Entropy Traces In Lagrangian and Eulerian Calculations

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Outline

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Introduction

The Big Picture

- There exists a common difficulty in the numerical solution of gasdynamic problems involving strong shockwaves.
- At boundaries and near the intersections of shockwaves, regions of anomalously high temperature appear.
- Often thought of as a feature of Lagrangian schemes, but occurs equally in Eulerian schemes if diffusion is sufficiently small.
- The difficulty is universal among all types of shock-capturing codes and if an assessment of temperature variation is important, casts doubt on the use of this otherwise robust and reliable class of methods.

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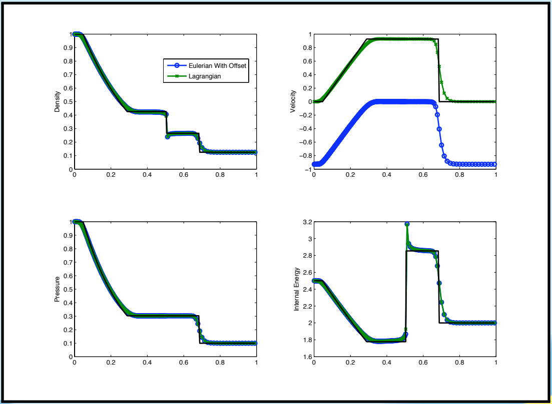
Sod's Problem

- To test this, compare Sod's shocktube problem for both types of methods, offsetting the velocity for the Eulerian method by the speed of the entropy wave.



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Governing Equations

- Without loss of generality, only the 1D Euler Equations in a fixed frame are shown, in vector notation as

$$\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = 0$$

or, expanded as

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho u \\ E\end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix}\rho u \\ \rho u^2 + p \\ \rho u H\end{bmatrix} = \begin{bmatrix}0 \\ 0 \\ 0\end{bmatrix},$$

with $H = \frac{E+p}{\rho}$ and closure from the ideal gas law,

$$p = (\gamma - 1)\left(E - \frac{1}{2}\rho u^2\right)$$

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Space-time Discretization

First-Order Godunov-type Methods

- Discretize in time explicitly with forward Euler time-stepping and in space with a Godunov-type scheme as

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{f}_{i+\frac{1}{2}}^n(\mathbf{u}_i^n, \mathbf{u}_{i+1}^n) - \mathbf{f}_{i-\frac{1}{2}}^n(\mathbf{u}_{i-1}^n, \mathbf{u}_i^n)\right)$$

  with the flux $\mathbf{f}_{i+\frac{1}{2}}^n(\mathbf{u}_i^n, \mathbf{u}_{i+1}^n)$ coming from the solution to the Riemann problem.
- In this work, both an exact and approximate (Roe) Riemann solver are used.
- 2^{nd}-order (or "high-resolution") methods do not alleviate wall heating; they instead preserve errors for much longer time than 1^{st}-order methods.

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A Canonical Example

The wall heating 'phenomenon'?

- Occurs in stagnation regions of a flow field.
- Manifests itself as a density defect, much larger than a typical numerical error.
- Since temperature and density are inversely proportional, this results in a large overshoot in temperature.
- Many stagnation regions are near walls, hence **wall heating phenomenon**.

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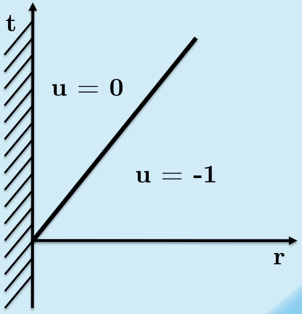
Isolating Wall Heating

The Noh Problem

- Notorious difficulty encapsulated by William Noh (1986)
- Describes the implosion of a strong shockwave by imposing an inward velocity.
- Exists in three dimensions with radial, cylindrical, and spherical symmetry.



