

# LA-UR-13-26741

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Title: An Hourglass Control Method for Three Dimensional Lagrangian Hydrodynamics

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# An Hourglass Control Method for Three Dimensional Lagrangian Hydrodynamics

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MultiMat 2013 Conference

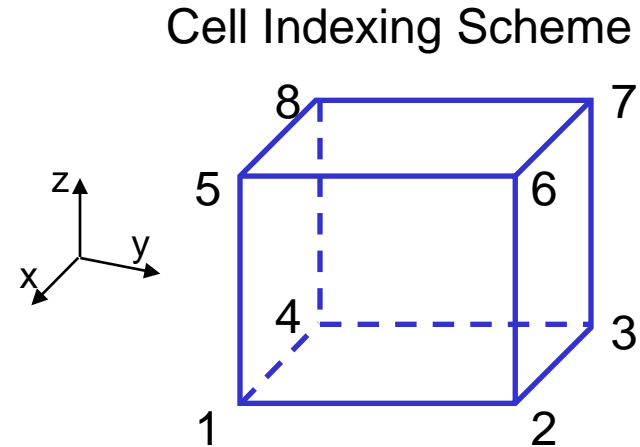
# Outline

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- Cercion 3D code description
  - Calculation of nodal forces
  - Artificial viscosity treatment
  - Energy equation
  - Time integration method
- Hourglass Control Technique
- Test Problems
  - Saltzman piston
  - 3D Sedov
  - 3D Noh
  - Verney imploding shell
- Conclusions

# The hydrodynamics in Cercion 3D is solved on a staggered grid consisting of hexahedral cells with eight nodes

- 3D Cartesian geometry
- Block structured mesh
  - Hexahedral cells with six faces
  - Fixed connectivity among mesh blocks
  - Velocities at the nodes
- Cell oriented data structures
  - C implementation
  - Fortran-type array indexing
  - Storage for nodal quantities such as position and velocity components
  - Cell-centered quantities such as density, pressure and volume



# A finite element approach is used to calculate the cell-centered velocity gradient and nodal forces

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The velocity gradient at the cell center can be calculated from the cell volume,  $V$ , and nodal velocities,  $u_{iI}$

$$\bar{u}_{i,j} = \frac{1}{V} u_{iI} B_{jI}$$

## Tensor Indexing Conventions

- Uppercase index denotes the cell node (1 thru 8)
- Lowercase index denotes spatial dimension (1 thru 3)

The nodal forces associated with a particular cell are determined from the cell-centered Cauchy stress tensor,  $T_{ij}$

$$f_{iI} = -\bar{T}_{ij} B_{jI}$$

$$\bar{T}_{ij} = \tau_{ij} - (p + q)\delta_{ij}$$

The B matrix (3 x 8) is calculated using the finite element method of Flanagan and Belytschko (1981)

For symmetric  $\bar{T}_{ij}$  on any given cell

$$\sum_{I=1}^8 f_{iI} = 0$$

ensuring momentum conservation for the scheme

# The B matrix and cell volume can be expressed in terms of the nodal coordinates using six basis vectors for the hexahedron

Basis vectors associated with shear, strain, rotation and hourglass modes

Node	$\Lambda_{1I}$	$\Lambda_{2I}$	$\Lambda_{3I}$	$\Gamma_{1I}$	$\Gamma_{2I}$	$\Gamma_{3I}$	$\Gamma_{4I}$
1	-1	-1	-1	1	1	1	-1
2	1	-1	-1	1	-1	-1	1
3	1	1	-1	-1	-1	1	-1
4	-1	1	-1	-1	1	-1	1
5	-1	-1	1	-1	-1	1	1
6	1	-1	1	-1	1	-1	-1
7	1	1	1	1	1	1	1
8	-1	1	1	1	-1	-1	-1

Note  $\Gamma_{4I}$  is not used in calculating  $C_{IJK}$

physical

hourglass

$$C_{IJK} = \frac{1}{192} e_{ijk} \left( 3\Lambda_{iI}\Lambda_{jJ}\Lambda_{kK} + \Lambda_{iI}\Gamma_{kJ}\Gamma_{jK} + \Gamma_{kI}\Lambda_{jJ}\Gamma_{iK} + \Gamma_{jI}\Gamma_{iJ}\Lambda_{kK} \right)$$

B matrix

Cell volume

$$B_{iI} = \begin{bmatrix} y_J z_K \\ z_J x_K \\ x_J y_K \end{bmatrix} C_{IJK}$$

$$V = x_I y_J z_K C_{IJK}$$

$$C_{IJK} = C_{KIJ} = C_{JKI}$$

$$\frac{\dot{V}}{V} = \bar{u}_{i,i} \text{ ensuring GCL}$$

# Nodal forces are calculated to filter the hourglass modes

- Flanagan and Belytschko (1981) method of identifying the portion of the nodal velocity field attributed to hourglass modes

$$u_{iI}^{HG} = u_{iI} - \bar{u}_i - \bar{u}_{i,j} (x_{jI} - \bar{x}_j)$$

- Margolin and Pyun (1987) method of directly filtering the nodal velocities at every cycle

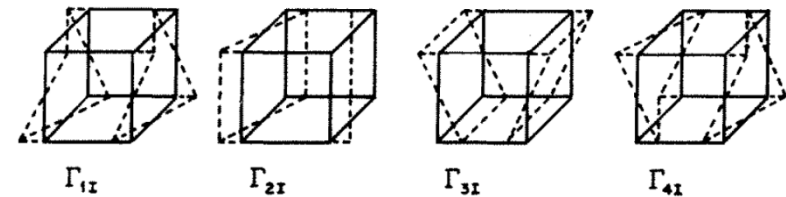
$$u_{iI}^* = u_{iI} - k u_{iI}^{HG}$$

- Nodal forces for hourglass dissipation in Cercion 3D

$$f_{iI}^{HG} = \frac{kM}{\Delta t} \left[ \bar{u}_i + \bar{u}_{i,j} (x_{jI} - \bar{x}_j) - u_{iI} \right]$$

$k$  is the single free parameter in the model

Illustration of the hourglass modes (4) associated with x component of nodal velocity field



There are a total of 12 hourglass modes for the hexahedron

Literature examples of 3D hourglass dissipation forces inspired by Margolin and Pyun

Anderson, Elliott and Pember (JPC 2004)

P. Wang (JPC 2010)

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# A non-mimetic form of the internal energy equation was implemented in Cercion 3D

