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Title:	A Comparative Study of Eulerian and Lagrangian Hydrodynamics Methods for Multimaterial Compressible Flow.
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A Comparative Study of Eulerian and Lagrangian Hydrodynamics Methods for Multimaterial Compressible Flow.

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We present a comparative study of various numerical methods to solve the multimaterial compressible Euler equations either with an Eulerian or Lagrangian formulation. We assume a single velocity field and rely on pressure relaxation techniques to close the system of equations. We test the following methods and algorithms on a two-materials shock tube test problem and compare the results with the analytical solution:

- Eulerian six-equations models with pressure relaxation (Saurel et al. 2009) using a Godunov method with HLLC Riemann solver with and without interface treatment,
- Staggered Lagrangian with standard predictor/corrector scheme with Tipton's closure model (Shashkov 2008),
- Cell-centered Lagrangian Godunov method with an acoustic Riemann solver with Tipton's closure model,
- Eulerian method as Lagrange plus remap with Tipton's closure model.

Tipton's closure model is a relaxation method in which the pressure is relaxed with a viscosity-like term to obtain the material volume fractions and thermodynamic state variables in the mixed cell. We observe different time history for the thermodynamic state variables in the mixed cell for the various methods and algorithms.

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Outline of this Presentation

- **Governing equations and multi-material cell notation**
- **Eulerian Formulation**
  - Classification of methods based on material treatment: sharp versus diffuse interface
  - Five-Equation and Six-Equation Models with Godunov method using MUSCL Hancock scheme with HLLC Riemann Solver
- **Lagrangian Formulation**
  - Staggered formulation with standard predictor/corrector scheme with Tipton's model
  - Cell-centered formulation with Godunov method with Tipton's model
- **1D Sod Shock Tube for Two Materials**
  - Comparison of staggered versus cell-centered Lagrangian formulation
  - Comparison of Lagrange+Remap with diffuse and sharp Eulerian methods
- **Conclusions and Future Work**

Governing Equations in 1D

- **No gravity, inviscid, ρ density, u velocity, p pressure, E total energy, e specific internal energy** $E = e + \frac{1}{2}u^2$

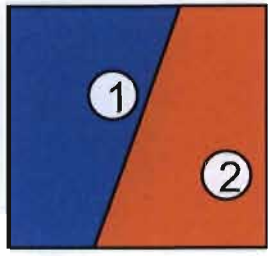
	Eulerian	Lagrangian
Mass	$\frac{\partial(\rho)}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0$	$\rho \frac{D}{Dt}\left(\frac{1}{\rho}\right) - \frac{\partial u}{\partial x} = 0$
Momentum	$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = 0$	$\rho \frac{Du}{Dt} + \frac{\partial p}{\partial x} = 0$
Energy	$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho E + p)u}{\partial x} = 0$	$\rho \frac{DE}{Dt} + \frac{\partial}{\partial x}(pu) = 0$

+ Equation of State $p = \rho e(\gamma - 1)$

Mixture of Multi-Materials

- **Material components indices** k
- **Volume fraction** α_k
  - Ratio of volume of component k to the total cell volume

$$\sum_k \alpha_k = 1$$

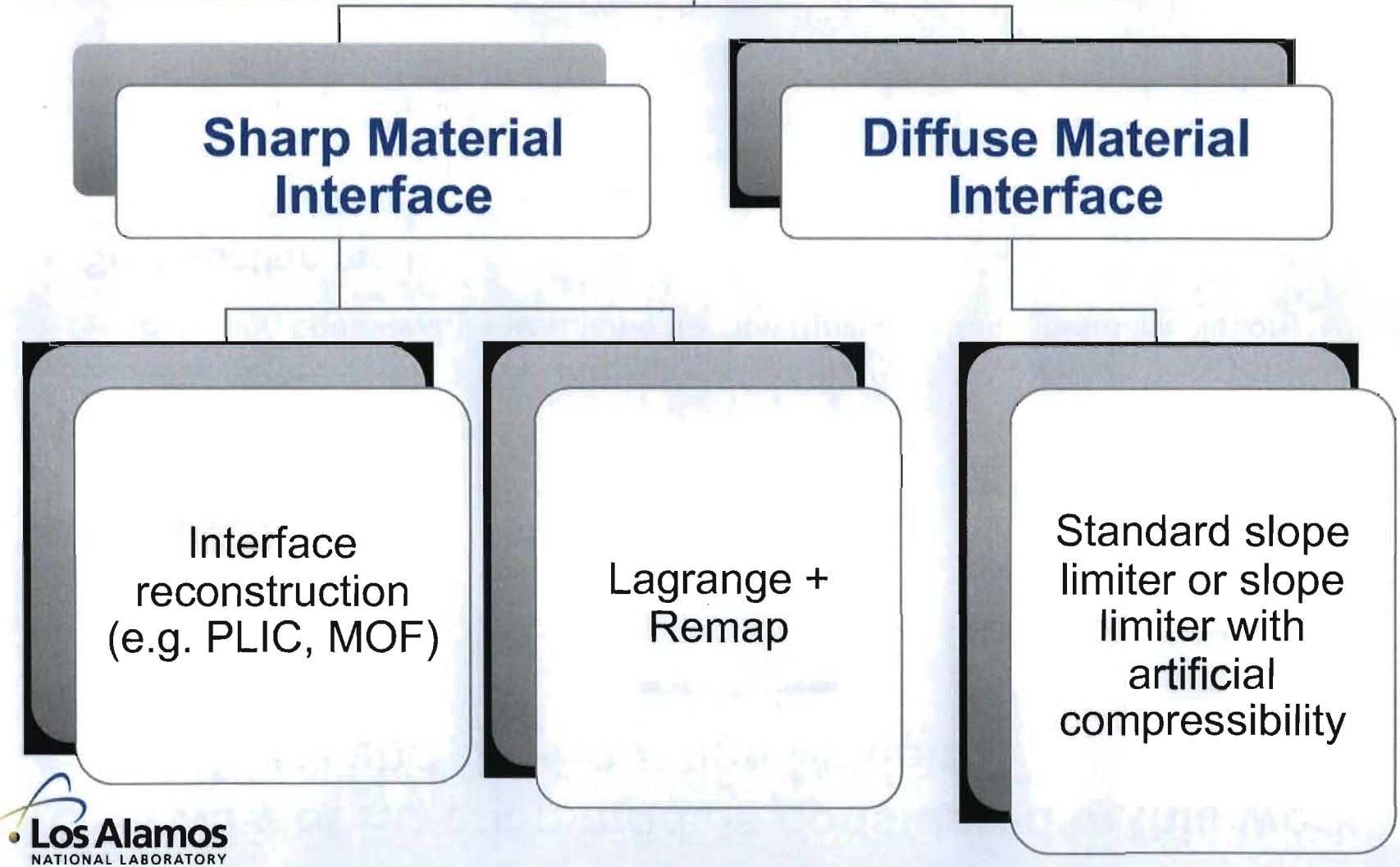


- **Mixture density** $\rho = \sum_k (\alpha_k \rho_k)$
- **Mass fraction** $m_k = \dfrac{(\alpha\rho)_k}{\rho}$
- **Mixture Specific Internal Energy**
  - Each material satisfies its pure material equation of state

$$e = \sum_k m_k e_k(\rho_k, p)$$

- **Here, we consider 1D flow, single velocity, 2 materials (k=2) and perfect gas equation of state**

Eulerian Methods for Multimaterial Flows



Overview of Eulerian models considered in this work
Four-, Five- and Six-Equation Models

- **Single velocity**
  - Reduced models derived by Kapila (2001) from general Baer-Nunziato model (1986)
- **Four-Equation models**
  - Pressure-Temperature equilibrium
- **Five-Equation models**
  - Single pressure - pressure equilibrium condition
  - Evolution equation for the volume fraction (uniform strain, thermal isolation)
- **Six-Equation model**
  - Two pressures with relaxation step
  - Two specific internal energy equations
  - Evolution equation for volume fraction
  - Additional equation for mixture total energy
  - Saurel, Petitpas, Berry, J. Comp. Physics, 228, 2009
- **Hyperbolic, non-conservative**

Five equation Eulerian models

- **Uniform Strain Model** (Grove and Masser, NECDC 2008)
  - Five-equation transport model (Allaire et al. 2002, Murrone and Guillard, 2005)

$$\frac{D\alpha_1}{Dt} = 0 \qquad \frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = 0 \qquad c^2 = \sum_k m_k c_k^2$$

- **Thermal Isolation Model** (Grove and Masser, NECDC 2008)
  - Also known as the Five-equation reduced model of Murrone and Guillard (JCP 2005)
  - Equivalent to six-equation model of Saurel et al. (JCP 2009) in the asymptotic limit when the pressure is relaxed

$$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = \frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}\frac{\partial u}{\partial x} \qquad \frac{1}{\rho c^2} = \sum_k \frac{\alpha_k}{\rho_k c_k^2}$$

Eulerian Numerics

- **2nd order Godunov method (e.g. MUSCL Hancock scheme)**
- **Riemann solver (e.g. HLLC, acoustic)**
- **Interface Preserver (IP) – minimizing the diffusion at interface**
  - IP applies the single material contact steepener of Yang (JCP 1990) to material interfaces
  - IP steepens the volume fractions gradients in order to keep the mass diffusion to a minimum
  - 5 Eq., 6 Eq. models with IP (Francois et al. MULTIMAT 2009)
- **Sharp interface – a single mixed cell**
  - Interface reconstruction (e.g. Youngs, 1982, PLIC Rider and Kothe 1998, MOF Dyadechko and Shashkov, 2005)
  - Pressure relaxation algorithm (Miller and Puckett 1996)

Staggered Lagrangian Method

- **Velocity at nodes and pressure at cell-centers**
- **Standard predictor-corrector time integration scheme (Shashkov, 2008)**
  - Half-time step: node position, cell volume, densities, pressure (adiabatic approximation)
  - Final update: velocity, node position, cell volume, densities, specific internal energies, pressure
  - Pressure augmented by artificial viscosity (von Neumann and Richtmyer)
- **Each material has its own mass, material interface may not coincide with mesh faces (mixed cells)**
- **Closure model: find mixture pressure and advance in time energy and density for each material**

Cell-centered Lagrangian method

- **Velocity and pressure at cell-centers**
- **2nd order Godunov method with acoustic Riemann solver**
- **Predictor-corrector time integration scheme (Maire and Shashkov, 2008)**
  - Half-time step: mass, momemtum, energy update with Riemann states u* and p* from time n data
  - Final update: mass, momemtum, energy update with Riemann states u* and p* from time n+1/2 data
- **Each material has its own mass, material interface may not coincide with mesh faces (mixed cells)**
- **Tipton's model for pressure relaxation after predictor and corrector steps**

Tipton's closure model

- **Pressure relaxation method**
  - "Artificial viscosity"-like term for relaxation

$$p_k^n - \left(\rho_k^n c_k^{n^2}\right)\left(1 + \frac{L^n}{c_k^n \delta t}\right)\left(\frac{\delta V_k^{n+1/2}}{V_k^n}\right) = p^{n+1/2}$$

