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A High-Resolution Godunov Method for Reactive and Nonreactive Multi-Material Flow on Overlapping Grids

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Project Overview

- Develop software tools for the numerical solution of the reactive Euler equations with a general equation of state and various reaction rate models.

  Include...
  - AMR to resolve contacts/shocks/detonations with numerical efficiency
  - Sub-CFL time step resolution of fast chemical reactions
  - Overlapping grids to handle complex two- and three-dimensional moving geometries
  - Parallel processing and three-dimensional moving geometry (in progress)

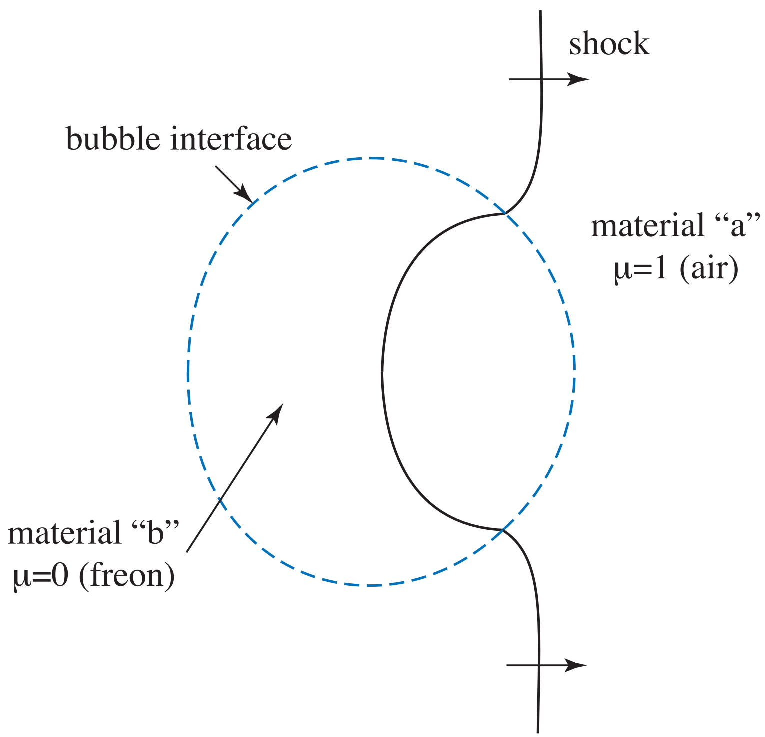
- Study detonation dynamics in homogeneous and heterogeneous explosives.

  For example...
  - Explore paths to detonation of reactive samples at critical conditions subject to an initial stimuli
  - Explore detonation interactions with rigid and compliant boundaries and with moving rigid (and deformable) objects

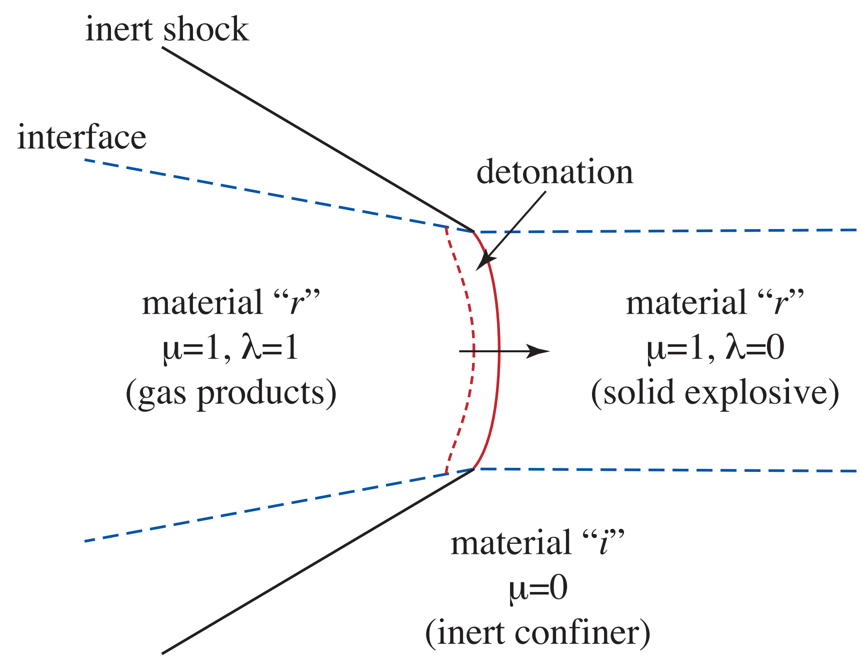
- Explore features and limitations of existing models, e.g. ignition & growth, explore new models, e.g. multiphase, and multi-material flows (in progress).

Compressible Multi-Material Flows

Non-reactive case:
e.g. shock-bubble interaction



Reactive case:
e.g. explosive rate stick



Mixture state variables:

- ρ density
- (u_1, u_2) velocity
- p pressure
- e internal energy

Species variables:

- μ mass fraction of material r
- λ mass fraction of gas products

Governing Equations

Multi-material reactive Euler equations (2-D):

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u_1\\ \rho u_2\\ \rho E\\ \rho\mu\\ \rho\lambda\end{pmatrix}+\frac{\partial}{\partial x_1}\begin{pmatrix}\rho u_1\\ \rho u_1^2+p\\ \rho u_1 u_2\\ u_1(\rho E+p)\\ \rho u_1\mu\\ \rho u_1\lambda\end{pmatrix}+\frac{\partial}{\partial x_2}\begin{pmatrix}\rho u_2\\ \rho u_1 u_2\\ \rho u_2^2+p\\ u_2(\rho E+p)\\ \rho u_2\mu\\ \rho u_2\lambda\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\\ \rho\mathcal{R}\end{pmatrix}$$

with

$$E=e(\rho,p,\mu,\lambda)+\frac{1}{2}(u_1^2+u_2^2),\qquad \mathcal{R}=\text{reaction rate}$$

Mixture EOS:

Mechanical: Thermal:

$$e_k=\frac{p_k v_k}{\omega_k}-\mathcal{F}_k\left(\frac{v_k}{v_{k,0}}\right)+Q_k \qquad p_k=\frac{\omega_k}{v_k}\left[C_{v,k}T_k+\mathcal{Z}_k\left(\frac{v_k}{v_{k,0}}\right)\right] \qquad k=s,\ g,\ i$$

Mixture rules:

$$e=\mu\left[(1-\lambda)e_s+\lambda e_g\right]+(1-\mu)e_i$$
$$v=\mu\left[(1-\lambda)v_s+\lambda v_g\right]+(1-\mu)v_i$$

Closure assumptions:

$$p=p_s=p_g=p_i$$
$$T=T_s=T_g=T_i$$

Reaction/EOS Models

Pressure-dependent rate law:

$$\mathcal{R} = \sigma(1-\lambda)^{\nu}(p - p_{\mathrm{ign}})^{n}$$

where

$$\sigma = \text{prefactor} \qquad \nu = \text{depletion exponent}$$
$$p_{\mathrm{ign}} = \text{ignition pressure} \qquad n = \text{pressure exponent}$$

