u}_z$$

Momentum equation

"Work"

$$\dot{w}_z = \frac{1}{M_z}\sigma_z : \left[\sum_i^z \mathbf{N}^i \mathbf{u}^i_s\right]$$
$$= \sigma_z : \dot{\gamma}$$

Strain equation

"Dissipation"

$$\dot{d}_z = \frac{1}{M_z}\sum_i^z \mathbf{N}^i \cdot \left(\delta^i_{sz}\sigma \cdot \delta^i_{sz}\mathbf{u}\right)$$

The Second Law

In a closed system $(\dot{j} = 0)$, the kinetic energy must dissipate into the internal, suggesting

$$\dot{d}_z \geq 0$$

It is sufficient (but not necessary) that

$$d^i = \hat{\mathbf{n}}^i \cdot \delta^i_{sz}\sigma \cdot \delta^i_{sz}\mathbf{u} \geq 0$$

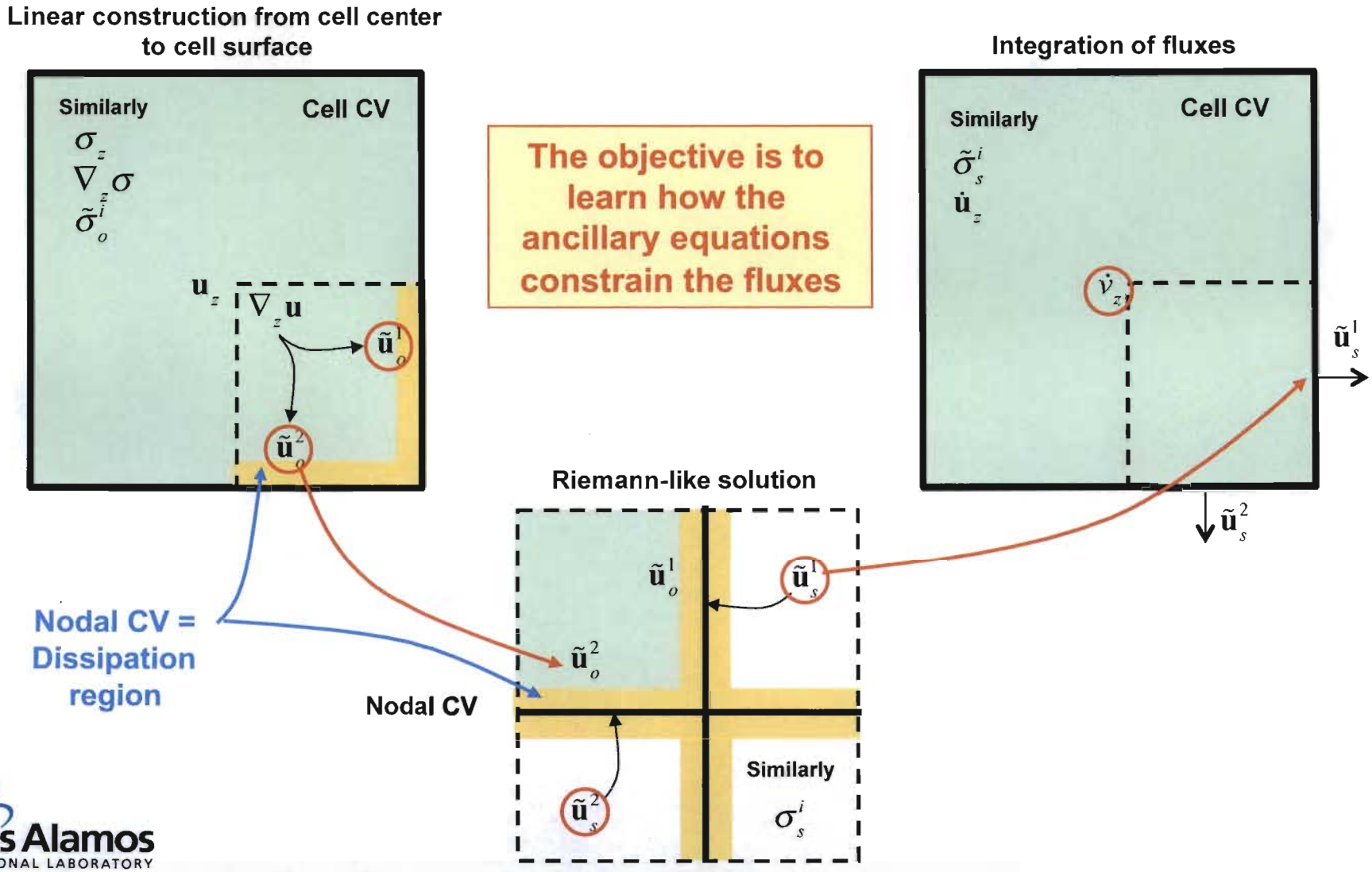
which is the "entropy condition"

Dissipation models similar to

$$\hat{\mathbf{n}}^i \cdot \delta^i_{sz}\sigma \sim \mu\delta^i_{sz}\mathbf{u}$$

are invoked to satisfy the entropy condition

Algorithmic roadmap
We begin with a description in terms of surface fluxes



Cells are divided into an equilibrium "core" and possibly non-equilibrium "shell" regions

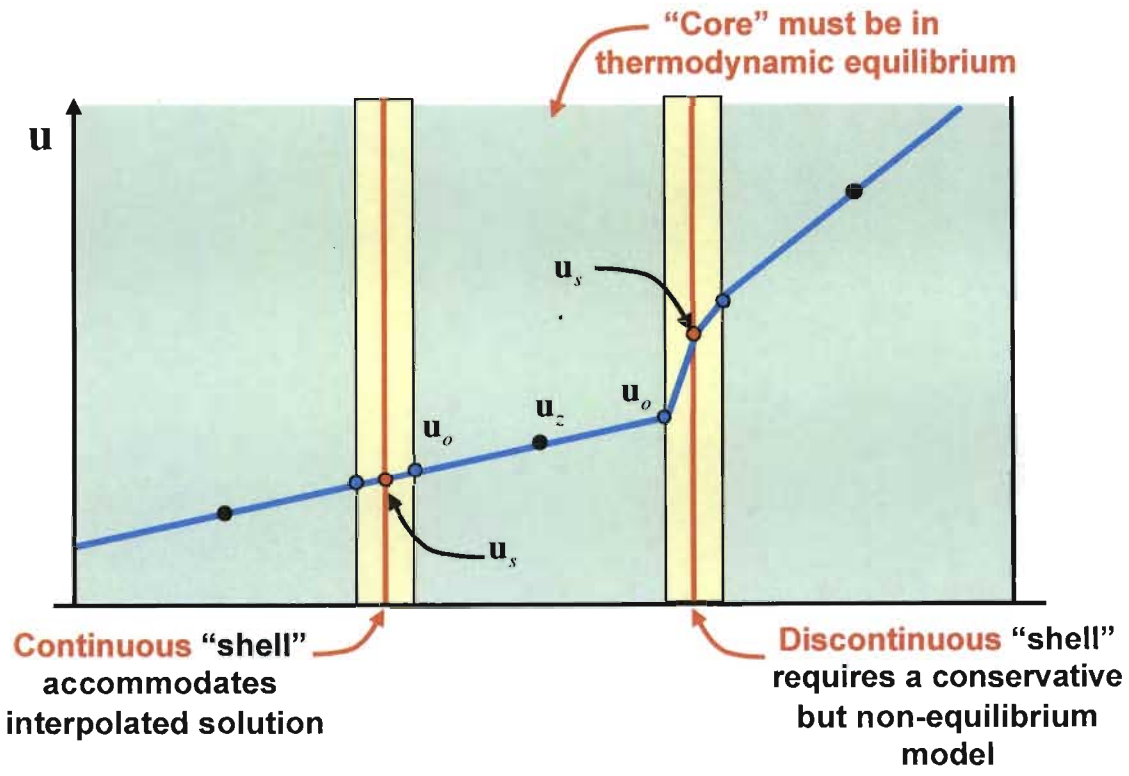
The finite volume integrals conserve momentum, but do not specify a functional form for velocity

