

Viscous Compaction Waves

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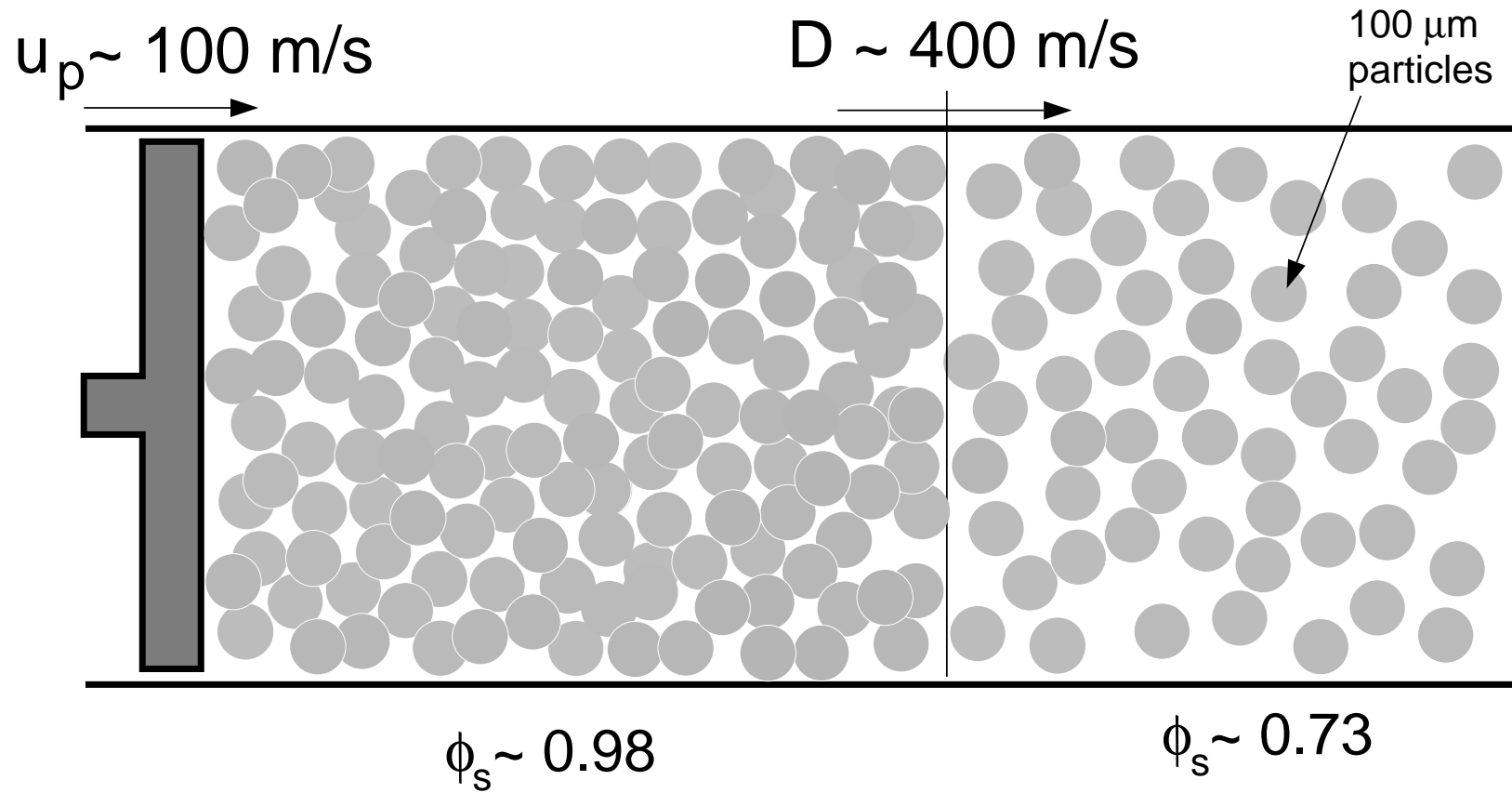
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Compaction Wave Schematic



Introduction

- Heterogeneous energetic solids composed of $100\ \mu m$ crystals in plastic binder.
- Engineering length scales on the order of many cm .
- Macrobehavior (ignition, etc.) strongly linked to microstructure.
- Continuum mixture models with non-traditional constitutive theories needed to capture grain scale physics.

Review

- Gokhale and Krier, *Prog. Energy Combust. Sci.*, 1982.
- Baer and Nunziato, *Int. J. Multiphase Flow*, 1986.
- Powers, Stewart, Krier, *Combust. Flame*, 1990.
- Saurel and Abgrall, *J. Comput. Phys.*, 1999.
- Bdzil, *et al. Phys. Fluids*, 1999, 2001.
- Gonthier and Powers, *J. Comput. Phys.*, 2000.
- Powers, *Phys. Fluids*, 2004.

Issues with Continuum Mixture Theories

- Well-posedness not always straightforward.
- Second law complicated.
- Shock jumps not clearly defined for non-conservative equations.
- Consequent numerical difficulties.

Inviscid Theory of Bdzil, *et al.*

- First theory to unambiguously satisfy the second law.
- Hyperbolic and well-posed for initial value problems.
- Fundamentally non-conservative.
- Some regularization needed for discontinuities.
- No viscous cutoff mechanism for multidimensional instabilities.
- Grid-dependent numerical viscosity problematic.