Mixture ideal-gas EOS:

$$\mathcal{F}_k = \mathcal{Z}_k = 0$$

which gives

$$e = pv\left\{\frac{\mu\left[(1-\lambda)C_{v,s} + \lambda C_{v,g}\right] + (1-\mu)C_{v,i}}{\mu\left[(1-\lambda)C_{v,s}\omega_s + \lambda C_{v,g}\omega_g\right] + (1-\mu)C_{v,i}\omega_i}\right\} + \mu(1-\lambda)\Delta Q$$

where

$$\Delta Q = \text{heat release} \qquad \left.\begin{array}{l} C_{v,k} = \text{specific heat} \\ \omega_k = \gamma_k - 1 \end{array}\right\} \quad k = s,\ g,\ i$$

Ignition-and-growth rate law (Lee & Tarver, 1980):

$$\mathcal{R} = \mathcal{R}_I + \mathcal{R}_{G_1} + \mathcal{R}_{G_2}$$

where

$$\begin{aligned} \mathcal{R}_I &= I(1-\lambda)^b(\max\{\rho-\rho_I,0\})^x & &\text{if } \lambda < \lambda_I & &\text{(hot spot ignition)} \\ \mathcal{R}_{G_1} &= G_1(1-\lambda)^c\lambda^d p^y & &\text{if } \lambda < \lambda_{G_1,\max} & &\text{(rapid growth)} \\ \mathcal{R}_{G_2} &= G_2(1-\lambda)^e\lambda^g p^z & &\text{if } \lambda > \lambda_{G_2,\min} & &\text{(slow growth)} \end{aligned}$$

Mixture JWL EOS:

$$\mathcal{F}_k(V) = A_k\left(\frac{V}{\omega_k} - \frac{1}{R_{1,k}}\right)\exp\left(-R_{1,k}V\right) + B_k\left(\frac{V}{\omega_k} - \frac{1}{R_{2,k}}\right)\exp\left(-R_{2,k}V\right)$$

$$\mathcal{Z}_k(V) = A_k\left(\frac{V}{\omega_k}\right)\exp\left(-R_{1,k}V\right) + B_k\left(\frac{V}{\omega_k}\right)\exp\left(-R_{2,k}V\right)$$

Remarks:

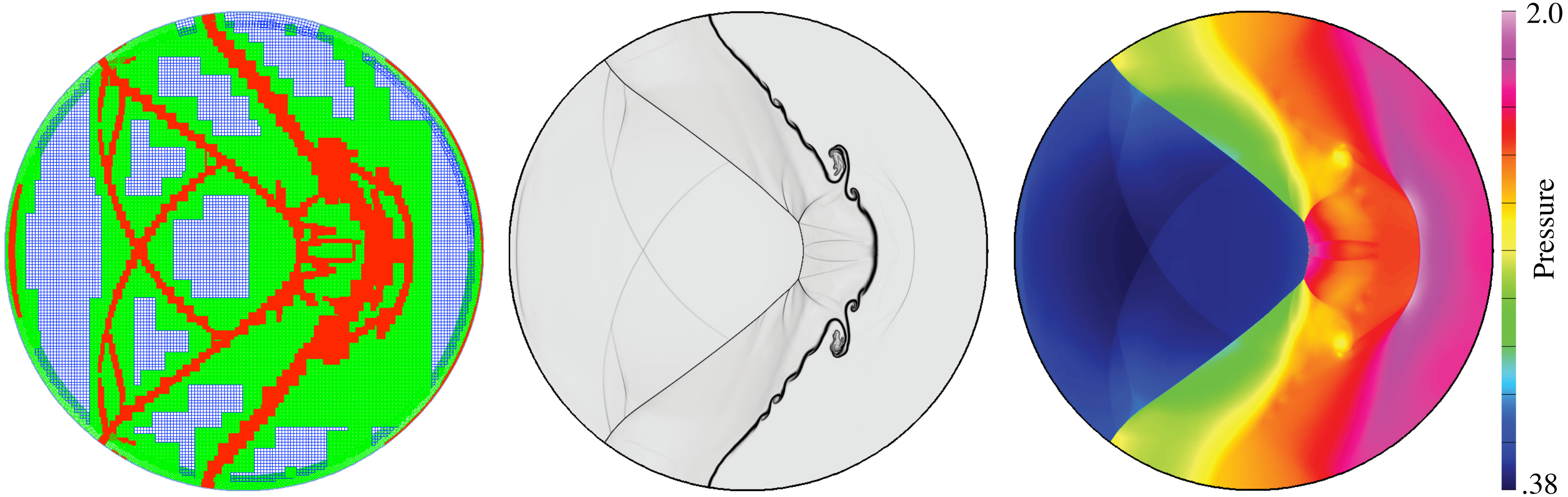
- internal energy $e(\rho, p, \mu, \lambda)$ defined implicitly
- rate and EOS parameters fit to data (e.g. the explosive PBX 9502)
- EOS parameters for the inert chosen to model *strong* or *weak* confinement

Numerical Method

Summary:

- Godunov-type, shock-capturing scheme on a domain discretized using composite overlapping grids (overset grids).
- Riemann problems handled using Roe approximate Riemann solvers (extended to handle the equation of state for the mixture).
- Reaction source term is handled with a Runge-Kutta error-control scheme.
- AMR is used to locally increase grid resolution near shocks, detonations and the material interface.
- An energy correction term is added (at the level of the truncation error) to suppress numerical errors in the pressure near the material interface.

Sample AMR grid and solution:



Basic time-stepping algorithm:

ReactiveEulerSolver$(\mathcal{G}, t_{\text{final}})$
{
  $t := 0; \quad n := 0;$
  $u^n :=$ **applyInitialCondition** $(\mathcal{G});$
  while $t < t_{\text{final}}$
    if $(n \bmod n_{\text{regrid}} == 0)$ *// rebuild the AMR grid*
      $e :=$ **estimateError**$(\mathcal{G}, u^n);$
      $\mathcal{G}^* :=$ **regrid**$(\mathcal{G}, e);$
      $u^* :=$ **interpolateToNewGrid**$(u^n, \mathcal{G}, \mathcal{G}^*);$
      $\mathcal{G} := \mathcal{G}^*; \quad u^n := u^*;$
    end
    $\Delta t :=$ **computeTimeStep**$(\mathcal{G}, u^n);$
    $u^{n+1} :=$ **advanceSolution**$(\mathcal{G}, u^n, \Delta t);$ *// reactive Euler time step*
    interpolate$(\mathcal{G}, u^{n+1});$
    applyBoundaryConditions$(\mathcal{G}, u^{n+1}, t + \Delta t);$
    $t := t + \Delta t; \quad n := n + 1;$
  end
}

Adaptive mesh refinement (AMR):