Within the core, the velocity field can be a linear function through the center of mass (CM), without altering the cell average

Slopes within cells are determined by fitting a linear solution to adjacent cells

Continuity of the function and slope between cells determines the discontinuities (jumps)

These must be treated with a non-equilibrium model



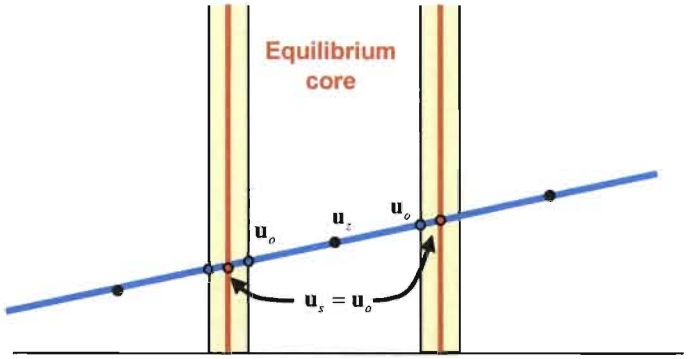
Velocity and stress cannot be distributed independently in the core without giving rise to unintended dissipation

The core is not a modeling abstraction, but represents the state of the cell under conditions of smooth flow when there should be no entropy production

Since stress is not conserved, what functional form should it have?

A linear distribution is often assumed

The requirement for thermodynamic equilibrium in the core places constraints on this



In the absence of discontinuities, the surface fluxes reduce to

$$\sigma_s^i \to \sigma_o^i \quad \& \quad \mathbf{u}_s^i \to \mathbf{u}_o^i$$

the numerical entropy condition for the cell should vanish

$$\dot{D}_z = \sum_i^z \mathbf{N}^i \cdot \left(\sigma_o^i - \sigma_z^i\right) \cdot \left(\mathbf{u}_o^i - \mathbf{u}_z^i\right) \to 0$$

Since this is the divergence of

$$\mathbf{d}_z = \left(\sigma_o^i - \sigma_z^i\right) \cdot \left(\mathbf{u}_o^i - \mathbf{u}_z^i\right)$$

the integral will vanish if

$$\mathbf{d}_z = constant$$

at the surface of the cell

If velocity is linear, then the stress is constrained by the above relationship

In our calculations, we satisfy this by assuming a constant stress in the cell

$$\sigma_o^i = \sigma_z^i$$

The curl and divergence identities constrain the fluxes on the nodal control volume - consider the curl of the velocity gradient

We need to show that the difference equations satisfy

$$\nabla_z \times \nabla_p \mathbf{u}_o = 0$$

The second-order operators are evaluated on a staggered grid

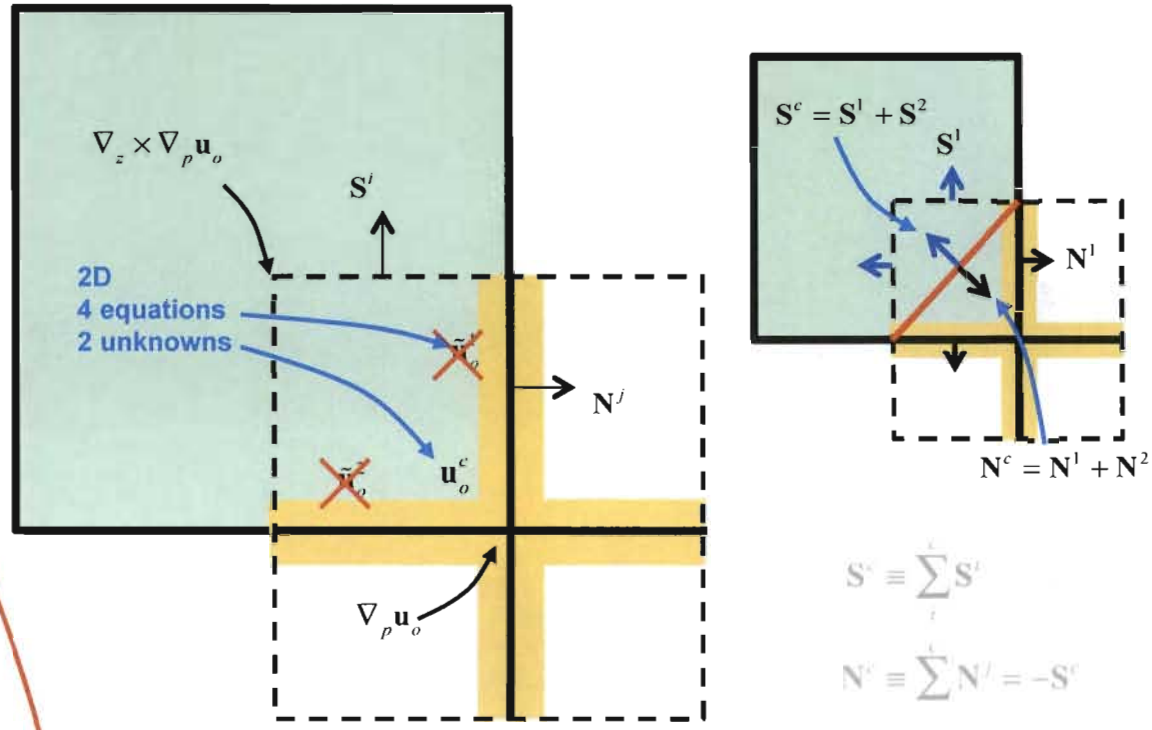
$$\nabla_z \times \nabla_p \mathbf{u}_o \rightarrow \frac{1}{V_z} \sum_c \frac{1}{V_{p(c)}} \left[\mathbf{N}^c \times \left(\sum_j^c \mathbf{S}^j \mathbf{u}_o^j \right) \right]$$

If there exists a corner velocity such that

$$\mathbf{S}^c \mathbf{u}_o^c = \sum_j^c \mathbf{S}^j \tilde{\mathbf{u}}_o^j$$

then each term vanishes because $\mathbf{N}^c$ & $\mathbf{S}^c$ are parallel

$$\mathbf{N}^c \times \left(\sum_j^c \mathbf{S}^j \tilde{\mathbf{u}}_o^j \right) \rightarrow \mathbf{N}^c \times \mathbf{S}^c \mathbf{u}_o^c$$



