An Algorithm For Time Evolving Volume Fractions in Mixed Zones in Lagrangian Hydrodynamics Calculations

Numerical Methods For Multi-Material Fluid Flows
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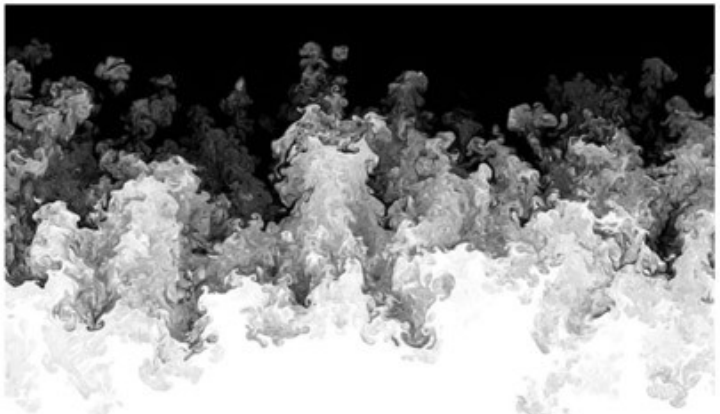
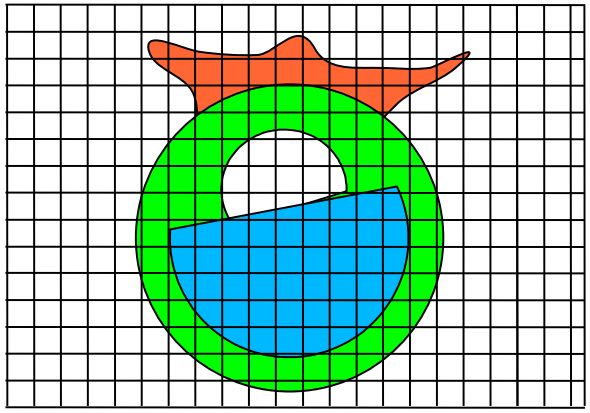
Mixed zones inevitably develop in all but the simplest problems



3D Rayleigh-Taylor calculation

- **Rayleigh-Taylor, Richtmeyer-Meshkov, and Kelvin-Helmholtz instabilities all generate vorticity that tangle Lagrangian meshes.**



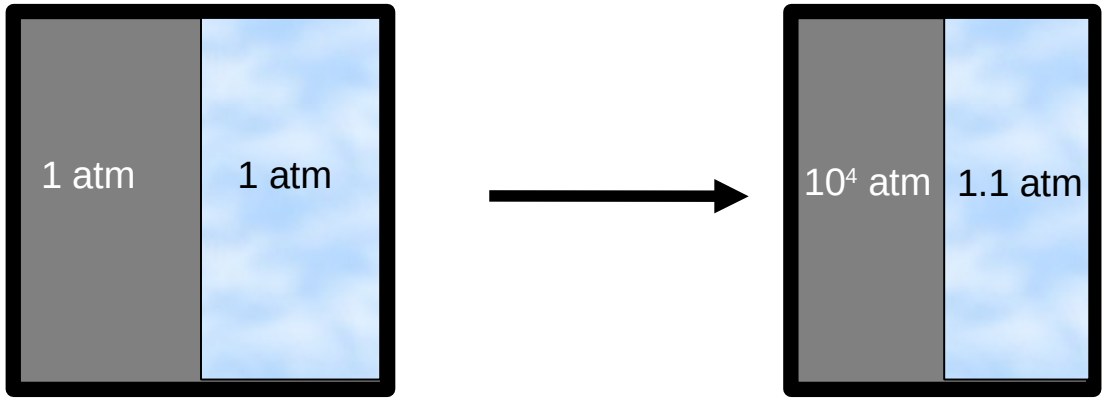
2D example of complicated geometry

- **It is often easier to create a mesh for complicated geometries using mixed zones from the beginning.**

Mixed zone issues are most severe in multi-physics problems.