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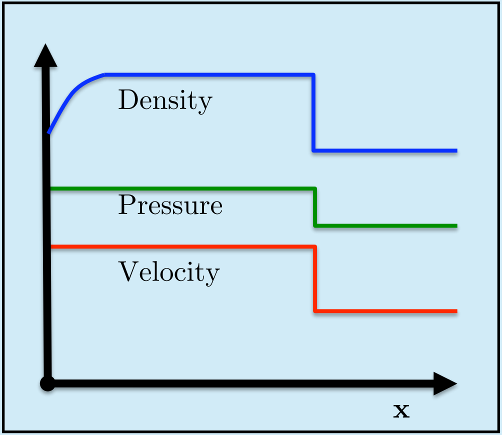
Representative Solutions



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Current Remedies

- Most current remedies use a type of energy diffusion, adjusting the energy equation in some form (Noh 1986, Xu and Hu 1998, Menikoff 1994)
- Within this category, there are also pressure type fixes (Fedkiw 1999) and Riemann Solver type fixes (Glaister 1988, Donat and Marquina 1996)

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Foundations of Wall Heating

Initial Setup

- Start with the Noh problem under planar symmetry, with initial state $\mathbf{u}_0$ defined by $[\rho_0, u_0, p_0]^T$.
- Define the uniform state produced by the shock as $\mathbf{u}_1$.
- Define a shock Courant number $\nu = S\frac{\Delta t}{\Delta r}$ for shock speed S.
- After one timestep of a Godunov-type finite volume method, the new state in the cell just right of the origin will be

$$\mathbf{u}(\nu) = \nu\mathbf{u}_1 + (1-\nu)\mathbf{u}_0.$$

- Thus all conserved variables change by an amount directly proportional to the timestep.

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Initial Theory

- Pressure, however, does not change linearly, but as

$$p(\nu) = \nu p_1 + (1-\nu)p_0 + \left(\frac{\gamma-1}{2}\right)\frac{\nu(1-\nu)\rho_0\rho_1 u_0^2}{(\nu\rho_1 + (1-\nu)\rho_0)}.$$

  which is greater than a linearly interpolated pressure.
- This higher pressure is then used in the second timestep and results in an excessive pressure gradient, expelling gas away from the center.
- The result is the removal of too much mass with no future mechanism for recovery.
- We refer to this numerical phenomenon as nonlinear mixing.

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A Linear Equation of State?

- To test if the problem truly is caused by pressure convexity, introduce a linear equation of state such that

$$p(\nu) = \nu p_1 + (1 - \nu)p_0.$$

- For simplicity and dimensional consistency, use

$$p = (\gamma - 1)E.$$

- This could also be viewed as a linear relationship between internal energy and total energy.

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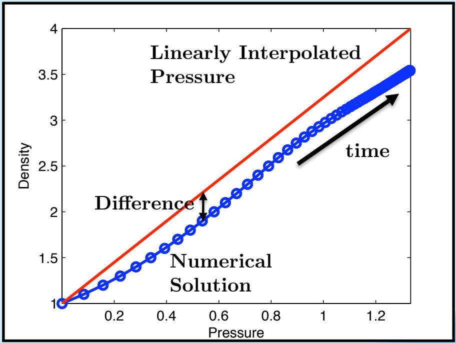
Wall Cell Results

- How different are the results from a linearly interpolated pressure?
- This can be measured this with a $\rho - p$ plot from the cell next to the wall.



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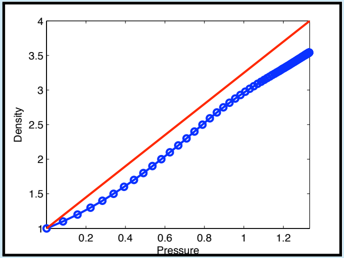
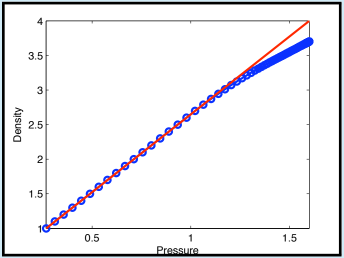
Wall Cell Results

Traditional Noh Problem -Shock speed of $\frac{1}{3}$



Ideal EOS



Linear EOS

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So what went wrong?

