A Comparative Study of Thermodynamic Closures for Multimaterial Cells in Lagrange-Plus-Remap Algorithms

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Outline

Introduction

- Hydrocodes may employ a homogenized picture of multimaterial cells to perform updates of momentum and energy equations.
- These schemes require a closure model to distribute the changes in volume and internal energy of a mixed cell to its material components.
- Los Alamos National Laboratory's Eulerian AMR code, xRage, implements four closure models in a conservative, Lagrange–plus–Remap context:
  - two uniform strain variants
  - Tipton pressure relaxation
  - pressure–temperature equilibrium
- We briefly describe each of these four closure models
- We compare these closure models on a set of test problems ranging from one–dimensional, two–material shock tube problems to two–dimensional solid impact problems.

Lagrange-Plus-Remap Algorithm

- The xRage hydro algorithm employs a MUSCL-Hancock method with an acoustic Riemann solver for Lagrangian updates
- The advective (Remap) phase uses donor cell advection with three possible interface treatments
  - diffuse treatment (NOIP)
  - interface preserver (IP)
  - volume–of-fluids (VOF)
- xRage historically relied on assumption of pressure, temperature and velocity equilibrium in mixed cells; recently, the pressure and temperature assumptions have been relaxed
- xRage supports a large suite of Equation of State (EOS) models and additional capabilities (strength, high explosives, radiation diffusion, etc)

"The RAGE radiation-hydrodynamic code", M. Gittings, R. Weaver, M. Clover, et al, Computational Science and Discovery, 1(1), 015005.

Pressure–Temperature Equilibrium

At appropriate length and time scales, (fluid) material interfaces exhibit pressure and temperature equilibrium (PTE). The assumption of this equilibrium in mixed cells leads to a system of two equations for the common pressure and temperature of the mixed cell.

- The specific volumes satisfy

$$V = \sum_k \mu_k V_k \left(P, T\right)$$

- The specific internal energies satisfy

$$e = \sum_k \mu_k e_k \left(P, T\right)$$

Here $\mu_k = m_k/m$. In each mixed cell, we solve for P and T, then evaluate material volumes and energies. Note: $N + 2$ inputs, $2N + 2$ outputs.

Uniform Strain Models

With PTE, material volumes (W_k) and specific internal energies (e_k) in mixed cells were determined by the equilibrium assumption. With the alternative closure models we consider, the mixed cell material volumes and energies are tracked with the flow.

- A material pressure is determined by a direct EOS call:

$$P_k = P_k\left(\rho_k, e_k\right)$$

  with the micro–density defined as $\rho_k = m_k / W_k$

- Applying a uniform strain assumption to the Gibbs relation for an individual material leads to the definition of a homogenized cell pressure

$$P = \sum_k \phi_k P_k$$

  with volume fractions defined as $\phi_k = W_k / W$.

Galera-Maire-Breil's Model

- After performing a Lagrangian update to cell-based momentum and energy quantities (including velocity and specific internal energy updates), a heating term for a mixed cell can be estimated

$$\delta Q = m(e^{n+1} - e^n) + P^n(W^{n+1} - W^n)$$

- Galera, Maire and Breil (2010) update material energies with

$$m_k \left(e_k^{n+1} - e_k^n\right) + P_k^n \left(W_k^{n+1} - W_k^n\right) = \phi_k \delta Q$$

  which follows from an assumption of an equal time rate of volumetric heating for both the mixed cell and the materials.

"A two-dimensional unstructured cell-centered multi-material ALE scheme using VOF interface reconstruction", S. Galera, P.H. Maire, J. Breil, JCP, 229(16), 5755-5787

Alternative Uniform Strain Model

We have found that the Galera-Maire-Breil Uniform Strain formulation performs very well in most cases. However, we have developed a slightly different treatment that has shown promise for high Atwood number flows.