Viscous Extension

$$\frac{\partial}{\partial t} (\rho_s \phi_s) + \nabla \cdot (\rho_s \phi_s \mathbf{u}_s) = \mathcal{C},$$

$$\frac{\partial}{\partial t} (\rho_g \phi_g) + \nabla \cdot (\rho_g \phi_g \mathbf{u}_g) = -\mathcal{C},$$

$$\frac{\partial}{\partial t} (\rho_s \phi_s \mathbf{u}_s) + \nabla \cdot \left(\rho_s \phi_s \mathbf{u}_s \mathbf{u}_s^T + \phi_s (p_s \mathbf{I} - \boldsymbol{\tau}_s) \right) = \mathcal{M},$$

$$\frac{\partial}{\partial t} (\rho_g \phi_g \mathbf{u}_g) + \nabla \cdot \left(\rho_g \phi_g \mathbf{u}_g \mathbf{u}_g^T + \phi_g (p_g \mathbf{I} - \boldsymbol{\tau}_g) \right) = -\mathcal{M},$$

Viscous Extension (cont.)

$$\frac{\partial}{\partial t} \left(\rho_s \phi_s \left(e_s + \frac{1}{2} \mathbf{u}_s \cdot \mathbf{u}_s \right) \right) + \nabla \cdot \left(\rho_s \phi_s \mathbf{u}_s \left(e_s + \frac{1}{2} \mathbf{u}_s \cdot \mathbf{u}_s \right) + \phi_s \mathbf{u}_s \cdot (p_s \mathbf{I} - \boldsymbol{\tau}_s) + \phi_s \mathbf{q}_s \right) = \mathcal{E},$$

$$\frac{\partial}{\partial t} \left(\rho_g \phi_g \left(e_g + \frac{1}{2} \mathbf{u}_g \cdot \mathbf{u}_g \right) \right) + \nabla \cdot \left(\rho_g \phi_g \mathbf{u}_g \left(e_g + \frac{1}{2} \mathbf{u}_g \cdot \mathbf{u}_g \right) + \phi_g \mathbf{u}_g \cdot (p_g \mathbf{I} - \boldsymbol{\tau}_g) + \phi_g \mathbf{q}_g \right) = -\mathcal{E},$$

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s) = -\frac{\rho_s \mathcal{F}}{\phi_s},$$

$$\frac{\partial}{\partial t} (\rho_s \phi_s \eta_s + \rho_g \phi_g \eta_g)$$

$$+ \nabla \cdot (\rho_s \phi_s \mathbf{u}_s \eta_s + \rho_g \phi_g \mathbf{u}_g \eta_g) \geq -\nabla \cdot \left(\frac{\phi_s \mathbf{q}_s}{T_s} + \frac{\phi_g \mathbf{q}_g}{T_g} \right).$$

Constitutive Equations

$$\phi_g + \phi_s = 1,$$

$$\psi_s = \hat{\psi}_s(\rho_s, T_s) + B(\phi_s), \quad \psi_g = \psi_g(\rho_g, T_g),$$

$$p_s = \rho_s^2 \left. \frac{\partial \psi_s}{\partial \rho_s} \right|_{T_s, \phi_s}, \quad p_g = \rho_g^2 \left. \frac{\partial \psi_g}{\partial \rho_g} \right|_{T_g},$$

$$\eta_s = - \left. \frac{\partial \psi_s}{\partial T_s} \right|_{\rho_s, \phi_s}, \quad \eta_g = - \left. \frac{\partial \psi_g}{\partial T_g} \right|_{\rho_g},$$

$$\beta_s = \rho_s \phi_s \left. \frac{\partial \psi_s}{\partial \phi_s} \right|_{\rho_s, T_s},$$

$$e_s = \psi_s + T_s \eta_s, \quad e_g = \psi_g + T_g \eta_g,$$

Constitutive Equations (cont.)

$$\boldsymbol{\tau}_s = 2\mu_s \left(\frac{(\nabla \mathbf{u}_s)^T + \nabla \mathbf{u}_s}{2} - \frac{1}{3}(\nabla \cdot \mathbf{u}_s)\mathbf{I} \right),$$

$$\boldsymbol{\tau}_g = 2\mu_g \left(\frac{(\nabla \mathbf{u}_g)^T + \nabla \mathbf{u}_g}{2} - \frac{1}{3}(\nabla \cdot \mathbf{u}_g)\mathbf{I} \right),$$

$$\mathbf{q}_s = -k_s \nabla T_s, \quad \mathbf{q}_g = -k_g \nabla T_g,$$

$$\mathcal{C} = \mathcal{C}(\rho_s, \rho_g, T_s, T_g, \phi_s),$$

$$\mathcal{M} = p_g \nabla \phi_s - \delta(\mathbf{u}_s - \mathbf{u}_g) + \frac{1}{2}(\mathbf{u}_s + \mathbf{u}_g)\mathcal{C},$$

$$\mathcal{E} = \mathcal{H}(T_g - T_s) - p_g \mathcal{F} + \mathbf{u}_s \cdot \mathcal{M} + \left(e_s - \frac{\mathbf{u}_s \cdot \mathbf{u}_s}{2} \right) \mathcal{C},$$

$$\mathcal{F} = \frac{\phi_s \phi_g}{\mu_c} (p_s - \beta_s - p_g).$$

Equations of State

Modified Tait equation for solid (correction courtesy D. W. Schwendeman)

$$\psi_s(\rho_s, T_s, \phi_s) = c_{vs} T_s \left(1 - \ln \left(\frac{T_s}{T_{s0}} \right) + (\gamma_s - 1) \ln \left(\frac{\rho_s}{\rho_{s0}} \right) \right) + \frac{1}{\gamma_s} \frac{\rho_{s0}}{\rho_s} \varepsilon_s + q$$
$$+ \frac{(p_{s0} - p_{g0}) (2 - \phi_{s0})^2}{\rho_{s0} \phi_{s0} \ln \left(\frac{1}{1 - \phi_{s0}} \right)} \ln \left(\left(\frac{2 - \phi_{s0}}{2 - \phi_s} \right) \frac{(1 - \phi_s)^{\frac{1 - \phi_s}{2 - \phi_s}}}{(1 - \phi_{s0})^{\frac{1 - \phi_{s0}}{2 - \phi_{s0}}}} \right)$$