$$\mathbf{S}^c \equiv \sum_j^c \mathbf{S}^j$$

$$\mathbf{N}^c \equiv \sum_j^c \mathbf{N}^j = -\mathbf{S}^c$$

The terms vanish if the fluxes are replaced by a corner velocity

$$\mathbf{u}_o^j \neq \tilde{\mathbf{u}}_o^j$$

$$\mathbf{u}_o^j = \mathbf{u}_o^c \quad \forall j \in c$$

Then

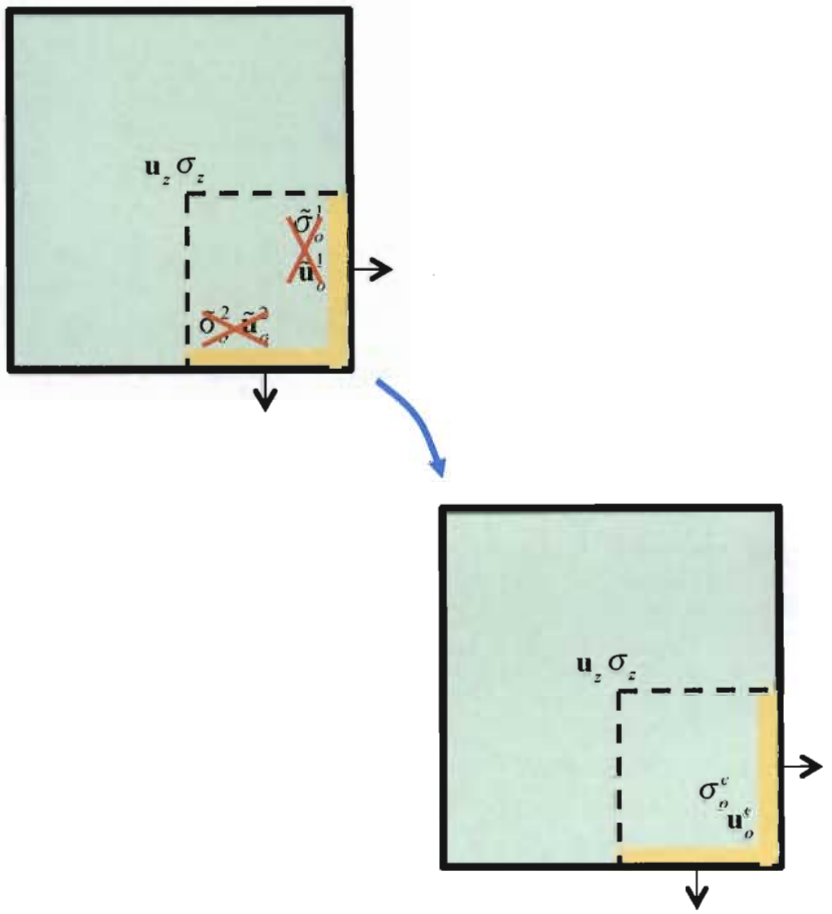
$$\nabla_z \times \nabla_p \mathbf{u}_o = 0$$

This means that the fluxes cannot be specified independently and some information must be discarded

$\mathbf{u}_o^c$ is the fundamental quantity

Nodal control volume: Constraints imposed by the ancillary equations change the conceptual picture of the differencing scheme

Relation	Constraint
$\nabla_z \times \left(\nabla_p \mathbf{u}_o \right) = 0$	$\mathbf{u}_o^j \rightarrow \mathbf{u}_o^c$
$\nabla_z \cdot \left(\nabla_p \times \mathbf{u}_o \right) = 0$	$\mathbf{u}_o^j \rightarrow \mathbf{u}_o^c$
Rotational equilibrium	σ *symmetric*
$\nabla_z \times \left(\nabla_p \cdot \sigma_o \right) = 0$	$\sigma_o^j \rightarrow \sigma_o^c$ *symmetric*
$\nabla_z \cdot \left(\nabla_p \times \sigma_o \right) = 0$	$\sigma_o^j \rightarrow \sigma_o^c$ *symmetric*
Thermodynamic equilibrium in core	$\left(\sigma_o^i - \sigma_z^i \right) \cdot \left(\mathbf{u}_o^i - \mathbf{u}_z^i \right) = constant$



First order case

$\mathbf{u}_o^c \rightarrow \mathbf{u}_z$

We will compare 2 methods to calculate the corner velocity – neither of which is completely satisfactory (see test problems)

Divergence method

This method demands only consistency with the divergence integral

$$V_z \nabla \cdot \mathbf{u} = \sum_i^z \mathbf{N}^i \cdot \mathbf{u}_o^c$$

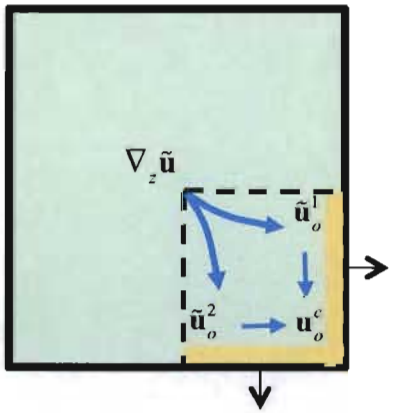
$$= \sum_i^z \mathbf{N}^i \cdot \tilde{\mathbf{u}}_o^i$$

This results in a simple set of equations

$$\hat{\mathbf{n}}^i \cdot \mathbf{u}_o^c = \hat{\mathbf{n}}^i \cdot \tilde{\mathbf{u}}_o^i$$

that is easily solved in each corner

Note that tangential information is discarded

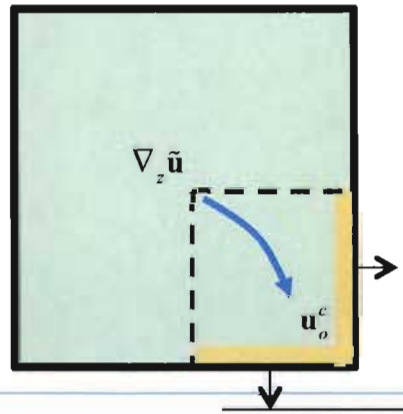


Gradient method

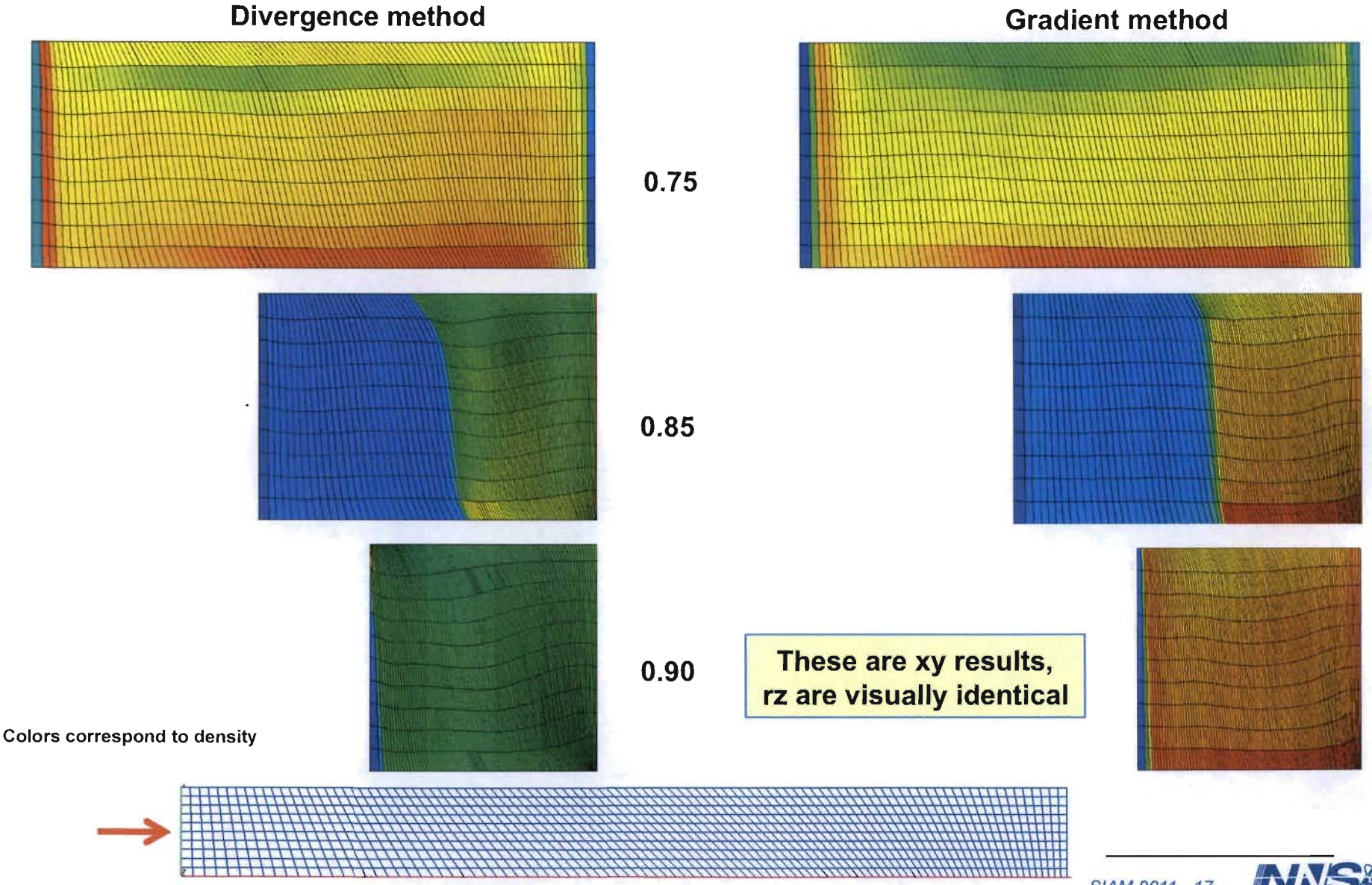
From monotonic reconstruction directly calculate