Too simple a model of mixed zone behavior can lead to unphysical results

- **Imagine a zone containing half air and half aluminum by volume, both at 1 atmosphere pressure, room temperature.**
- **Squeeze the zone slightly to 95% of its original volume.**
- **If we do not change the volume fractions of the air and aluminum, the result is a zone with an unreasonably high pressure in the aluminum.**



$$P_{Al} = P_{air} \qquad P_{Al} >> P_{air}$$

We use a single zone containing both air and aluminum as our test problem

- **The zone is crushed from the right at a constant speed of 4,000 m/s. This is between the sound speeds of air and aluminum.**
- **Intuitively, we expect the air should compress a great deal before the aluminum compresses appreciably**
- **The air pressure and aluminum pressure should equilibrate at high compression**
- **We use a tabular equation of state for air (LEOS #2260), and a linear polynomial equation of state for Al:**

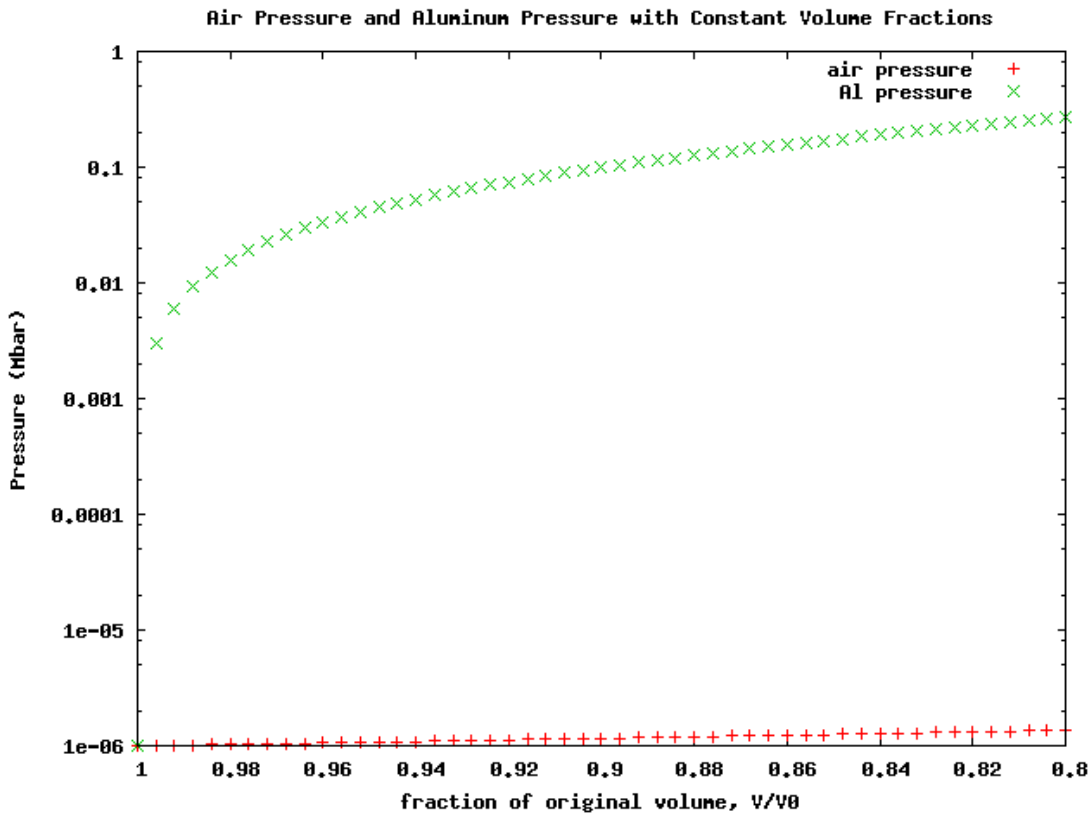
$P = a_1\mu + a_2\mu^2 + a_3\mu^3 + (b_0 + b_1\mu)\,E$, where $\mu = \rho/\rho_0 - 1$, and $\rho_0 = 2.7$ g/cc,

$a_1 = 7.4\text{x}10^{11}$ Pa, $a_2 = 6.0\text{x}10^{11}$ Pa, $a_3 = 1.9\text{x}10^{11}$ Pa,

$b_0 = 2.0$, $b_1 = 0.5$

Model #0: Constant volume fractions

- In this approximation, we do not change the volume fraction of either species during compression.
- The unphysically large pressure in the aluminum appears immediately.
- The air has hardly compressed at all, even though there is a 10,000x pressure ratio.
- pressure relaxation is too slow to matter when shocks are involved.