Virial equation for gas

$$\psi_g(\rho_g, T_g) = c_{vg} T_g \left(1 - \ln \left(\frac{T_g}{T_{g0}} \right) + (\gamma_g - 1) \left(\ln \left(\frac{\rho_g}{\rho_{g0}} \right) + b_g (\rho_g - \rho_{g0}) \right) \right)$$

Viscous Dissipation Function

$$\Phi_s = 2\mu_s \underbrace{\left(\underbrace{\frac{\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T}{2}}_{\text{strain rate}} - \underbrace{\frac{1}{3}(\nabla \cdot \mathbf{u}_s) \mathbf{I}}_{\text{mean strain rate}} \right)}_{\text{deviatoric strain rate}} :$$

$$\underbrace{\left(\underbrace{\frac{\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T}{2}}_{\text{strain rate}} - \underbrace{\frac{1}{3}(\nabla \cdot \mathbf{u}_s) \mathbf{I}}_{\text{mean strain rate}} \right)}_{\text{deviatoric strain rate}} .$$

- similar expression for Φ_g .

Dissipation: Clausius-Duhem Equation

$$\begin{aligned}
 I \equiv (-\mathcal{C}) & \left(\frac{\beta_s}{\rho_s T_s} + \frac{e_s - e_g - p_g(1/\rho_g - 1/\rho_s)}{T_g} + \eta_g - \eta_s \right) \\
 & + \delta \frac{(\mathbf{u}_s - \mathbf{u}_g) \cdot (\mathbf{u}_s - \mathbf{u}_g)}{T_g} \\
 & + \mathcal{H} \frac{(T_g - T_s)^2}{T_g T_s} \\
 & + \frac{\phi_s \phi_g}{\mu_c} \frac{(p_s - \beta_s - p_g)^2}{T_s} \\
 & + \frac{\phi_s \Phi_s}{T_s} + \frac{\phi_g \Phi_g}{T_g} \\
 & + \frac{k_s \phi_s \nabla T_s \cdot \nabla T_s}{T_s^2} + \frac{k_g \phi_g \nabla T_g \cdot \nabla T_g}{T_g^2} \geq 0.
 \end{aligned}$$

Characteristics

- Three real characteristics $u_s, u_s, u_g,$
- Three associated eigenvectors,
- Not enough eigenvectors for eleven equations:
parabolic,
- Eight additional conditions from boundary conditions
on $T_s, T_g, u_s, u_g.$

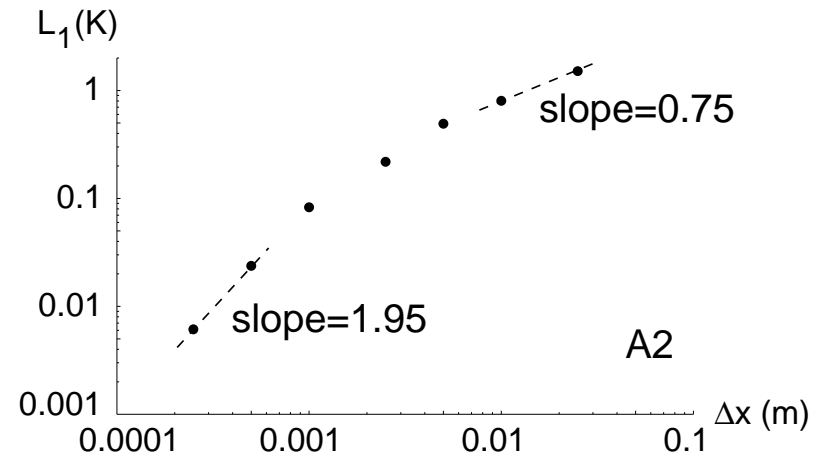
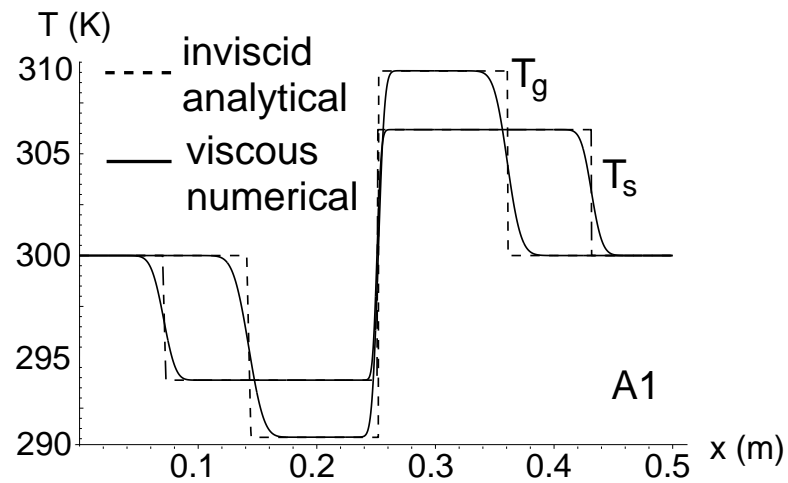
Numerical Method

- One-Dimensional: Fortran 90 code
 - Second order central spatial discretization
 - High order implicit integration in time with DLSODE
- Two-Dimensional: FEMLAB software tool
 - Finite element method for the form