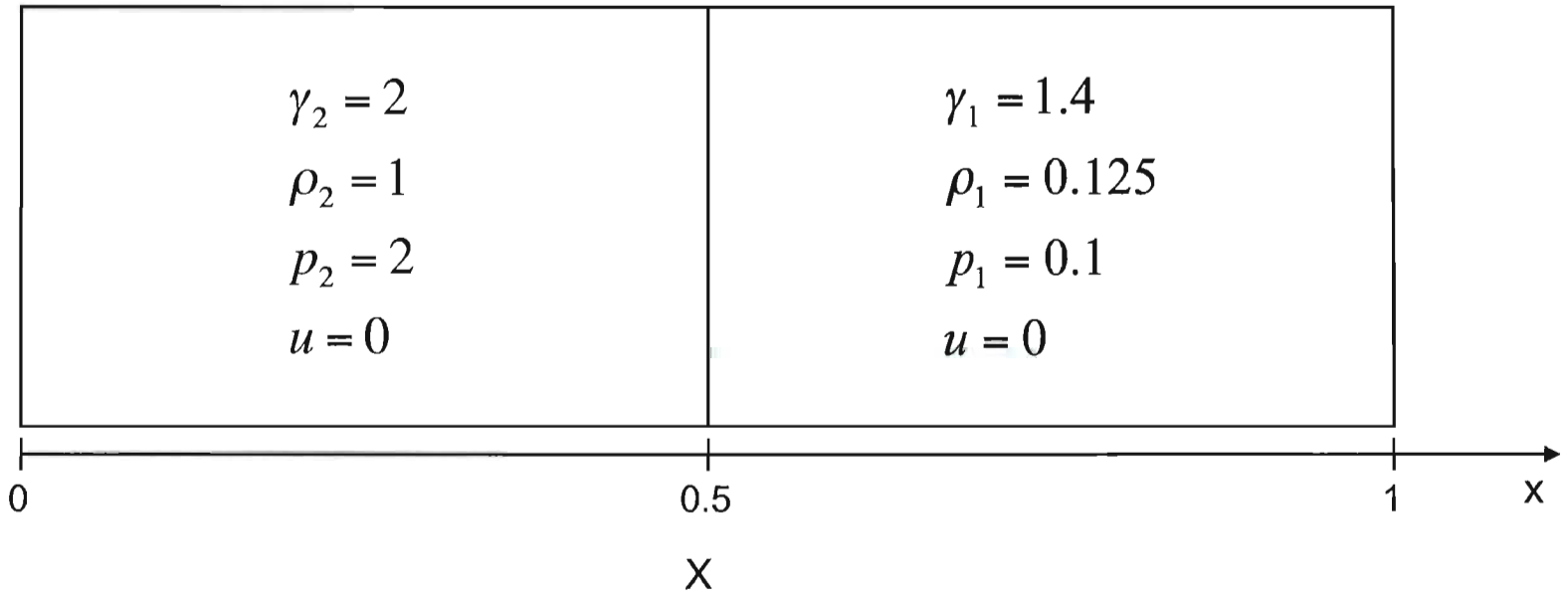
$$\delta V^{n+1/2} = \sum_k \delta V_k^{n+1/2}$$

c	Speed of sound
L	Length (cell-length)
V	Volume
k	Material index

- **Staggered Lagrangian scheme**
  - Tipton's model for pressure relaxation after half-time step
  - Consistent internal energies with total energy conservation
- **Cell-centered Lagrangian scheme**
  - Tipton's model after predictor and corrector steps
  - Conservation of total energy by redistributing discrepancy in total internal energies to either material internal energies based on the sign of the discrepancy

Two Materials Sod Shock Tube

- Non-dimensional Initial Conditions
- Perfect gas with different gammas
- 1D, Final time t=0.2

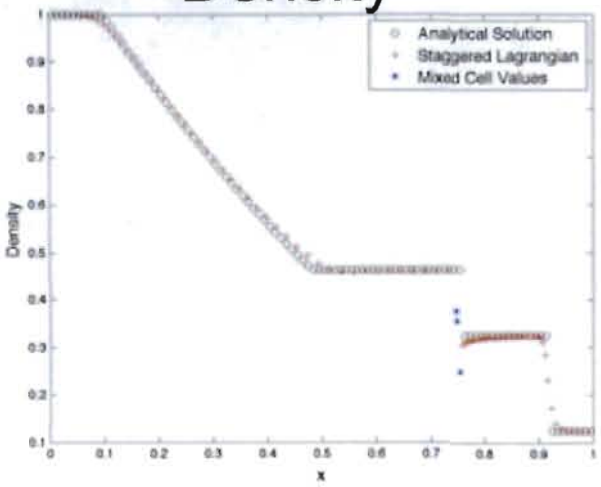


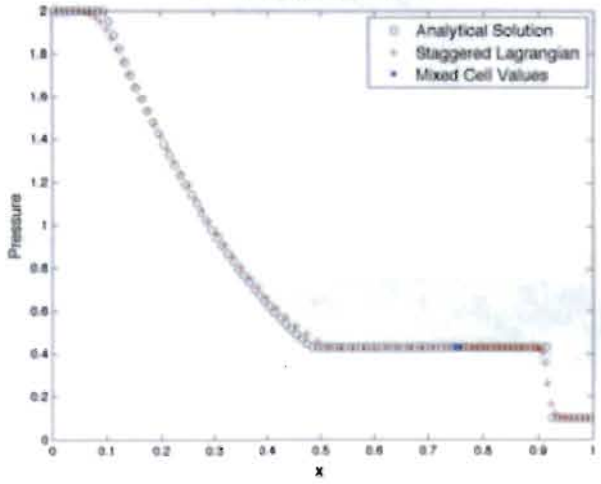
Two-materials Sod - Density and Pressure Plots at t=0.2
Staggered versus cell-centered Lagrangian formulation

Density

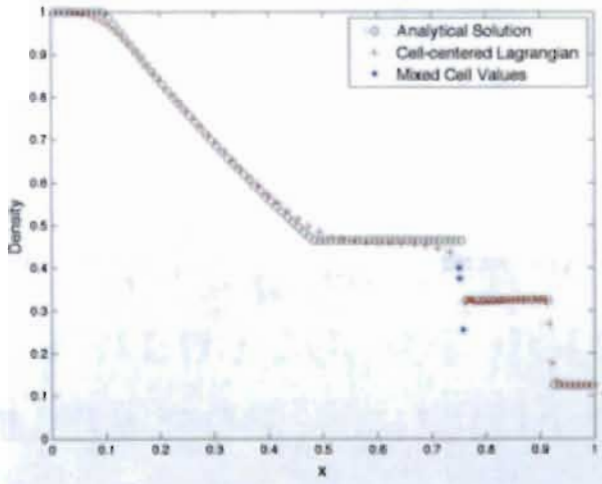
Pressure

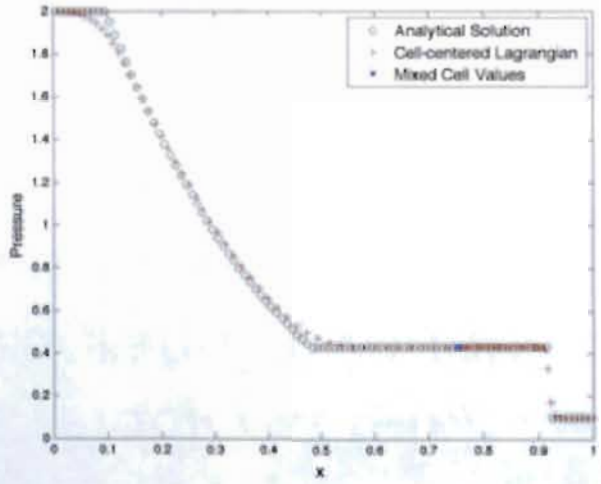
Staggered





Cell-centered



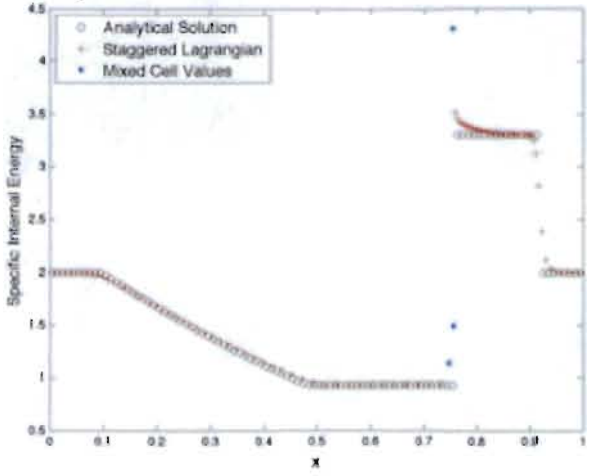


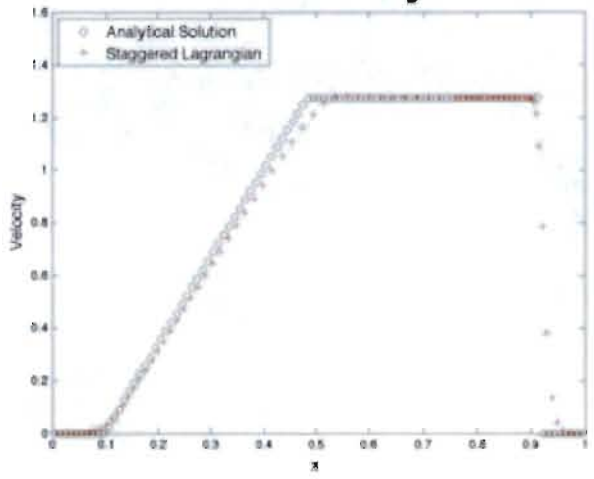
Two-materials Sod – Energy and Velocity at t=0.2
Staggered versus cell-centered Lagrangian formulation