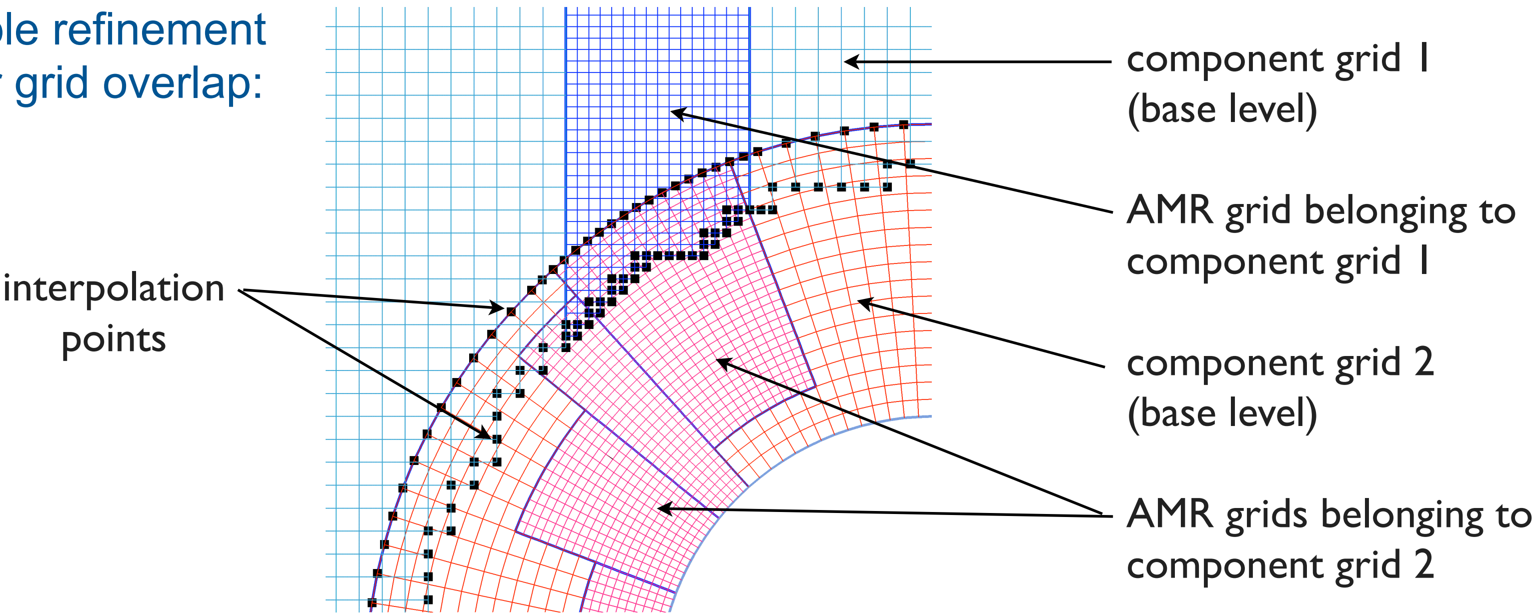
For each component grid at a fixed time...

- compute error estimate $e_{i,j}$ based on second differences of the components of the solution and on the reaction rate

$$e_{i,j} = \sum_{k=1}^{m} s_k \left(|\Delta_r^2 U_{i,j}^{(k)}| + |\Delta_s^2 U_{i,j}^{(k)}| \right) + s_R |\tau_{i,j}|$$

- smooth $e_{i,j}$ and interpolate to the overlap (if any) from neighboring component grids
- build refined (child) grid patches that cover all cells with $e_{i,j} > \text{tol}$
- interpolate solution from the coarse (parent) grid or copy solution from old child grids, if they exist

Sample refinement near grid overlap:



Component grid time step:

Overlapping grid...

$$\mathcal{G} = \{\mathbf{G}_g\}, \quad g = 1, \ldots, \mathcal{N} \qquad \text{Includes base grids + AMR grids}$$

Mapping...

$$\mathbf{x} = \mathbf{G}_g(\mathbf{r}, t), \qquad \mathbf{x} = \text{physical space}, \quad \mathbf{r} \in [0,1]^2 = \text{computational space}$$

Mapped equations...

$$\frac{\partial}{\partial t}\mathbf{u} + \frac{1}{J}\frac{\partial}{\partial x_1}\hat{\mathbf{f}}_1(\mathbf{u}) + \frac{1}{J}\frac{\partial}{\partial x_2}\hat{\mathbf{f}}_2(\mathbf{u}) = \mathbf{h}(\mathbf{u})$$

where

$$\hat{\mathbf{f}}_1 = a_{2,2}\,\mathbf{f}_1(\mathbf{u}) - a_{1,2}\,\mathbf{f}_2(\mathbf{u}), \quad \hat{\mathbf{f}}_2 = a_{1,1}\,\mathbf{f}_2(\mathbf{u}) - a_{2,1}\,\mathbf{f}_1(\mathbf{u}), \quad \text{(mapped fluxes)}$$

and

$$a_{i,j} = \frac{\partial x_i}{\partial r_j}\,, \quad J = \left|\frac{\partial(x_1, x_2)}{\partial(r_1, r_2)}\right| \quad \text{(metrics and jacobian are given by } \mathbf{G}_g\text{)}$$

Fractional-step scheme...

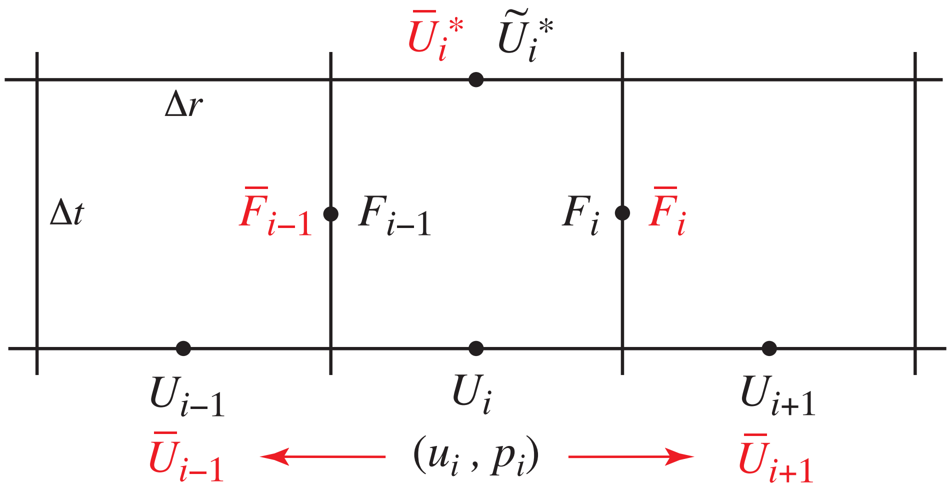
$$U_{\mathbf{i}}^{n+1} = \mathcal{S}_h(\Delta t/2)\,\mathcal{S}_f(\Delta t)\,\mathcal{S}_h(\Delta t/2)\,U_{\mathbf{i}}^n, \qquad U_{\mathbf{i}}^n = \text{cell average of } \mathbf{u} \text{ at } \mathbf{r}_{\mathbf{i}},\ t_n$$

Convective term update: $U^*_{\mathbf{i}} = \mathcal{S}_f(\Delta t)\, U_{\mathbf{i}}$

Godunov schemes (e.g. 1D)...

$$\tilde{U}^*_i = U_i - \frac{\Delta t}{J\Delta r}\left(F_i - F_{i-1}\right) \qquad \bar{U}^*_i = U_i - \frac{\Delta t}{J\Delta r}\left(\bar{F}_i - \bar{F}_{i-1}\right)$$

(standard Godunov) (adjusted for uniform pressure-velocity flow)



Energy correction...