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Symmetric strain rate tensor

$$\dot{\epsilon}_{i,j} = \frac{1}{2}(\bar{u}_{i,j} + \bar{u}_{j,i})$$

Anti-Symmetric strain rate tensor

$$\dot{\omega}_{i,j} = \frac{1}{2}(\bar{u}_{i,j} - \bar{u}_{j,i})$$

Semi-discrete energy equation where all quantities are cell-centered at time  $n$

$$\rho \frac{De}{Dt} = -(p + q)(\dot{\epsilon}_{1,1} + \dot{\epsilon}_{2,2} + \dot{\epsilon}_{3,3}) + \tau_{11}\dot{\epsilon}_{1,1} + \tau_{22}\dot{\epsilon}_{2,2} + \tau_{33}\dot{\epsilon}_{3,3} + 2(\tau_{12}\dot{\epsilon}_{1,2} + \tau_{23}\dot{\epsilon}_{2,3} + \tau_{31}\dot{\epsilon}_{3,1})$$

Artificial viscosity model with both linear and quadratic terms

$$q = \rho(C_1 U^2 - C_2 Ua) \quad \text{for } U < 0 \text{ otherwise } q=0$$

$$U = V^{1/3} \sum_i \dot{\epsilon}_{i,i}$$

$a$  is the sound speed

$$C_1 = 2.0$$

$$C_2 = 0.1$$



# The Lagrangian equations of motion are integrated in time with a two step Runge-Kutta method

**Advancing cell-centered stress deviators  
from time  $n$  to  $n+1$  in two steps**

$$\tau_{ij}^p = \tau_{ij}^n + \Delta t \left[ 2\mu \left( \dot{\varepsilon}_{ij}^n - \dot{\varepsilon}_{kk}^n \delta_{ij} / 3 \right) + \dot{w}_{ik}^n \tau_{kj}^n + \dot{w}_{jk}^n \tau_{ki}^n \right]$$
$$\tau_{ij}^{n+1} = \tau_{ij}^n + \frac{\Delta t}{2} \left[ 2\mu \left( \dot{\varepsilon}_{ij}^p - \dot{\varepsilon}_{kk}^p \delta_{ij} / 3 \right) + \dot{w}_{ik}^p \tau_{kj}^p + \dot{w}_{jk}^p \tau_{ki}^p + \frac{(\tau_{ij}^p - \tau_{ij}^n)}{\Delta t} \right]$$

**Advancing the nodal velocity components  
from time  $n$  to  $n+1$  in two steps**

$$u_i^p = u_i^n + \frac{\Delta t}{M} \sum_C f_i^n$$
$$u_i^{n+1} = u_i^n + \frac{\Delta t}{2M} \left( \sum_C f_i^n + \sum_C f_i^p \right)$$

**$M$  is the fixed nodal mass and  $C$  is the set  
of eight cells that surround the node**

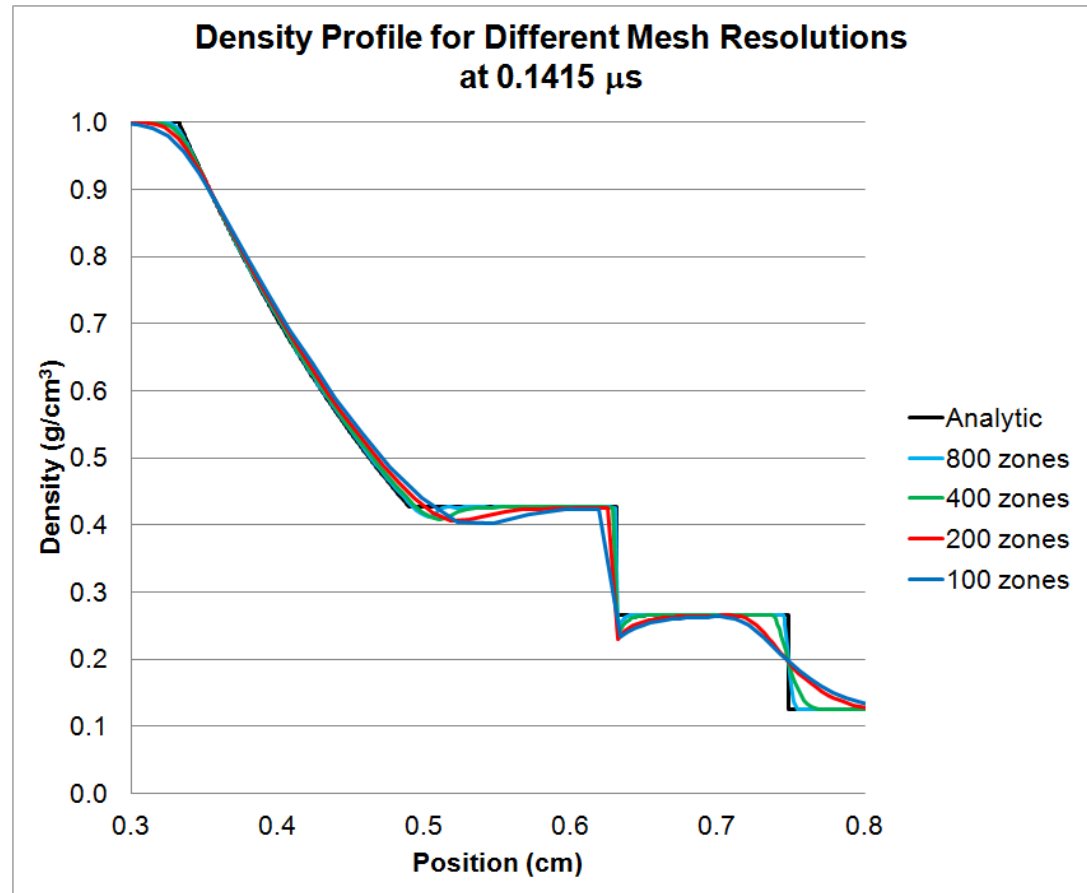
*Similar predictor-corrector update for the energy equation*