Specific Internal Energy

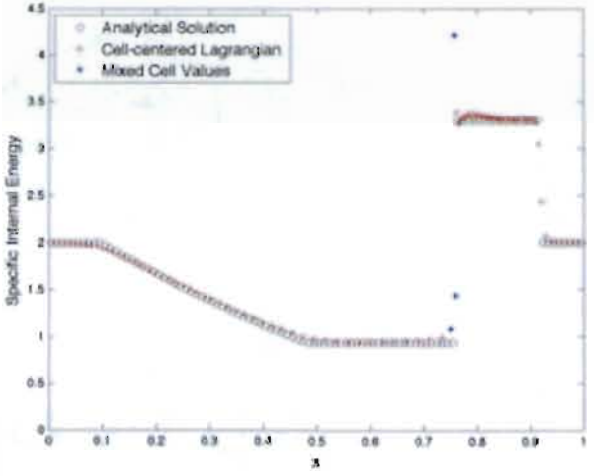
Velocity

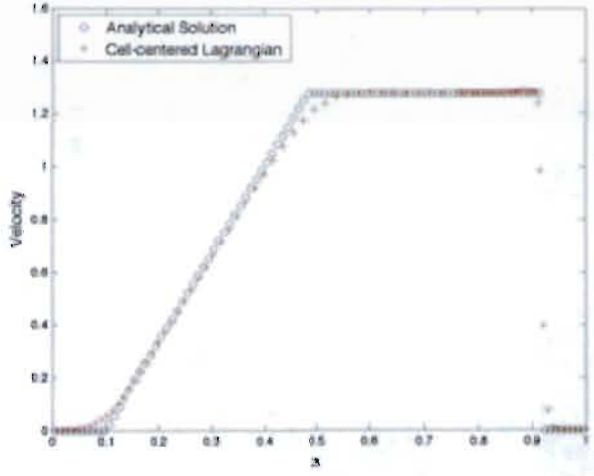
Staggered





Cell-centered

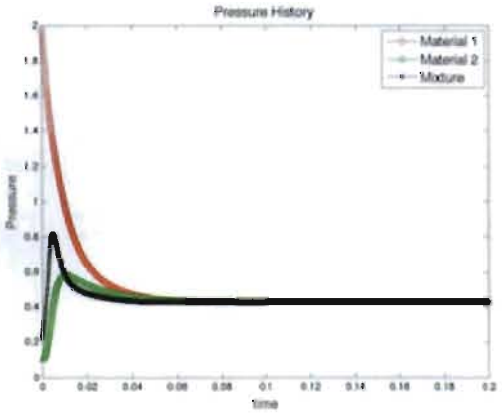


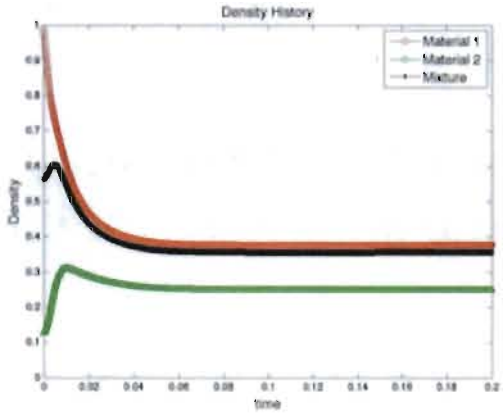


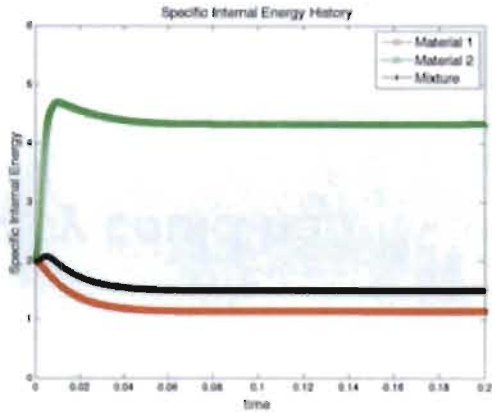
Time-history plots in the mixed cell with Tipton's model
Staggered versus cell-centered Lagrangian formulation

Pressure | Density | Specific Internal Energy

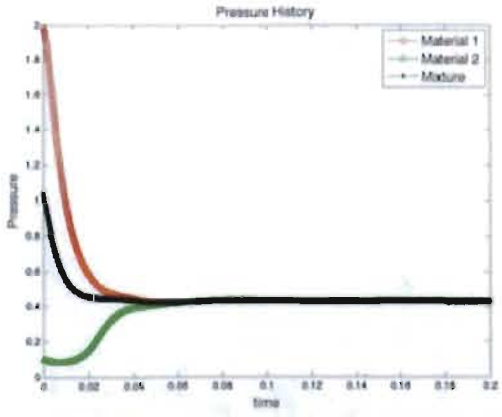
Staggered

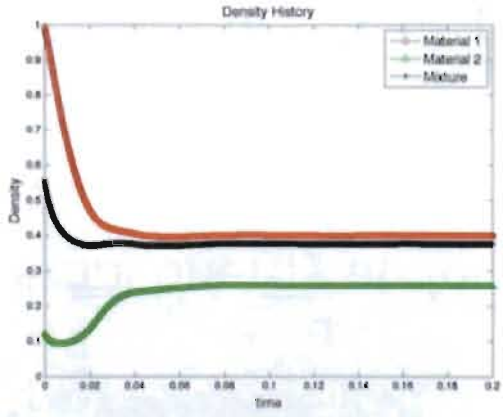


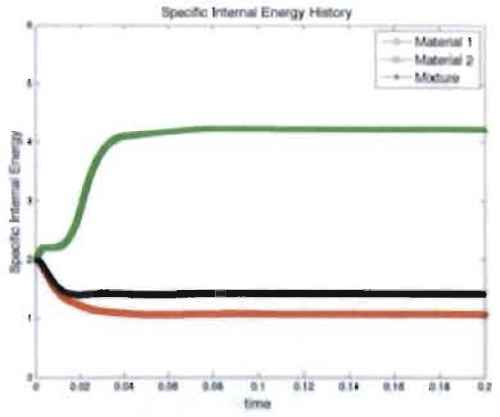




Cell-centered



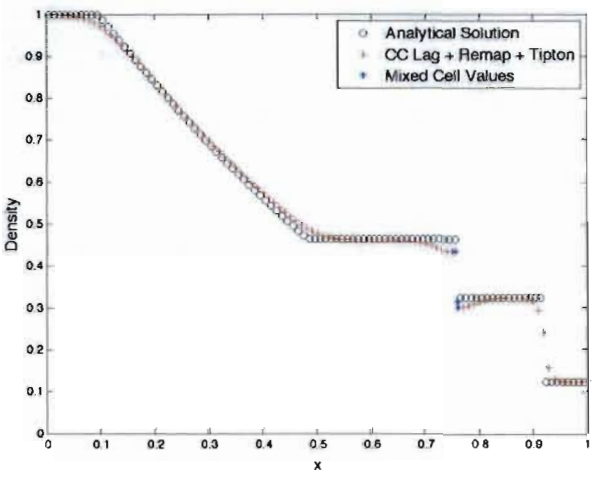


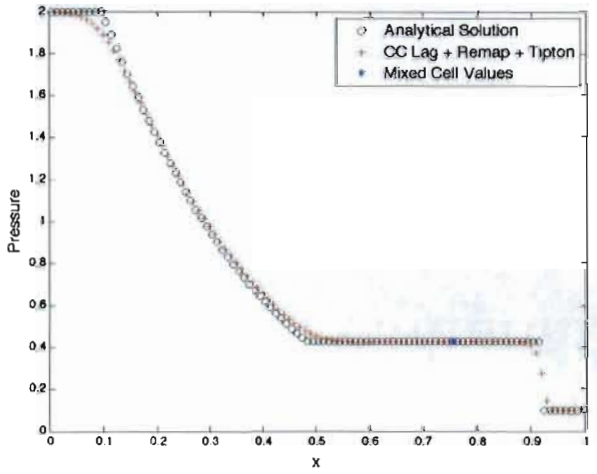


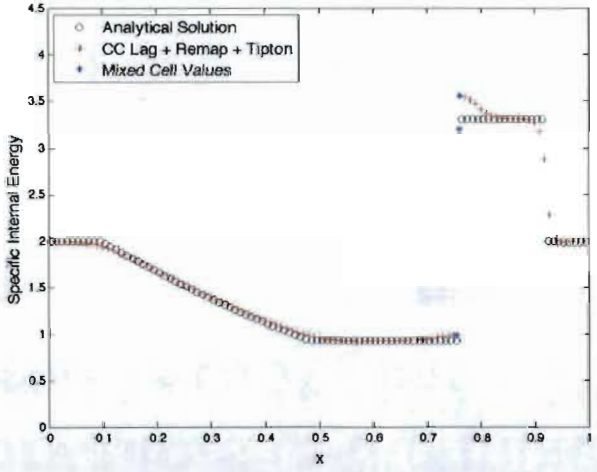
Staggered versus cell-centered Lagrangian formulation Remarks

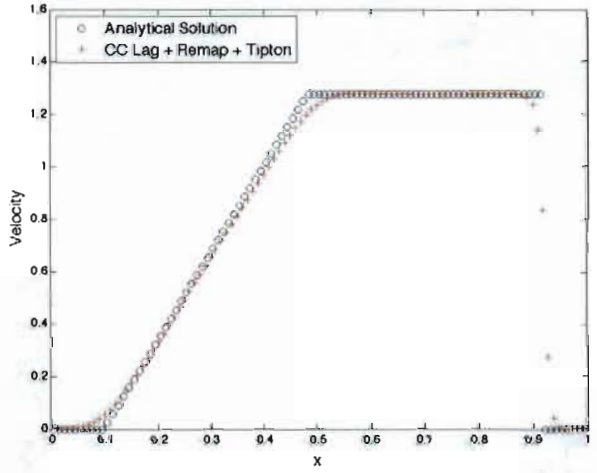
- Difference in specific internal energy at time t=0.2
- Difference in history plots for mixed cells thermodynamics quantities
- Transient pressure in mixed cell is always bounded between the two materials pressure ($p_1 < p_{mix} < p_2$) for cell-centered formulation, not the case for staggered formulation
- Other correction algorithm for energy discrepancy could be designed and give other time-history behavior

Cell-centered Lagrangian + 2nd order Remap with Tipton's closure model



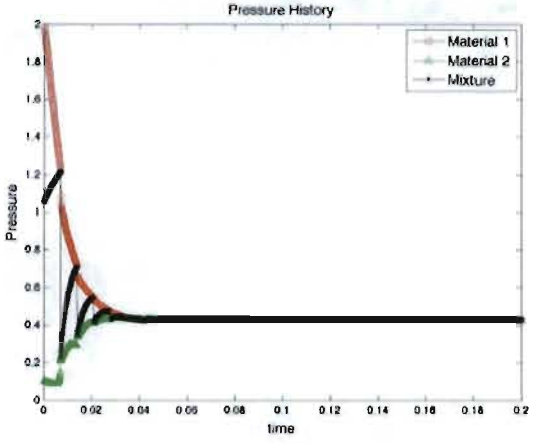




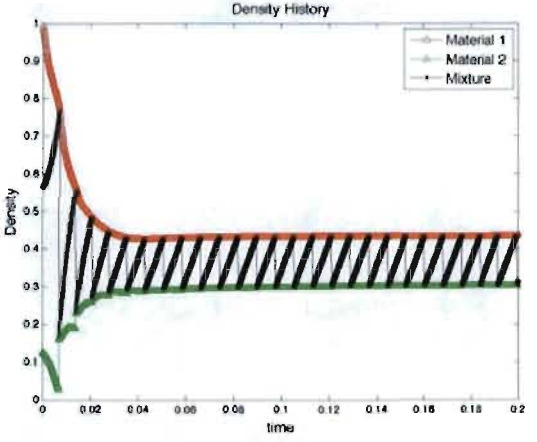


Time-history plots in the mixed cell with Tipton's model Cell-centered Lagrangian + 2nd order remap

