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An Hourglass Control Method for Three Dimensional Lagrangian Hydrodynamics

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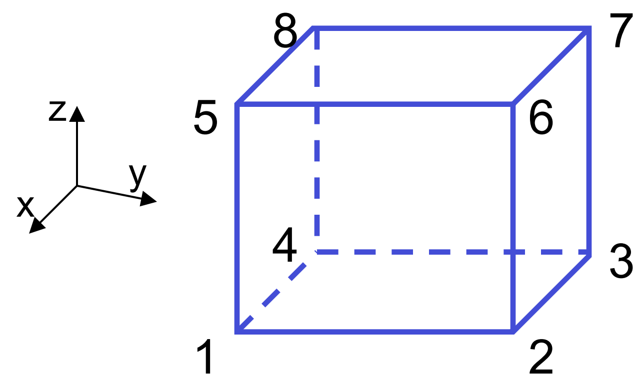
Outline

- 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

Cell Indexing Scheme



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

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

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

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

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

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

Tensor Indexing Conventions

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

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	Λ_{1I}	Λ_{2I}	Λ_{3I}	Γ_{1I}	Γ_{2I}	Γ_{3I}	Γ_{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

physical hourglass

Note Γ_{4I} is not used in calculating C_{IJK}

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

B matrix

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

Cell volume

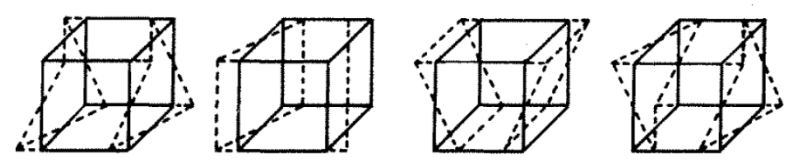
$$V = x_I y_J z_K C_{IJK}$$

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

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

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



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

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

There are a total of 12 hourglass modes for the hexahedron

- Nodal forces for hourglass dissipation in Cercion 3D

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

k is the single free parameter in the model

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

Symmetric strain rate tensor

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

Anti-Symmetric strain rate tensor

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

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

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

Artificial viscosity model with both linear and quadratic terms

$$q = \rho\left(C_1 U^2 - C_2 U a\right)$$ for $U < 0$ otherwise $q=0$

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

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

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

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

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

$$u_{i}^{p} = u_{i}^{n} + \frac{\Delta t}{M}\sum_{C} f_{i}^{n}$$

$$u_{i}^{n+1} = u_{i}^{n} + \frac{\Delta t}{2M}\left(\sum_{C} f_{i}^{n} + \sum_{C} f_{i}^{p}\right)$$

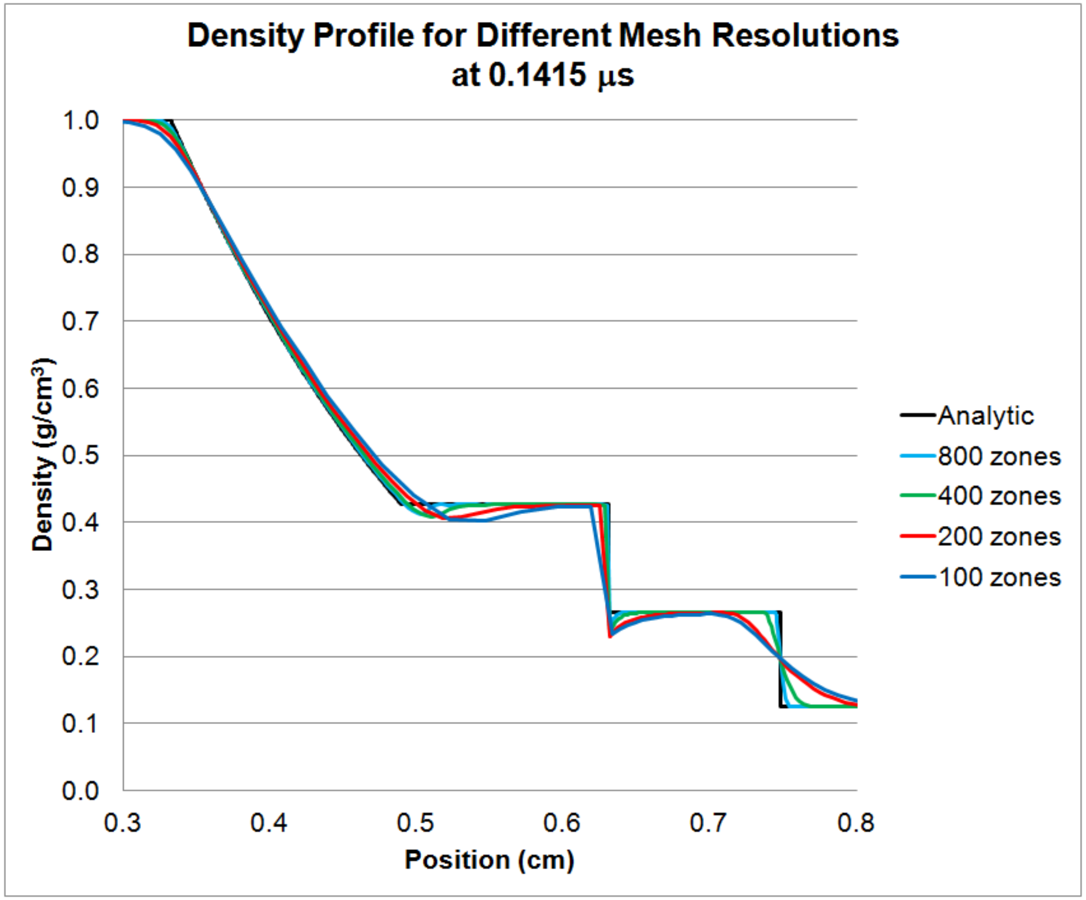
***M* is the fixed nodal mass and *C* is the set of eight cells that surround the node**