$$\mathbf{g}_z = \nabla_z \tilde{\mathbf{u}}$$

$$\mathbf{u}_o^c = \mathbf{u}_z + \left(\mathbf{x}_p - \mathbf{x}_z\right) \cdot \mathbf{g}_z$$

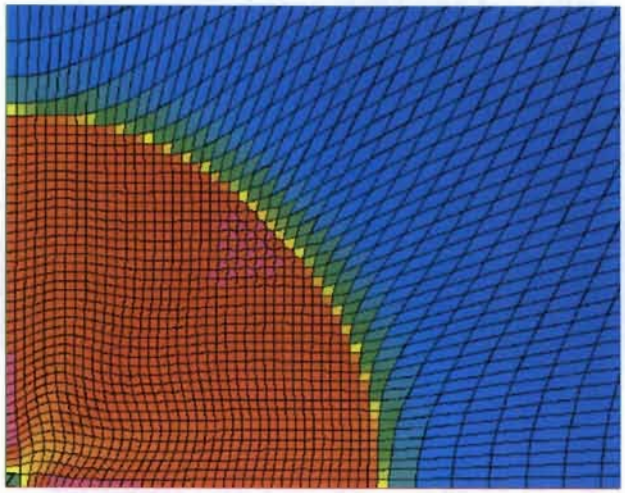


The Gradient method performs significantly better on the Saltzman problem - but there are issues (later)

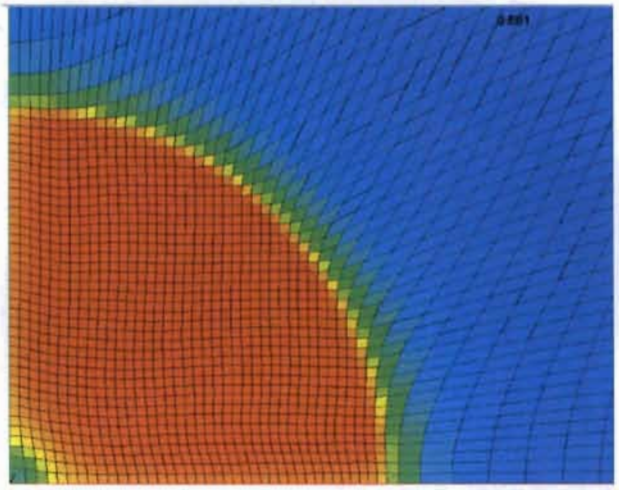


The Gradient method also significantly improves results on the Noh (xy) problem on a box grid

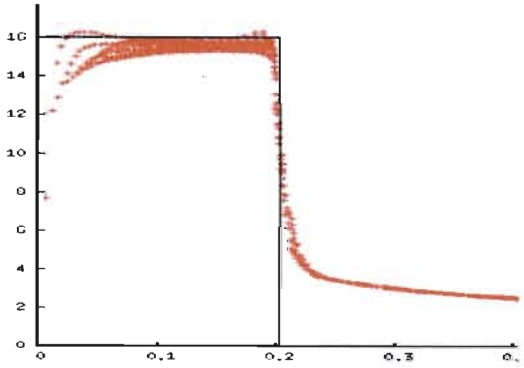
Divergence method



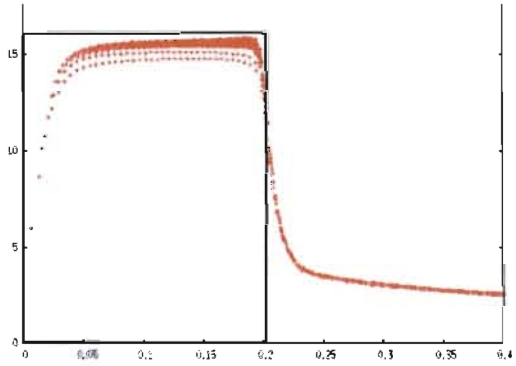
Gradient method



Density



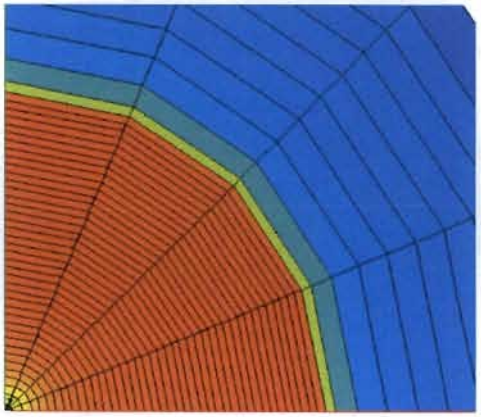
Density vs Distance



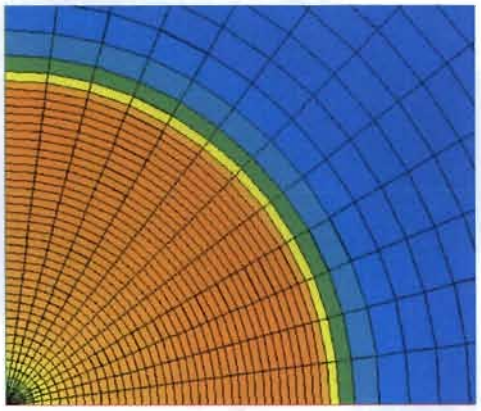
However, the Gradient results were disappointing on the Noh (xy) problem on a polar grid

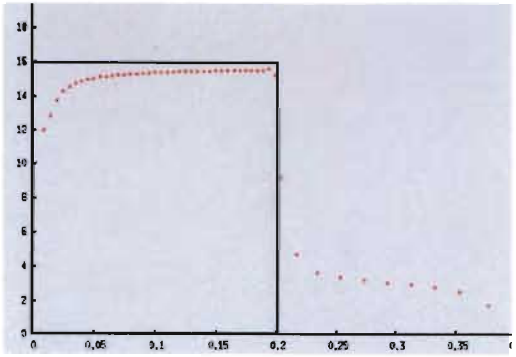
Divergence method good even at poor angular resolution