We need to change the volume fractions, $f_i = V_i / V_z$, during the Lagrangian step

- **Need to take into account the differences in bulk modulus, *K***

$$P^{n+1} = P^n + \Delta V \frac{\partial P}{\partial V}$$

$$K \equiv -V \frac{\partial P}{\partial V}$$ definition of bulk modulus

$$P^{n+1} = P^n - \frac{\Delta V}{V} K$$

$K_{air} = 1.4\text{x}10^5$ Pa
$K_{Al} = 7.6\text{x}10^{10}$ Pa

} Variations in *K* between materials are large

- **We introduce $\beta_i = \partial V_i / \partial V_z$, the change of volume for the *i*th species in a zone, per the change in the total zone volume, V_z.**

- **As part of the Lagrangian step, we now require**

$$v_i' = v_i + \beta_i \Delta v_z$$

now, $P_i^{n+1} = P_i^n + \beta_i \Delta v_z K_i / f_i V_z$

We assume some constraints on β

- **β must be positive**
  - **if** $\Delta v_z > 0$, **all the** $\Delta v_i > 0$
  - **This prohibits some ideas, like setting** $\beta = P$**, because material in tension has** $P < 0$.
- $\Sigma\, \beta_i = 1$ **in order to conserve volume**

Model #1: Determine β by bulk modulus weighting

- **We insist on preserving the pressure difference between the two species, which leads to a bulk modulus weighted algorithm.**

Pressure difference at the beginning of the step has to be the same as at the end

(1) $\Delta P = P_{air} - P_{Al}$ $\quad \Delta P' = P'_{air} - P'_{Al}$ and we require $\Delta P = \Delta P'$

(2) $$\Delta P' = P_{air} - \beta_{air} \frac{\Delta V_z}{f_{air} V_z} K_{air} - \left(P_{Al} - \beta_{Al} \frac{\Delta V_z}{f_{Al} V_z} K_{Al} \right)$$

Combining these we get

(3) $$\frac{\beta_{air} K_{air}}{f_{air}} = \frac{\beta_{Al} K_{Al}}{f_{Al}}$$

Using $\sum \beta_i = 1$ gives

$$\beta_{air} = \frac{\frac{f_{air}}{K_{air}}}{\frac{f_{air}}{K_{air}} + \frac{f_{Al}}{K_{Al}}}$$

For N materials, we get

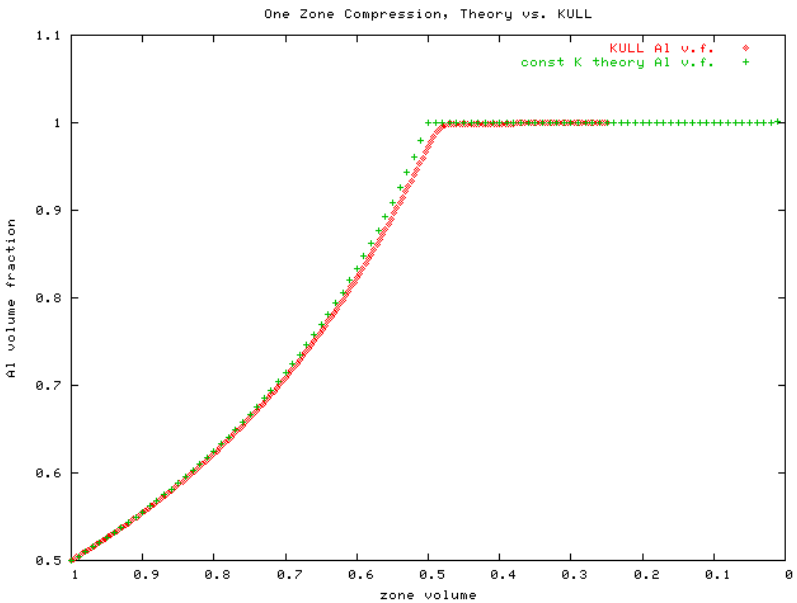
$$\beta_i = \frac{\frac{f_i}{K_i}}{\sum_{j=1}^{N} \frac{f_j}{K_j}}$$