Similar predictor-corrector update for the energy equation

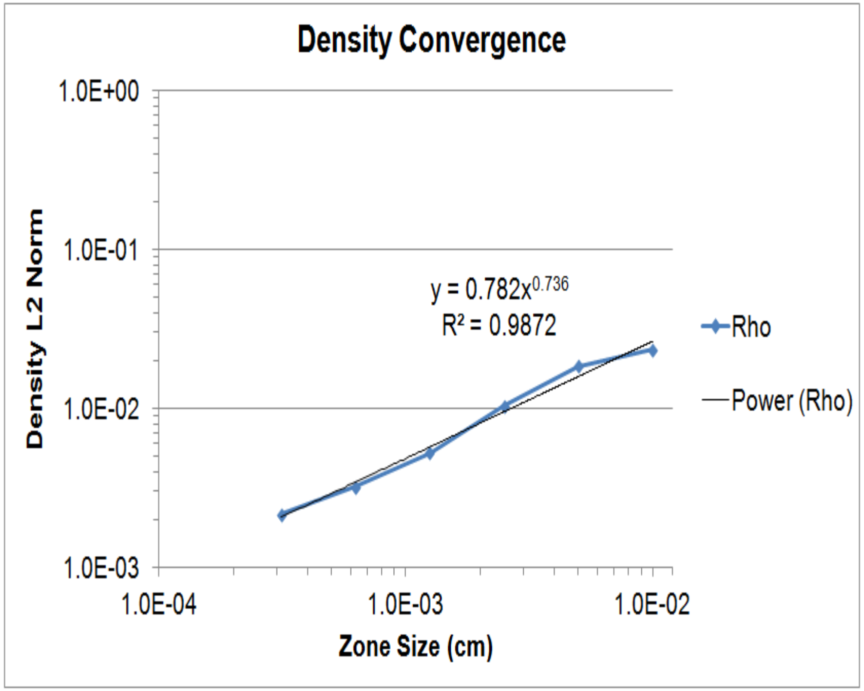
The locations of the shock and contact discontinuity for the Sod test problem are captured by the code

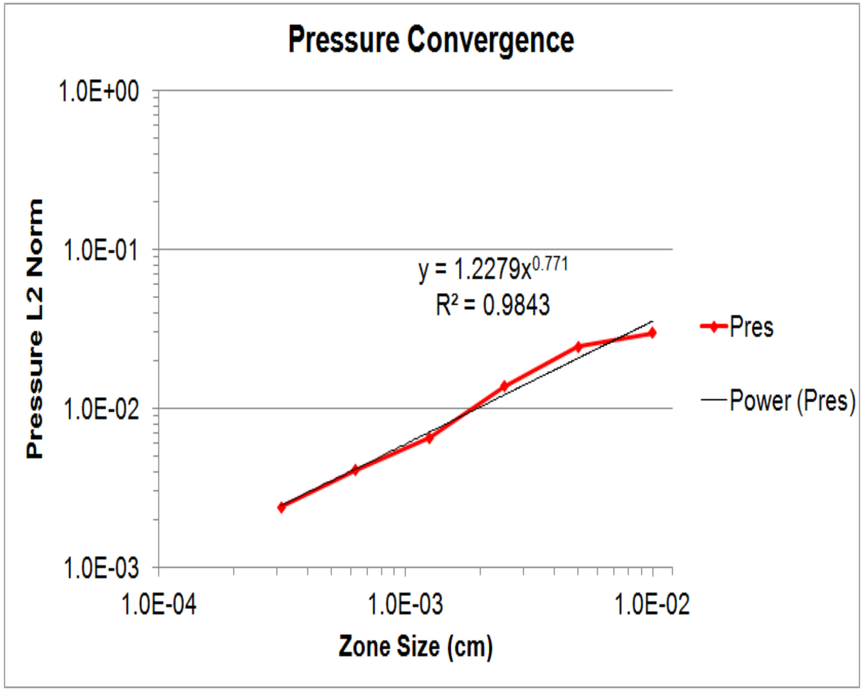
Setup

- An initial discontinuity between two ideal gas regions (γ=1.4)
- Region 1
  - density of 1 g/cm^3
  - pressure of 1 Mbar
- Region 2
  - density of 0.125 g/cm^3
  - pressure of 0.1 Mbar
- The solution is obtained at 0.1415 μs