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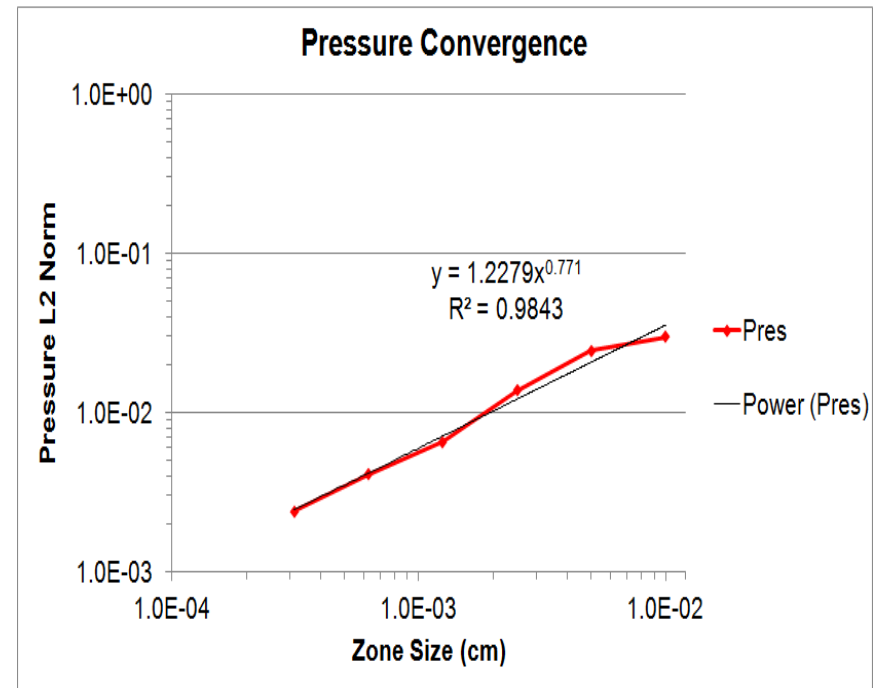
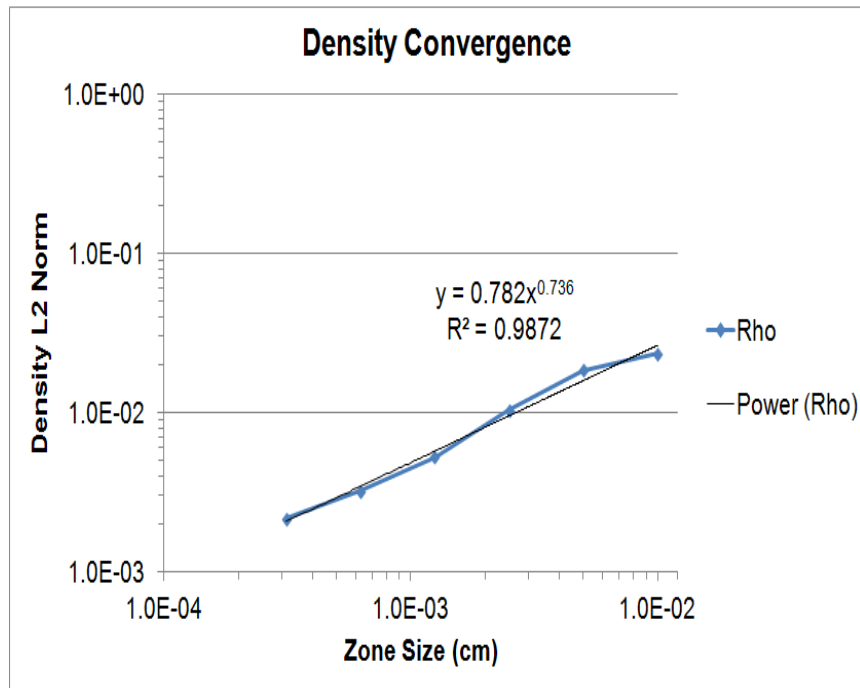
# The locations of the shock and contact discontinuity for the Sod test problem are captured by the code

## Setup

- An initial discontinuity between two ideal gas regions ( $\gamma=1.4$ )
- Region 1
  - density of 1 g/cm<sup>3</sup>
  - pressure of 1 Mbar
- Region 2
  - density of 0.125 g/cm<sup>3</sup>
  - pressure of 0.1 Mbar
- The solution is obtained at 0.1415  $\mu$ s