- **Simple, conceptually pleasing**
- **Fixes high pressure problem in compression**
- **Introduces a problem under a driven expansion**

A simple model predicts bulk modulus weighting's performance in the one-zone compression test

- **Assume constant κ, 2-component system, constant compression (a simplified air/Al one-zone test), and β as defined by bulk modulus.**
- **Then:** $V_z = 1 - v\,t$ $\quad \frac{dV_1}{dt} = \frac{-v\,V_1}{V_1 + \frac{\kappa_1}{\kappa_2} V_2}$ $\quad \frac{dV_2}{dt} = \frac{-v\,V_2}{V_1 \frac{\kappa_2}{\kappa_1} + V_2}$
- **Which can be integrated and re-arranged to get**

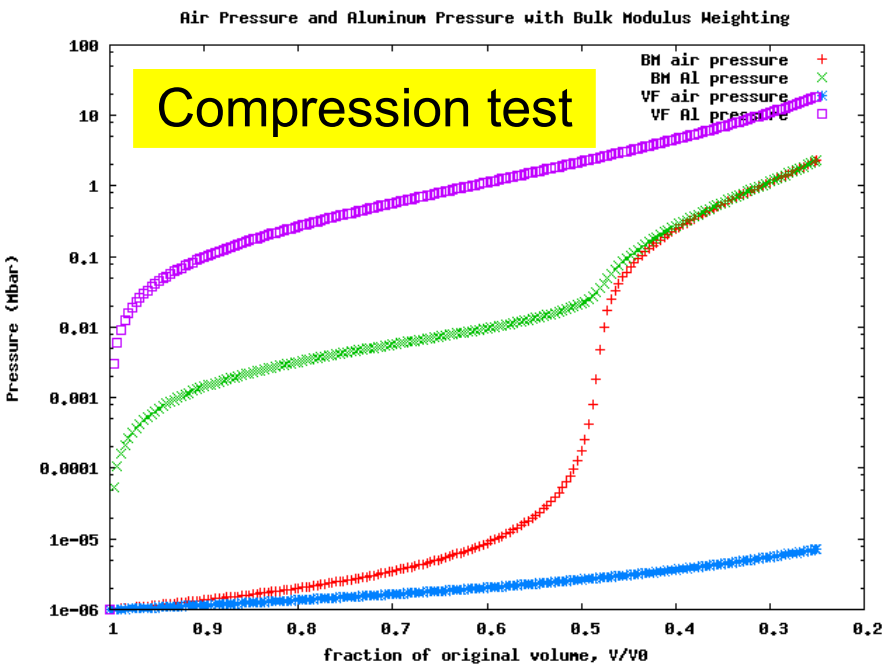
$V_1 + V_2^0 \left(\frac{V_1}{V_1^0} \right)^a = V_z^0 - v\,t$, where a = κ_1/κ_2 ~ 10^6 for 1=Al and 2=air



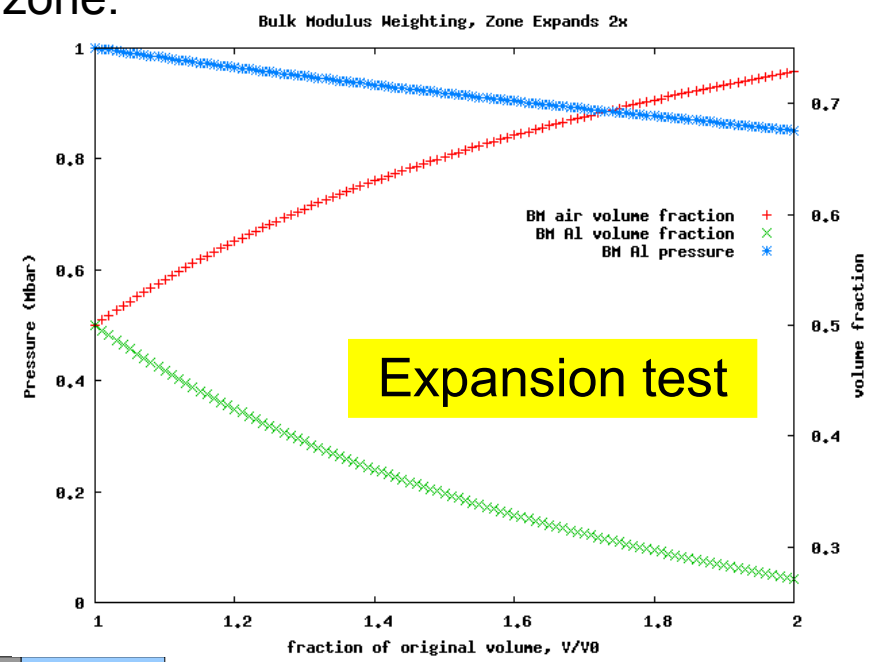
KULL reproduces the simple model very closely. Differences are due to non-constant κ and artificial viscosity.