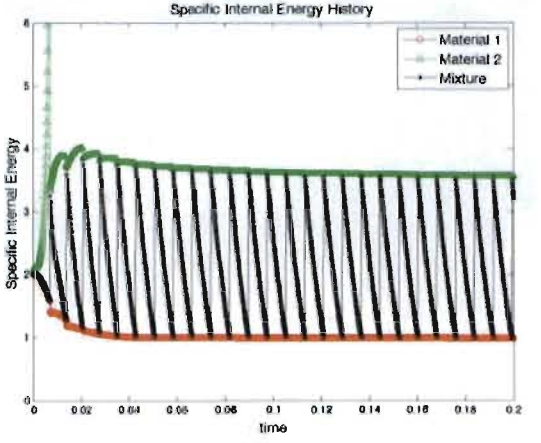
Pressure



Density



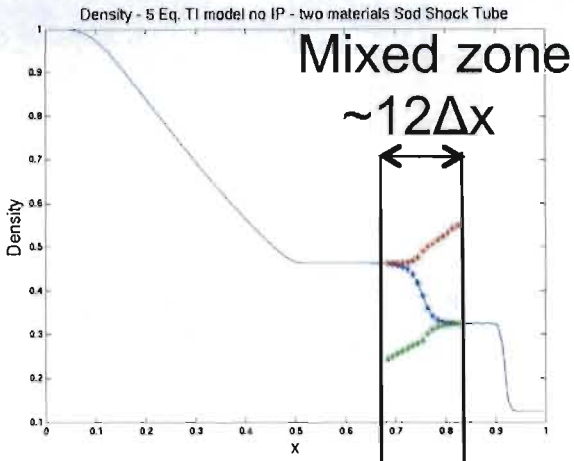
Specific Internal Energy

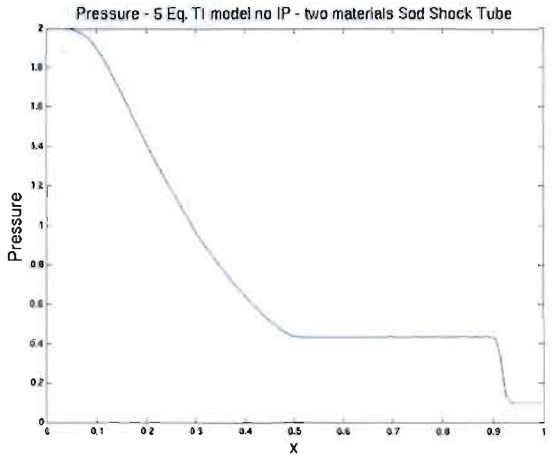


- As interface moves within the mixed cell, the mixture pressure varies between p_1 and p_2 $\quad p = \sum_k (\alpha_k p_k)$
- Spike in specific internal energy depends on relaxation

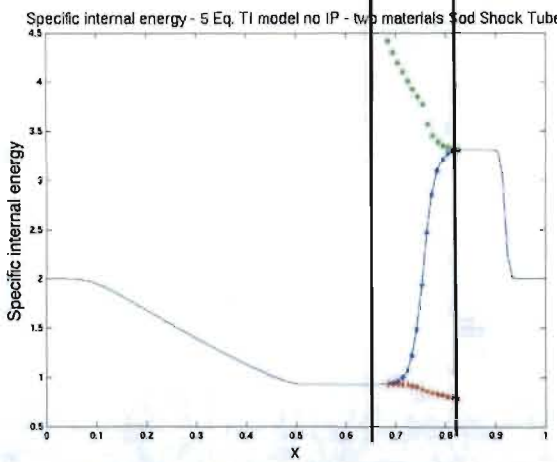
Two Materials Sod Shock Tube at t=0.2
Eulerian method with 5 Equation TI model no IP

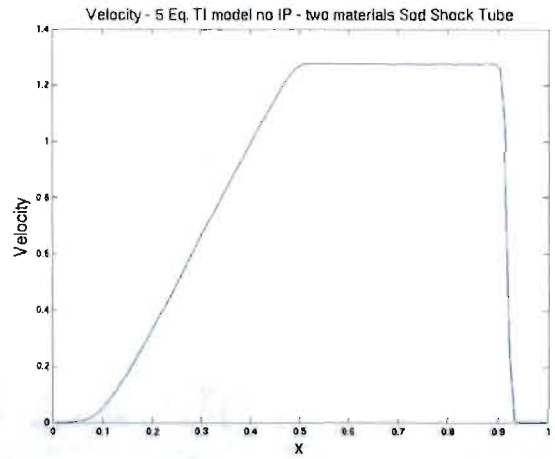
$$\rho = \sum_k (\alpha_k \rho_k)$$





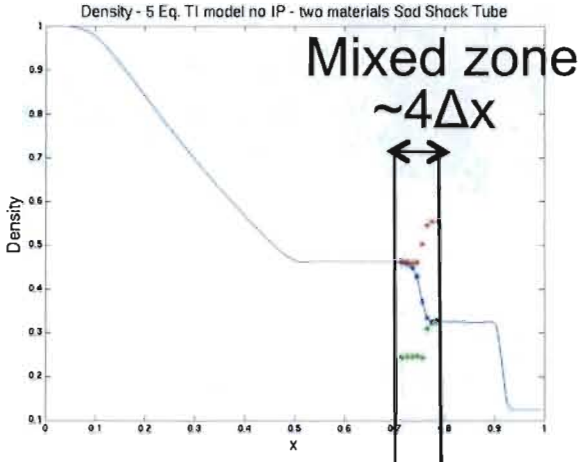
$$e = \sum_k m_k e_k(\rho_k, p)$$

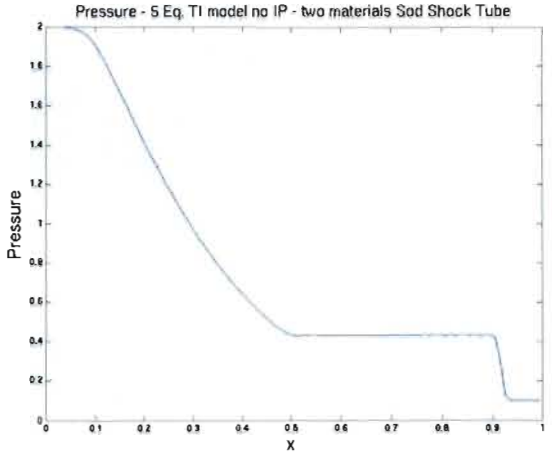




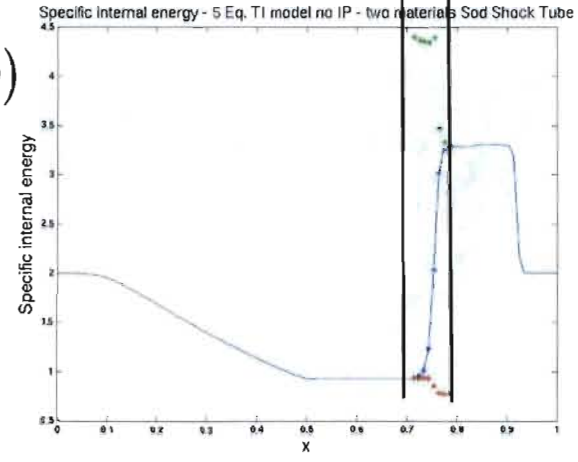
Two Materials Sod Shock Tube at t=0.2
Eulerian method with 5 Equation TI model with IP

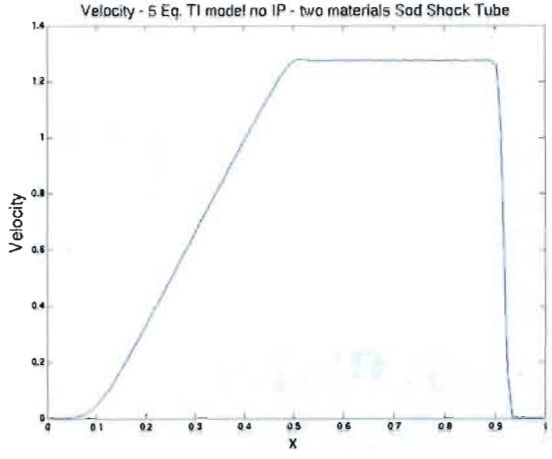
$$\rho = \sum_k (\alpha_k \rho_k)$$





$$e = \sum_k m_k e_k (\rho_k, p)$$



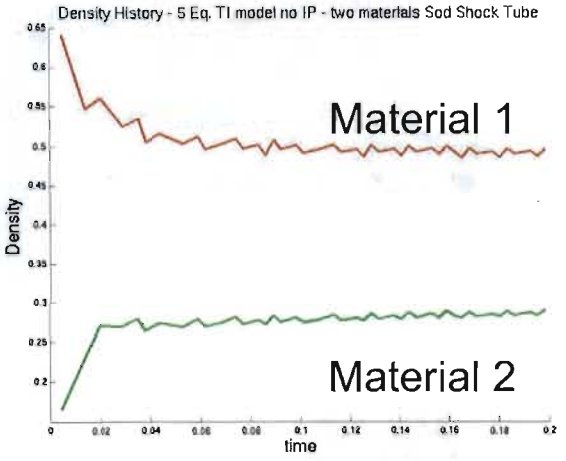


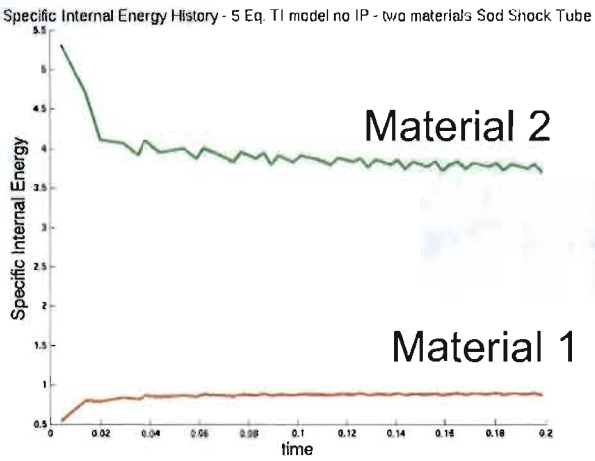
Tentative time-history plots for Eulerian method with 5 Equation TI model - Interface identified for $0.4 < \alpha < 0.6$