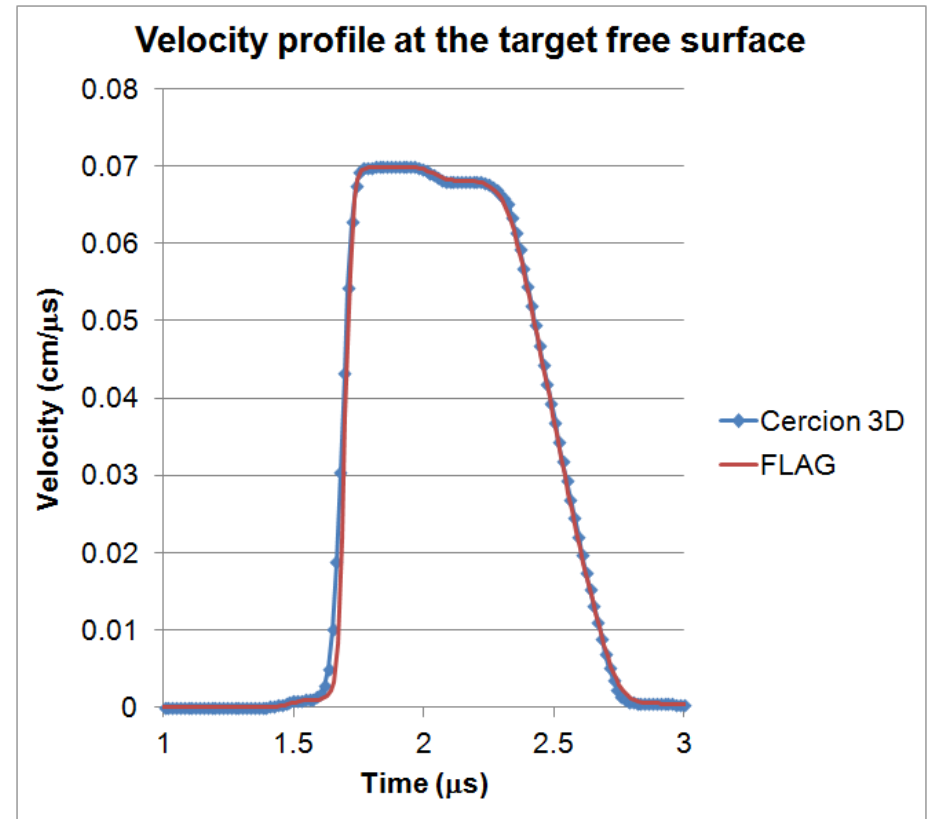


# Both pressure and density converge to approximately first order in spatial resolution



# Flyer plate problem tests the material strength treatment in the code

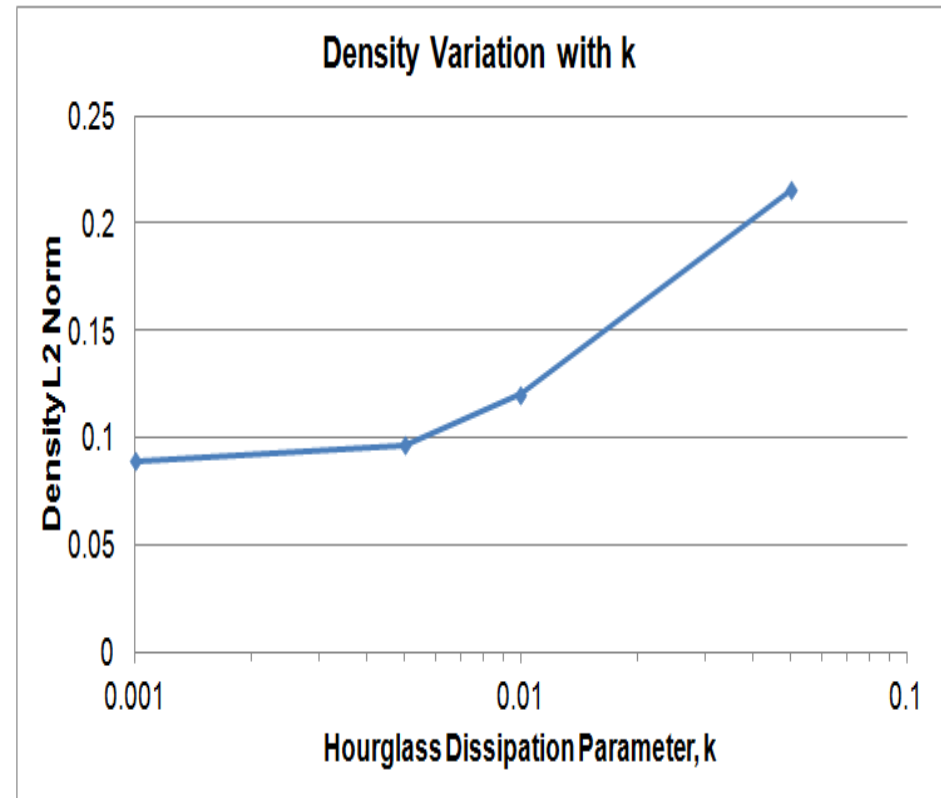
- Cylindrical geometry with 1 radial zone
- Aluminum target
  - 1 cm thick with 200 axial zones
- Aluminum projectile
  - 0.2 cm thick with 40 axial zones
- Gruneisen EOS
  - $\rho_0=2.707$
  - $C_0=0.5386$
  - $S_1=1.339$
  - $\gamma_0=1.97$
  - $b=0.48$
- Material strength model
  - yield strength of 0.0004 Mbar
  - shear modulus of 0.271 Mbar
- Companion FLAG 2D calculation



# The Saltzman piston problem provides a means to determine acceptable values of the hourglass dissipation parameter, $k$

- Caramana *et al.* (2000)
- Skewed piston
  - square cross section of 0.1 cm by 0.1 cm
  - 1 cm in length
  - Fixed velocity of 1 cm/ $\mu$ s on left boundary
  - Initial density of 1 g/cm<sup>3</sup>
- 0.7  $\mu$ s run time
- 100 x 10 x 10 cells

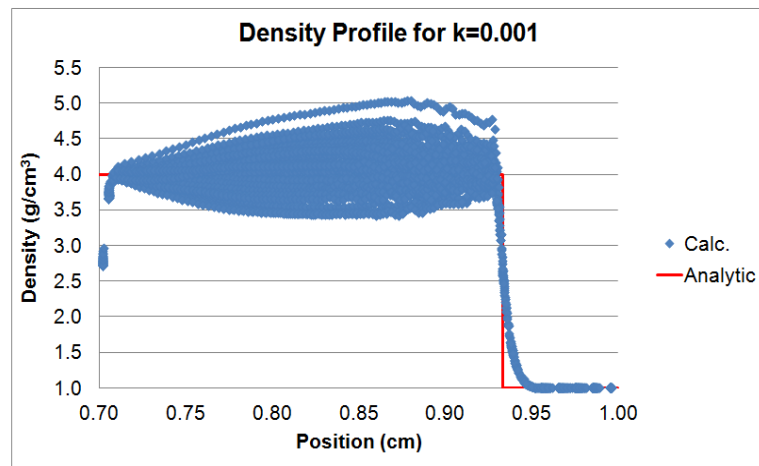
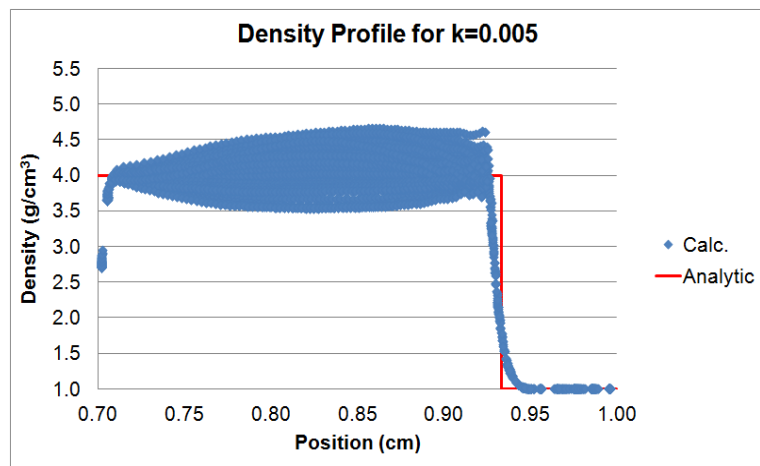
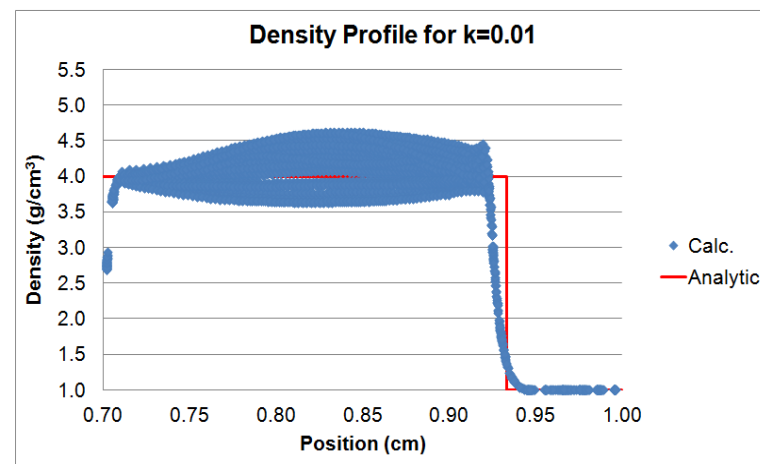
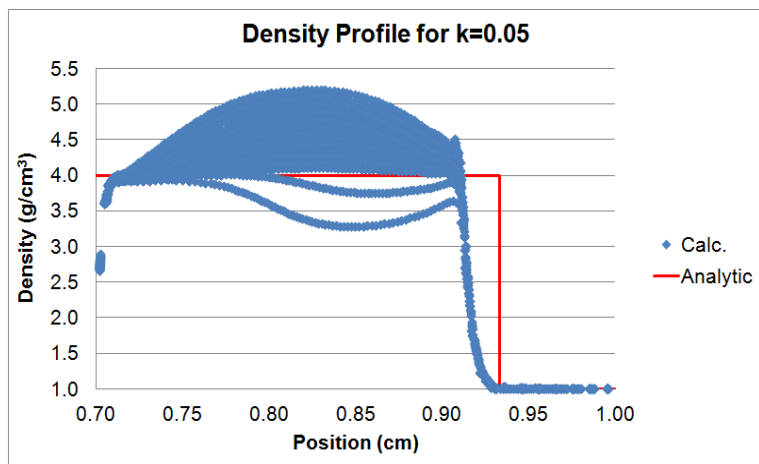
$$\begin{aligned}x &= 0.01i + 0.01(10 - k)(5 - j)/5 \sin(0.01\pi i) \quad \text{for } 0 \leq j \leq 5 \\x &= 0.01i + 0.01k(j - 5)/5 \sin(0.01\pi i) \quad \text{for } 6 \leq j \leq 10 \\y &= 0.01j \\z &= 0.01k\end{aligned}$$