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

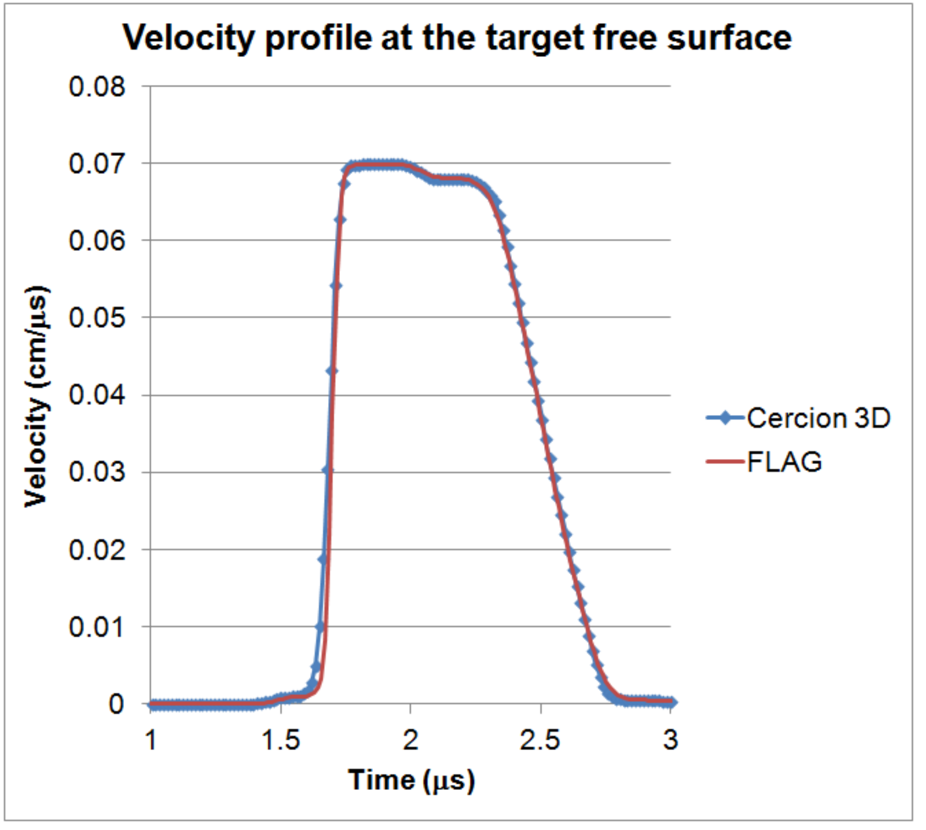




Flyer plate problem tests the material strength treatment in the code

- 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

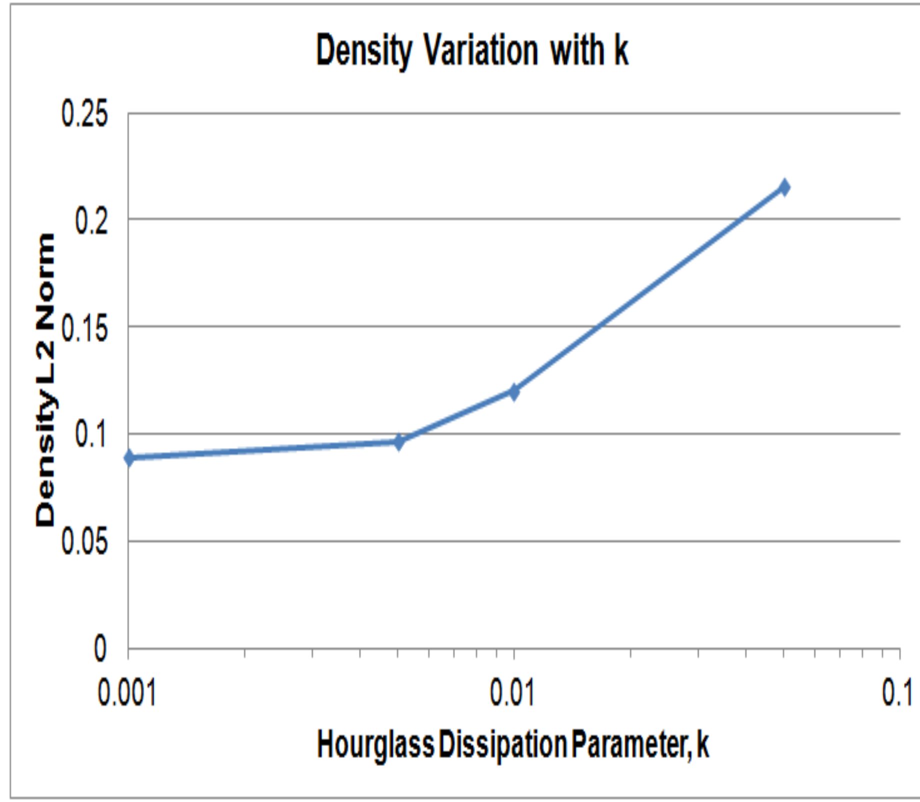
  ρ_0=2.707
  C_0=0.5386
  S_1=1.339
  γ_0=1.97
  b=0.48
- Material strength model
  - yield strength of 0.0004 Mbar
  - shear modulus of 0.271 Mbar
- Companion FLAG 2D calculation



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/μs on left boundary
  - Initial density of 1 g/cm^3
- 0.7 μs run time
- 100 x 10 x 10 cells