- We update material energies using

$$m_k \left(e_k^{n+1} - e_k^n\right) + P_k^n \left(W_k^{n+1} - W_k^n\right) = \mu_k \delta Q$$

  which relies on the heating assumption

$$T_k \frac{dS_k}{dt} = T \frac{dS}{dt}$$

- Compare this to the assumption of an equal time rate of volumetric heating

$$\rho_k T_k \frac{dS_k}{dt} = \rho T \frac{dS}{dt}$$

  Here, a mixed cell with $\rho/\rho_k \gg 1$ may exhibit extreme shock heating of the lighter materials.

Tipton's Model

Physically, both the uniform strain and pressure–temperature equilibrium assumptions leave a lot to be desired. Material interfaces do obtain both pressure and temperature equilibrium, but at time scales that may not be relevant for applications of interest. Pressure–relaxation models have been employed to provide more physically realistic material interface treatments.

- In Tipton's model, the material volume updates take the form

$$\Delta W_k = \left(\frac{P_k - \bar{P}}{K_k} \right) W_k + \phi_k \frac{K}{K_k} \Delta W$$

- An isentropic assumption is applied to the specific internal energy updates

$$m_k \Delta e_k = -\hat{P} \Delta W_k$$

Tipton's Model

- The Tipton model relies on a characteristic length scale L, that appears in the bulk modulus terms

$$K_k = \left(\rho c^2\right)_k \left(1 + \frac{L}{c_k \Delta t}\right)$$

- This model also makes use of homogenized cell quantities

$$K = \left(\sum_k \frac{\phi_k}{K_k}\right)^{-1}, \quad \bar{P} = \sum_k \phi_k \frac{K}{K_k} P_k$$

- The pressure that appears in the specific internal energy updates (see references for additional details) can be expressed as

$$\hat{P} = \bar{P} - \frac{\Delta W}{W} K$$

Tipton's Model

- Final Tipton note: the Tipton update is equivalent to one iteration of the Miller–Puckett Pressure Equilibration algorithm.

"Closure models for multimaterial cells in arbitrary Lagrangian–Eulerian hydrocodes", M.Shashkov, International Journal for Numerical Methods in Fluids, 56(8) (2008) 1497–1504

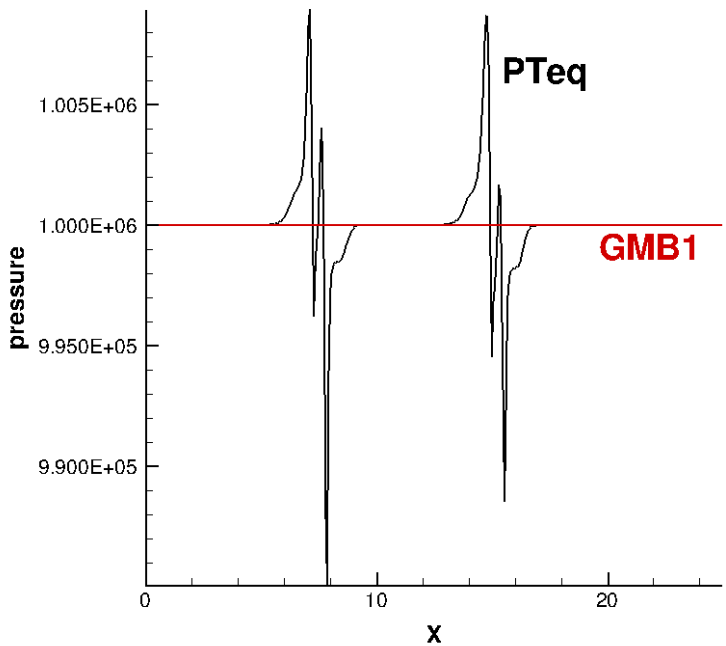
"A comparative study of multimaterial Lagrangian and Eulerian methods with pressure relaxations", M.François, M.Shashkov, T.Masser, E.Dendy, Computers and Fluids, 83 (2013) 126–136

"A high-order Godunov method for multiple condensed phases", G.H. Miller, E.G. Puckett, JCP, 128(1), 134-164