*$k=0.005$  was chosen for the other test problems in this work*

# The calculated shock position is sensitive to the value of $k$

Time = 0.7  $\mu$ s

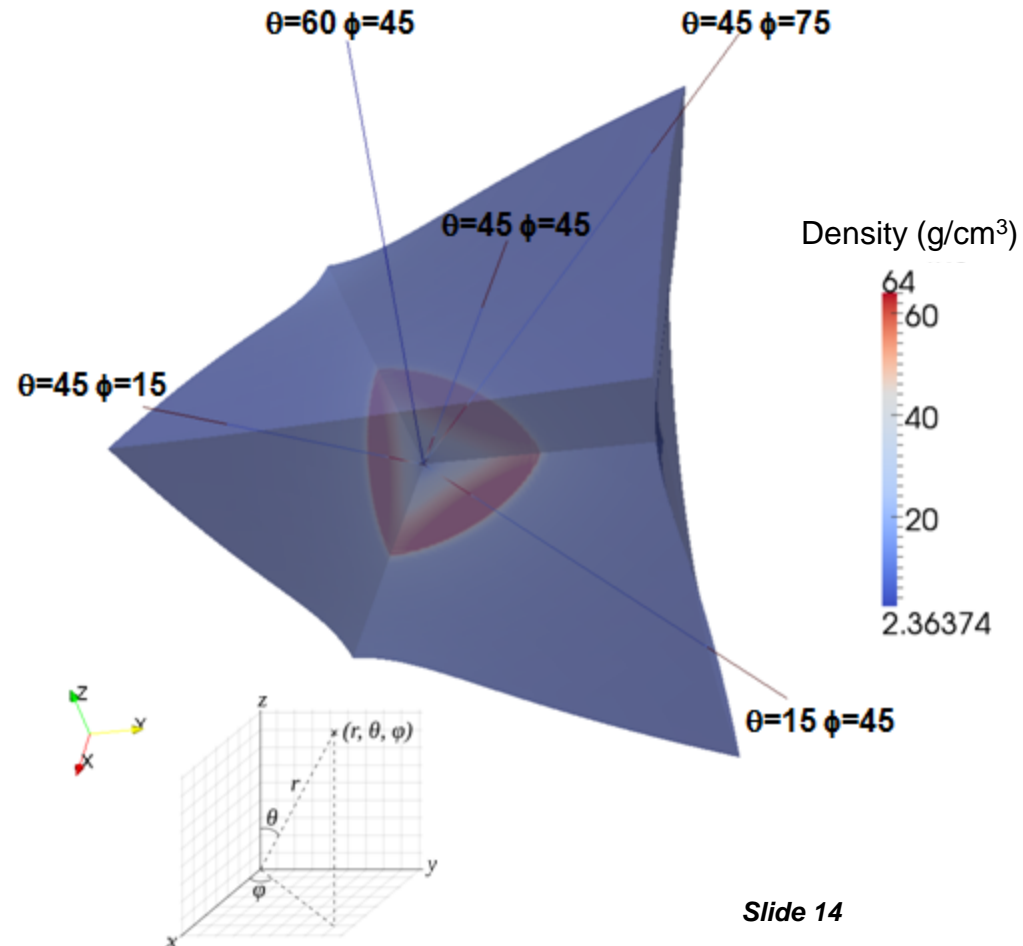


# The 3D Noh problem was simulated with Cercion 3D

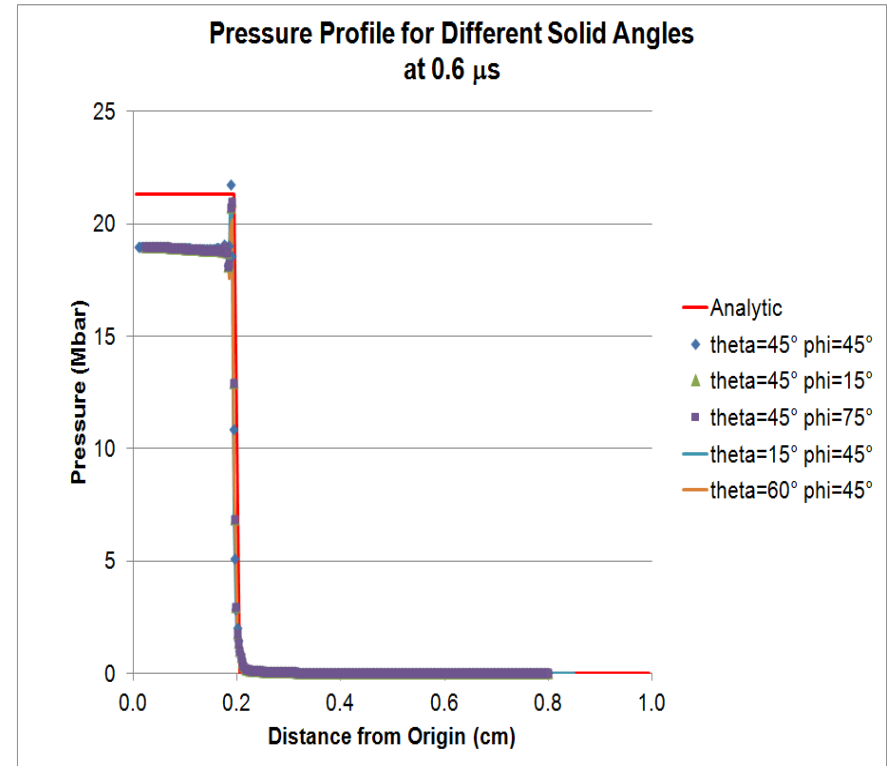
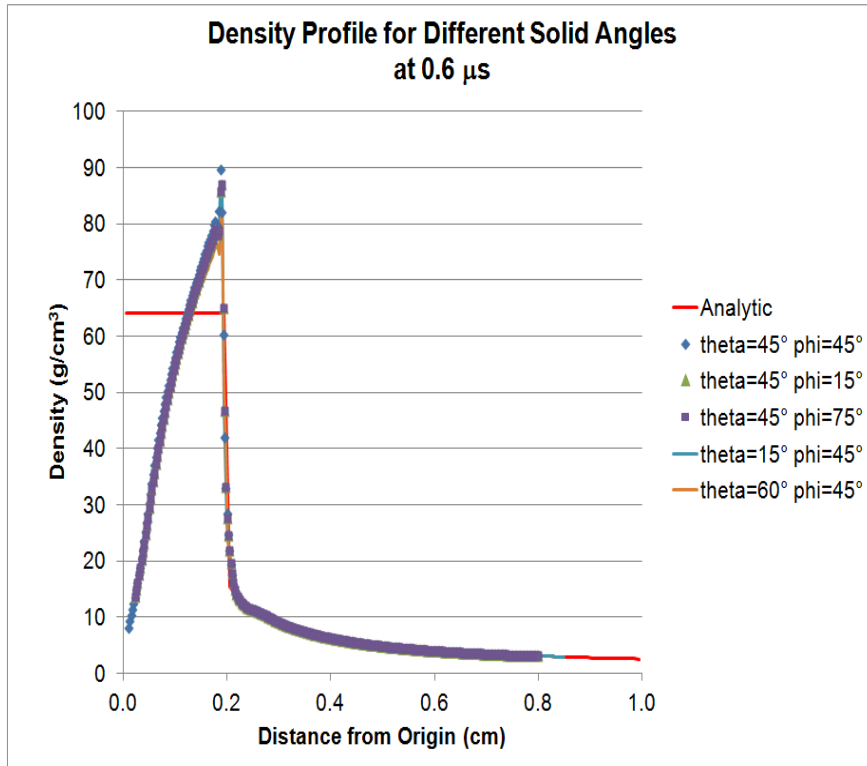
## Setup