- There is at least one more mechanism at work.
- Previous work (Roberts, 1996, Arora and Roe, 1996, Karni and Čanić, 1997, Xu and Hu, 1998) suggests that this could be due to the slowly moving shock or similar phenomena.
- We relate this also to the 'start-up error', which is common in all codes and directly related to the transition of a shock into a stable cycle.

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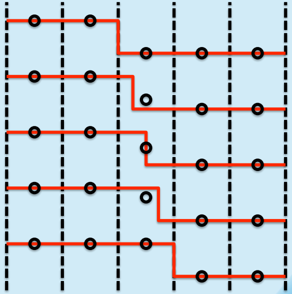
Underlying Theory (Arora and Roe, 1996)

- For a single captured shock to be located anywhere on a 1D grid, at least one internal value is needed.
- If we regard the figure as snapshots of the moving shock, it appears that this shock structure will be periodic, with period

$$T_S = \frac{\Delta x}{S}$$



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A Note on 'Shock Transition'

- Single shocks eventually propagate with a periodic shock structure.
- This is proceeded by a transient phase following start-up.
- During both phases, spurious waves are emitted and then propagate as physical waves.

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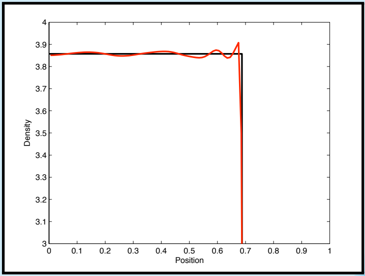
Slowly Moving Shocks

- If the shock speed is slow, oscillations occur behind the shock caused by spurious waves in the solution to the Riemann Problem.
- These waves have a long timescale, and are preserved by the numerical scheme.
- For a fast shock, these waves are still present but on a short timescale; thus they are not preserved by the numerical scheme, hence no observed oscillations.



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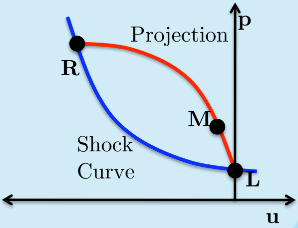
Entropy Traces

- Entropy traces occur for a simple wave when internal states do not lie on the path connecting external states.
- Here, a left and right state and the Shock curve connecting them is shown.



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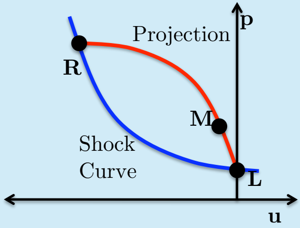
Entropy Traces

- After one step, the internal state lies on the curve described earlier, here referred to as the Projection curve.
- The solution to future Riemann problems will then contain spurious waves of the other families, which will continue to propagate and result in potential errors.



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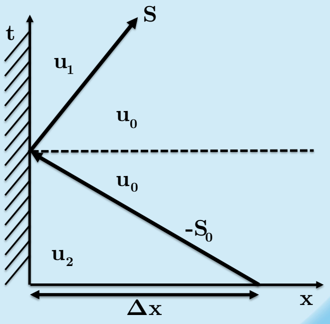
Entropy Traces

- To investigate start-up error as a mechanism for wall heating, the 'reflecting Noh problem' was developed.
- This is similar to the original Noh problem, but allows for the start-up error to be observed before contacting the wall.



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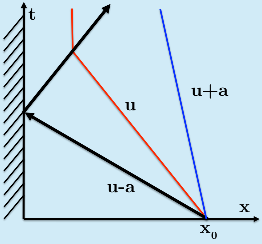
Entropy Traces

- Based on the previous analysis, a wave diagram similar to the one on the right is expected.
- The spurious contact discontinuity propagates an error towards the wall, but it is intercepted by the reflecting shock.
- A density defect should then occur away from the wall at the point of intersection, within the stagnation region.