$$\Delta E^*_i = \tilde{\rho}_i e\big(\tilde{\rho}_i, \tilde{p}_i + \Delta p_i, \tilde{\mu}_i, \tilde{\lambda}_i\big) - \tilde{\rho}_i \tilde{e}_i, \qquad \Delta p_i = p_i - \bar{p}_i$$

Update...

$$U^*_i = \tilde{U}^*_i + \Delta G^*_i\,, \qquad \text{where} \quad \Delta G^*_i = \big[0,\,0,\,\Delta E^*_i,\,0,0\big]^T$$

Energy-corrected scheme: test cases

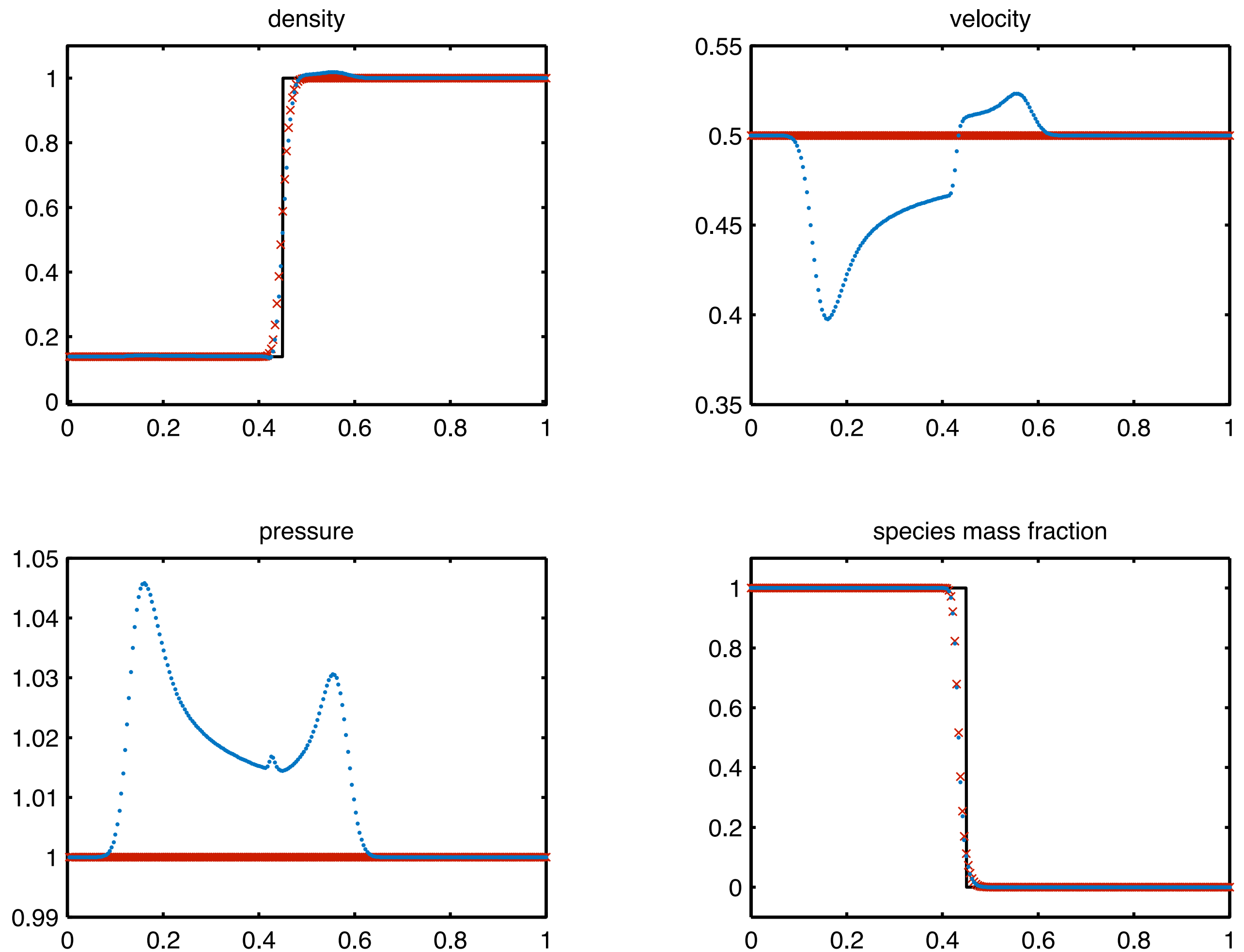
1D Riemann problem...

$$(\rho_L, u_L, p_L, \mu_L) = (0.138, 0.5, 1.0, 1.0)$$

for $x < 0.4$ at $t = 0$ (helium on the left)

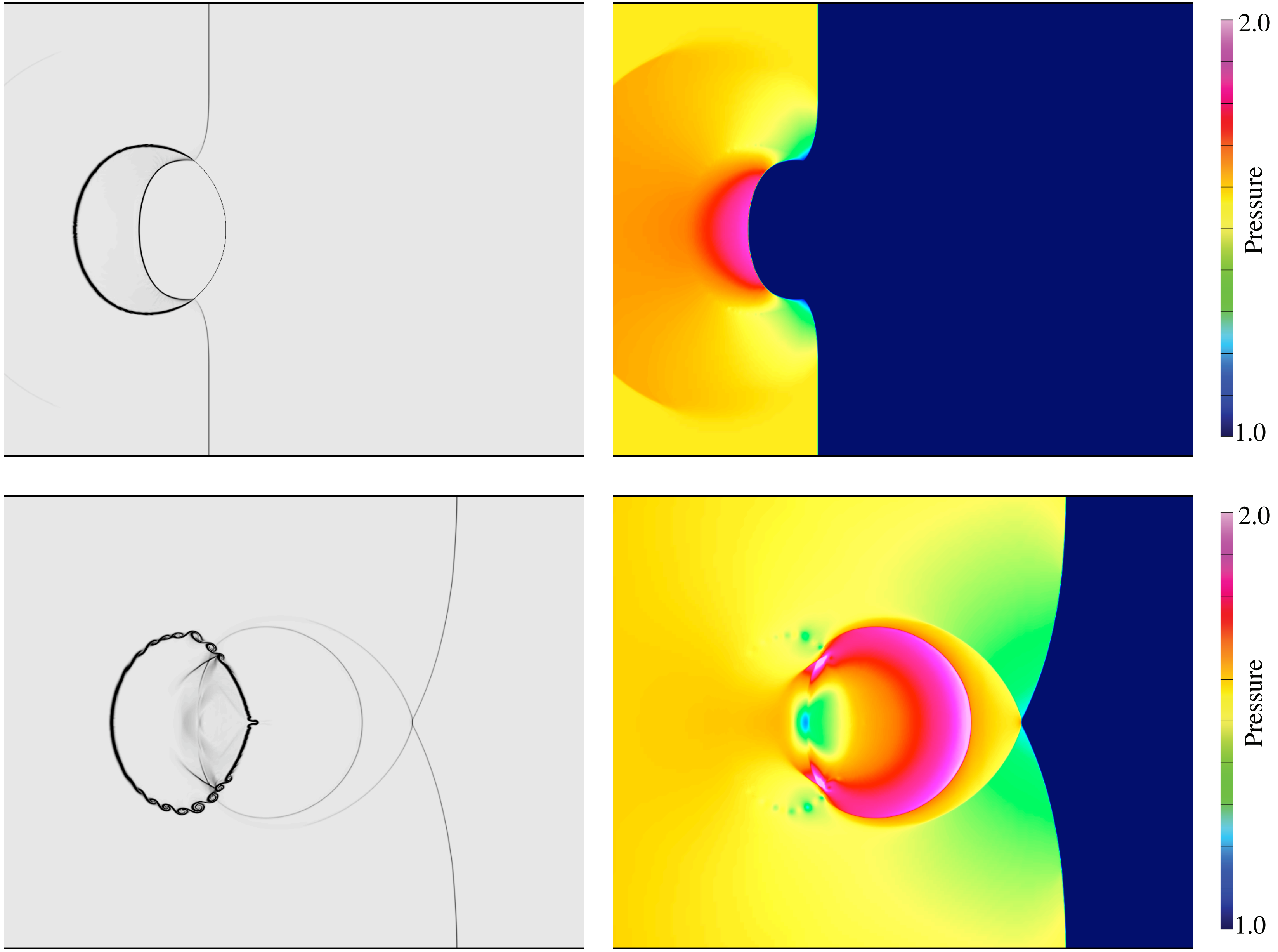
$$(\rho_R, u_R, p_R, \mu_R) = (1.0, 0.5, 1.0, 0.0)$$