- 1 cm octant with 60 x 60 x 60 cells
- 1 cm/ $\mu$ s initial velocity directed toward the origin
- Uniform initial pressure of zero and density of 1 g/cm<sup>3</sup>
- Ideal gas with  $\gamma=5/3$

Density contours for 3D Noh problem at 0.6  $\mu$ s showing the locations of five probe lines

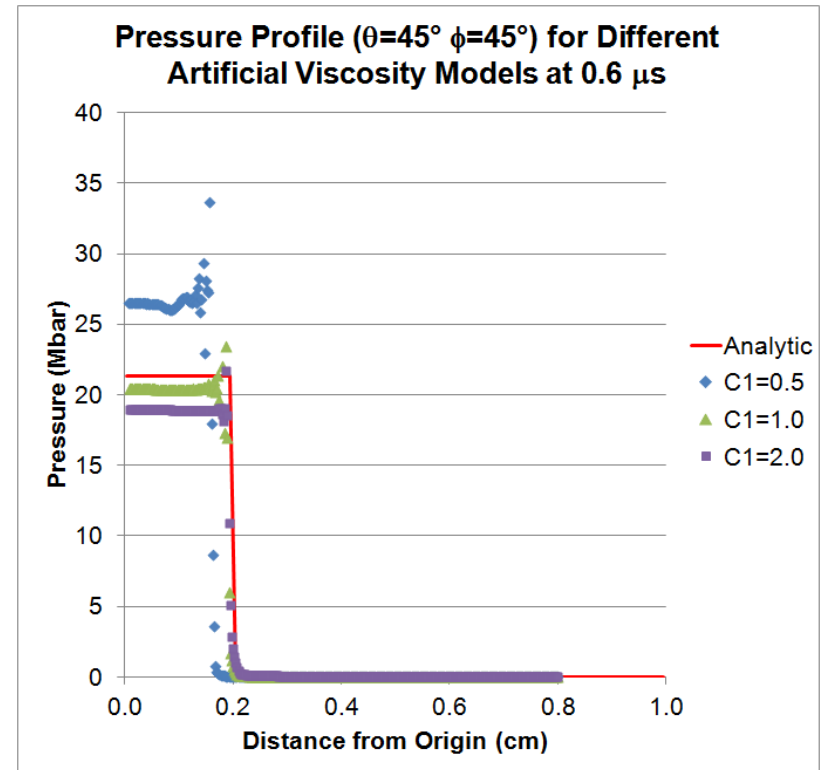
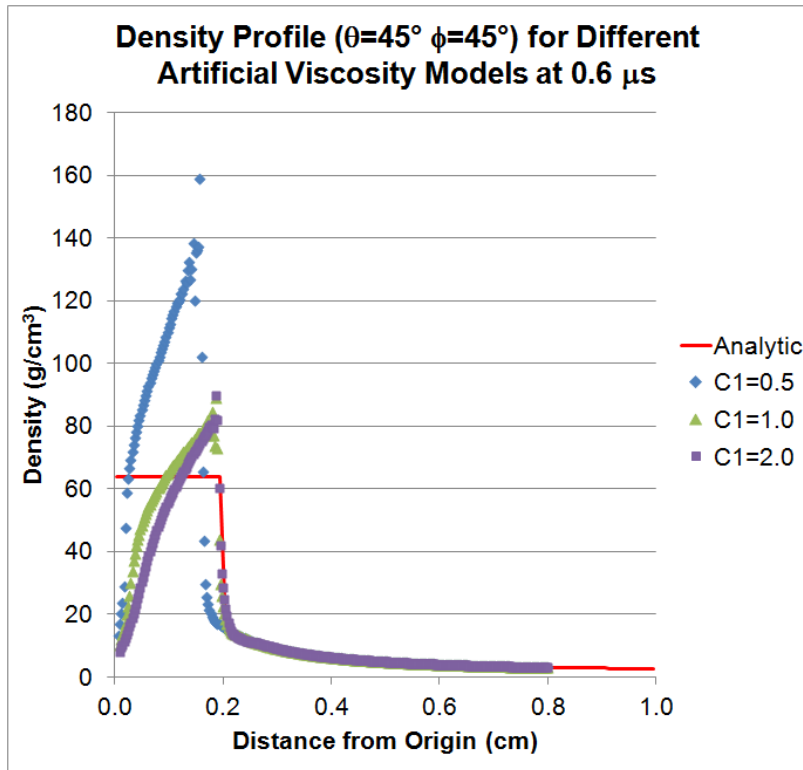