Gradient method converges with increasing angular resolution

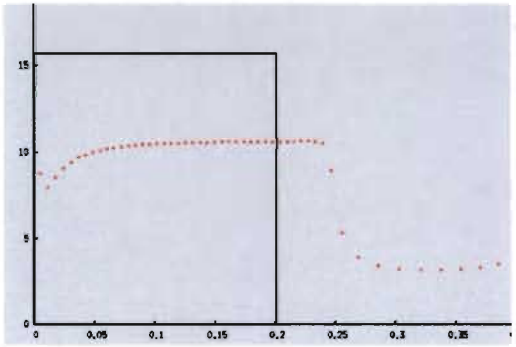


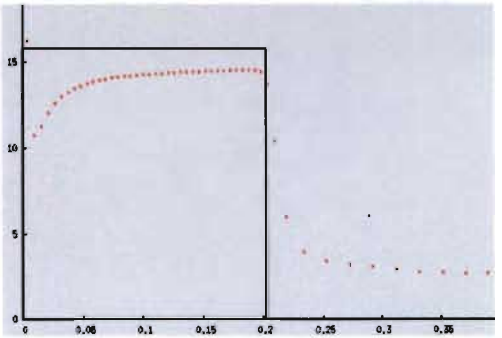
Density





Density vs Distance





The curl and divergence identities also constrain the fluxes on the cell control volume – consider the curl of the momentum equation

We need to show that the difference equations satisfy $\rho\dot{\mathbf{u}} = \nabla\bullet\sigma$

$$\nabla\times\left(\rho\dot{\mathbf{u}}\right) = \nabla\times\nabla\bullet\sigma = 0$$

The second-order operators are evaluated on a staggered grid

$$\nabla_p\times\left(\nabla_z\cdot\sigma\right)\rightarrow\frac{1}{V_p}\sum_c^p\frac{1}{V_{z(c)}}\left[\mathbf{S}^c\times\left(\sum_j^c\mathbf{N}^j\cdot\tilde{\sigma}_s^j\right)\right]$$

If we can show there exists a corner stress tensor such that

$$\mathbf{N}^c\cdot\sigma^c = \sum_j^c\mathbf{N}^j\cdot\tilde{\sigma}_s^j$$

then the stress factors out and each term vanishes

$$\mathbf{S}^c\times\left(\sum_j^c\mathbf{N}^j\cdot\tilde{\sigma}_s^j\right)\rightarrow\mathbf{S}^c\times\mathbf{N}^c\cdot\sigma^c = 0$$

because $\mathbf{N}^c$ & $\mathbf{S}^c$ are parallel

The terms vanish if the tensor is **non-symmetric**. Then

$$\nabla_p\times\left(\nabla_z\cdot\sigma\right) = 0$$

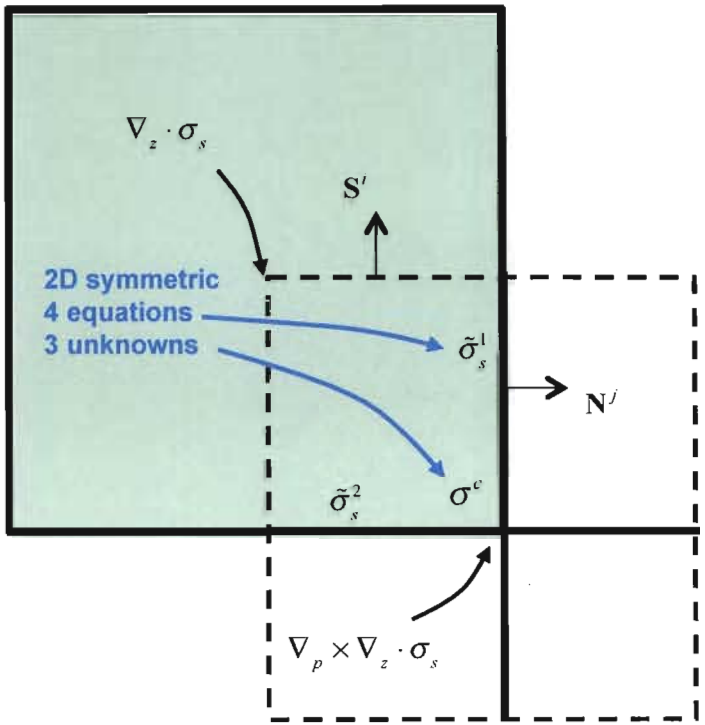
for

$$\sigma_s^j = \tilde{\sigma}_s^j$$

If we require **symmetry**, the system is over determined and the terms vanish only if we replace the fluxes by a corner stress

$$\sigma_s^j \neq \tilde{\sigma}_s^j$$

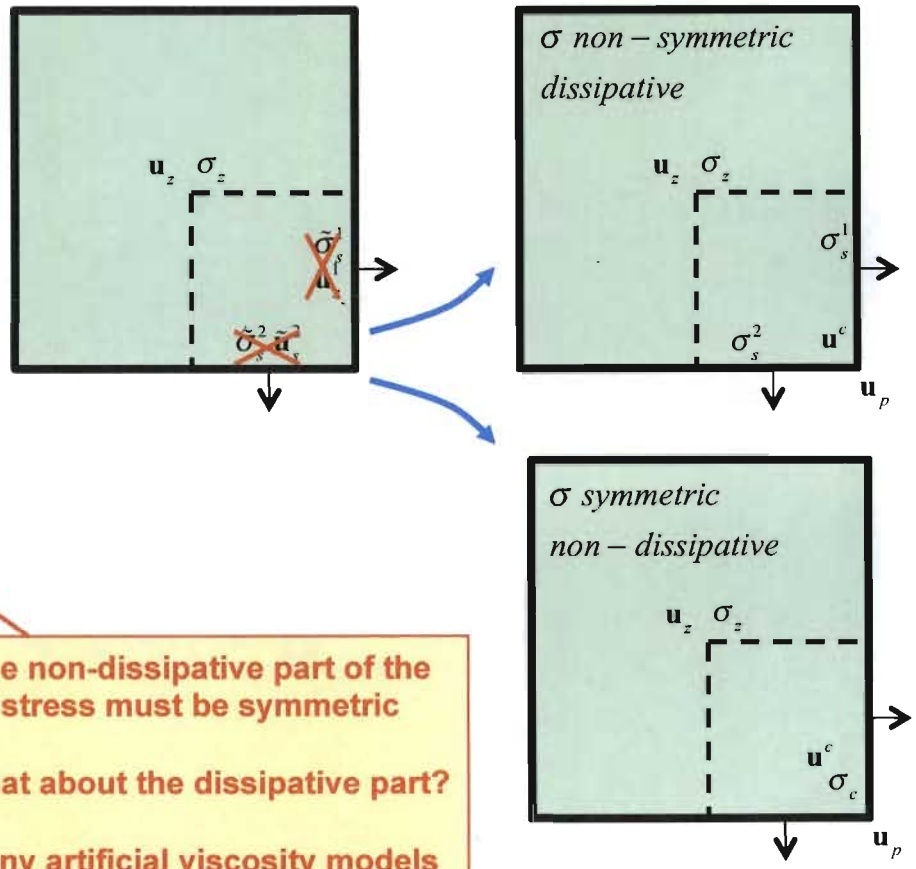
$$\sigma_s^j = \sigma^c \quad \forall j\in c$$



To satisfy rotational equilibrium, at least the **non-dissipative** part of the stress must be symmetric

Cell control volume: Constraints imposed by the ancillary equations change the conceptual picture of the differencing scheme

Relation	Constraint
Geometric volume compatibility	$\mathbf{u}_s \rightarrow \hat{\mathbf{n}}\hat{\mathbf{n}} \cdot \mathbf{u}_p$
$\nabla_p \times \left(\nabla_z \mathbf{u}_s \right) = 0$	$\mathbf{u}_s \rightarrow \mathbf{u}^c$
$\nabla_p \cdot \left(\nabla_z \times \mathbf{u}_s \right) = 0$	$\mathbf{u}_s \rightarrow \mathbf{u}^c$
Rotational equilibrium	$\sigma \; symmetric\left(S\right)$
$\nabla_p \times \left(\nabla_z \cdot \sigma_s \right) = 0$	$\sigma_s \rightarrow \begin{cases} \tilde{\sigma}_s & NS \\ \sigma^c & NS \; or \; S \end{cases}$
$\nabla_p \cdot \left(\nabla_z \times \sigma_s \right) = 0$	$\sigma_s \rightarrow \begin{cases} \tilde{\sigma}_s & NS \\ \sigma^c & NS \; or \; S \end{cases}$



The non-dissipative part of the stress must be symmetric

What about the dissipative part?