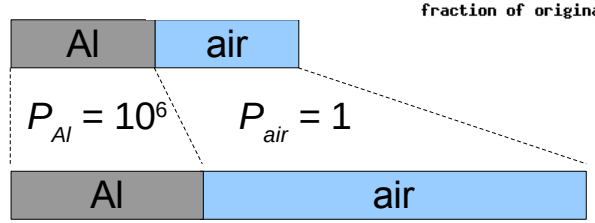
Bulk modulus weighting reduces pressure error but introduces unphysical behavior in driven expansion

Compression is much more as we would physically expect



But when the zone is expanding, the air expands more than the aluminum. In our driven expansion test, we have P_{Al} = 1 Mbar and P_{air} = 1 bar, each occupying half of the zone.

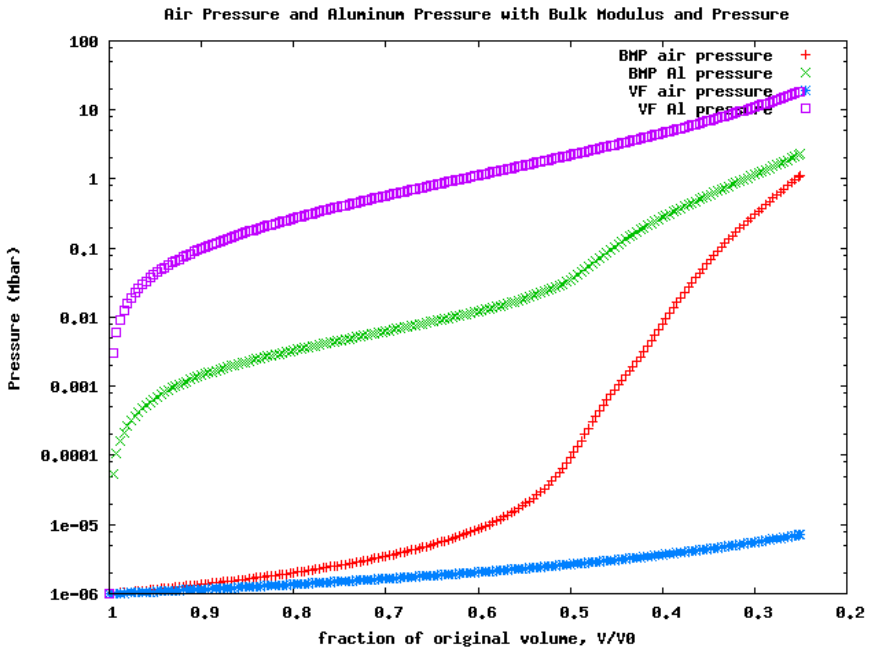




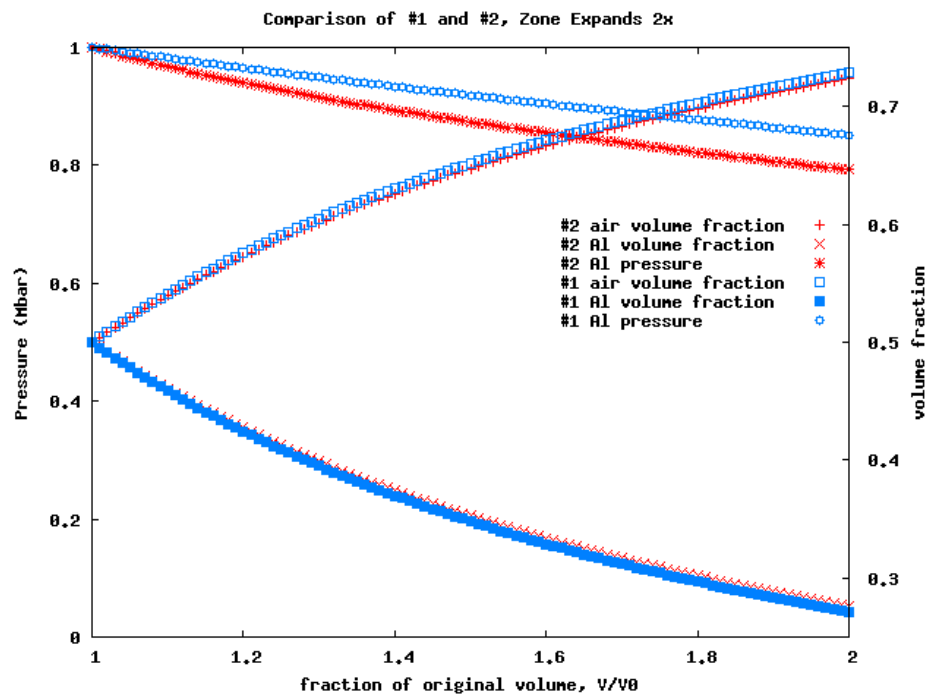
Model #2: Find β by bulk modulus and pressure

- **We thought that factoring in the pressure might lead to a better response in expansion. High pressure materials should expand as much or more than lower pressure materials in the same zone.**

We tried $$\beta_i = \frac{f_i P_i}{K_i}$$



The compression test results are not as satisfying as model #1.