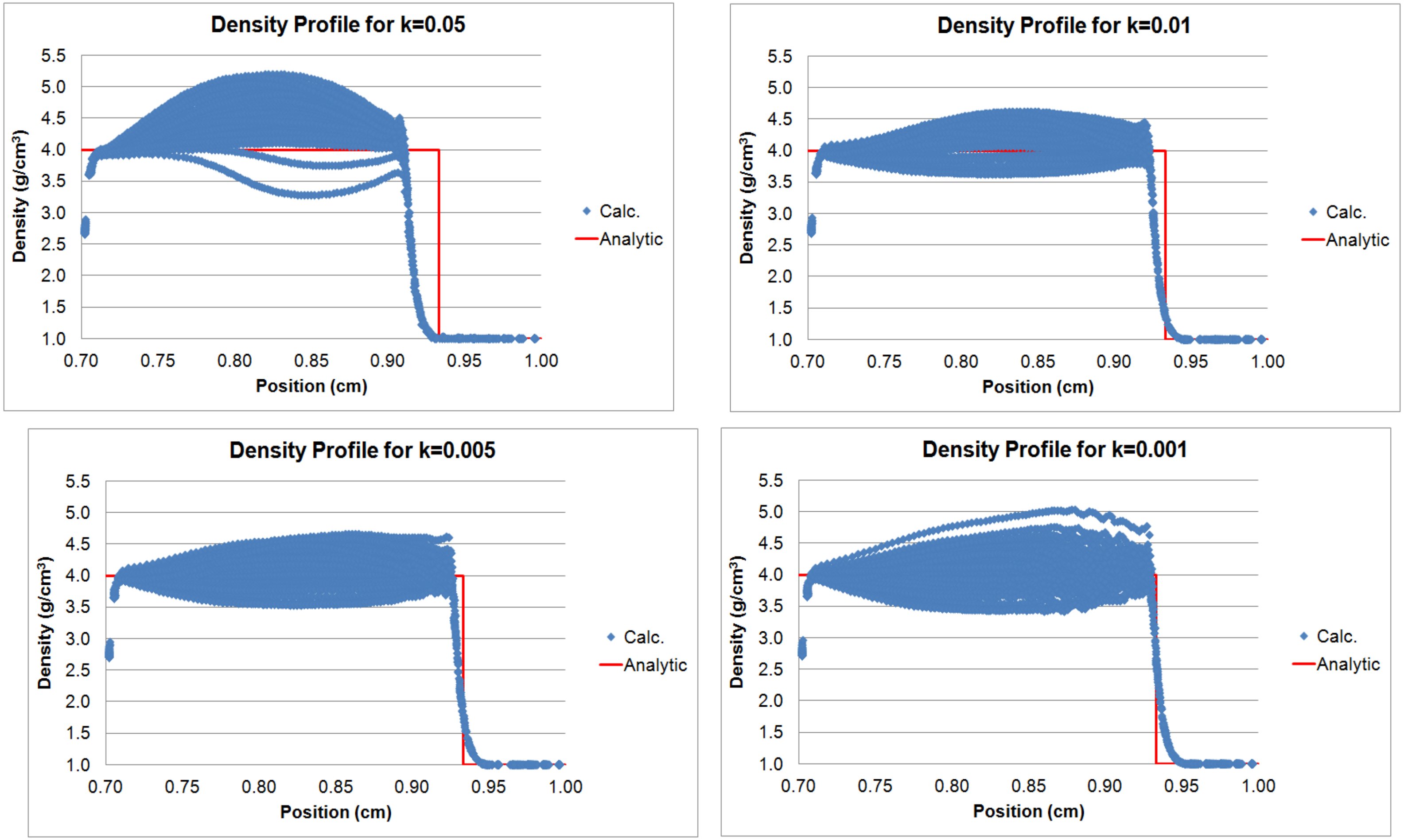
$$x = 0.01i + 0.01(10-k)(5-j)/5\sin(0.01\pi i) \quad \text{for } 0 \le j \le 5$$
$$x = 0.01i + 0.01k(j-5)/5\sin(0.01\pi i) \quad \text{for } 6 \le j \le 10$$
$$y = 0.01j$$
$$z = 0.01k$$