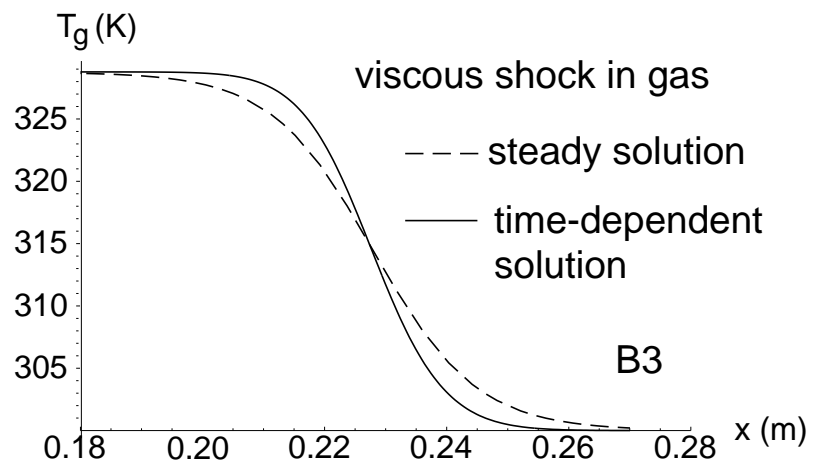
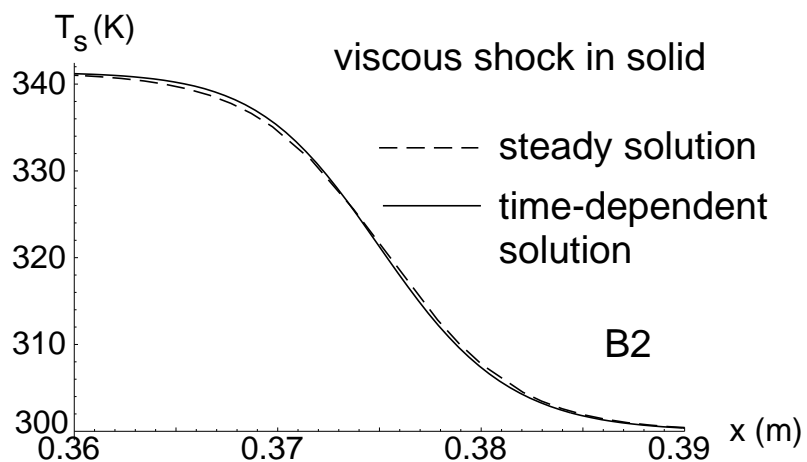
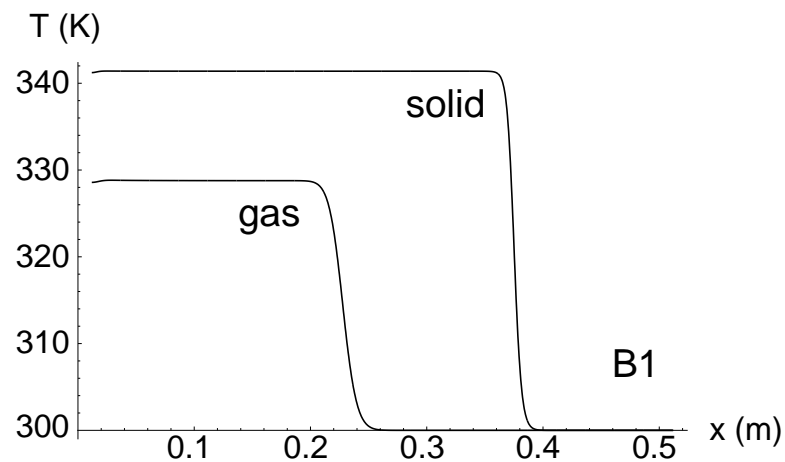
$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{q}) = \mathbf{s}(\mathbf{q}).$$