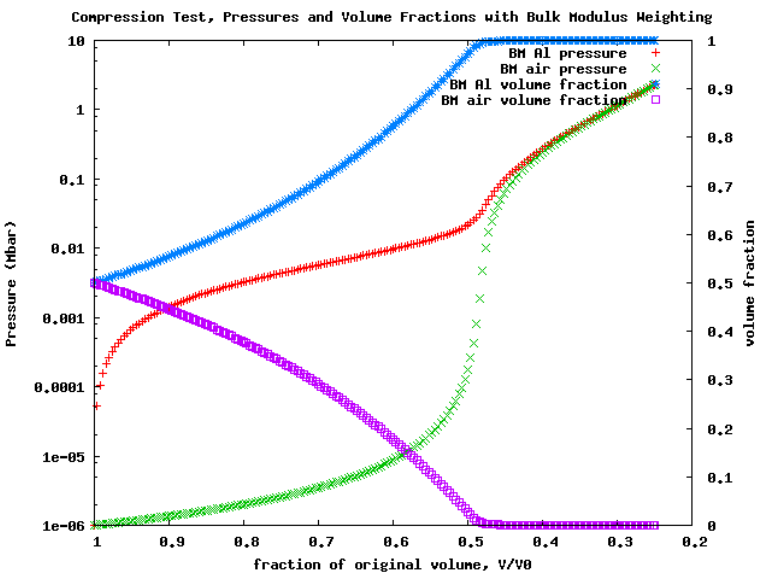


The new scheme improves the behavior in expansion, but not a lot

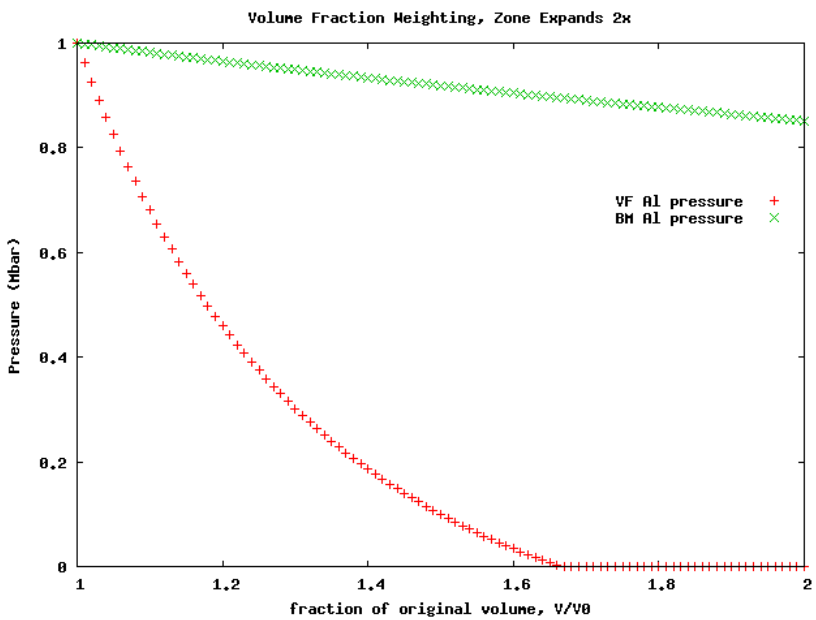
Model #3: Hybrid Algorithm

$$\beta_i = \begin{cases} \dfrac{f_i}{K_i}, & \Delta V_z < 0 \\ f_i, & \Delta V_z > 0 \end{cases}$$

- **Bulk modulus in compression**