# Numerical results for 3D Noh problem are relatively symmetric





# The numerical solution is sensitive to the artificial viscosity model



Artificial Viscosity Model

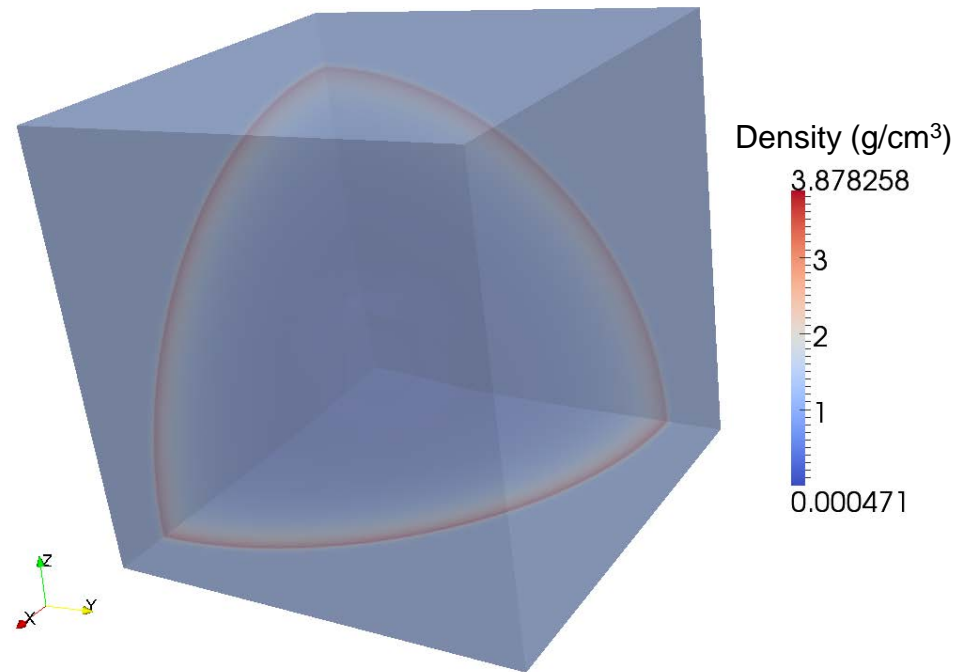
$$q = \rho(C_1 U^2 - C_2 U a)$$

# The 3D Sedov blast wave problem is a stringent test of numerical methods in the code

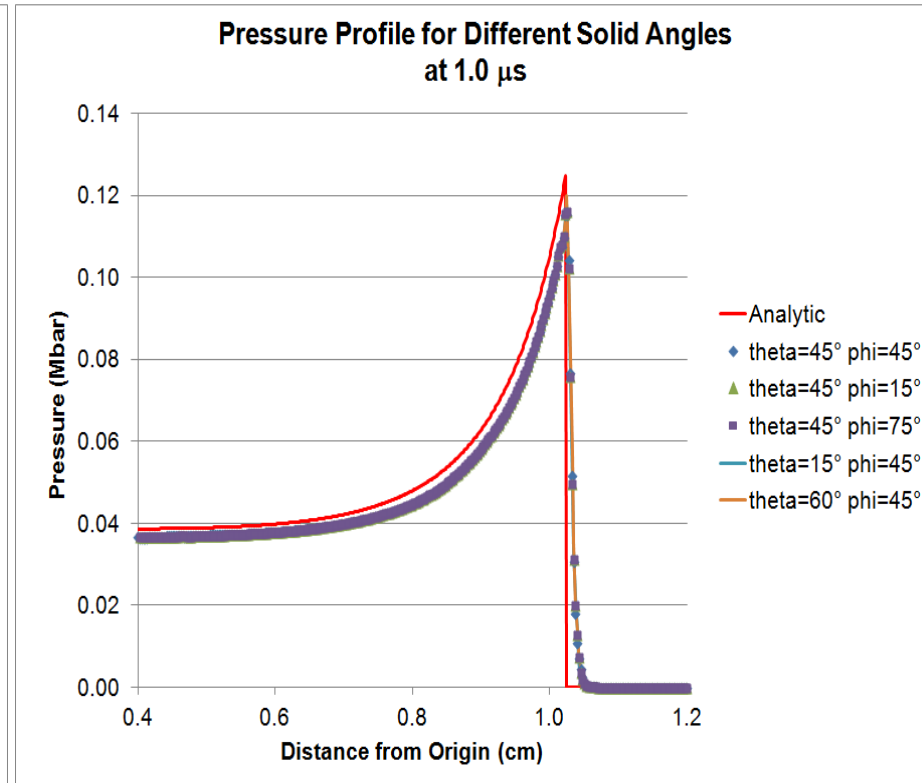
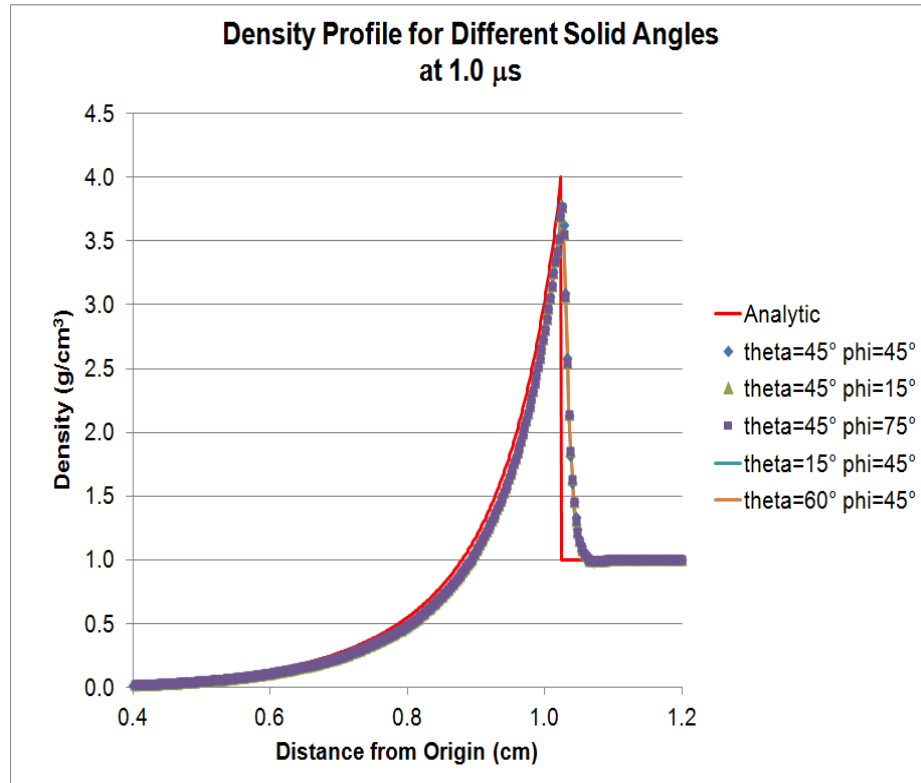
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Density contours for 3D Sedov problem at  $1.0 \mu\text{s}$

- An ideal gas ( $\gamma=5/3$ )
- A 1.2 cm octant (80 x 80 x 80 cells)
- Energy source at the origin
  - 56 kJ
- The solution is obtained at  $1.0 \mu\text{s}$



The calculated blast front leads the analytic solution by a small amount but the symmetry of the front is good



# The Verney problem tests the ability of the code to convert kinetic energy into internal energy for a constant density implosion