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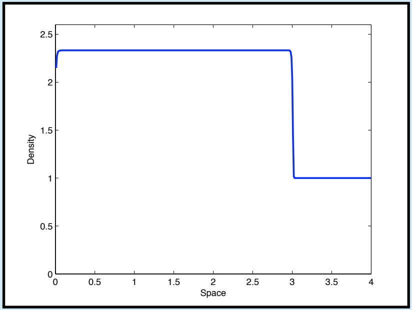
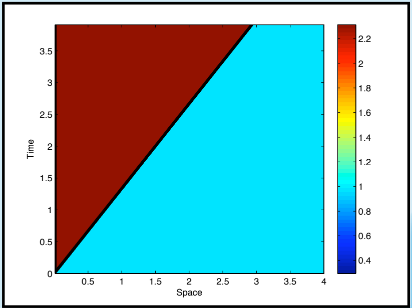
Sample Results

Density at Final Time



Density Contours



- Shock started 1 cell away.

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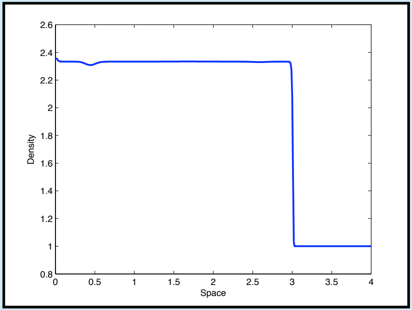
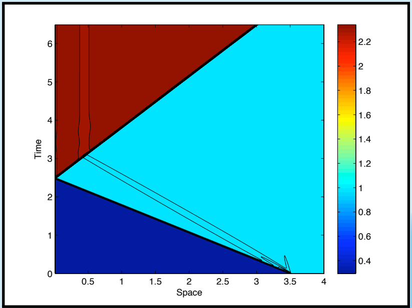
Sample Results

Density at Final Time



Density Contours



- Shock started 350 cells away.

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A Wall Heating-Free System

- To further demonstrate that the 'start-up' error is a entropy trace, devise a three-wave system whose projections lie exactly on the shock curve.
- One such system is the one shown below,

$$\begin{bmatrix} u \\ a \\ b \end{bmatrix}_t + \begin{bmatrix} \frac{1}{2}\left(u^2 + a^2 + b^2\right) \\ ua \\ ub \end{bmatrix}_x = \mathbf{0}$$

- This system has eigenvalues $u - c, u, u + c$ for $c^2 = a^2 + b^2$ and a linear (identical) shock and expansion curve.

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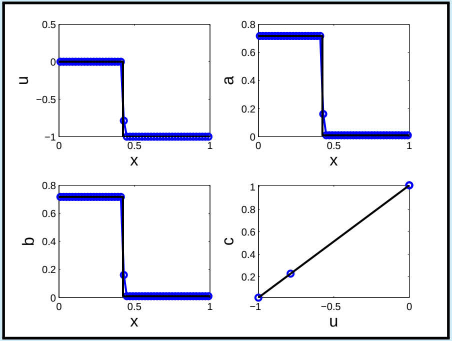
A Wall Heating-Free System

A Single Slow Shock



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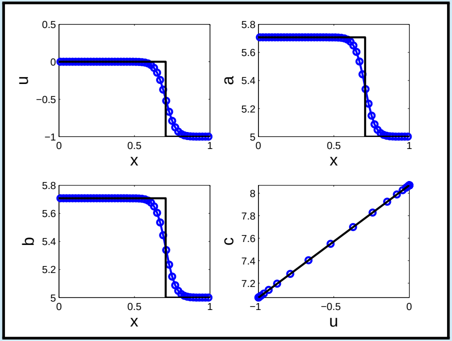
A Wall Heating-Free System

A Single Fast Shock



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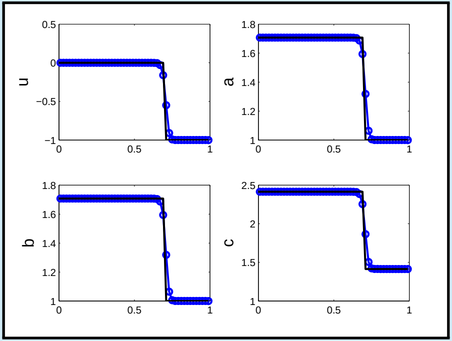
A Wall Heating-Free System

A Noh Problem



- Here 50 cells are shown with $\mathbf{u}(x,0) = [-1,1,1]^T$ and a wall boundary condition on the left side.