for $x \geq 0.4$ at $t = 0$ (air on the right)



Solution at t=0.1: black = exact, blue = Godunov w/out correction, red = Godunov w/ correction

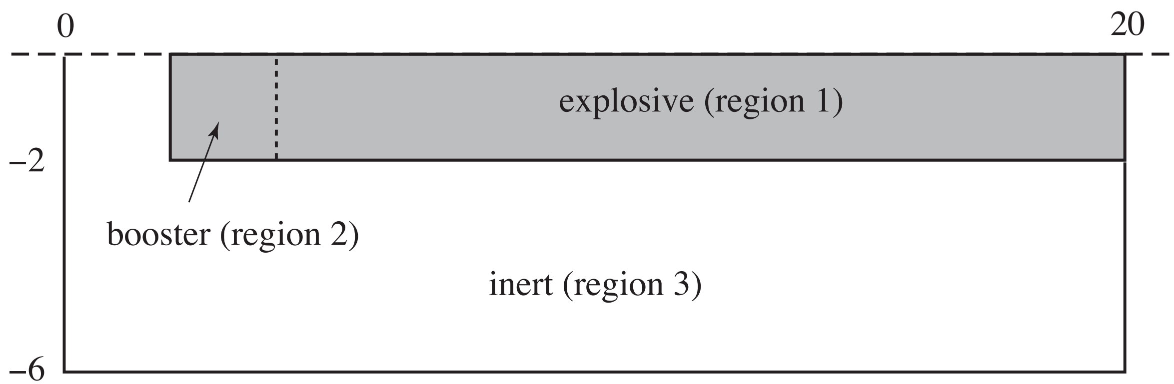
2D shock-bubble interaction...



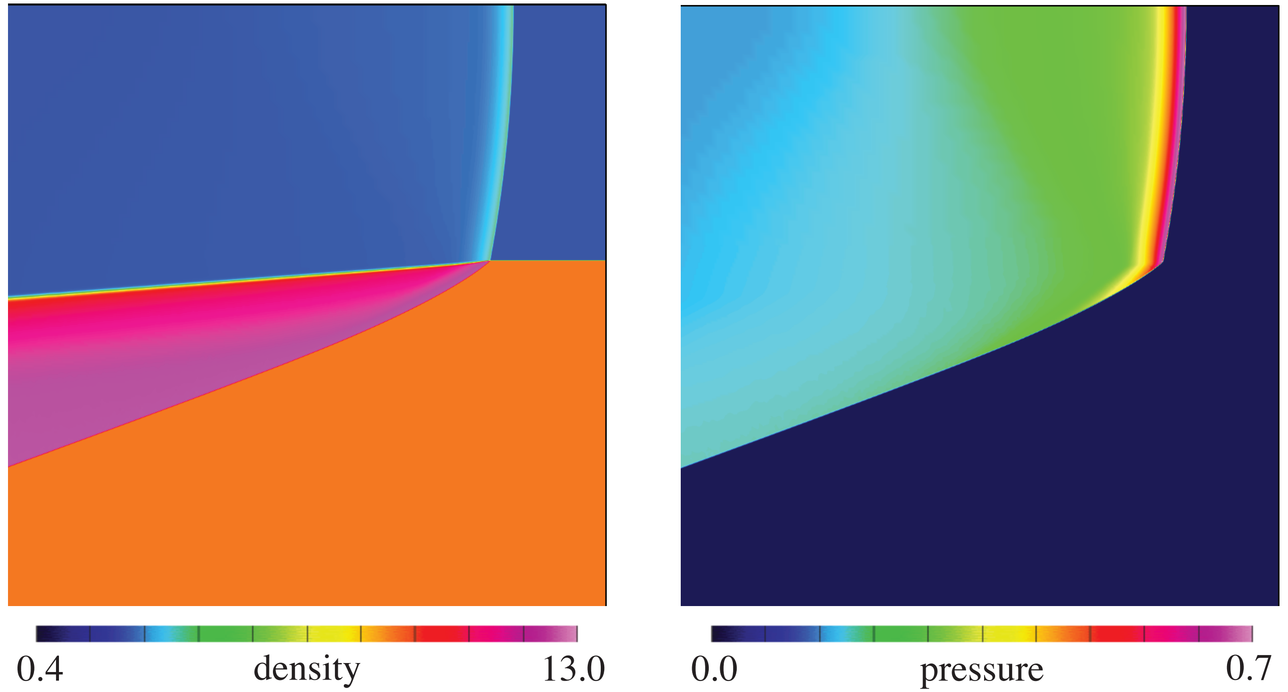
Refrigerant-filled bubble in air: numerical schlieren (left) and pressure (right).

2D explosive rate stick...

Initial state



Downstream steady state



Numerical Results

The numerical method has been used to study a number of problems involving both reactive and nonreactive flow, including...