- Unstructured mesh

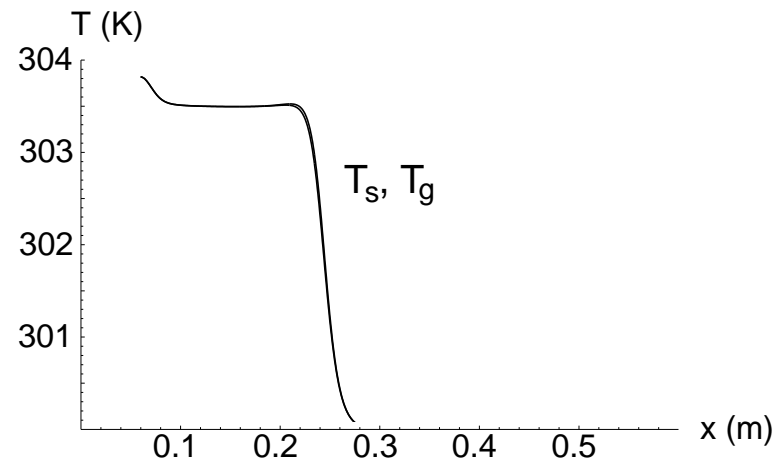
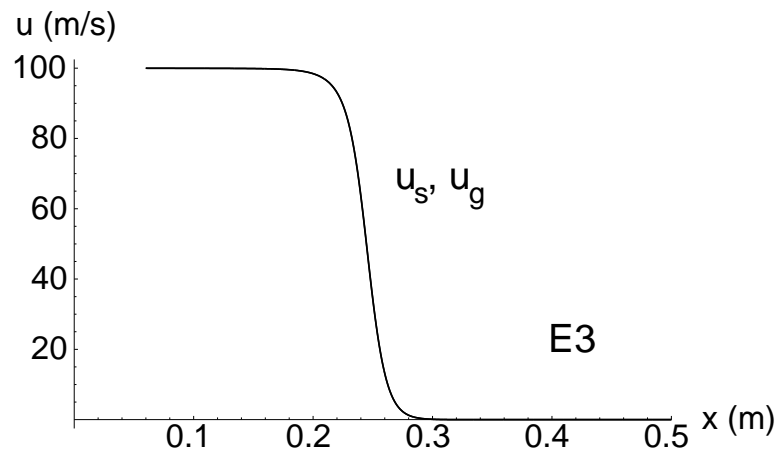
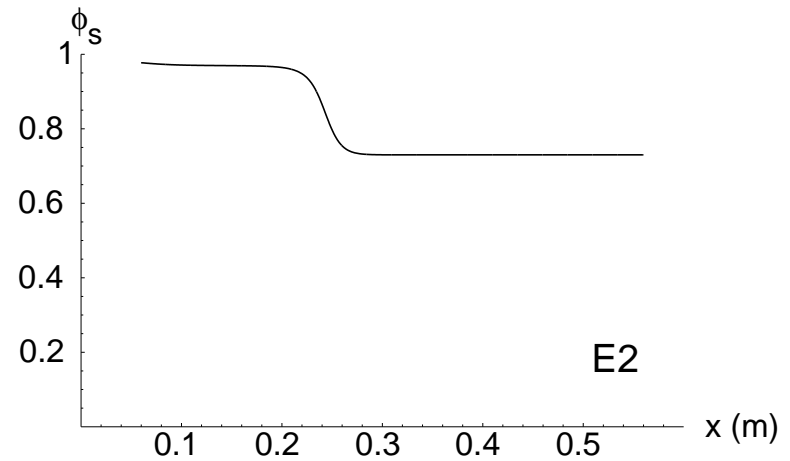
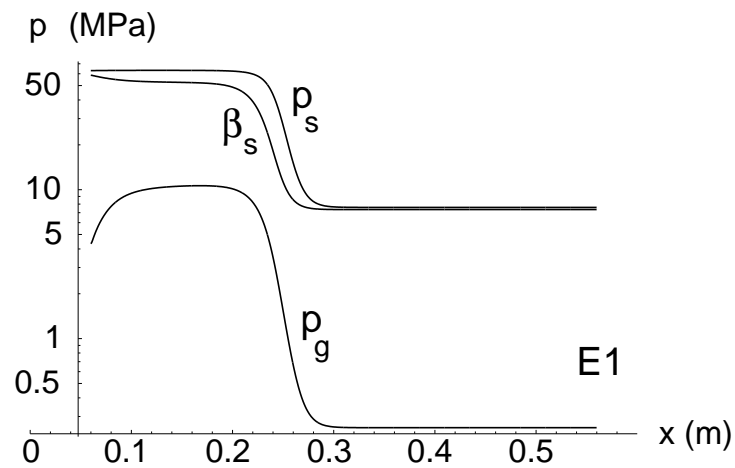
1D Verification: Shock Tube