Many artificial viscosity models are NS, but theoretical justification needs work

Geometric volume compatibility (GVC) constrains not only the velocity flux $\mathbf{u}_s^i$ but also the surface area vectors $\mathbf{N}^i$

The fluxed volume change must be constrained to equal the geometric volume change of the cell

$$\Delta V_z = \sum_i^z \mathbf{N}^i \cdot \mathbf{u}_s^i$$

In plane (xy) geometry this can be accomplished by constraining

$$\mathbf{u}_s^i \rightarrow \hat{\mathbf{n}}^i \hat{\mathbf{n}}^i \cdot \mathbf{u}_p^i$$

$$\mathbf{N}^i = \frac{1}{2}\left(\mathbf{N}^n + \mathbf{N}^{n+1}\right)$$

KEY POINT

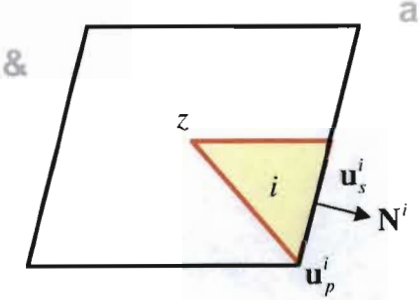
The compatible surface areas are

$$\mathbf{N}^i = \begin{cases} \mathbf{A} & 1D\,planar \\ \frac{1}{2}\left(r^{n+1} + r^n\right)\mathbf{A} & 1D\,cylindrical \\ \frac{1}{3}\left[\left(r^{n+1}\right)^2 + \left(r^n\right)^2 + \left(r^{n+1}r^n\right)\right]\mathbf{A} & 1D\,spherical \\ \frac{1}{2}\left(\mathbf{A}^{n+1} + \mathbf{A}^n\right) & 2Dxy \\ \frac{1}{6}\left[2\left(\bar{r}^{n+1}\mathbf{A}^{n+1} + \bar{r}^n\mathbf{A}^n\right) + \bar{r}^{n+1}\mathbf{A}^n + \bar{r}^n\mathbf{A}^{n+1}\right] & 2Drz \\ \frac{1}{2}\left(\mathbf{A}^{n+1} + \mathbf{A}^n\right) & 3Dxy \end{cases}$$

in which $\bar{r}^i = \frac{1}{3}\left(2r_p + r_{p\pm1}\right) = \frac{1}{3}\left(r_p + 2r_j\right)$

In curvilinear geometry, things are much more complicated, especially for axi-symmetric (rz) geometry

The problem was solved in seminal work by Whalen with later contributions from Loubere & Shashkov



and

$$\mathbf{A}^i = \begin{cases} \pm\hat{\mathbf{x}} & 1D\,planar \\ \pm\hat{\mathbf{r}} & 1D\,cylindrical \\ \pm\hat{\mathbf{r}} & 1D\,spherical \\ L^i\hat{\mathbf{n}}^i & 2Dxy \\ L^i\hat{\mathbf{n}}^i & 2Drz \\ A^i\hat{\mathbf{n}}^i & 3Dxy \end{cases}$$

$$\sum_i^z \mathbf{A}^i = 0$$

$$\sum_i^z \mathbf{N}^i \neq 0$$

Expressions in 3D are actually more complicated

1D Coggeshall problem is an example of adiabatic compression - It is a severe test of slope limiters and curvilinear formulation

The results should be flat and they are

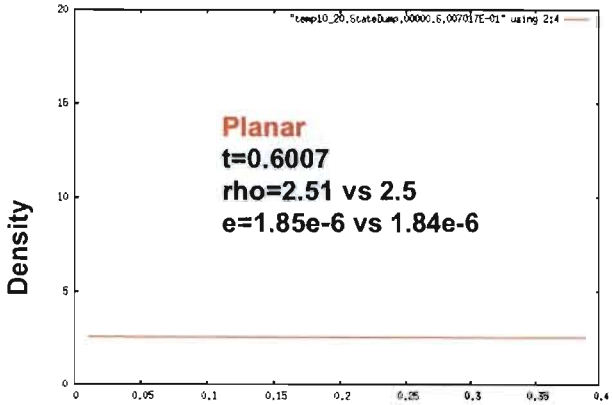
Initial conditions

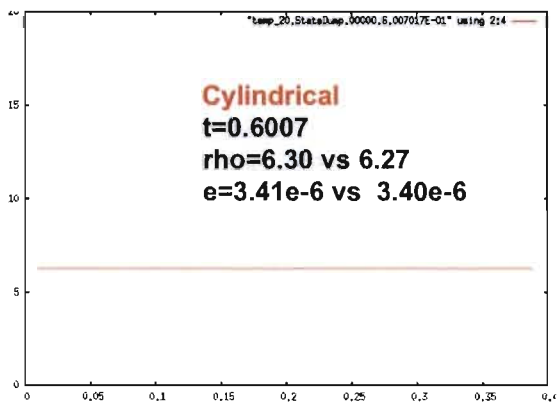
$$u_p^{00} = -x_p^{00}$$
$$\rho_z^{00} = 1$$
$$e_z^{00} = 10^{-6}$$
$$p_z^{00} = (\gamma - 1)\rho_z^{00} e_z^{00}$$
$$\gamma = 5/3$$

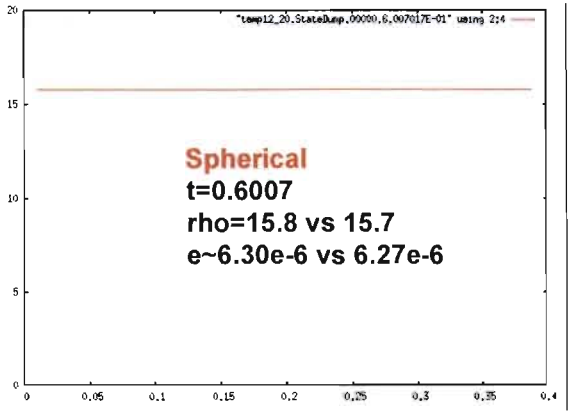
Coarse zoning: 20 cells
dtmax=1e-3

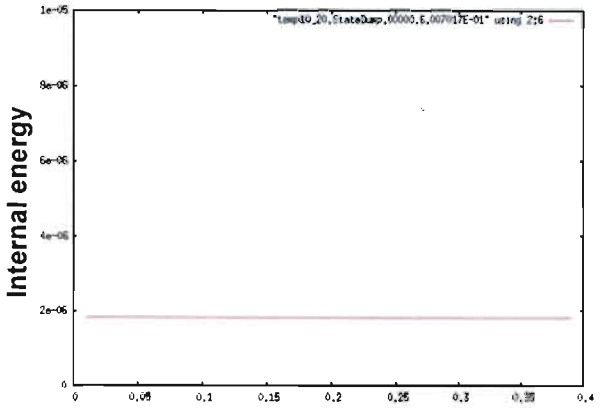
Analytic solution

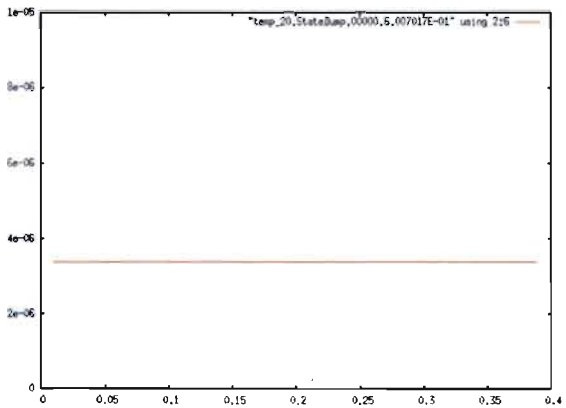
$$u_p(t) = -x_p^{00}$$
$$\rho_z(t) = \rho_z^0 / (1-t)^{\alpha}$$
$$e_z(t) = e^0 / (1-t)^{\alpha(\gamma-1)}$$
$$\alpha = \{1,2,3\}$$