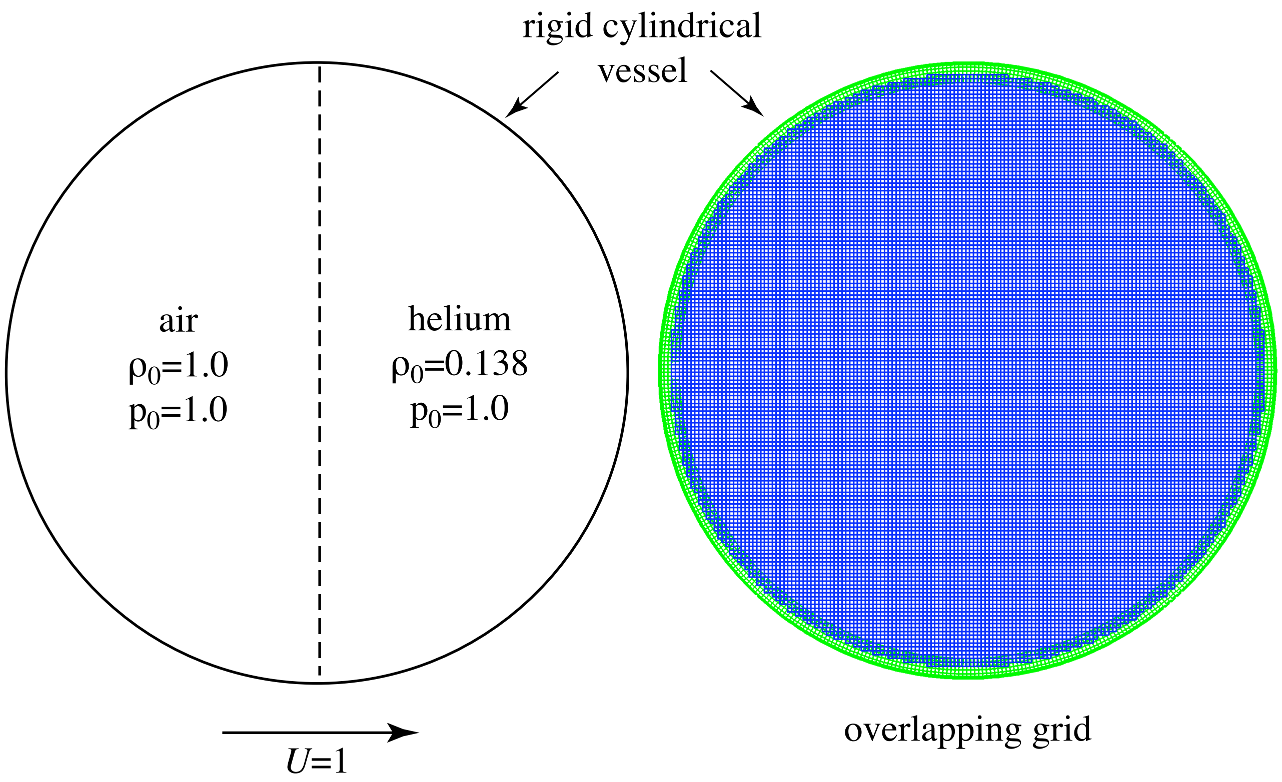
- Shock interaction with curved gas inhomogeneities.
- Interface interaction with rigid confinements.
- Detonation diffraction in expanding and converging geometries.
- Detonation failure and re-birth in various expanding configurations.
- Detonation interactions with compliant boundaries.

Focus on 2 problems...

- Impulsive motion of a two-fluid system in a rigid vessel (nonreactive).
- Detonation diffraction at a 90 degree corner (reactive).

Two-fluid system in a rigid vessel:

Initial geometry and base grid...



EOS model...

ideal gas: $\gamma = 1.4$, $C_v = 0.720$ for air, and $\gamma = 1.67$, $C_v = 3.11$ for helium.

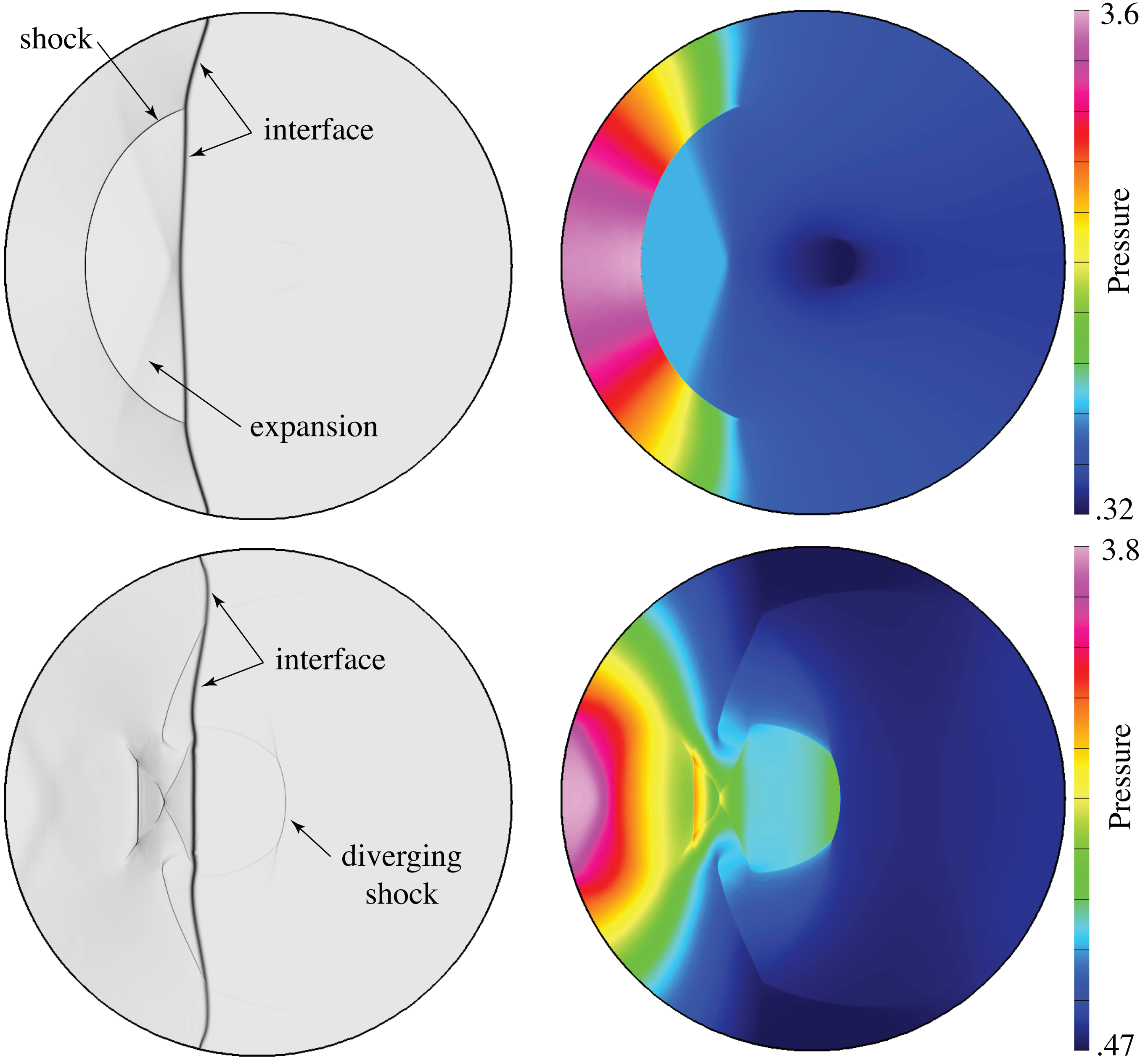
AMR...

up to 2 AMR grid levels with refinement factor=4

Solution behavior (early times)...