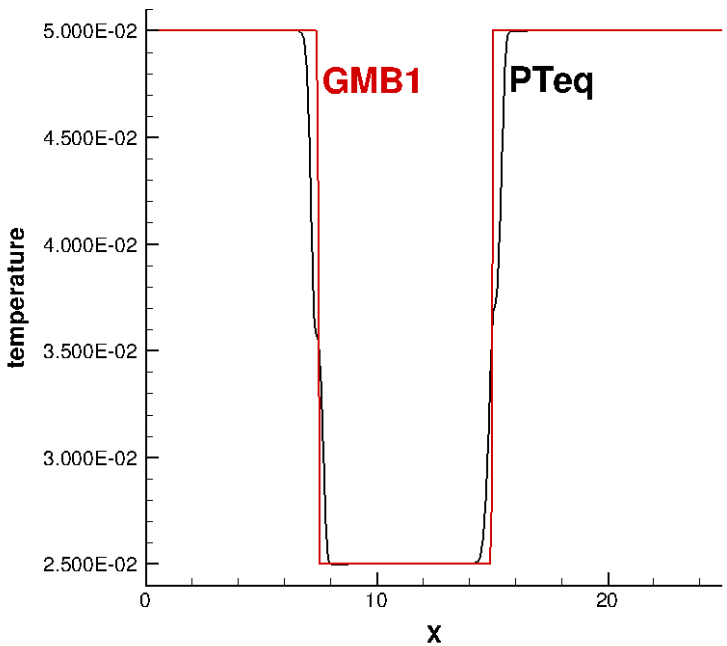
Numerical Tests

Hot Air Problem

- Galilean translation over periodic domain of material interfaces
- Exploit $C_{v,1}T_1 = C_{v,2}T_2$ to create a temperature discontinuity at an interface with uniform density, velocity and pressure.
- All multi–pressure models produce similar results