1D Verification: Piston-Driven Shock

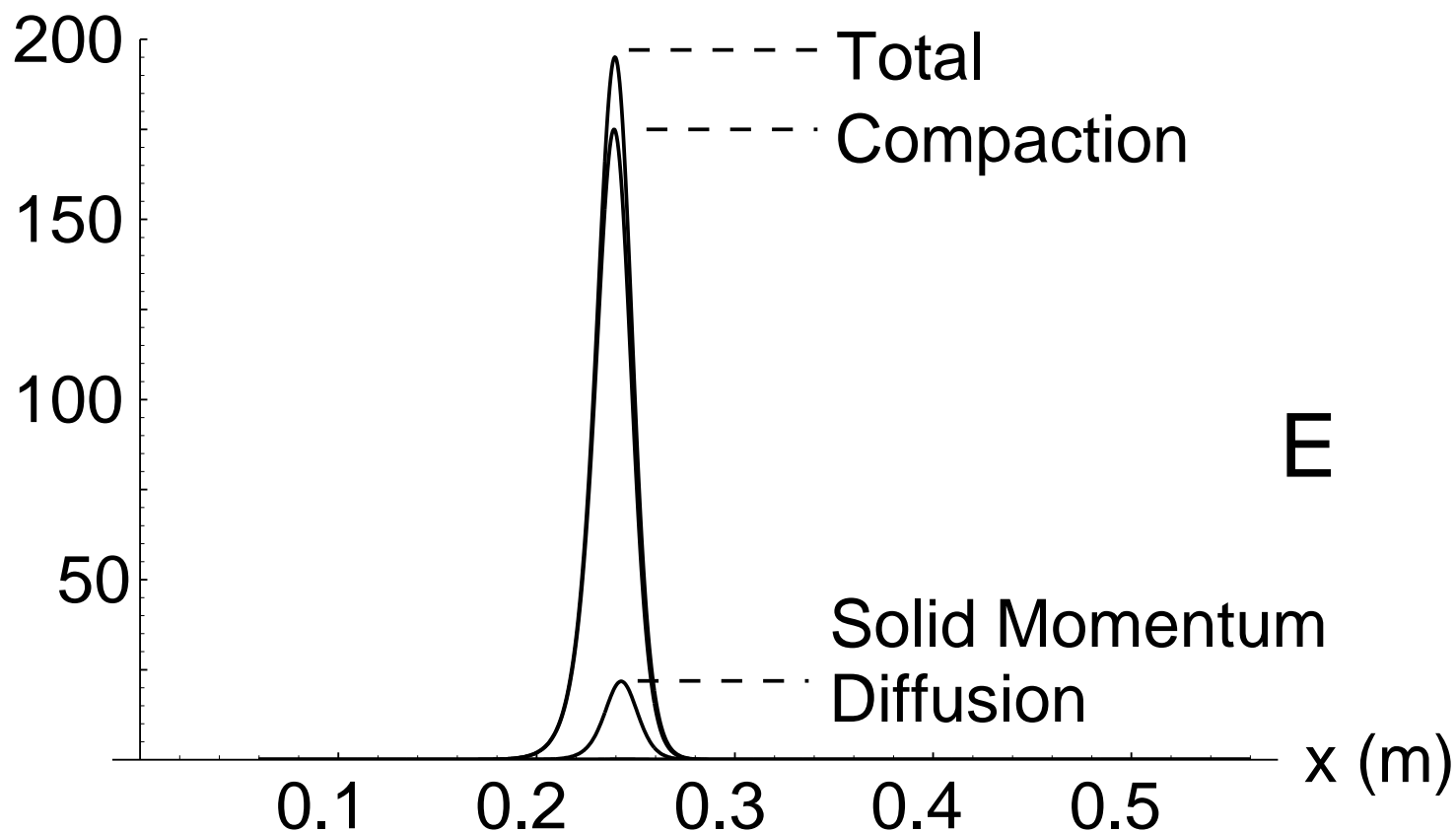


1D Subsonic Piston-Driven Compaction

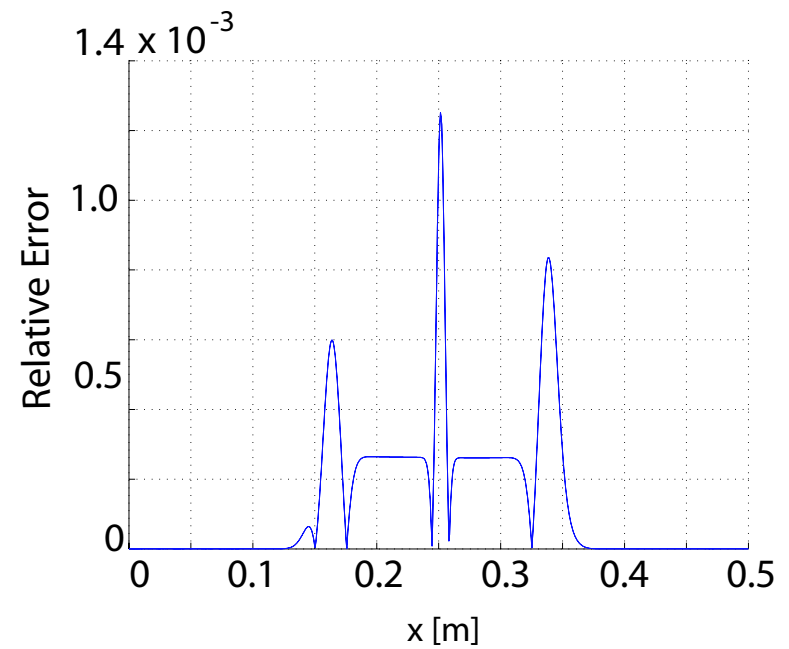
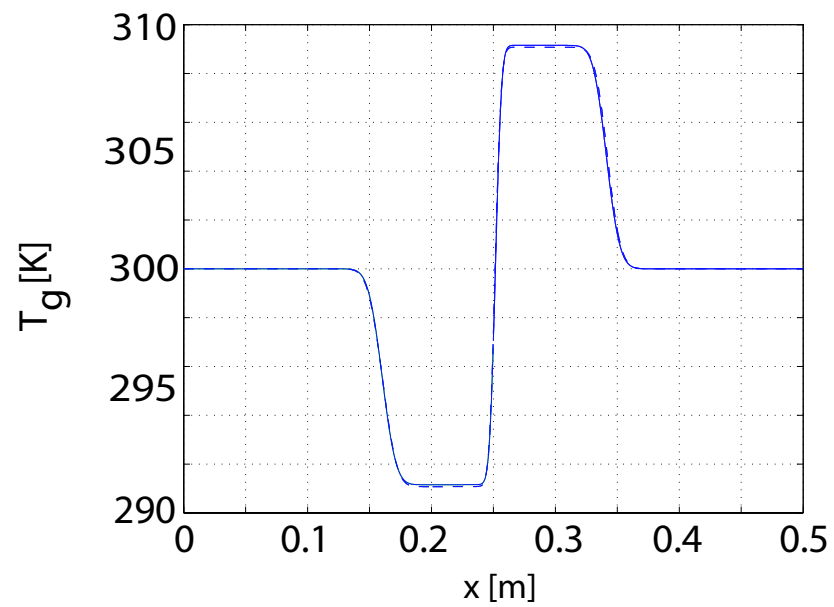


1D Dissipation: Subsonic Case

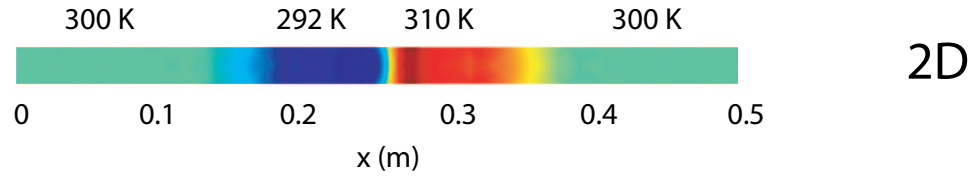
I (MW/m³/K)