- **Constant volume fraction in expansion**
- **Best match to our physical intuition**



The compression test results are good, as before.

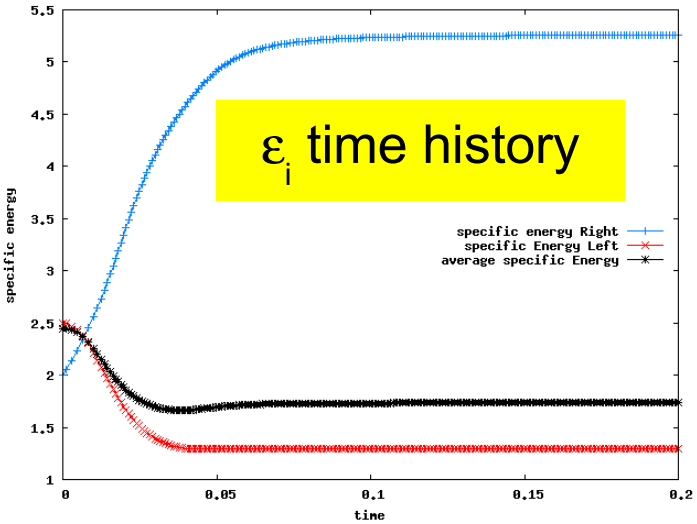


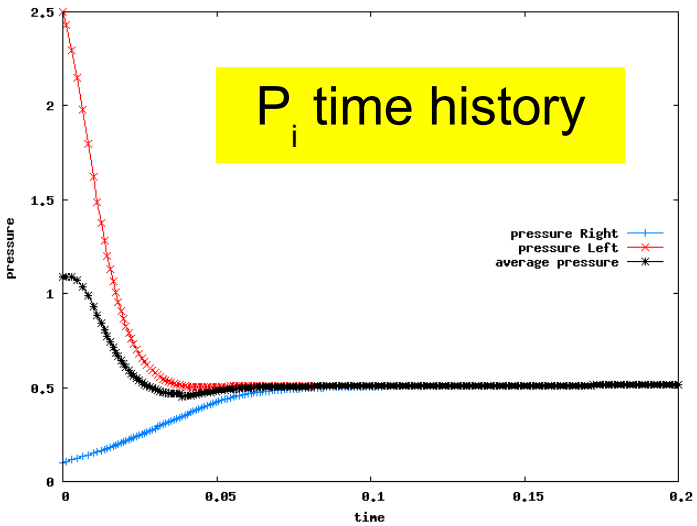
Expansion results are much improved over models #1 and #2.