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A Wall Heating-Free System

Observations

- For a single shock moving across a grid, all internal states lie exactly on the shock curve.
- For the slowly moving shock, there is no entropy trace or spurious oscillations.
- Since there is no entropy trace or nonlinear mixing, there is no wall heating observed.

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Summary

- Whenever entropy is created by numerical error, it is propagated along particle paths as though it had been created physically.
- The simplest example of this is wall heating, exemplified by the Noh problem.
- Two mechanisms behind this phenomenon are examined and isolated.
- The explanations were validated by constructing examples of artificial conservation laws from which the mechanisms were absent, and then verifying that the phenomenon did not occur.
- These errors derive from insisting on the narrowest possible shock profiles, and so we are currently looking at various shock-broadening mechanisms.

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An Alternate Form of Pressure?

- An alternative description of pressure comes from defining a convective equation for pressure of the form

$$\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right) p_{\mathrm{nc}} + (p + (\gamma - 1)p_{\mathrm{nc}})\frac{\partial u}{\partial x} = 0$$

  where p_{nc} refers to 'nonconservative' pressure.
- p_{nc} is then a linearly interpolated pressure.

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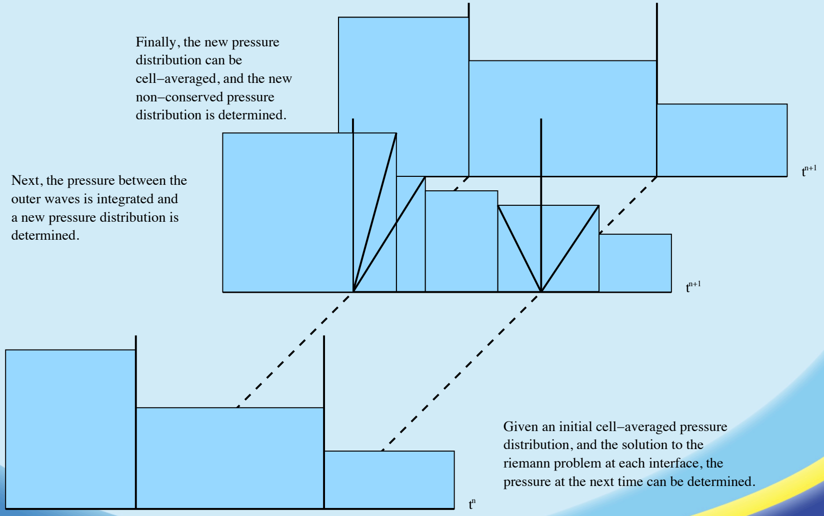
Determining Nonconservative Pressure



Finally, the new pressure distribution can be cell–averaged, and the new non–conserved pressure distribution is determined.

Next, the pressure between the outer waves is integrated and a new pressure distribution is determined.

Given an initial cell–averaged pressure distribution, and the solution to the riemann problem at each interface, the pressure at the next time can be determined.

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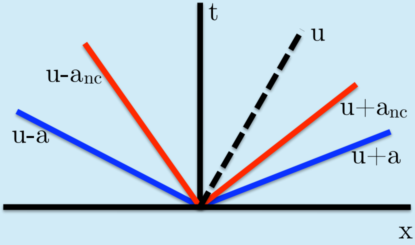
Non-conservative Pressure



- Introducing p_{nc} into the system results in slower propagating waves.
- This prevents mass and other conserved quantities from propagating as fast.

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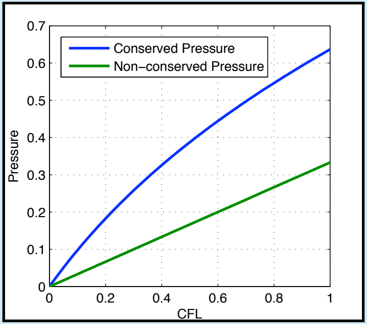
Non-conservative Pressure



- After one timestep, plotting pressure against CFL number shows the expected nonlinear relationship in ‘conserved’ pressure and linear relationship in ‘non-conserved’ pressure.