Pressure



Temperature

Two–material Sod Problem: Temperature Profiles

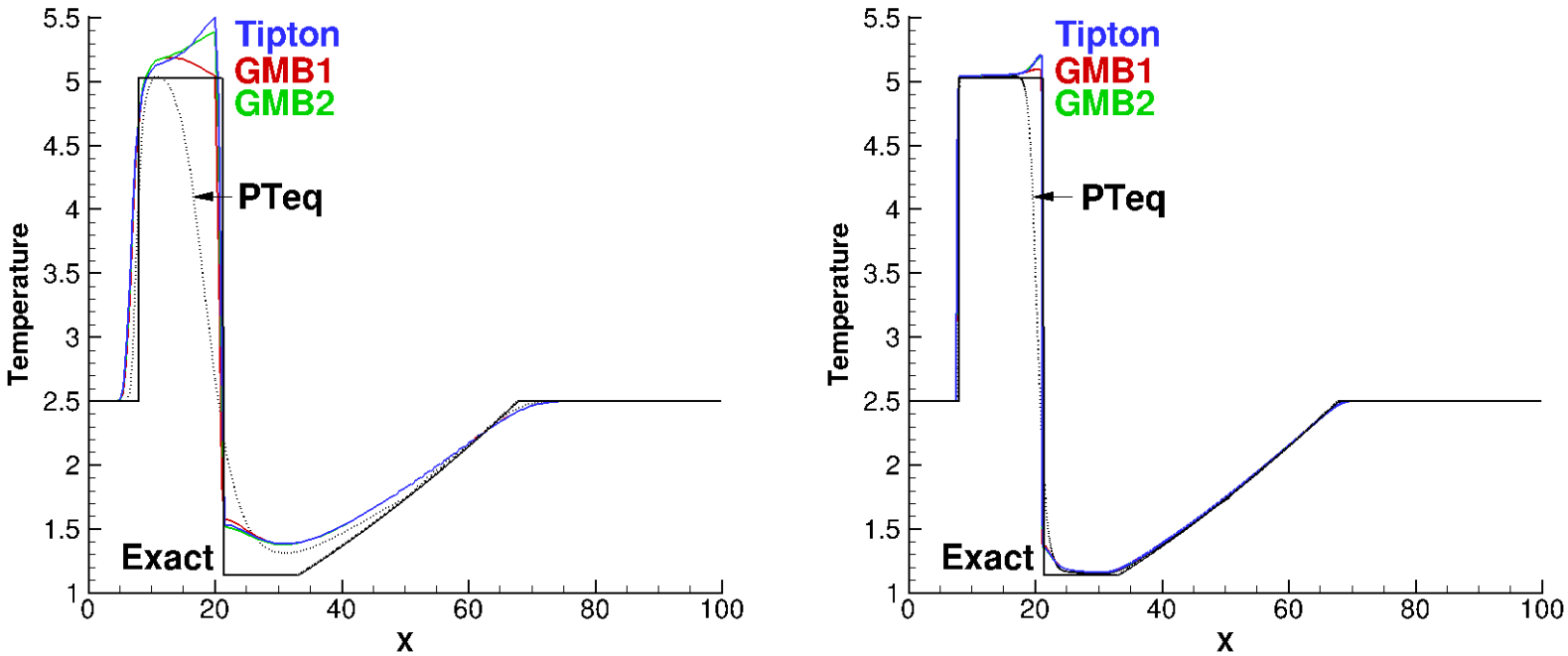


Figure 1: Resolution: Left 200. Right 2000

Two–material Sod Problem: Maximum Temperatures

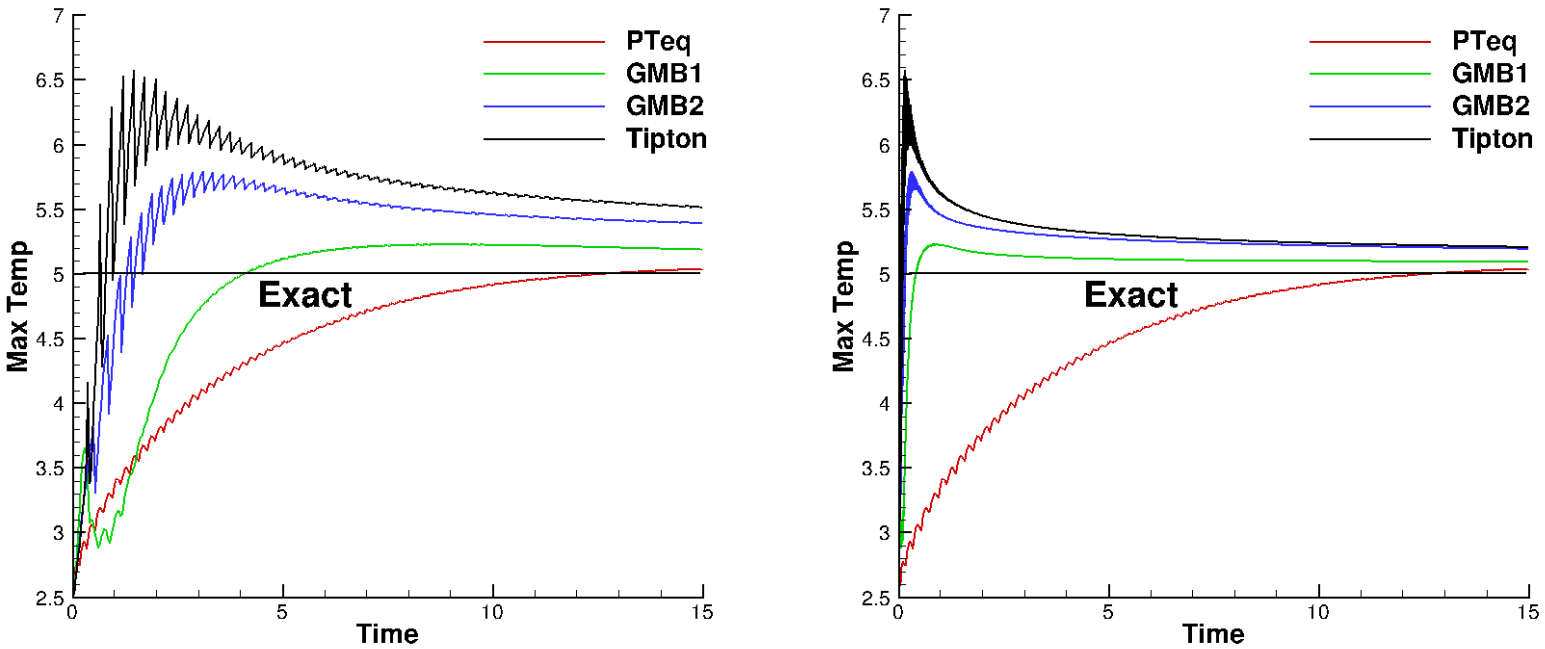
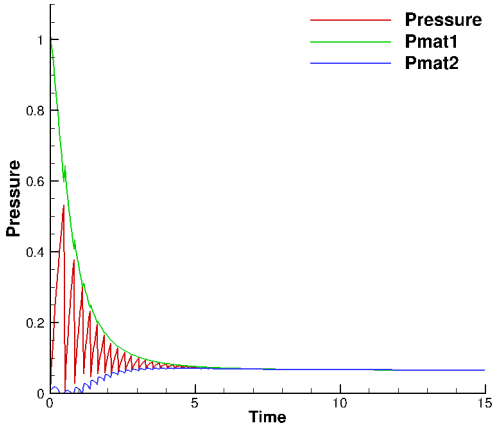
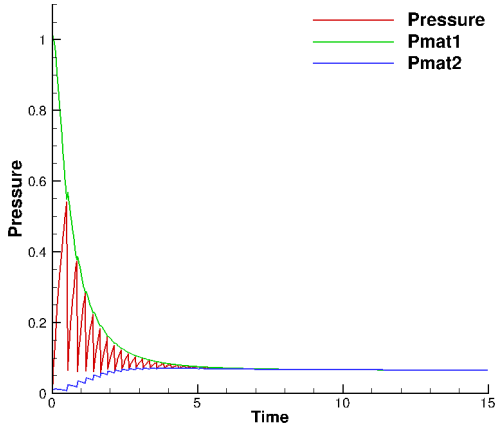