- Imploding steel shell

- inner radius of 8 cm
- 0.5 cm thick

- Initial velocity profile

$$u = u_0^2 (r_0 / r)^2$$

- $u_0 = 0.14$  cm/ $\mu$ s
- results in constant density implosion

- Simple strength model

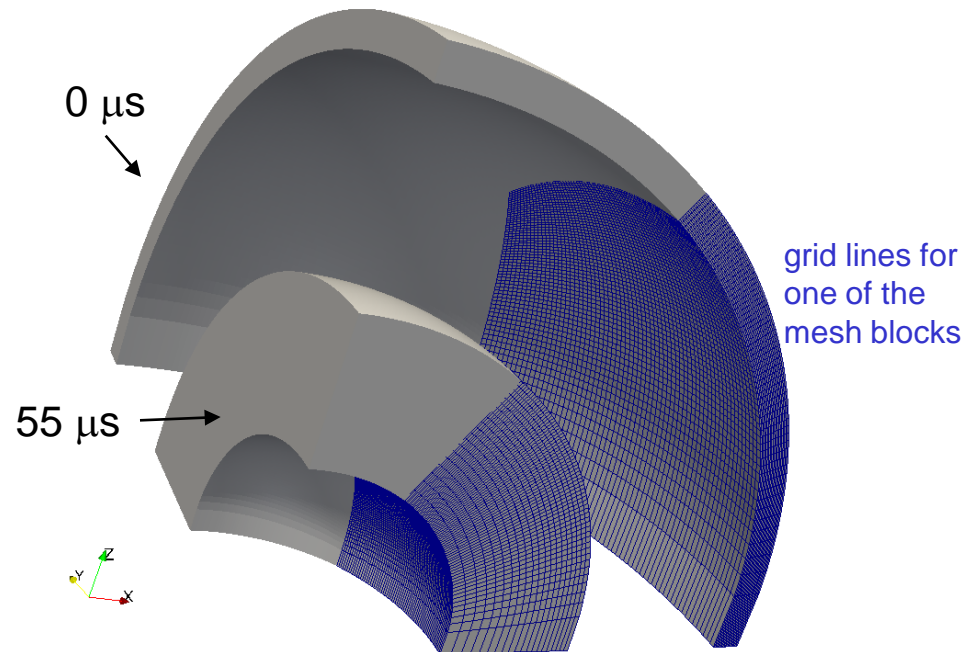
- shear modulus,  $\mu = 0.895$  Mbar
- yield stress of 0.050 Mbar

- Gruneisen EOS

$$\begin{aligned}\rho_0 &= 7.90 \\ C_0 &= 0.457 \\ S_1 &= 1.49 \\ \gamma_0 &= 1.93 \\ b &= 0.50\end{aligned}$$

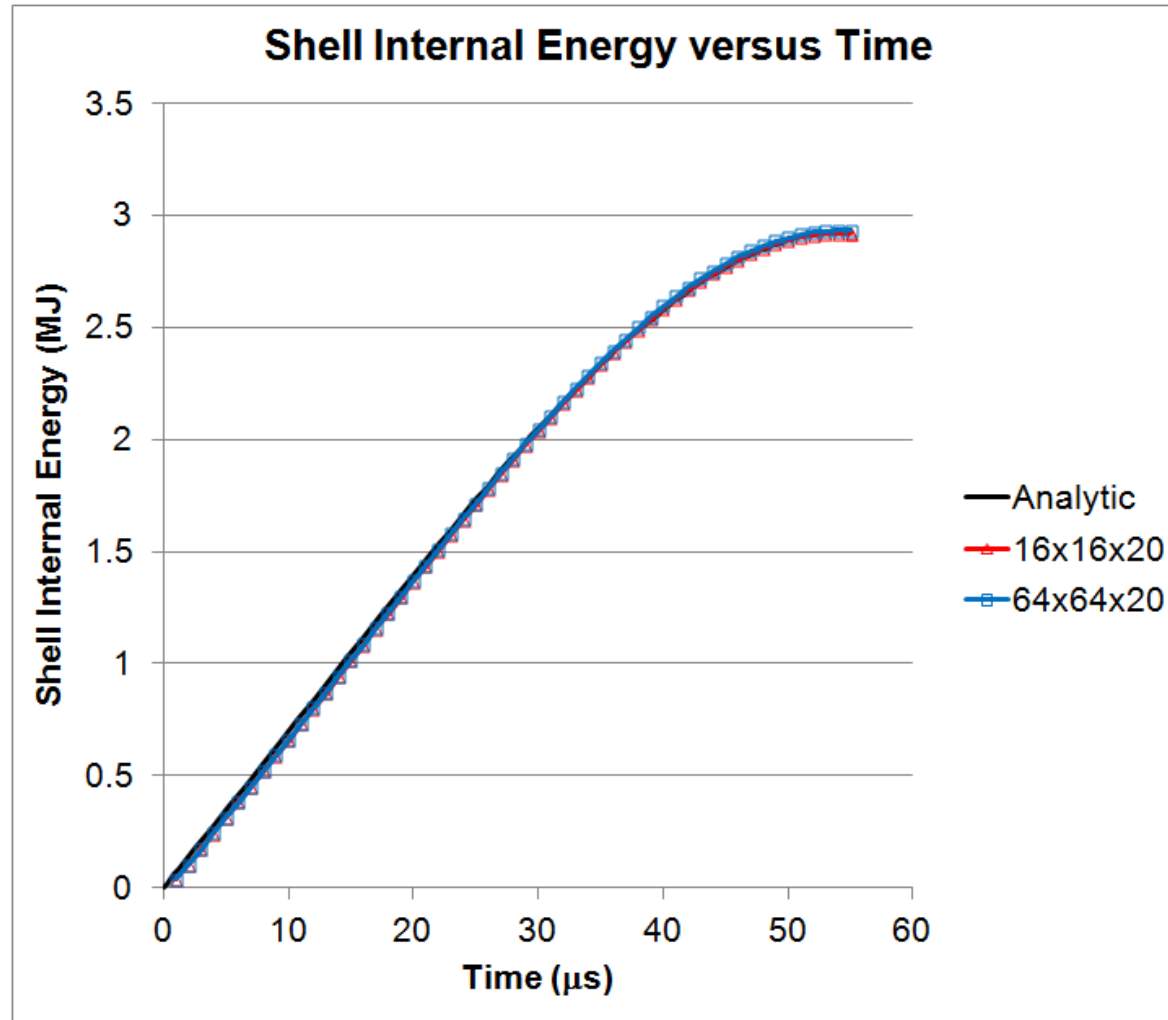
- Analytic solution from Weseloh (2007)

Computational mesh for the Verney test problem at 0  $\mu$ s and 55  $\mu$ s



- 3 mesh blocks with 64 x 64 x 20 cells each
- Parallelization using OpenMP

The calculated internal energy history of the shell agrees well with the analytic solution



# Conclusions

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- A finite element approach is used to calculate the cell-centered velocity gradient and nodal forces for Lagrangian hydrodynamics in Cercion 3D
- A simple model is used to calculate nodal forces that dissipate hourglass modes
- The optimum hourglass dissipation parameter,  $k$ , is determined from simulations of the 3D Saltzman piston problem and is less than the typical value used for 2D simulations
- Excellent agreement with the analytic solution is achieved for the Sod shock tube problem and approximate first order convergence is demonstrated
- The calculated blast front for the Sedov problem leads the analytic solution by a small amount but the symmetry of the front is good
- Cercion 3D captures the time evolution of the shell internal energy in the Verney test problem