time = 0.25

time = 0.50

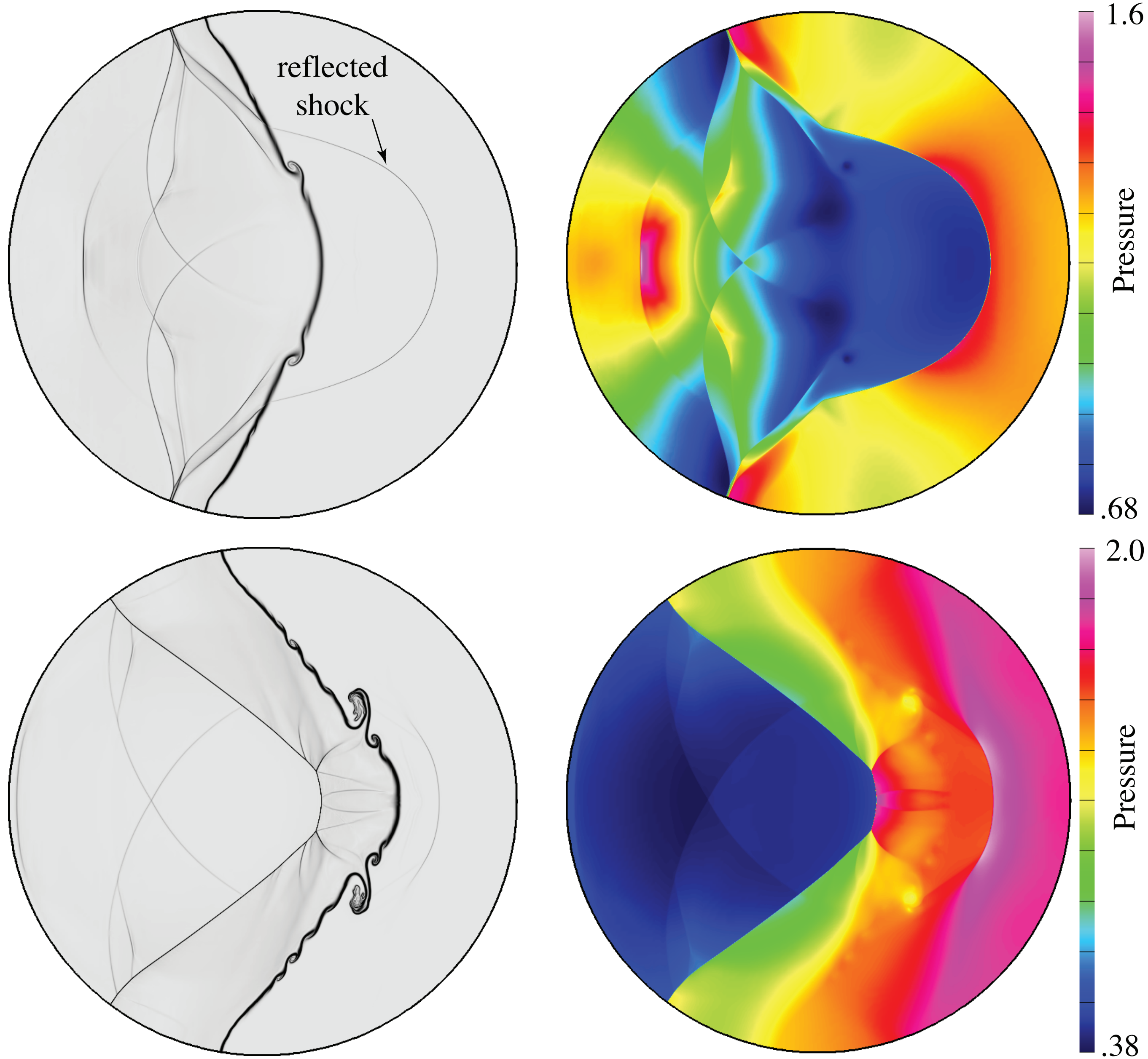


Two-fluid system in a rigid vessel: numerical schlieren (left) and pressure (right).

Solution behavior (late times)...

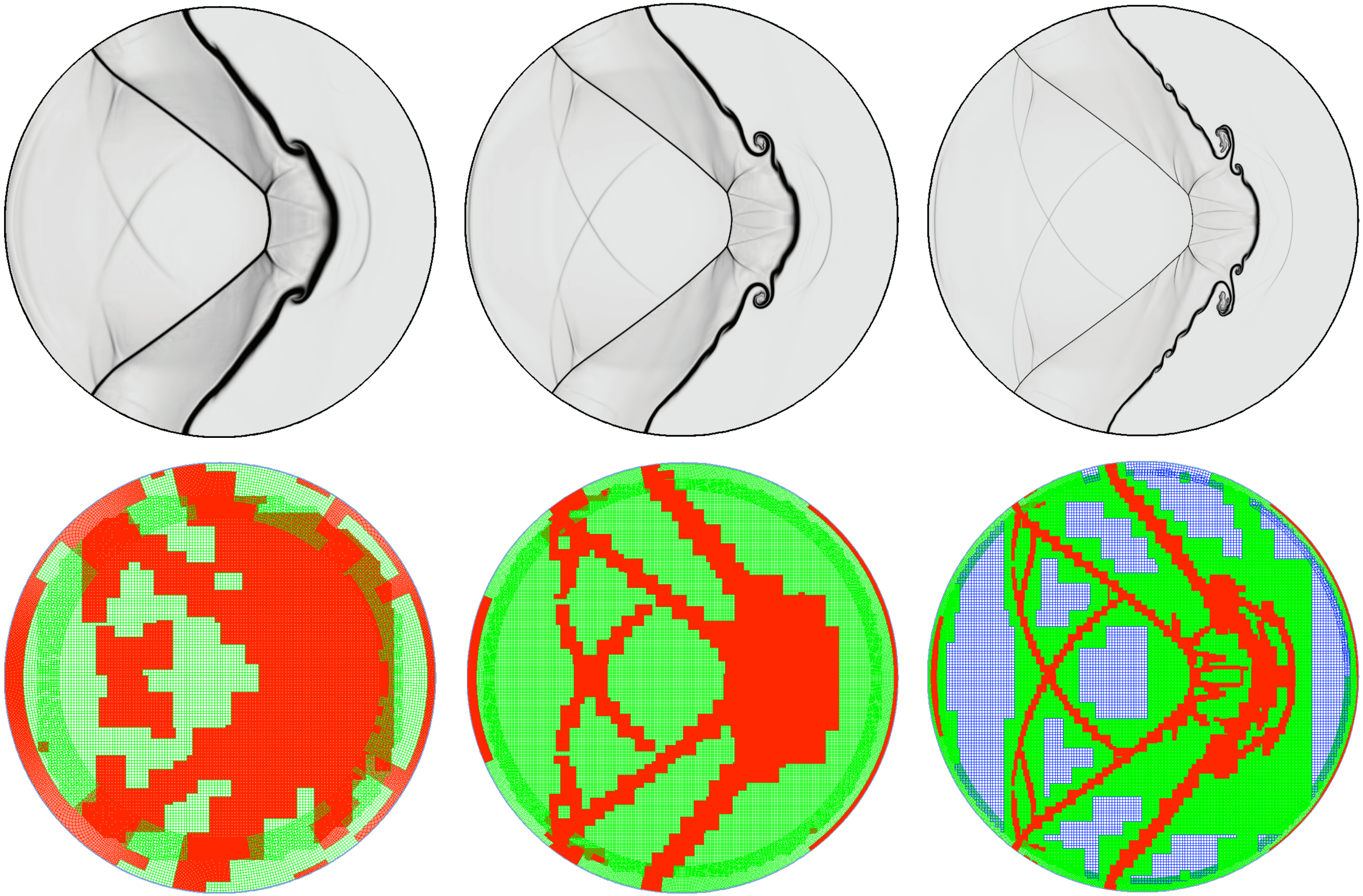
time = 0.75

time = 1.00



Two-fluid system in a rigid vessel: numerical schlieren (left) and pressure (right).