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 μs

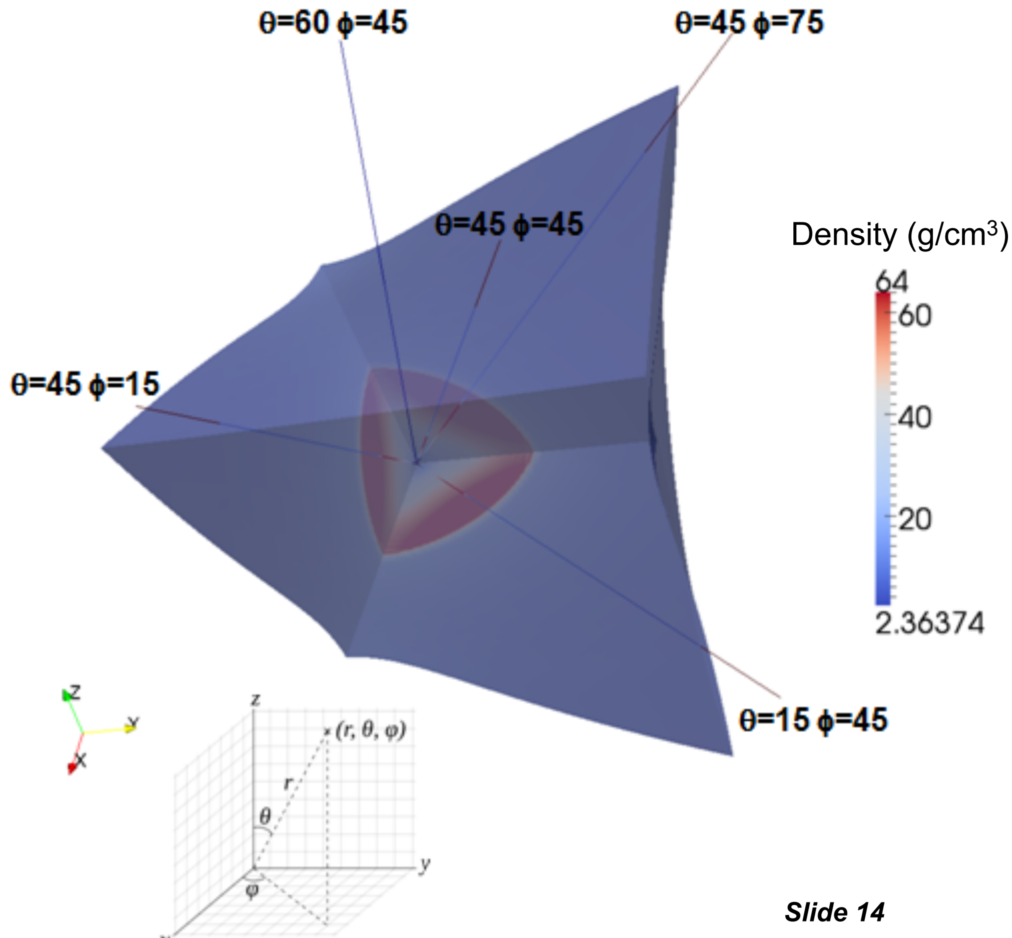


The 3D Noh problem was simulated with Cercion 3D

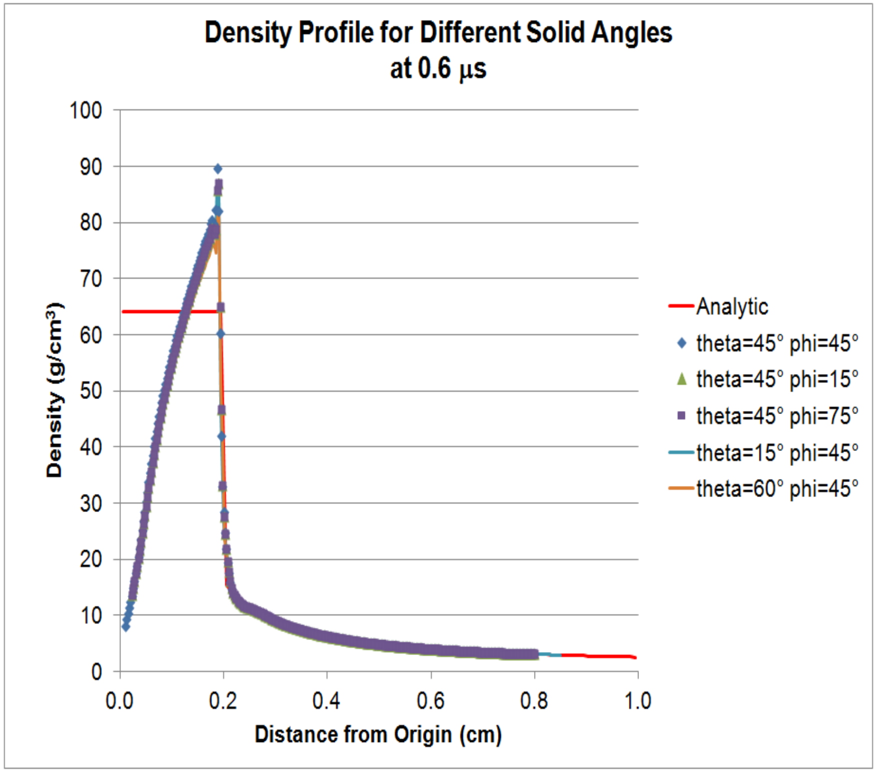
Setup

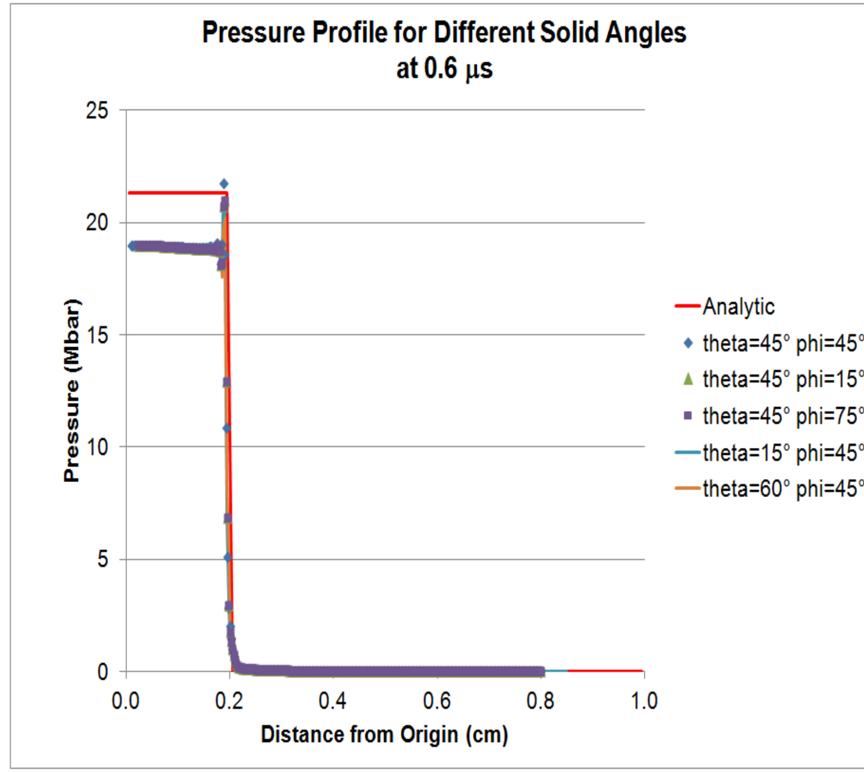
- 1 cm octant with 60 x 60 x 60 cells
- 1 cm/μs initial velocity directed toward the origin
- Uniform initial pressure of zero and density of 1 g/cm^3
- Ideal gas with γ=5/3

Density contours for 3D Noh problem at 0.6 μs showing the locations of five probe lines