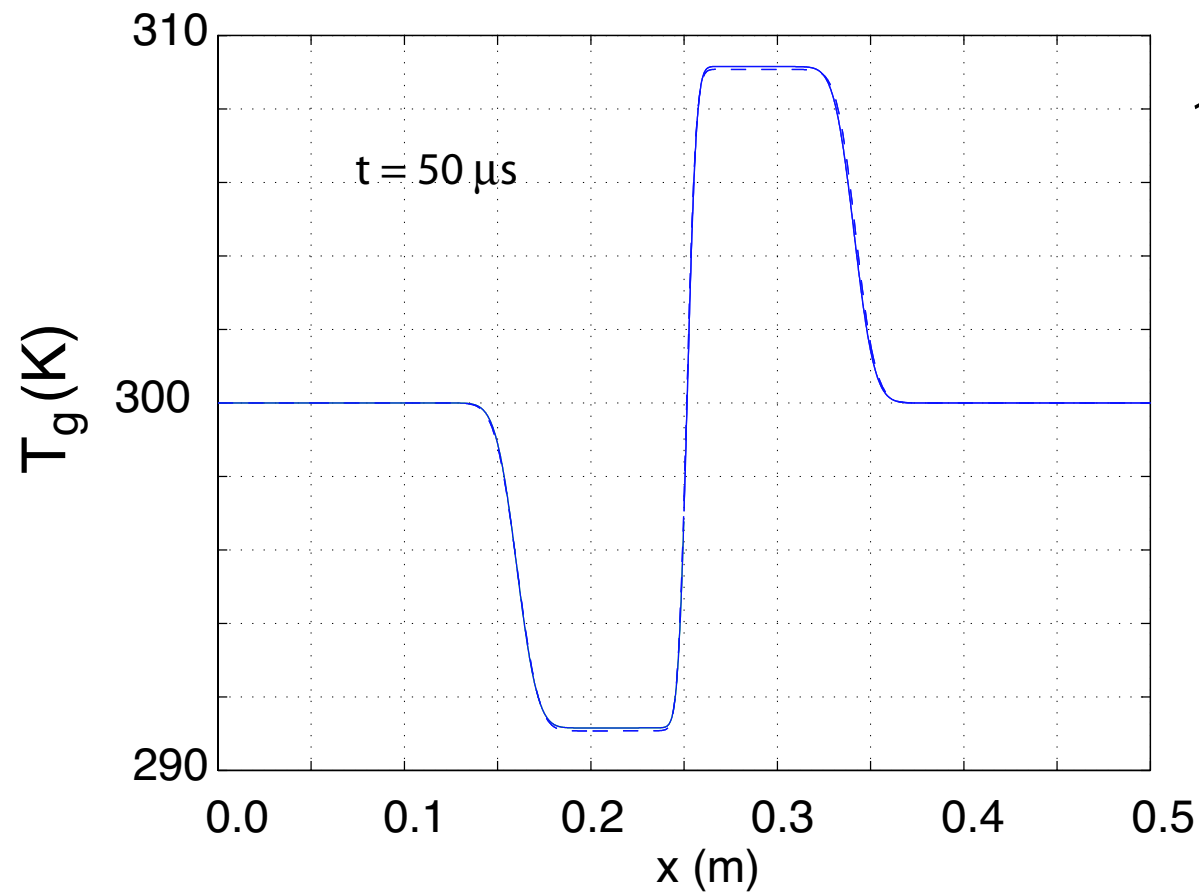
FEMLAB vs. F90 Verification: 1D Shock Tube