Density

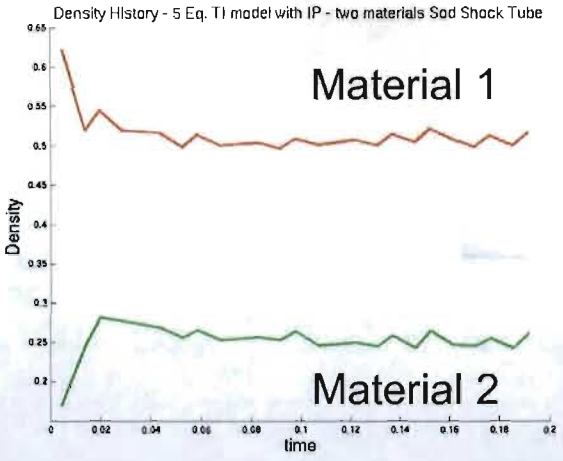
Specific Internal Energy

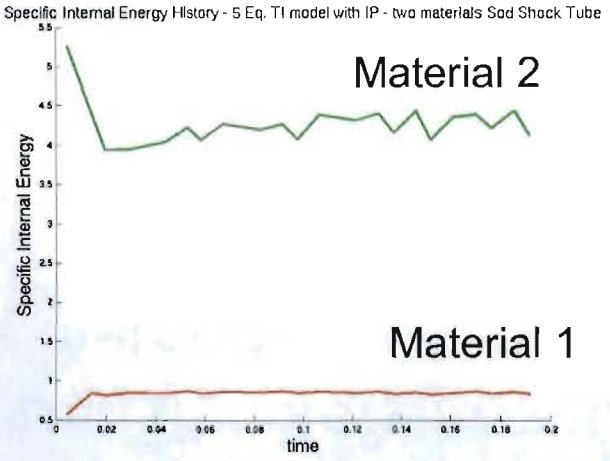
No IP



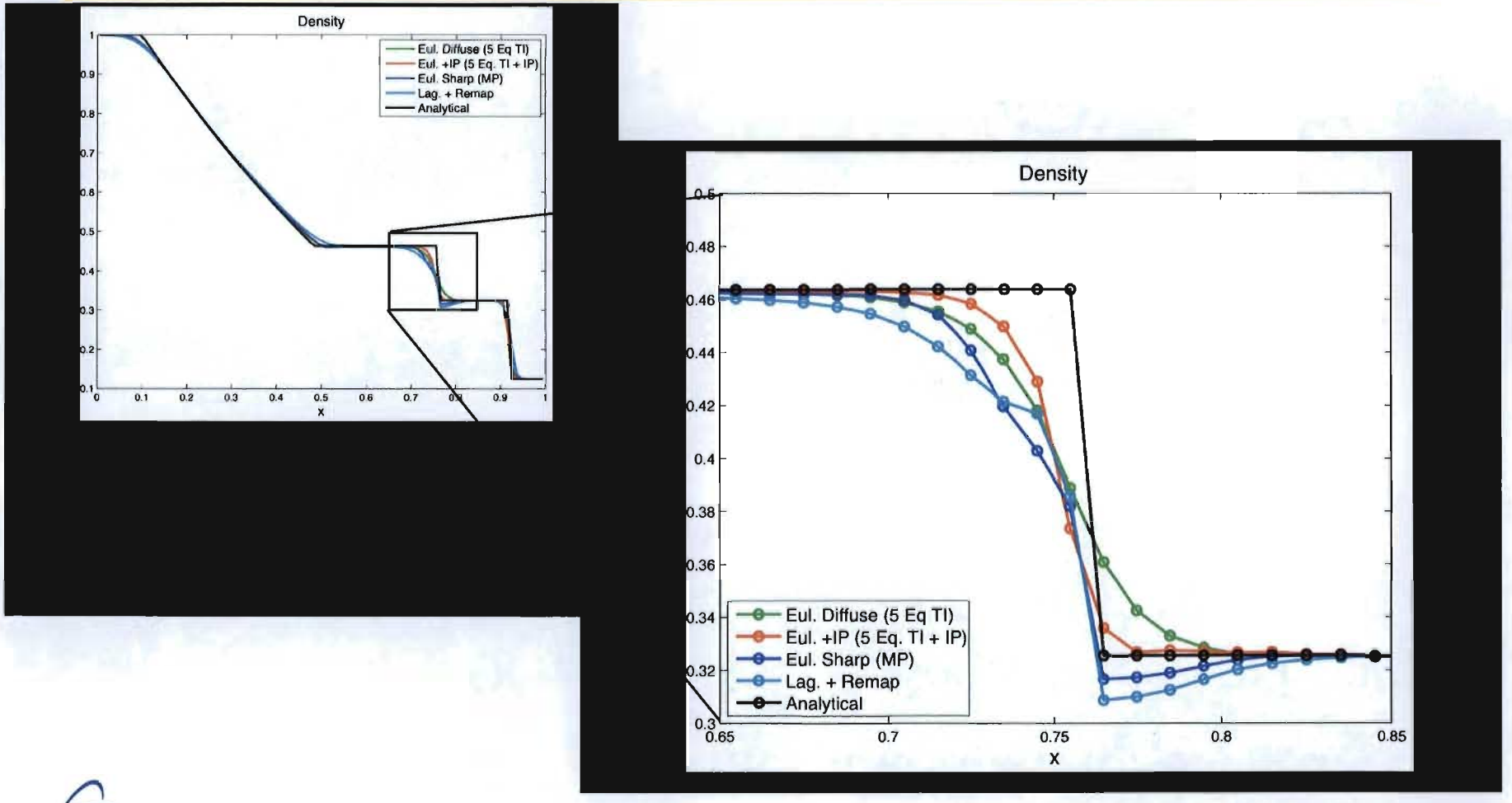


With IP

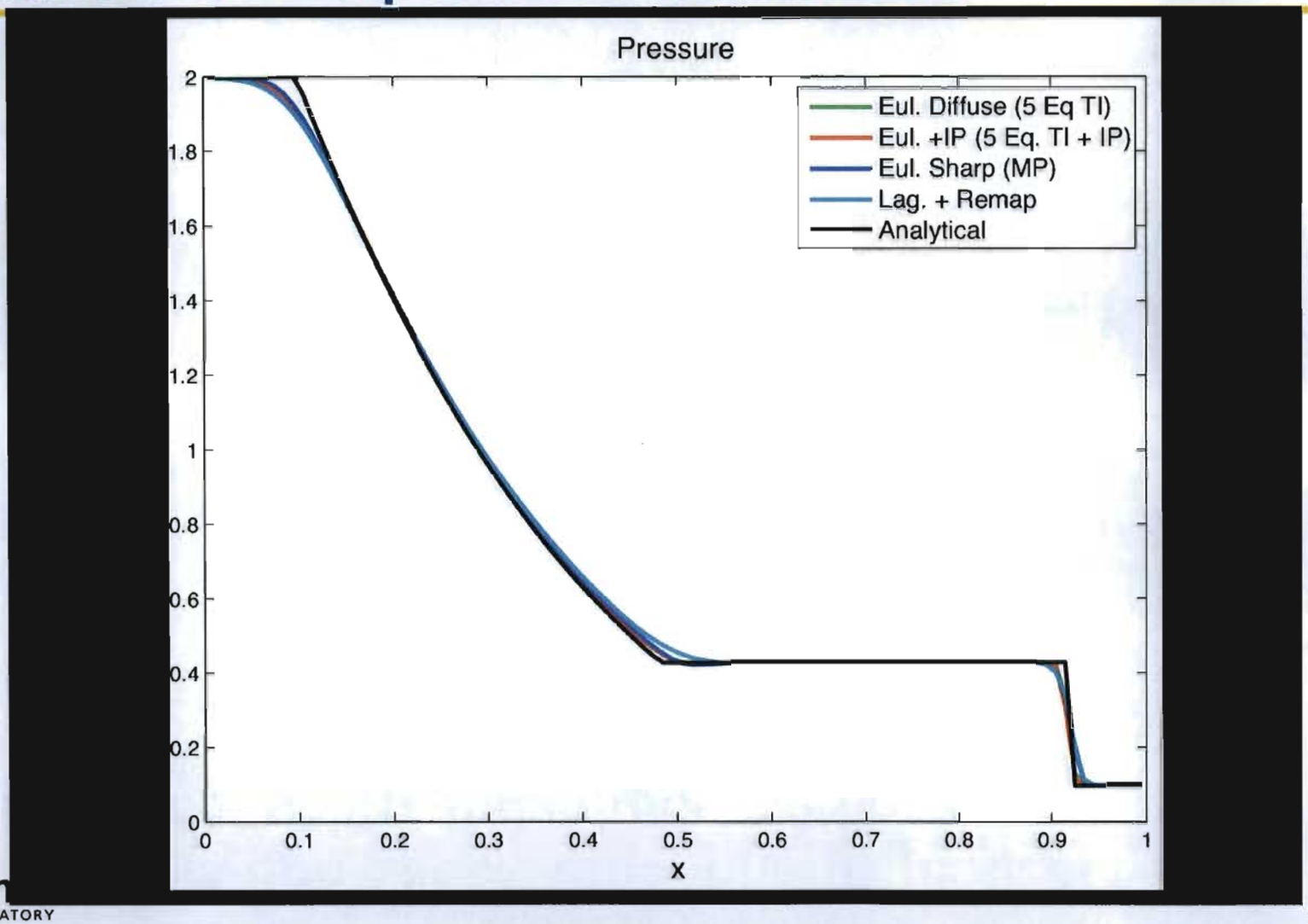




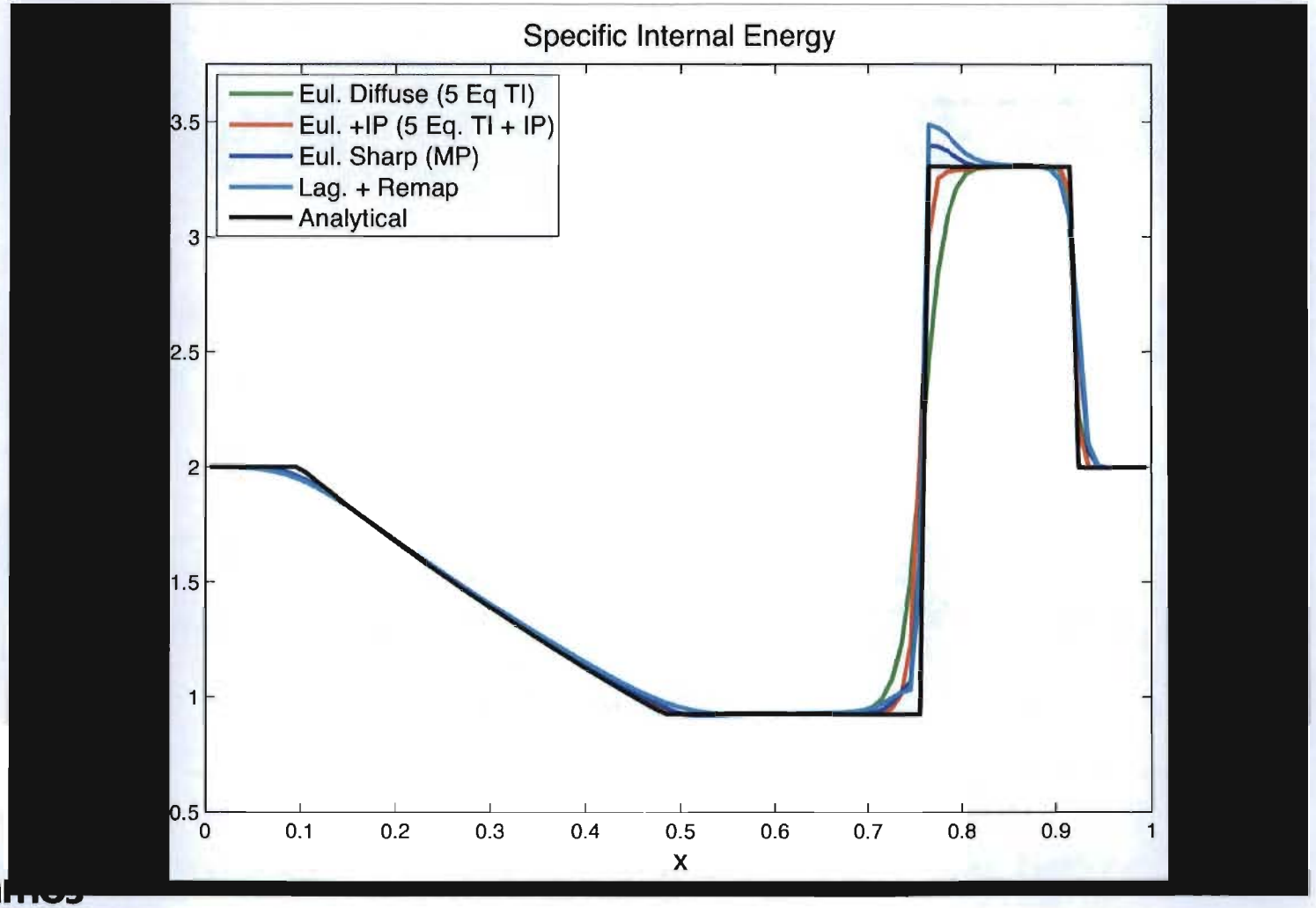
Two-materials Sod Shock Tube - Density plots at t=0.2
Comparison of sharp and diffuse methods