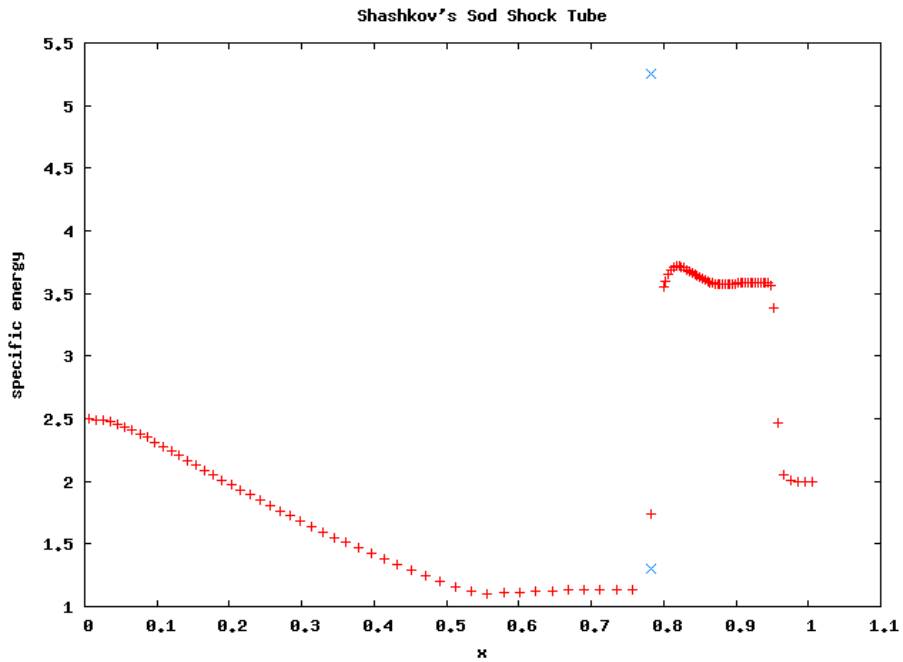
Shashkov's version of the Sod shock tube provides another mixed zone test

Left: γ=2, ρ=1, P=2.5

Right: γ=1.4, ρ=0.125, P=0.1

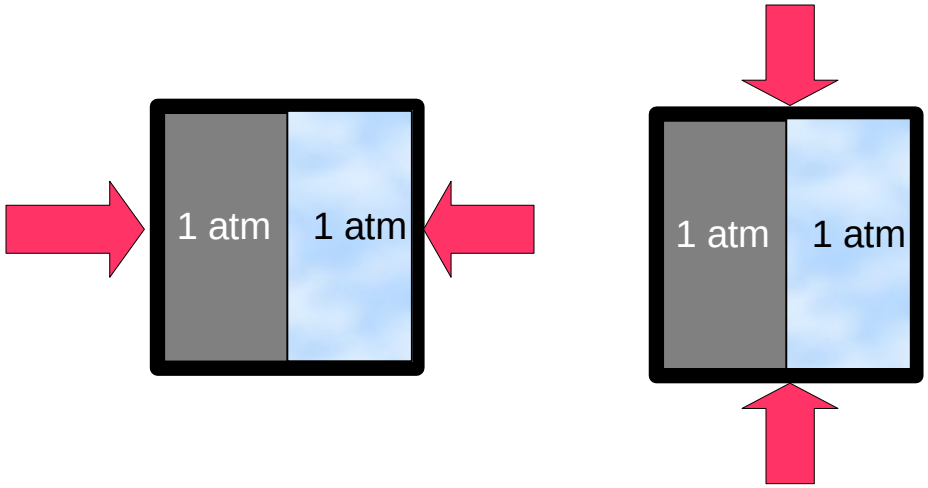






Mixed zone physics is an *approximation;* it is not possible to always get correct behaviour.

- **We assume no knowledge of the actual configuration of materials in the zone. In a real calculation we do not know the direction of the volume change.**
- **The two situations shown here should have different solutions.**



Sub-zonal algorithms like these are meant to keep a code running wtih reasonable correctness, not to produce high quality solutions inside a single zone.

Conclusions

- **Possibly a different method should be used to handle the driven expansion problem. The true solution is a shock within the zone, and probably requires relaxing $\beta_i > 0$. Our method won't do that but a Riemann solver approach (*e.g.*, Barlow's method) could.**
- **The hybrid approach, using constant volume fraction during expansion, and bulk modulus weighting during compression, gave us the best results.**
- **Mixed zone issues most commonly arise in problems involving more than just hydrodynamics. Radiation flow or chemical reactions make a calculation much more sensitive to how mixed zones are treated.**