Narrow 2D Shock Tube vs. 1D Shock Tube

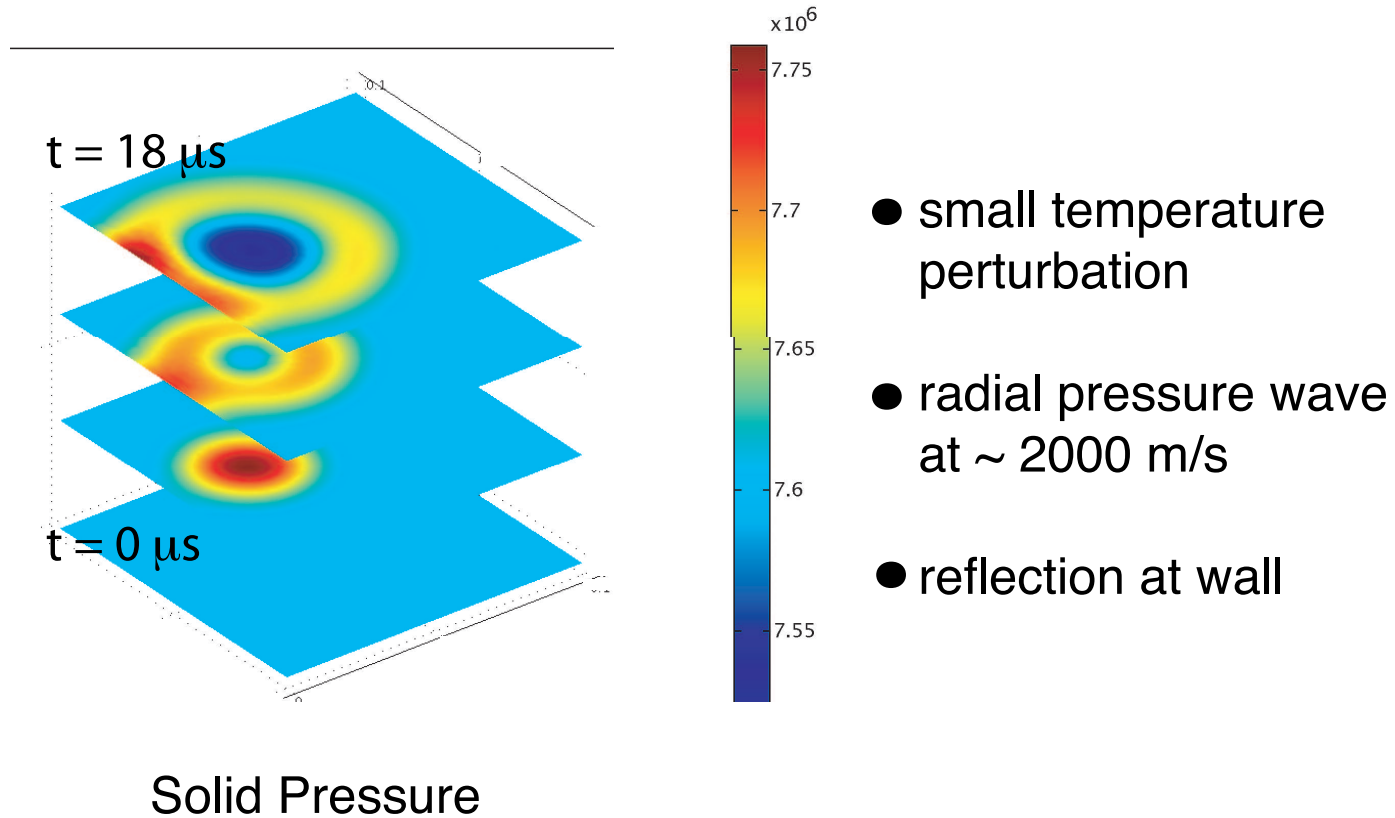


2D

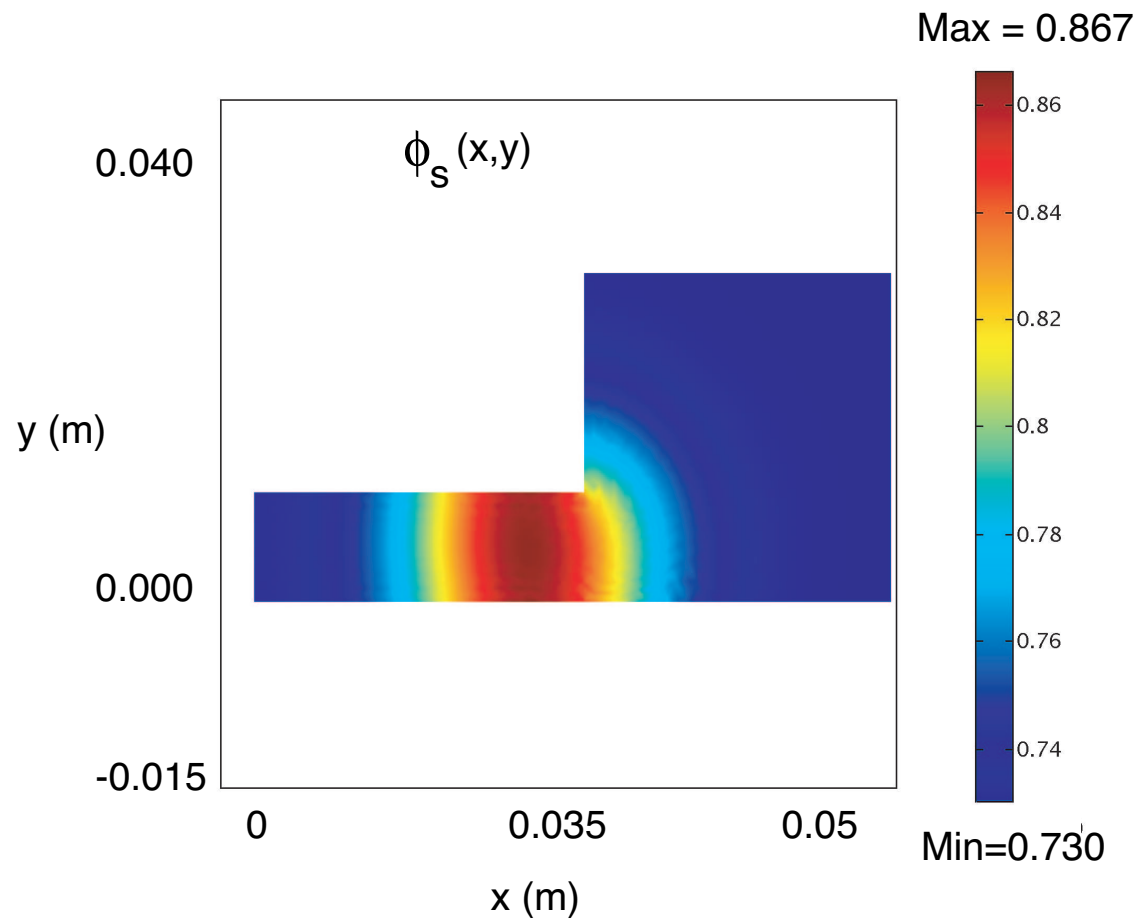


1D

Small Energy Pulse: 2D Response



Large Energy Pulse: 2D Response



Conclusions

- Diffusion enables use of simple numerical techniques.
- Diffusion suppresses short wavelength instabilities, e.g. Kelvin-Helmholtz.
- Diffusion suppresses subgranular length scales.
- Compaction dominates the dissipation.
- Rigorous subscale physical justification for diffusion models presently lacking.
- Such justification necessary for a validated model.