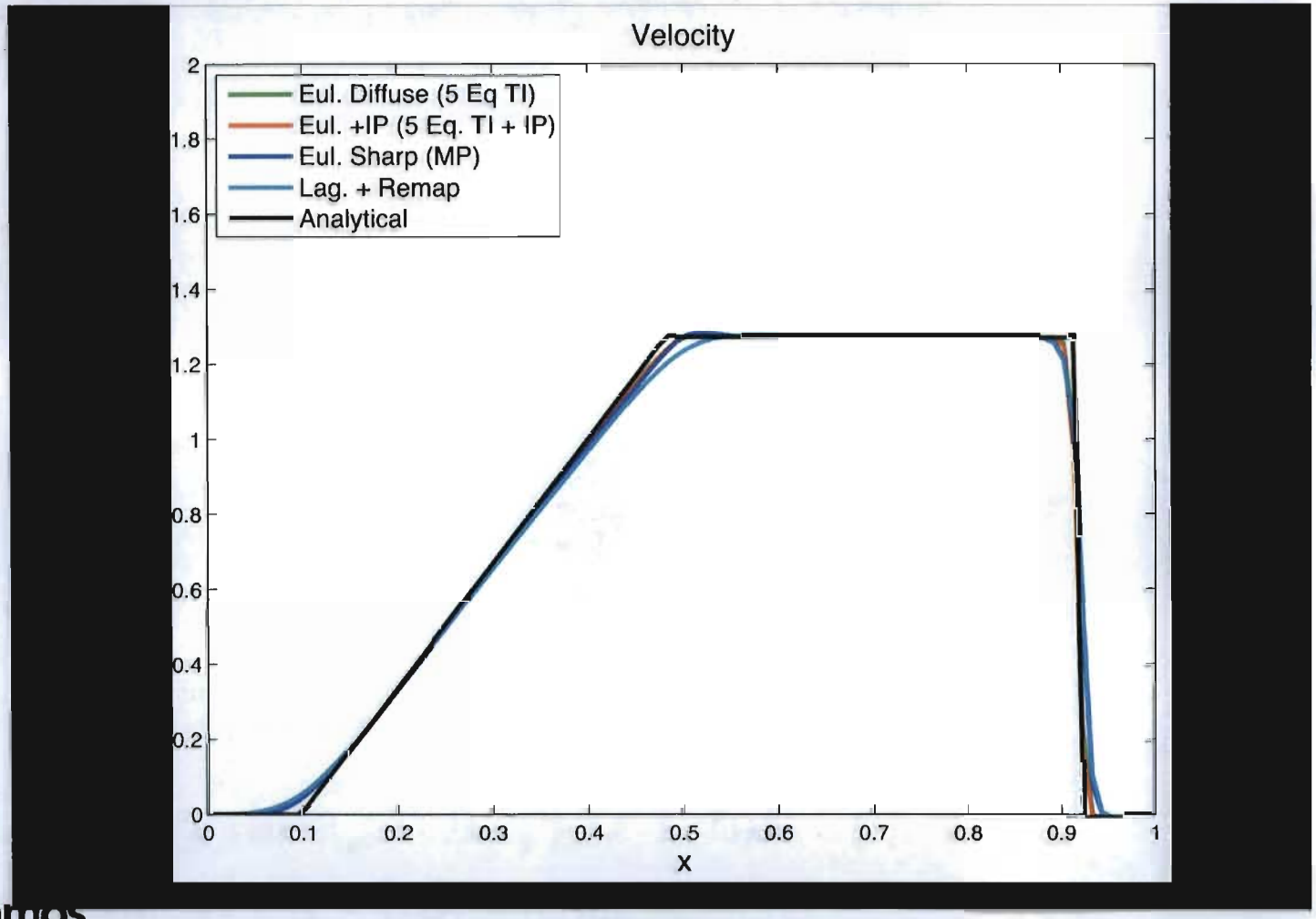
Two-materials Sod Shock Tube- Pressure plots at t=0.2
Comparison of sharp and diffuse methods



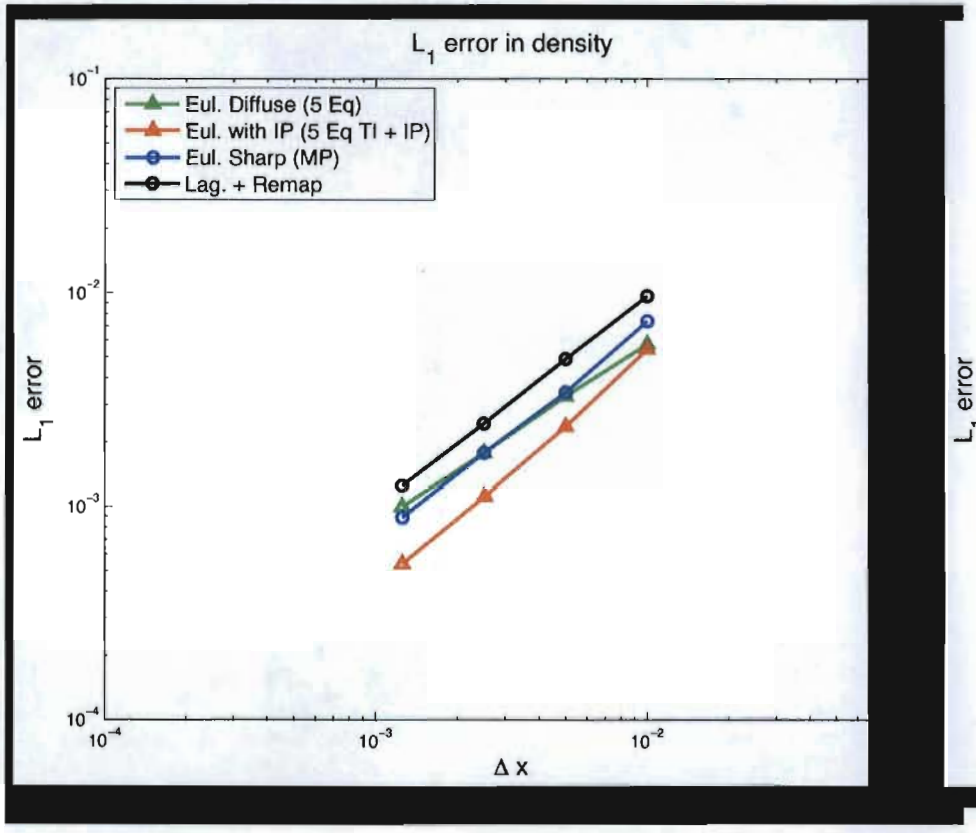
Two-materials Sod Shock Tube- Energy plots at t=0.2 Comparison of sharp and diffuse methods

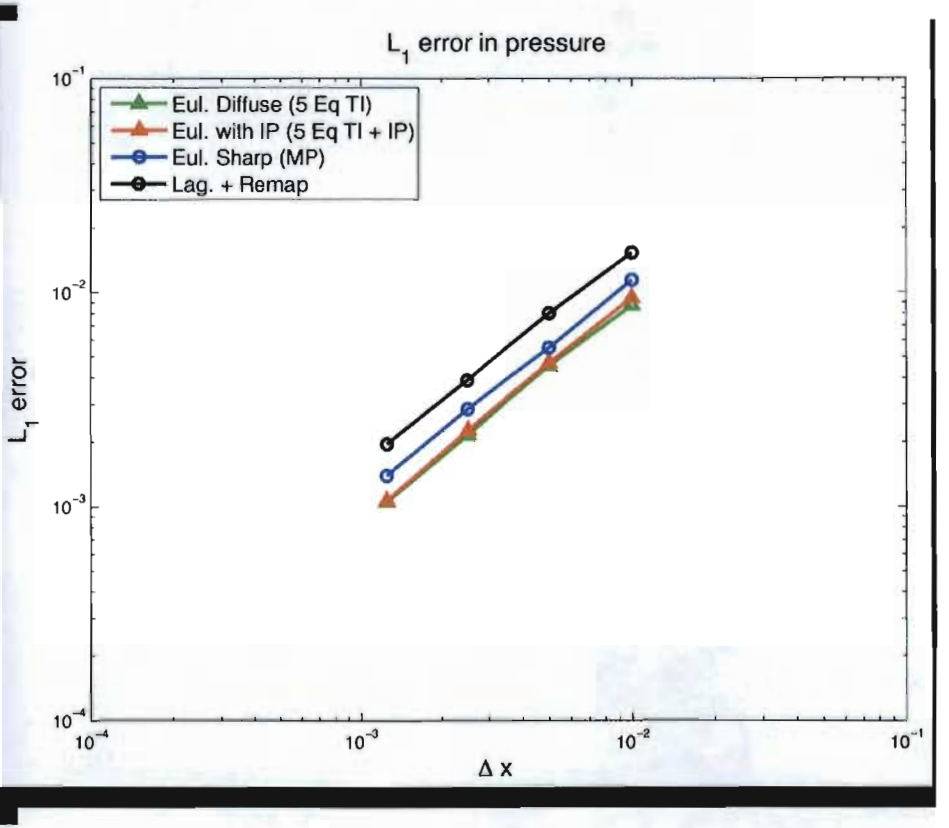


Two-materials Sod Shock Tube- Velocity plots at t=0.2 Comparison of sharp and diffuse methods