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Non-conservative Pressure

- To introduce this into the regular system, an additional wave of strength

$$\alpha = \frac{2}{(\gamma - 1)u^2}\Delta(p - p_{\mathrm{nc}})$$

- With an additional contribution to the flux as in

$$\hat{\mathbf{f}}(\mathbf{u}_L, \mathbf{u}_R) = \mathbf{f}(\mathbf{u}_L, \mathbf{u}_R, p_{\mathrm{nc}L}, p_{\mathrm{nc}R}) - \begin{bmatrix} 0 \\ 0 \\ |u| \end{bmatrix} \frac{\Delta(p - p_{\mathrm{nc}})}{2(\gamma - 1)}$$

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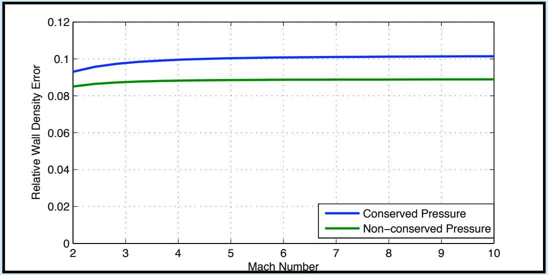
Results



- Here, relative density error at the wall, defined as

$$\text{error} = \frac{\rho_{\text{exact,wall}} - \rho_{\text{wall}}}{\rho_{\text{exact,wall}}}$$

is plotted for a range of Mach numbers, M_0.

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Diffusion

- Since the effect of non-conservative pressure is small, define a scalar diffusive flux of the form

$$f_{d,i+\frac{1}{2}} = -\frac{k_{i+\frac{1}{2}}}{\Delta x}((p_{\mathrm{nc}} - p)_{i+1} - (p_{\mathrm{nc}} - p)_i)$$

- Modify the energy equation to the form

$$E_t + (u(E+p))_x = \left(\frac{k}{\gamma - 1}(p_{\mathrm{nc}} - p)_x\right)_x$$

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Diffusion

- To determine k, define

$$C_{i+\frac{1}{2}} = k_{i+\frac{1}{2}} \frac{\Delta t}{(\Delta x)^2} \qquad 0 \leq C_{i+\frac{1}{2}} \leq \frac{1}{2}$$

- We propose the CFL dependent choice of

$$C_{i+\frac{1}{2}} = \mathrm{CFL}\frac{1}{2}\frac{|\Delta \mathbf{v}_{i+\frac{1}{2},2}|}{\sum_j |\Delta \mathbf{v}_{i+\frac{1}{2},j}|}$$

where $\Delta \mathbf{v} = \mathbf{L}\Delta \mathbf{u}$ are the wave strengths.

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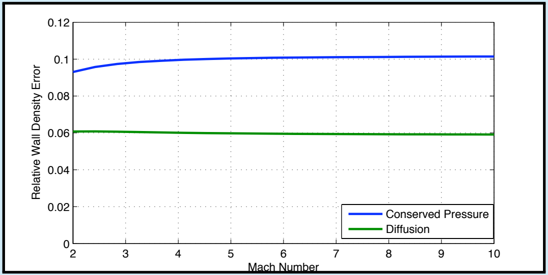
Results



- Using diffusion produces much more promising results, reducing error by roughly 40%.

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Observations

- While we are able to reduce the error significantly, the effects of diffusion on the rest of the solution have not been thoroughly examined.
- The exact placement of non-conservative pressure within the Riemann solver used also affects the solution.
- The choice of diffusive coefficient is fairly ad-hoc, and it is not clear how effective the current choice is in more complex problems.