Figure 2: Resolution: Left 200. Right 2000

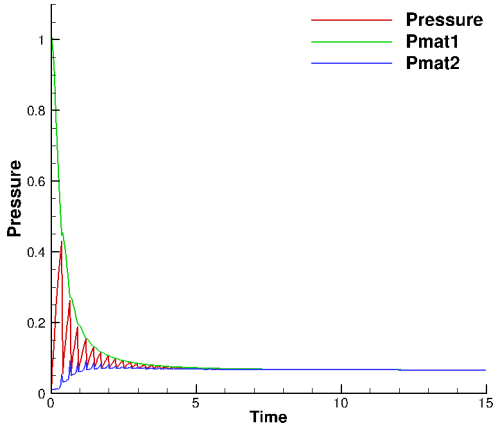
Two–material Sod Problem: Mixed Cell Pressures



GMB1



GMB2



Tipton

Table 1: Relaxation Times

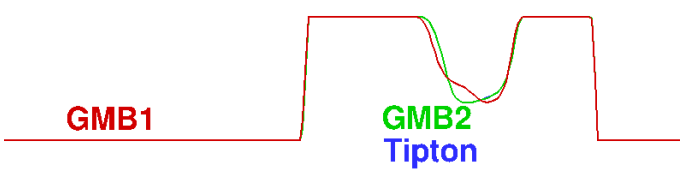
Resolution	GMB1	GMB2	Tipton
200	1.0797	1.0510	0.54736
2000	0.10797	0.1051	0.054736

Flyer Plate Test

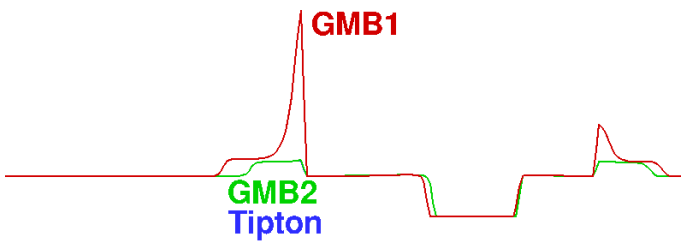
- Initial conditions: $P = 1$ bar, $T = 0.025$ eV uniform
- SESAME tabular equation of state, Steinberg-Guinan strength model is used for Cu
- Closure models and algorithms above have modifications for solid mechanics; velocities below in m/s.