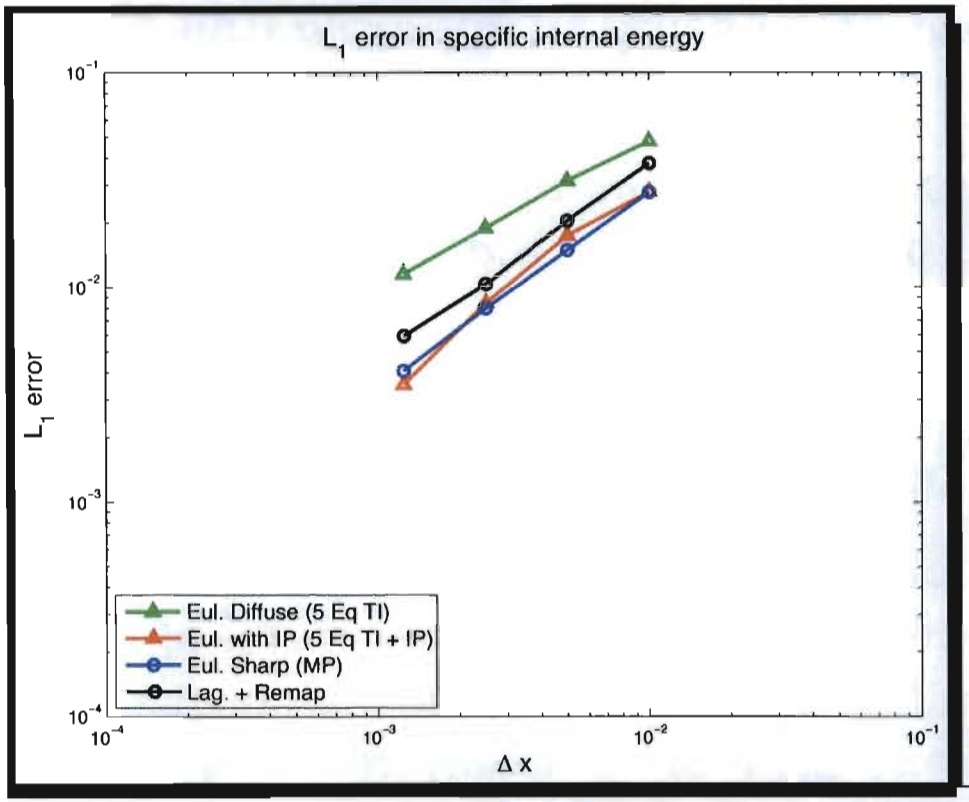


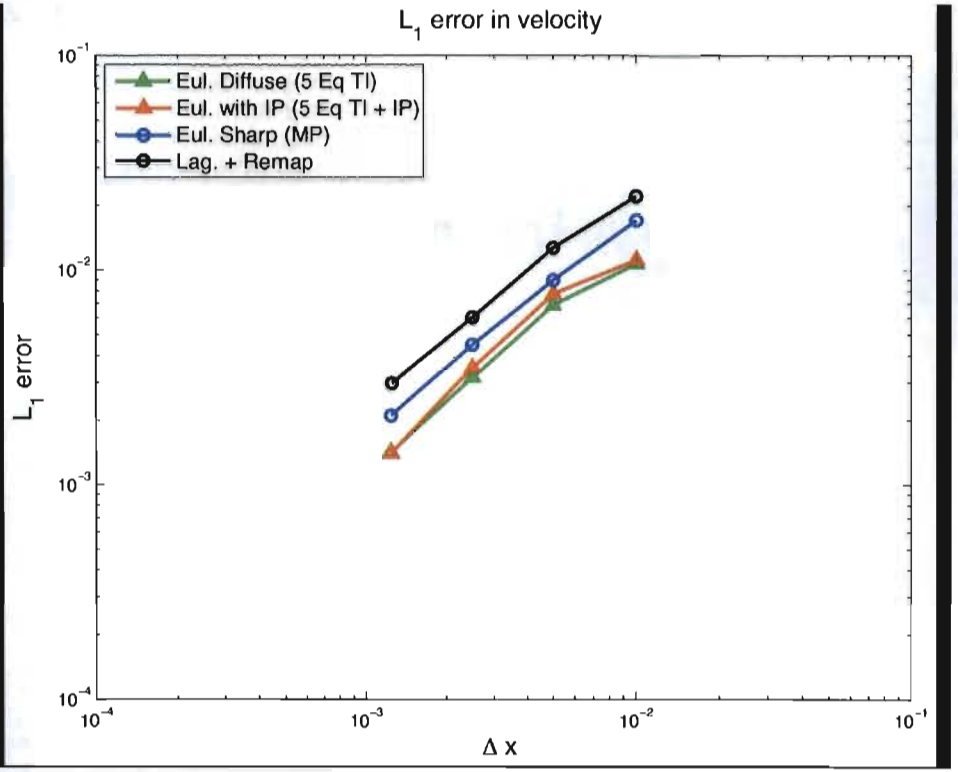
Two-materials Sod Shock Tube
L_1 Error for Density and Pressure at t=0.2





Two-materials Sod Shock Tube
L_1 Error for Energy and Velocity at t=0.2





Comparison of sharp and diffuse methods Remarks

- Both sharp interface method (Eul. Sharp (MP) and Lag. + Remap) exhibit a jump in density and specific internal energy over a single cell, however an overshoot in specific internal energy and an undershoot in density behind the interface are observed.
- The Eulerian diffuse methods do not exhibit overshoot/ undershoots, however the transition is smeared over a few cell across the interface.
- The Eulerian diffuse method with IP has less overall error in density, pressure, velocity and specific internal energy than the other methods.
- Sharp methods have less error only in specific internal energy.
- The Eulerian sharp method (MP) has slightly less error than the Lagrange + Remap error.

Conclusions and Future Work

- **We have compared fundamental Eulerian and Lagrangian algorithms and methods in 1D for multi-material compressible flow on the two materials Sod Shock Tube test problem.**
- **We found that:**
  - Interface steepening reduces numerical diffusion at the interface and leads to overall more accurate results than the other methods, however sharp interface methods can reproduce jump in density and specific internal energy.
  - Time history of the thermodynamic state variables in mixed cell varies with the various methods and algorithms.
- **Our focus for future work will be on pressure relaxation model**
  - **How can we create a dynamic relaxation model that meets specific requirements ? How much and how fast shall we relax ?**
  - **What is the equivalent of Tipton's model in Eulerian method ?**
  - **Additional test cases with various EOS**

EXTRA SLIDES

Five-Equation Model

$$
\begin{cases}
\dfrac{\partial \alpha_1}{\partial t} + u\dfrac{\partial \alpha_1}{\partial x} = 0 \\
\dfrac{\partial (\alpha\rho)_1}{\partial t} + \dfrac{\partial (\alpha\rho)_1 u}{\partial x} = 0 \\
\dfrac{\partial (\alpha\rho)_2}{\partial t} + \dfrac{\partial (\alpha\rho)_2 u}{\partial x} = 0 \\
\dfrac{\partial (\rho u)}{\partial t} + \dfrac{\partial (\rho u^2 + p)}{\partial x} = 0 \\
\dfrac{\partial (\rho E)}{\partial t} + \dfrac{\partial (\rho E + p) u}{\partial x} = 0
\end{cases}
$$

$$\rho = (\alpha\rho)_1 + (\alpha\rho)_2$$

$$e = m_1 e_1 + m_2 e_2 \qquad m_k = \frac{(\alpha\rho)_k}{\rho}$$

$$p = \frac{\rho e}{\dfrac{\alpha_1}{\gamma_1 - 1} + \dfrac{\alpha_2}{\gamma_2 - 1}}$$

$$E = e + \frac{1}{2}u^2$$

Six-Equation Model (Saurel et al., JCP, 228, 1678, 2009)

$$
\begin{cases}
\dfrac{\partial \alpha_1}{\partial t} + u\dfrac{\partial \alpha_1}{\partial x} = \mu(p_1 - p_2) \\
\dfrac{\partial(\alpha_1\rho_1)}{\partial t} + \dfrac{\partial(\alpha_1\rho_1 u)}{\partial x} = 0 \\
\dfrac{\partial(\alpha_2\rho_2)}{\partial t} + \dfrac{\partial(\alpha_2\rho_2 u)}{\partial x} = 0 \\
\dfrac{\partial(\rho u)}{\partial t} + \dfrac{\partial\left(\rho u^2 + (\alpha_1 p_1 + \alpha_2 p_2)\right)}{\partial x} = 0 \\
\dfrac{\partial(\alpha_1\rho_1 e_1)}{\partial t} + \dfrac{\partial(\alpha_1\rho_1 e_1 u)}{\partial x} + \alpha_1 p_1 \dfrac{\partial u}{\partial x} = -p_I \mu(p_1 - p_2) \\
\dfrac{\partial(\alpha_2\rho_2 e_2)}{\partial t} + \dfrac{\partial(\alpha_2\rho_2 e_2 u)}{\partial x} + \alpha_2 p_2 \dfrac{\partial u}{\partial x} = p_I \mu(p_1 - p_2)
\end{cases}
$$

$$p_I = \frac{Z_2 p_1 + Z_1 p_2}{Z_1 + Z_2} \qquad Z_k = \rho_k c_k$$

$$p = \alpha_1 p_1 + \alpha_2 p_2$$

Six-Equation Model (Saurel et al., JCP, 228, 1678, 2009)

- **Additional equation to numerically enforce conservation of energy**

$$\frac{\partial \rho\left(m_1 e_1 + m_2 e_2 + \frac{1}{2}u^2\right)}{\partial t} + \frac{\partial u\left(\rho\left(m_1 e_1 + m_2 e_2 + \frac{1}{2}u^2\right) + \left(\alpha_1 p_1 + \alpha_2 p_2\right)\right)}{\partial x} = 0$$

Godunov-type Method
MUSCL-Hancock Scheme (van Leer 1985, Toro 1999)

$$U_t + F(U)_x = 0$$

- **1. Data reconstruction**
  - Slope limiter
- **2. Half time step evolution**

$$\overline{U}_i^{L,R} = U_i^{L,R} - \frac{1}{2}\frac{\Delta t}{\Delta x}\left(F_i^R - F_i^L\right)$$

- **3. Solve Riemann Problem given left and right states to determine fluxes**
- **4. Update the variables in time**

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left(F_{i+1/2} - F_{i-1/2}\right)$$

Numerical Algorithm for Five-Equation Model

- **Conservative variables:** $\rho u, \rho E, (\alpha\rho)_1, (\alpha\rho)_2$

$$\mathsf{U} = \begin{pmatrix} \rho u \\ \rho\left(e + \frac{u^2}{2}\right) \\ (\alpha\rho)_1 \\ (\alpha\rho)_2 \end{pmatrix} \qquad \mathsf{F} = \begin{pmatrix} \rho u^2 + p \\ \left(\rho\left(e + \frac{u^2}{2}\right) + p\right)u \\ (\alpha\rho)_1 u \\ (\alpha\rho)_2 u \end{pmatrix}$$

- **Data reconstruction**
  - Minbee slope limiter $\rho, u, p, (\alpha\rho)_1, (\alpha\rho)_2$
- **Half time step evolution, compute Left and Right states of** U
- **HLLC Riemann solver**
- **Variable update**

$$\mathsf{U}_i^{n+1} = \mathsf{U}_i^n - \frac{\Delta t}{\Delta x}\left(\mathsf{F}_{i+1/2}^{HLLC} - \mathsf{F}_{i-1/2}^{HLLC}\right)$$

- **Volume fraction evolution**

$$\alpha_{1_i}^{n+1} = \alpha_{1_i}^n - \frac{\Delta t}{\Delta x}\left((u\alpha_1)_{i+1/2}^* - (u\alpha_1)_{i-1/2}^* - \alpha_{1_i}^n\left(u_{i+1/2}^* - u_{i-1/2}^*\right)\right)$$