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Comparison with Ideal EOS

EOS	Linear	Ideal
Pressure	$(\gamma-1)E$	$(\gamma-1)(E-1/2\rho u^2)$
Eigenvalues	$\frac{\gamma+1}{2}u \pm a, u$	$u \pm a, u$
Speed of Sound Squared	$\frac{\gamma p}{\rho} + \frac{(\gamma-1)^2}{4}u^2$	$\frac{\gamma p}{\rho}$
$\left(\frac{\rho_R}{\rho_L}\right)_{\max}$ across a shock	Infinite	$\frac{\gamma+1}{\gamma-1}$
$\left(\frac{p_R}{p_L}\right)_{\max}$ across a shock	Infinite	Infinite

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S and E Curves for the Linear EOS

Flux Jacobian

- Introduce the flux Jacobian $\mathbf{A} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} = \mathbf{R}\Lambda\mathbf{L}$ and defining an enthalpy $h = \frac{(E+p)}{\rho} = \frac{\gamma e}{\rho}$, the flux Jacobian is

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 \\ -u^2 & 2u & \gamma - 1 \\ -hu & h & \gamma u \end{bmatrix}$$

- with eigenvalues $\frac{(\gamma+1)}{2} u \pm a, u$ for a propagation speed

$$a = \sqrt{(\gamma - 1)\left(h + (\gamma - 1)\frac{u^2}{4}\right)}$$

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Wave Decomposition

Eigenvectors

$$\mathbf{L} = \begin{bmatrix} \frac{u(2a+(\gamma-1)u)^2}{8ah(\gamma-1)} & -\frac{(2a+(\gamma-1)u)^2}{8ah(\gamma-1)} & \frac{2(2a+(\gamma-1)u)}{8ah} \\ 1-\frac{u^2}{h} & \frac{u}{h} & -\frac{1}{h} \\ -\frac{u(2a-(\gamma-1)u)^2}{8ah(\gamma-1)} & \frac{(2a-(\gamma-1)u)^2}{8ah(\gamma-1)} & \frac{2(2a-(\gamma-1)u)}{8ah} \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} 1 & 1 & 1 \\ u-\frac{2(\gamma-1)h}{2a+(\gamma-1)u} & u & u+\frac{2(\gamma-1)h}{2a-(\gamma-1)u} \\ h-\frac{2(\gamma-1)uh}{2a+(\gamma-1)u} & 0 & h+\frac{2(\gamma-1)uh}{2a-(\gamma-1)u} \end{bmatrix}$$

This research was supported by the DOE NNSA/ASC under the Predictive Science Academic Alliance Program by grant number DEFC52-08NA28616.

Expansion Waves

Wave Jumps

- Similar to the ideal EOS, across a contact, $\mathrm{d}p$ and $\mathrm{d}u$ are both zero.
- For expansions, two relations arise:

$$\left(\frac{(\gamma-1)}{2}u \pm a\right)\mathrm{d}u = \frac{\mathrm{d}p}{\rho}$$

$$\mathrm{d}E = h\mathrm{d}\rho + \rho u \mathrm{d}u$$

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Expansion Waves

Expansion Curves

- With a great deal of algebra, a transcendental equation for the part of the expansion curve can be written as

$$\frac{\mathrm{d}a}{\mathrm{d}u} = \frac{(\gamma - 1)(\gamma u \pm a)}{2a}$$

- Further manipulation and integration gives

$$\left(\frac{p^*}{p_0}\right)^{\gamma-1} = \left(\frac{h^*}{h_0}\right)^{\gamma} \exp\left[-\int_{u_0}^{u^*} \frac{\gamma u \mathrm{d}u}{\frac{a(u)^2}{\gamma-1} - \frac{\gamma-1}{4}u^2}\right]$$

where the solution can be achieved numerically.