Air	Cu	Cu	Air
v=900	v=900	v=600	v=600

Density



Temperature



Flyer Plate Test: Maximum Temperatures

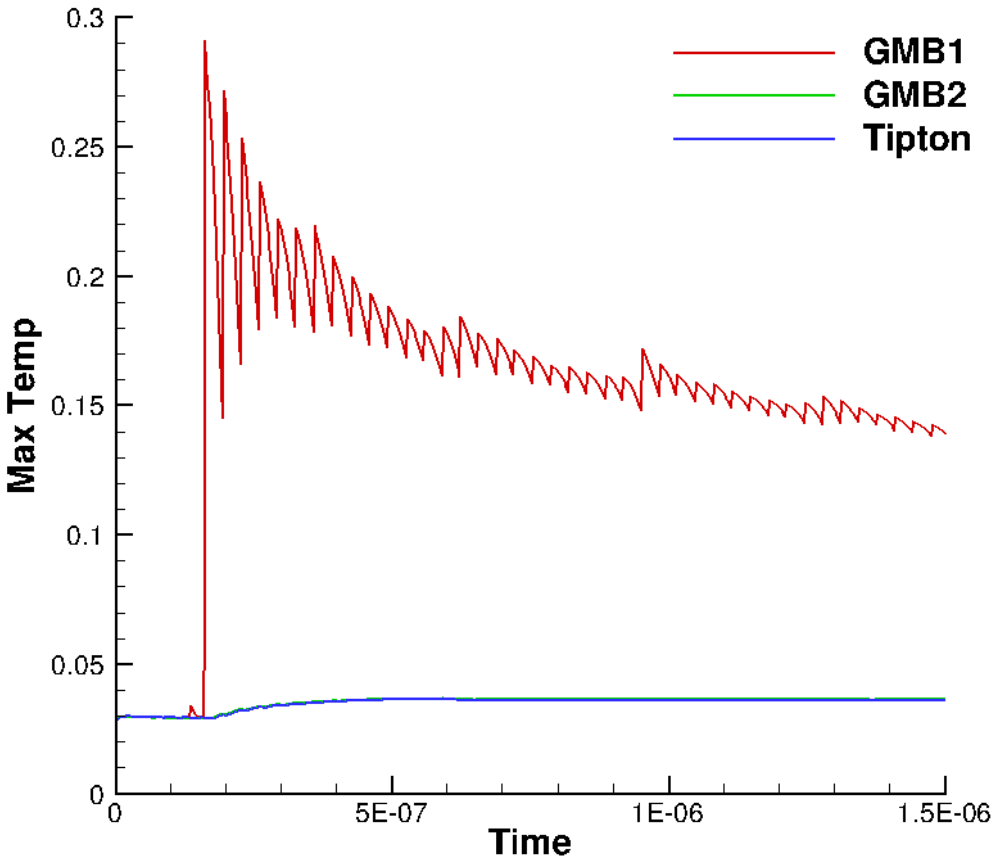


Figure 3: Maximum Temperatures

Conclusion and Future Work

Conclusions:

- We have implemented four distinct closure models in xRage
- Volumetric heating assumption may exhibit anomalous overheating in high Atwood number flows
- Pressure–relaxation model shown to equilibrate faster than purely non–equilibrium models, but not significantly faster

Future work:

- Investigate implicit closure models in xRage
- Investigate Tipton–like relaxation schemes for solid mechanics
- Verify the extensions of the models to solid mechanics and radiation hydrodynamics cases