Numerical Algorithm for Six-Equation Model

- **6 primitive variables:** $\alpha_1, \rho_1, \rho_2, u, p_1, p_2$
- **6 equations + 1 mixture total energy**
- **MUSCL Hancock: data reconstruction, half time step evolution**
- **HLLC Approximate Riemann Solver**
- **Variable update**

$$\mathsf{U}_i^{n+1} = \mathsf{U}_i^n - \frac{\Delta t}{\Delta x}\left(\mathsf{F}_{i+1/2}^{HLLC} - \mathsf{F}_{i-1/2}^{HLLC}\right)$$

$$\alpha_{1_i}^{n+1} = \alpha_{1_i}^n - \frac{\Delta t}{\Delta x}\left(\left(u\alpha_1\right)_{i+1/2}^* - \left(u\alpha_1\right)_{i-1/2}^* - \alpha_{1_i}^n\left(u_{i+1/2}^* - u_{i-1/2}^*\right)\right)$$

$$\left(\alpha\rho e\right)_{k_i}^{n+1} = \left(\alpha\rho e\right)_{k_i}^n - \frac{\Delta t}{\Delta x}\left(\left(\alpha\rho eu\right)_{k_{i+1/2}}^* - \left(\alpha\rho eu\right)_{k_{i-1/2}}^* - \left(\alpha p\right)_{k_i}^n\left(u_{i+1/2}^* - u_{i-1/2}^*\right)\right)$$

- **Relaxation step**

Saurel et al., J. Comp. Physics, 228, p. 1678-1712, 2009

Relaxation Step for solving Six-Equation Model

- **Relaxation step** $\sum_k \alpha_k = 1 \qquad V_k = \frac{1}{\rho_k}$

$$V_k(p) = V_k^0 \frac{p^0 + (\gamma_k - 1)\hat{p}_I}{p + (\gamma_k - 1)\hat{p}_I}$$

$$\sum_k (\alpha\rho)_k V_k(p) = 1$$

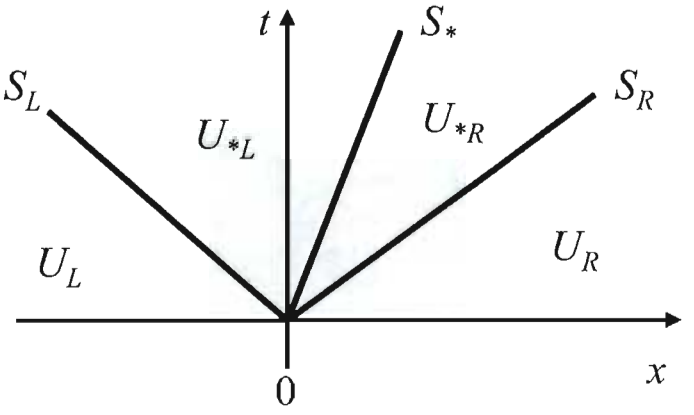
- **Solve for p by Newton's method**
- **Get new volume fractions** α_1, α_2
- **Reinitialization step**
  - Compute mixture pressure $$p = \frac{\rho e}{\frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}}$$
  - Reset internal specific energy $e_k = e_k(p, \alpha_k \rho_k, \alpha_k)$

Saurel et al., J. Comp. Physics, 228, p. 1678-1712, 2009

HLLC Approximate Riemann Solver (Toro et al. 1994)

- **Wave-speed estimates**

$$S_L = \min(u_L - c_L, u_R - c_R)$$
$$S_R = \max(u_L + c_L, u_R + c_R)$$
$$S_* = \frac{p_R - p_L + \rho_L u_L (S_L - u_L) - \rho_R u_R (S_R - u_R)}{\rho_L (S_L - u_L) - \rho_R (S_R - u_R)}$$



$$\mathsf{U}_{*K} = \begin{cases} \rho_K \left(\dfrac{S_K - u_K}{S_K - S_*} \right) S_* \\ \rho_K \left(\dfrac{S_K - u_K}{S_K - S_*} \right) \left(\dfrac{U_{2K}}{\rho_K} + (S_* - u_K) \left[S_* + \dfrac{p_K}{\rho_K (S_K - u_K)} \right] \right) \\ (\alpha_1 \rho_1)_K \left(\dfrac{S_K - u_K}{S_K - S_*} \right) \\ (\alpha_2 \rho_2)_K \left(\dfrac{S_K - u_K}{S_K - S_*} \right) \end{cases}$$

$$\mathsf{F}_{i+1/2}^{HLLC} = \begin{cases} \mathsf{F}_L & if \quad 0 \le S_L \\ F_L + S_L (\mathsf{U}_{*L} - \mathsf{U}_L) & if \quad S_L \le 0 \le S_* \\ F_R + S_R (\mathsf{U}_{*R} - \mathsf{U}_R) & if \quad S_* \le 0 \le S_R \\ \mathsf{F}_R & if \quad S_R \le 0 \end{cases}$$

$$K = L, R$$

Additional step in HLLC Approximate Riemann Solver

- **Additional variables:** $\alpha_k^*, \rho_k^*, u^*, p_k^*, e_k^*$

- **Volume fraction constant along fluid trajectories** $\alpha_{k_K}^* = \alpha_{k_K}$ $\quad K = L, R \quad k = 1,2$

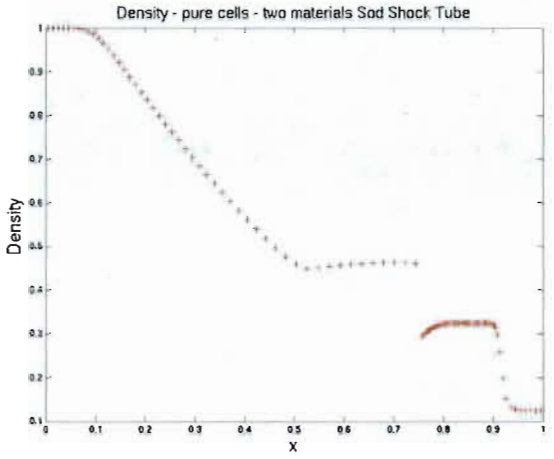
- **Density** $\rho_{k_K}^* = \rho_{k_K}\left(\frac{S_K - u_K}{S_K - S_*}\right)$

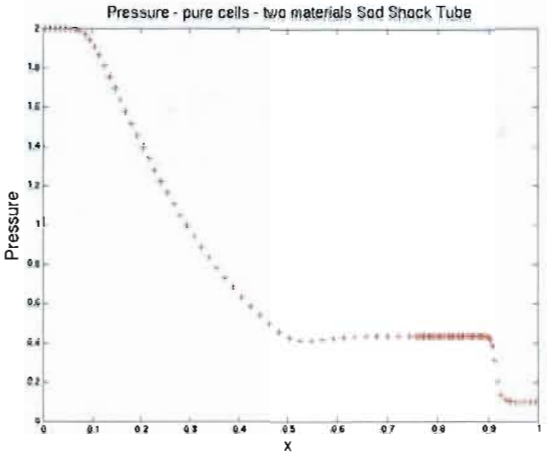
- **Internal energy jumps determined using Hugoniot relation**

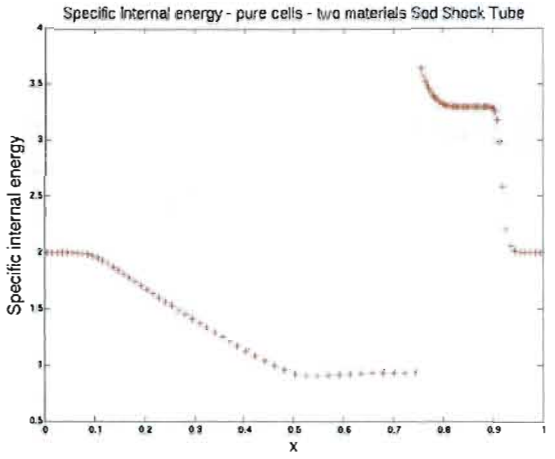
$$p_k^*(\rho_k^*) = p_k \frac{(\gamma_k - 1)\rho_k - (\gamma_k + 1)\rho_k^*}{(\gamma_k - 1)\rho_k^* - (\gamma_k + 1)\rho_k} \qquad e_{k_K}^* = e_{k_K}^*(p_k^*, \rho_k^*)$$

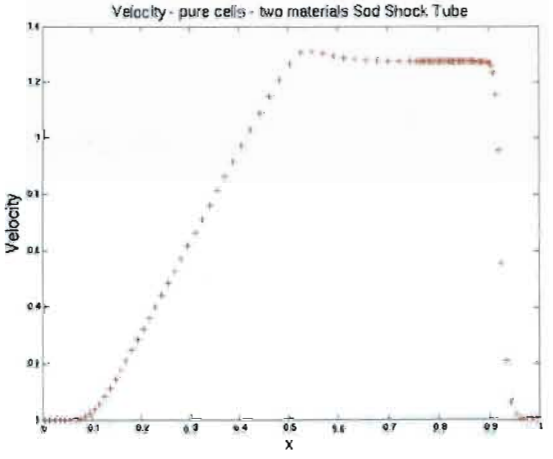
Saurel et al., J. Comp. Physics, 228, p. 1678-1712, 2009

Two Materials Sod Shock Tube at t=0.2
Staggered Lagrangian calculation with pure cells

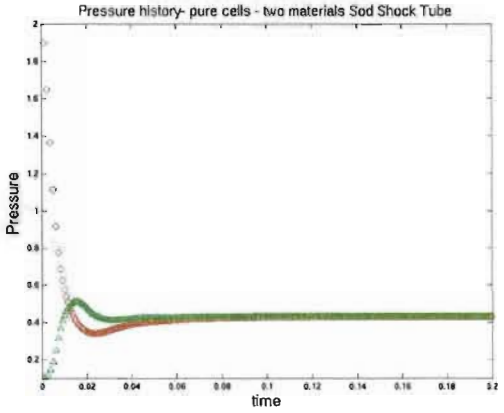
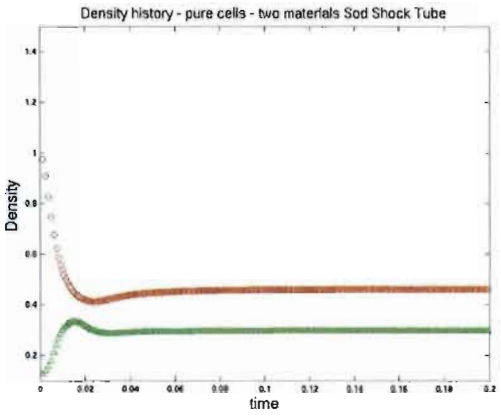
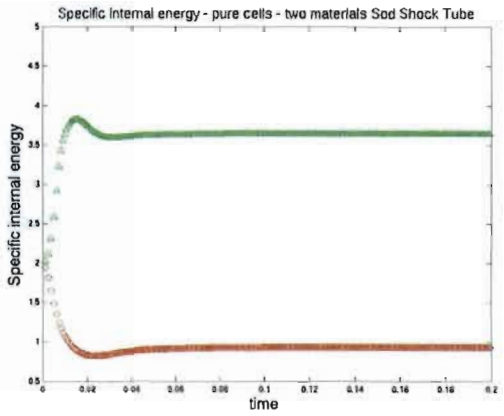








Lagrangian Calculation History

	Pressure	Density	Specific Internal Energy
Pure cells			
Tipton