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Shockwaves

Hugoniot Curves

- From the jump conditions, the Hugoniot Curve is

$$p^* = p + \rho[u]\left(\frac{(\gamma u^* - u)}{2} \pm \sqrt{\frac{(\gamma u^* - u)^2}{4} + (\gamma - 1)h}\right)$$

- The density can then be obtained from

$$\rho^* = \rho\left[\frac{u[p] - \gamma[up]}{u^*[p] - \gamma[up]}\right]$$

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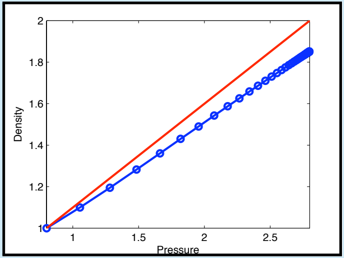
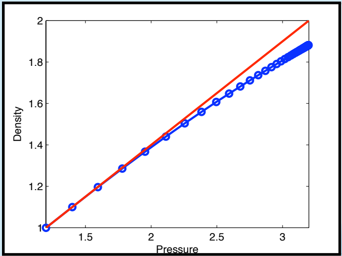
Wall Cell Results

Shock speed of 1



Ideal EOS



Linear EOS

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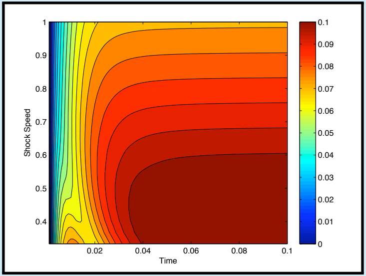
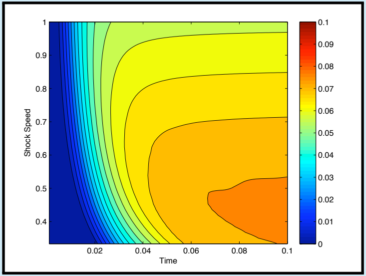
Error Contours



Ideal EOS



Linear EOS

- Here, a range of shock speeds are examined and error contours are plotted to get a feel for trends in the system.

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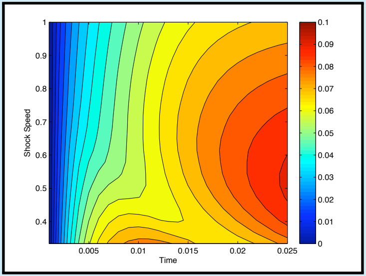
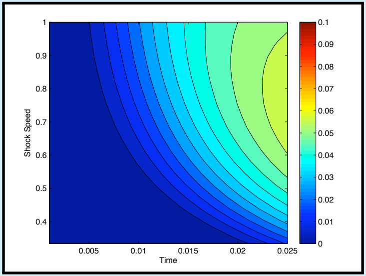
Error Contours



Ideal EOS



Linear EOS

- Taking a closer look, using a Linear EOS seems to eliminate one mechanism of error.
- However, some error at the wall still remains.

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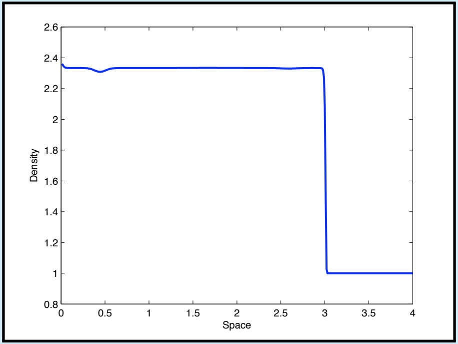
Initial Results

Reflecting Noh Problem



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Linear Shock Curve System

$$\mathbf{A} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} = \begin{bmatrix} u & a & b \\ a & u & 0 \\ b & 0 & u \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} -c & 0 & c \\ a & -b & a \\ b & a & b \end{bmatrix}$$

$$\mathbf{L} = \frac{1}{2c^2} \begin{bmatrix} -c & a & b \\ 0 & -2b & 2a \\ c & a & b \end{bmatrix}$$

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Linear Shock Curve System

Conditions Across a Wave

- Through a shock or an expansion, the conditions are

$$\frac{a}{b} = \text{constant} \qquad u \pm c = \text{constant}$$

- Across a contact wave, u and c are both constant.

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Linear Shock Curve System

An Entropy

- The entropy equation is

$$U_t + F_x \leq 0$$

with

$$U(\mathbf{u}) = \frac{1}{2}(u^2 + c^2)$$

and

$$F(\mathbf{u}) = \frac{1}{3}u^3 + uc^2$$

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