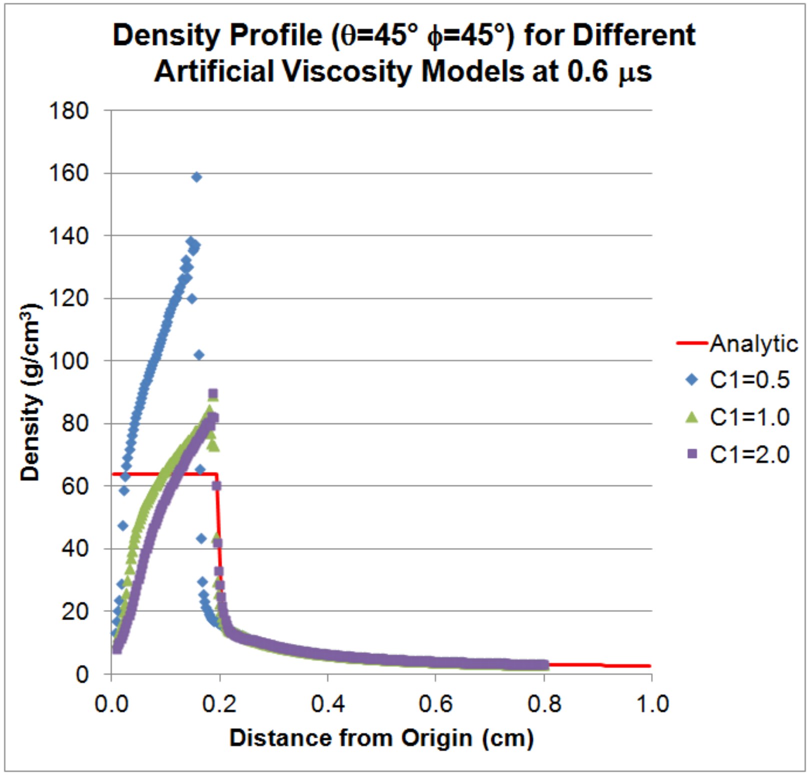


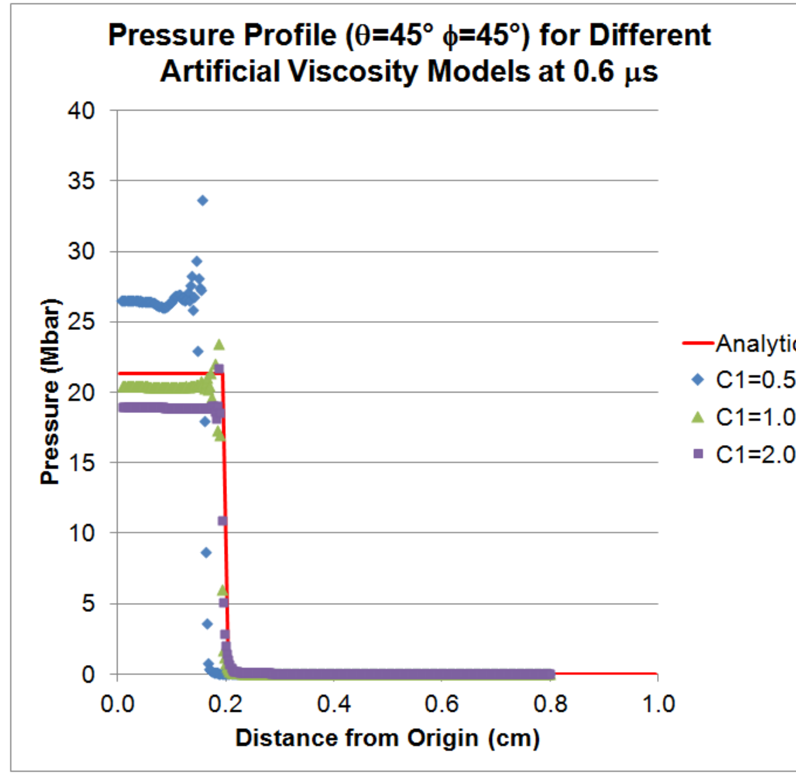
Numerical results for 3D Noh problem are relatively symmetric