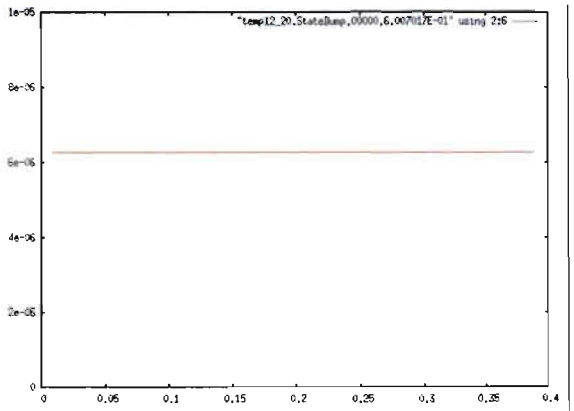










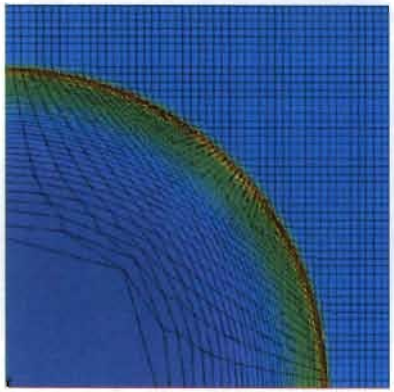


The Sedov problem is a sensitive test of the curvilinear formulation, volumetric compatibility, energy conservation, as well as robustness

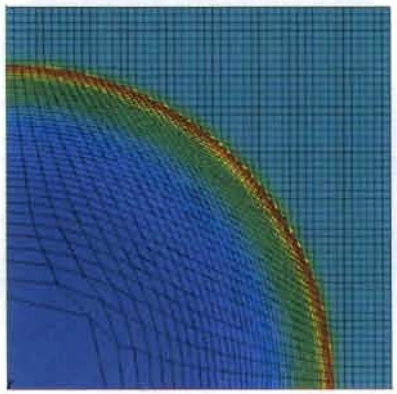
Divergence method xy result

Divergence method rz result

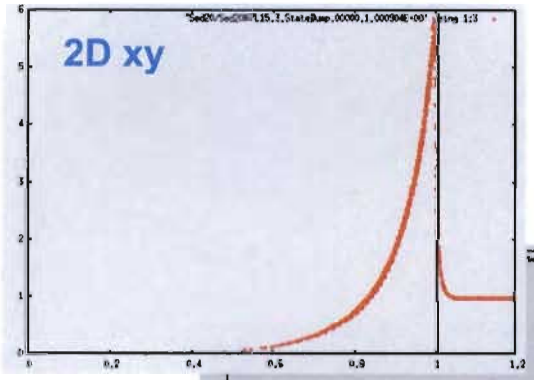
Gradient method was unable to run the problem

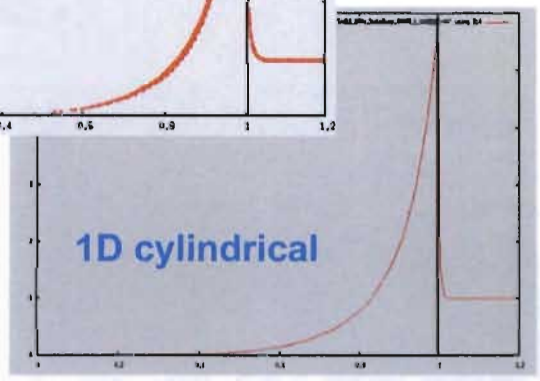


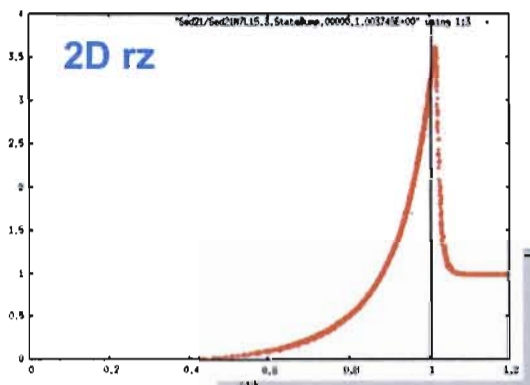
Density

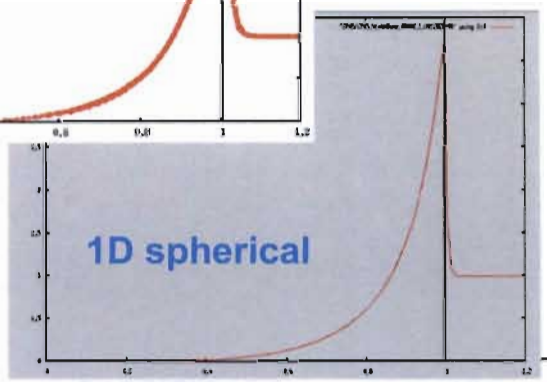


Density vs Distance









NNSA

A simplified tensor dissipation model is used for now – but should be replaced by a more physically inappropriate model

The stress jump at the discontinuity is assumed to be proportional to the strain rate

$$\delta\sigma = \dot{\sigma}\delta t = (\kappa \cdot \dot{\varepsilon})\delta t = (\kappa \cdot \varepsilon)$$

In the principal frame of the strain rate tensor, the pre-shock thickness in each direction is

$$L = a_i \delta t$$

in which a_i is the signal velocity

The deformation is

$$\delta L = \delta u_i \delta t$$

so that the strain tensor is

$$\varepsilon = \begin{bmatrix} \delta u_1/a_1 & 0 & 0 \\ 0 & \delta u_2/a_2 & 0 \\ 0 & 0 & \delta u_3/a_3 \end{bmatrix}$$

The modulus tensor is of the form

$$\kappa = \begin{bmatrix} \rho a_1^2 & 0 & 0 \\ 0 & \rho a_2^2 & 0 \\ 0 & 0 & \rho a_3^2 \end{bmatrix}$$

so the stress jump is

$$\delta\sigma = \begin{bmatrix} \rho a_1 \delta u_1 & 0 & 0 \\ 0 & \rho a_2 \delta u_2 & 0 \\ 0 & 0 & \rho a_3 \delta u_3 \end{bmatrix}$$

This can be expressed in an impedance form

$$\delta\sigma = \underline{\mu} \cdot \delta\mathbf{w}$$

In the principal frame of the strain rate tensor, the impedance tensor is

$$\underline{\mu} = \begin{bmatrix} \rho a_1 & 0 & 0 \\ 0 & \rho a_2 & 0 \\ 0 & 0 & \rho a_3 \end{bmatrix}$$

and

$$\delta\mathbf{w} = \begin{bmatrix} \delta u_1 & 0 & 0 \\ 0 & \delta u_2 & 0 \\ 0 & 0 & \delta u_2 \end{bmatrix}$$