Extra Slides

Closure Derivations

We begin with Gibbs relation in a single material cell

$$de = TdS - PdV$$

In mixed cells, individual materials should satisfy a similar relation

$$de_k = T_k dS_k - P_k dV_k$$

Energy conservation demands that component energy updates satisfy

$$\sum_k \mu_k \Delta e_k = \Delta e$$

Assume that isentropic and shock heating terms can be decoupled

$$\sum_k \mu_k T_k \Delta S_k = T \Delta S$$

$$\sum_k \mu_k P_k \Delta V_k = P \Delta V$$

Closure Derivations

The uniform strain assumptions (with cell pressure defined as volume-weighted average of material pressures) allow us to satisfy the pressure equation. To complete our closure model, we require a distribution of $\Delta Q = T\Delta S$ term to corresponding material terms, ΔQ_k, that satisfies

$$\sum_k \mu_k \Delta Q_k = \Delta Q$$

The Galera-Maire-Breil closure corresponds to the selection

$$\Delta Q_k = \frac{\phi_k}{\mu_k} \Delta Q$$

The alternative Uniform Strain treatment selects a simpler model

$$\Delta Q_k = \Delta Q$$

We have not found a similar algorithm in the literature.

Useful Representations

It may be useful to rewrite the material specific internal energy updates in terms of the energy and volume updates for the mixed cells.

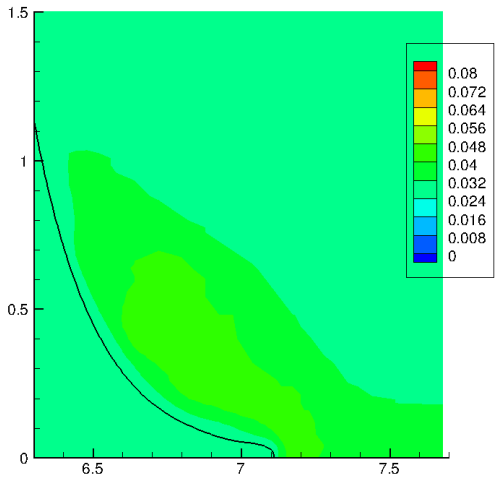
- The Galera-Maire-Breil model may be rewritten as

$$\mu_k \Delta e_k = \phi_k \left[\Delta e + (P - P_k) \, \Delta W \right]$$

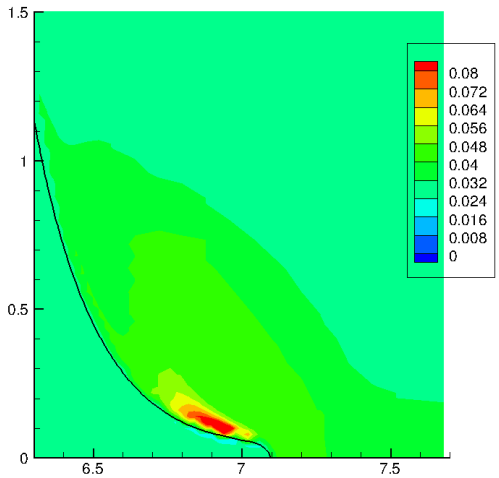
- The alternative Uniform Strain model may be rewritten as

$$\Delta e_k = \Delta e + \frac{\Delta W}{m} \left(P - \frac{\phi_k}{\mu_k} P_k \right)$$

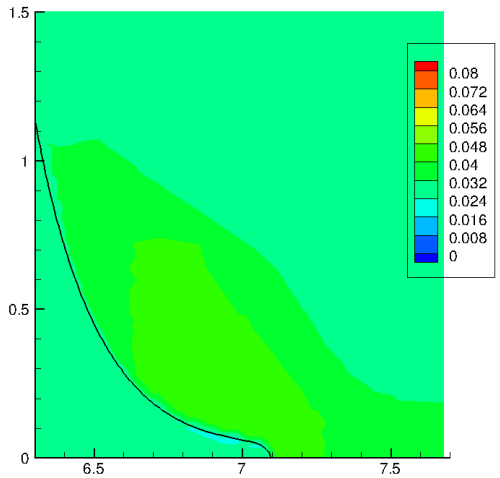
Copper Bar Impact



PTeq



GMB1



GMB2

Copper Bar Impact: Maximum Temperatures