The numerical solution is sensitive to the artificial viscosity model





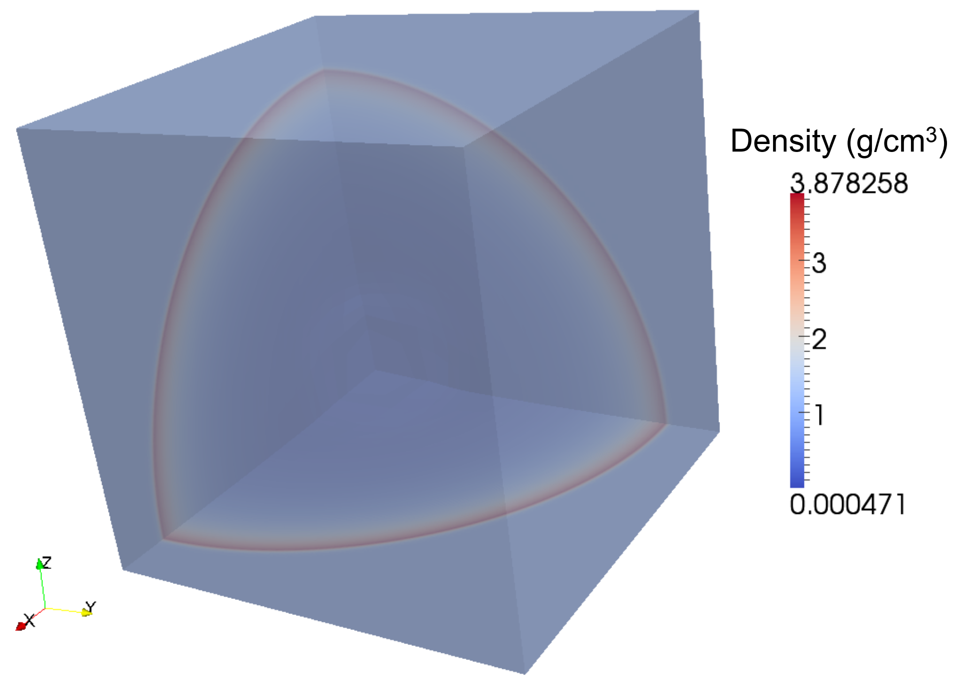
Artificial Viscosity Model

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

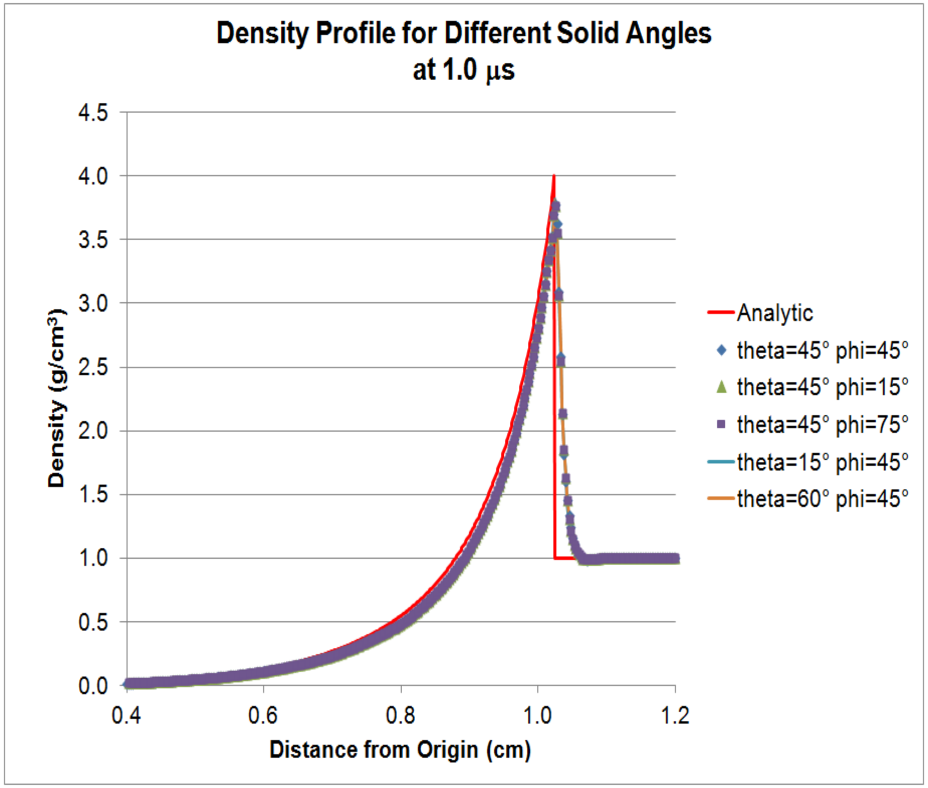
The 3D Sedov blast wave problem is a stringent test of numerical methods in the code

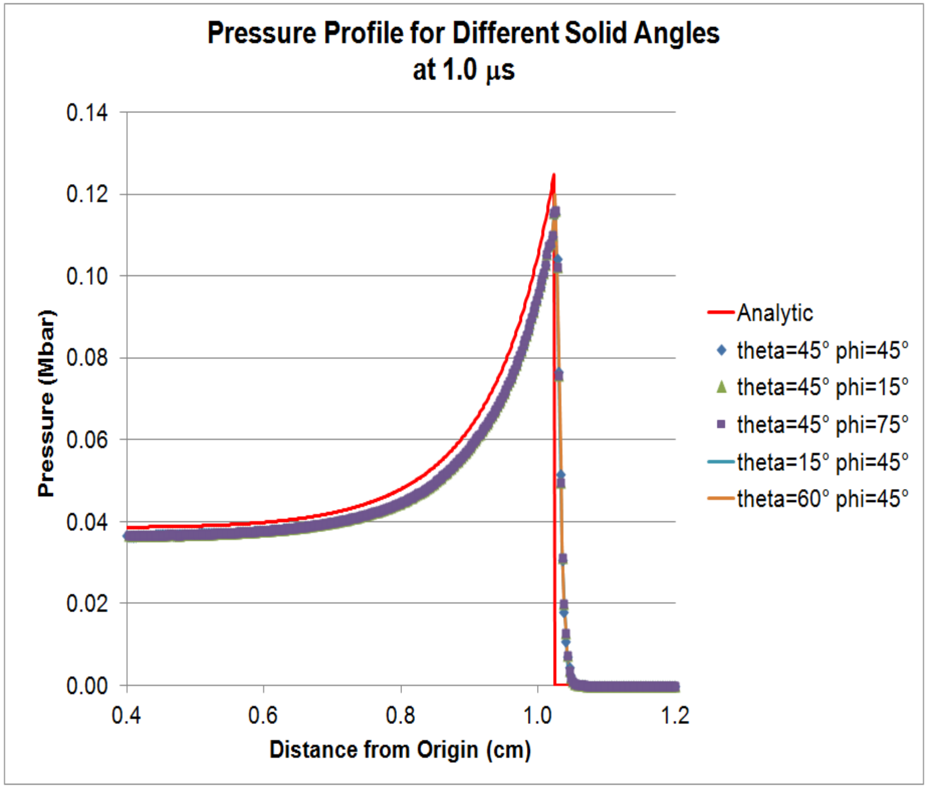
Density contours for 3D Sedov problem at 1.0 μs