We use a simplification that corresponds to the assumptions:

- **the most compressive strain rate is in the direction of the surface normal**
- **shear wave velocities in the tangential directions are negligible**

$$\underline{\mu} \rightarrow \begin{bmatrix} \mu = \rho a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

so that the normal stress jump can be expressed

$$\hat{\mathbf{n}}\hat{\mathbf{n}} : \delta\sigma = \mu\hat{\mathbf{n}} \cdot \delta\mathbf{u}$$

and the force density as

$$\hat{\mathbf{n}} \cdot \delta\sigma = \mu\hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \delta\mathbf{u})$$

The nodal solution is analogous to that of Maire but extended to tensors & multi-materials (not shown)

Substitute the dissipation expression

$$\mathbf{u}_s^i = \hat{\mathbf{n}}\hat{\mathbf{n}} \cdot \mathbf{u}_p^i$$

$$\hat{\mathbf{n}}^i \cdot \sigma_s^i = \hat{\mathbf{n}}^i \cdot \sigma_o^c + \mu^i \left(\mathbf{u}_p^i - \mathbf{u}_o^c \right) \cdot \hat{\mathbf{n}}^i \hat{\mathbf{n}}^i$$

into the flux conservation law

$$0 = \sum_i^p \mathbf{N}^i \cdot \sigma_s^i$$

$$= \mathbf{u}_p \cdot \sum_i^p N^i \mu^i \left(\hat{\mathbf{n}}^i \hat{\mathbf{n}}^i \right) + \sum_i^p N^i \left(\hat{\mathbf{n}}^i \cdot \sigma_o^c - \mu^i \mathbf{u}_o^c \right)$$

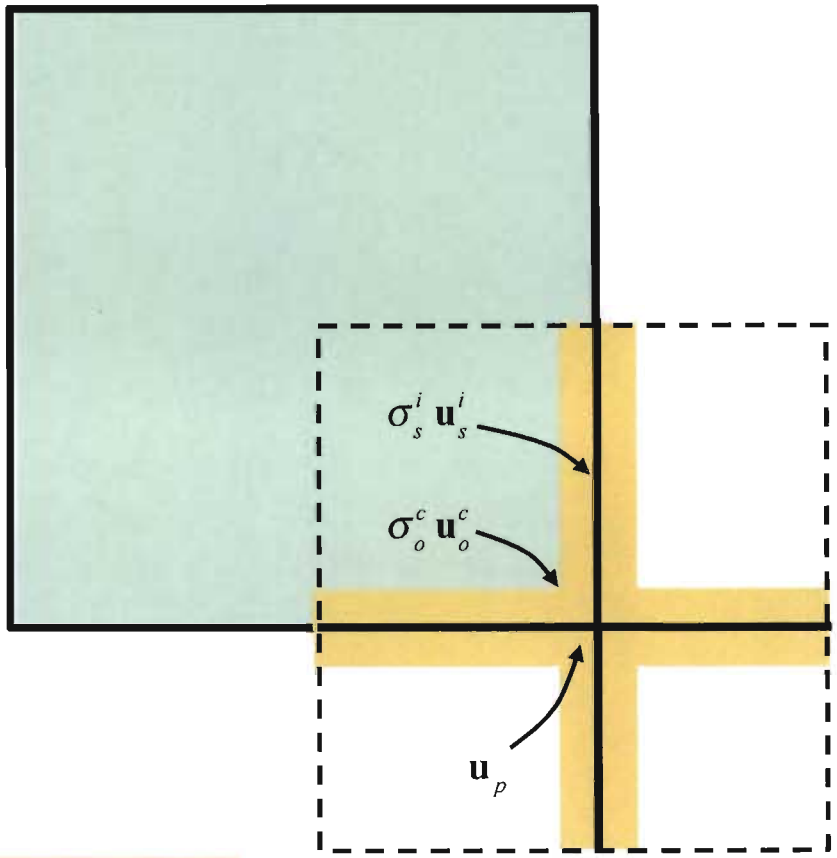
$$= [\mathbf{A}][\mathbf{u}_p] - [\mathbf{B}]$$

and solve for velocity

$$[\mathbf{u}_p] = [\mathbf{A}]^{-1}[\mathbf{B}]$$

then go back to solve for force

$$\hat{\mathbf{n}}^i \cdot \sigma_s^i = \hat{\mathbf{n}}^i \cdot \sigma_o^c + \mu^i \left(\mathbf{u}_p^i - \mathbf{u}_o^c \right) \cdot \hat{\mathbf{n}}^i \hat{\mathbf{n}}^i$$



Satisfies the rotational equilibrium requirement providing σ_o^c is symmetric

The final algorithmic details

Predictor-corrector scheme

Advance coordinates & areas

$$\mathbf{x}_z^{n+1} = \mathbf{x}_z^n + \delta t\, \mathbf{u}_p$$

$$\mathbf{N}^i \sim \frac{1}{2}\left(\mathbf{N}^n + \mathbf{N}^{n+1}\right)$$

Integrate evolution equations

Strain & volume

$$M_z \dot{\gamma}_z = \sum_i^z \mathbf{N}^i \mathbf{u}_s^i$$

$$M_z \dot{v}_z = \sum_i^z \mathbf{N}^i \cdot \mathbf{u}_s^i$$

$$v_z^{n+1} = v_z^n + \delta t\, \dot{v}_z$$

Momentum

$$M_z \dot{\mathbf{u}}_z = \sum_i^z \mathbf{N}^i \cdot \sigma_s^i$$

$$\mathbf{u}_z^{n+1} = \mathbf{u}_z^n + \delta t\, \dot{\mathbf{u}}_z$$

$$\mathbf{u}_z = \frac{1}{2}\left(\mathbf{u}_z^{n+1} + \mathbf{u}_z^n\right)$$

Total energy

$$M_z \dot{j}_z = \sum_i^z \mathbf{N}^i \cdot \sigma_s^i \cdot \mathbf{u}_s^i$$

$$j_z^{n+1} = j_z^n + \delta t\, \dot{j}_z$$

Necessary for kinetic energy definition

Calculate the energy partition

Kinetic energy

$$\dot{k}_z = \dot{\mathbf{u}}_z \cdot \mathbf{u}_z$$

Internal energy

$$\dot{e}_z = \dot{j}_z - \dot{k}_z$$

$$e_z^{n+1} = e_z^n + \delta t\, \dot{e}_z$$

Constitutive model

$$\sigma_z^{n+1} \sim \sigma_z^n + \delta t\, f\left(v, e, \gamma\right)$$

Summary: Because we are in relatively unexplored territory, we used a mimetic approach to guide the derivation of the difference scheme

The mimetic approach led to a much better understanding of what works or does not. In particular it constrained:

- Surface fluxes for cell & nodal control volumes
- Gradients in the equilibrium core
- Symmetry vs. non-symmetry of stress tensor
- Nodal velocity & entropy conditions
- Tensor impedance & entropy conditions

Historically, the weakest link in CCH has been the nodal solver

- It now lies in the 2nd order velocity construction that drives the Riemann solution
- The optimal solution remains to be determined

The test problems demonstrated:

- Elastic-plastic material: Verney, Howell
- Adiabatic flow: Coggeshall
- Robustness: pressurized ball, Saltzmann
- Multi-dimensional curvilinear formulation
  - 3D: Verney
  - 2D xy & rz: Sedov, Noh
  - 1D planar, cylindrical, spherical: Coggeshall, Sedov