- An ideal gas (γ=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 μs



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





The Verney problem testes 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

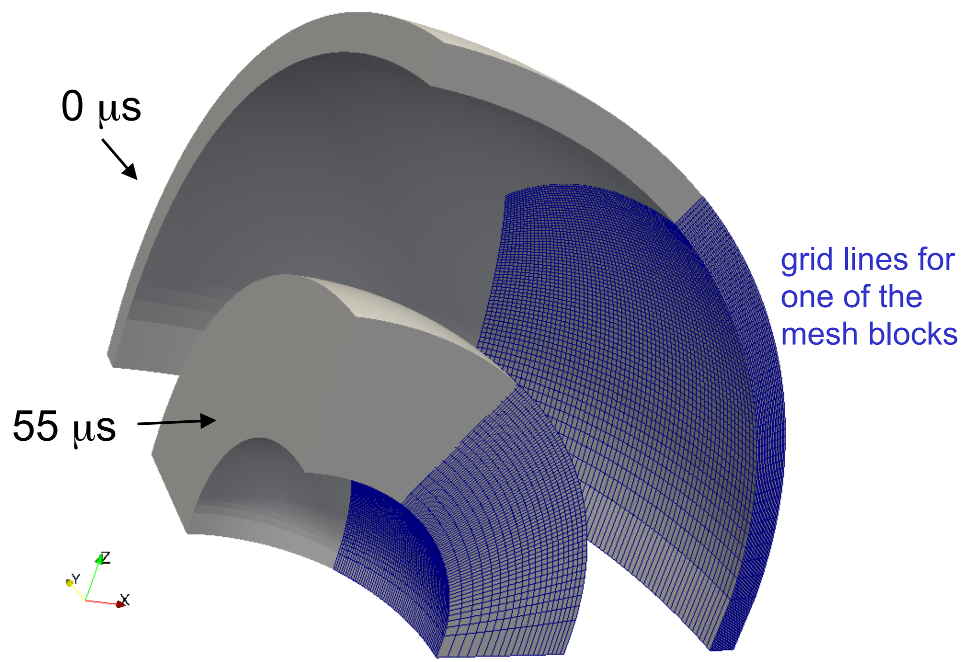
$$u = u_0^2 (r_0 / r)^2$$

  - u_0=0.14 cm/μs
  - results in constant density implosion
- Simple strength model
  - shear modulus, μ=0.895 Mbar
  - yield stress of 0.050 Mbar
- Gruneisen EOS

ρ_0=7.90
C_0=0.457
S_1=1.49
γ_0=1.93
b=0.50

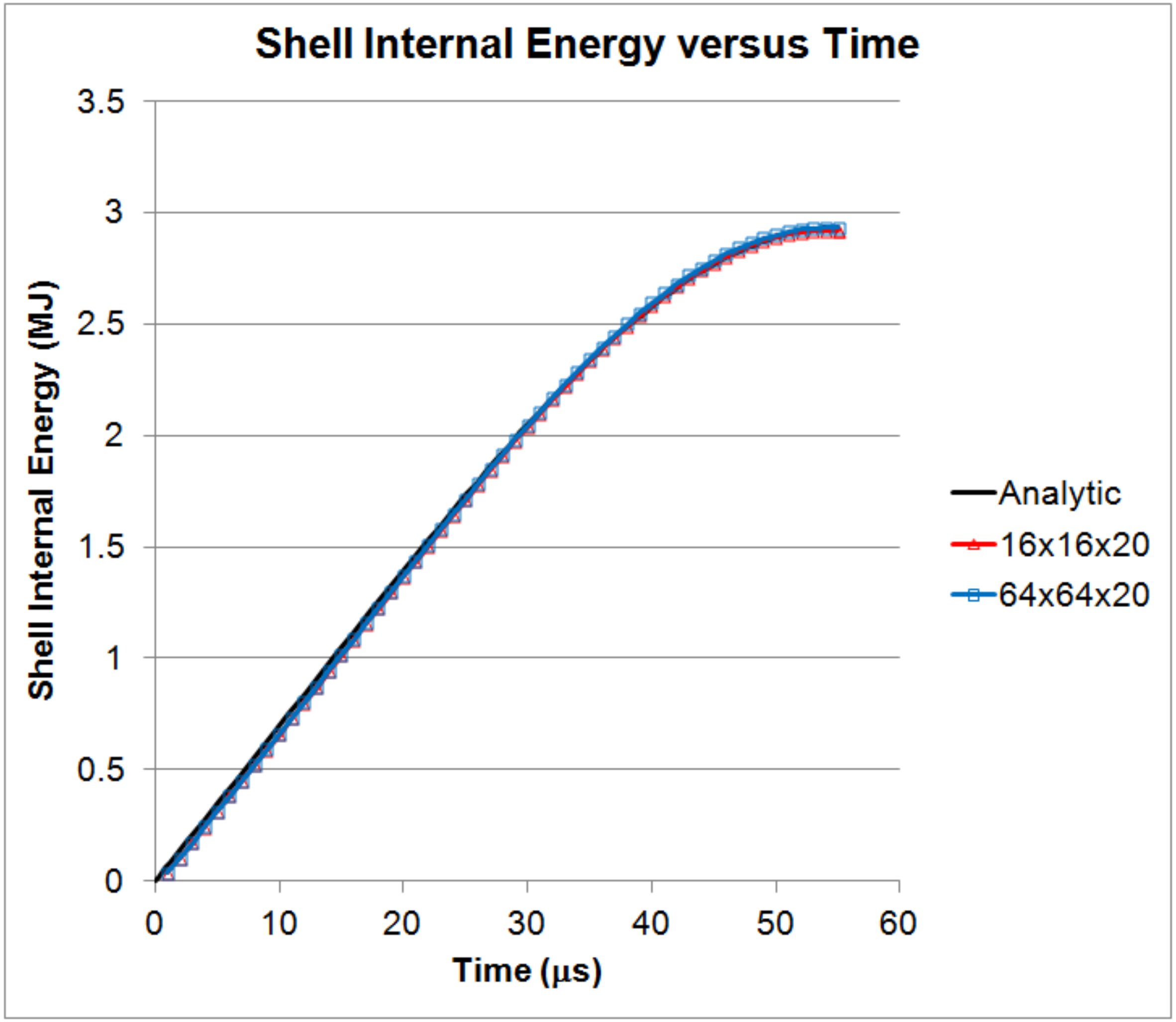
- Analytic solution from Weseloh (2007)

Computational mesh for the Verney test problem at 0 μs and 55 μs



- 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

- 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