Grid convergence...

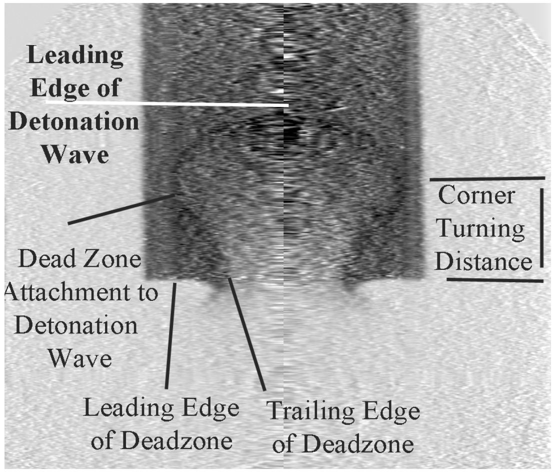


$h_{\mathrm{eff}} = h_0 = .0025$ $h_{\mathrm{eff}} = h_0/2$ $h_{\mathrm{eff}} = h_0/4$

Detonation diffraction at a 90-degree corner:

Motivation: Corner-turning experiments...

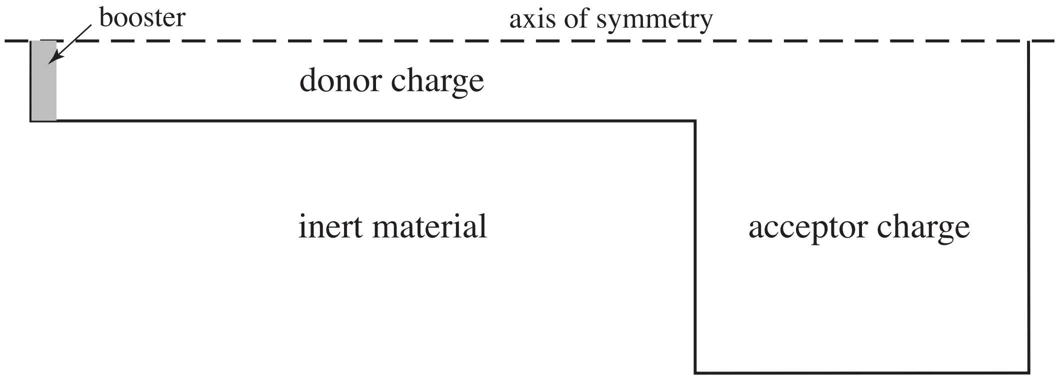
rate-stick charges.



Volume density image.

Eric N. Ferm, et al.
Proton Radiography Examination of Unburnt Regions in PBX 9502 Corner-Turning Experiments

Model geometry...



Reaction/EOS model...

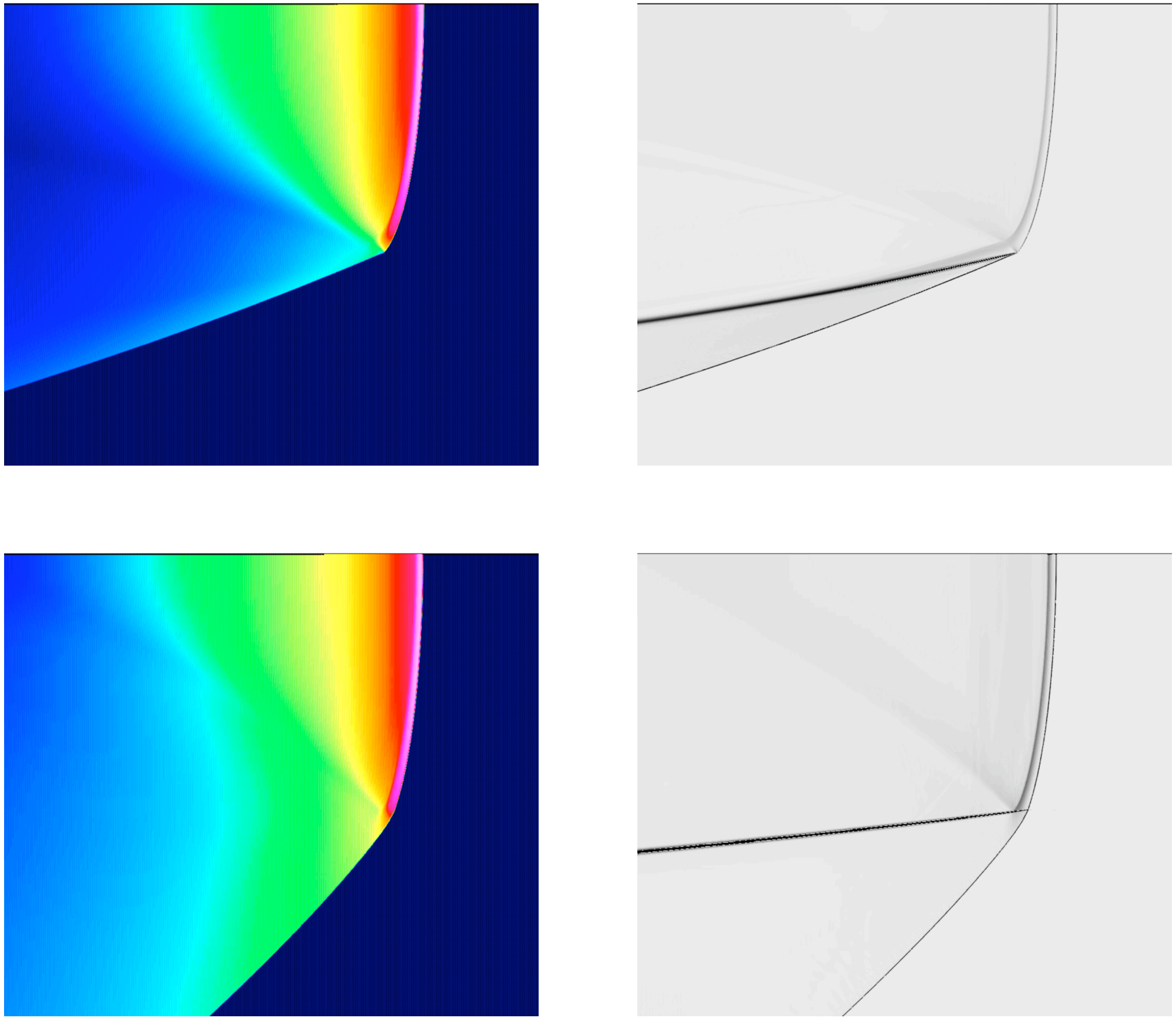
Ignition-and-growth model with reaction rate and EOS parameters calibrated to the explosive PBX 9502.

(Tarver & McGuire, 2002)

Base grid + AMR...

up to 2 AMR grid levels with refinement factor=4

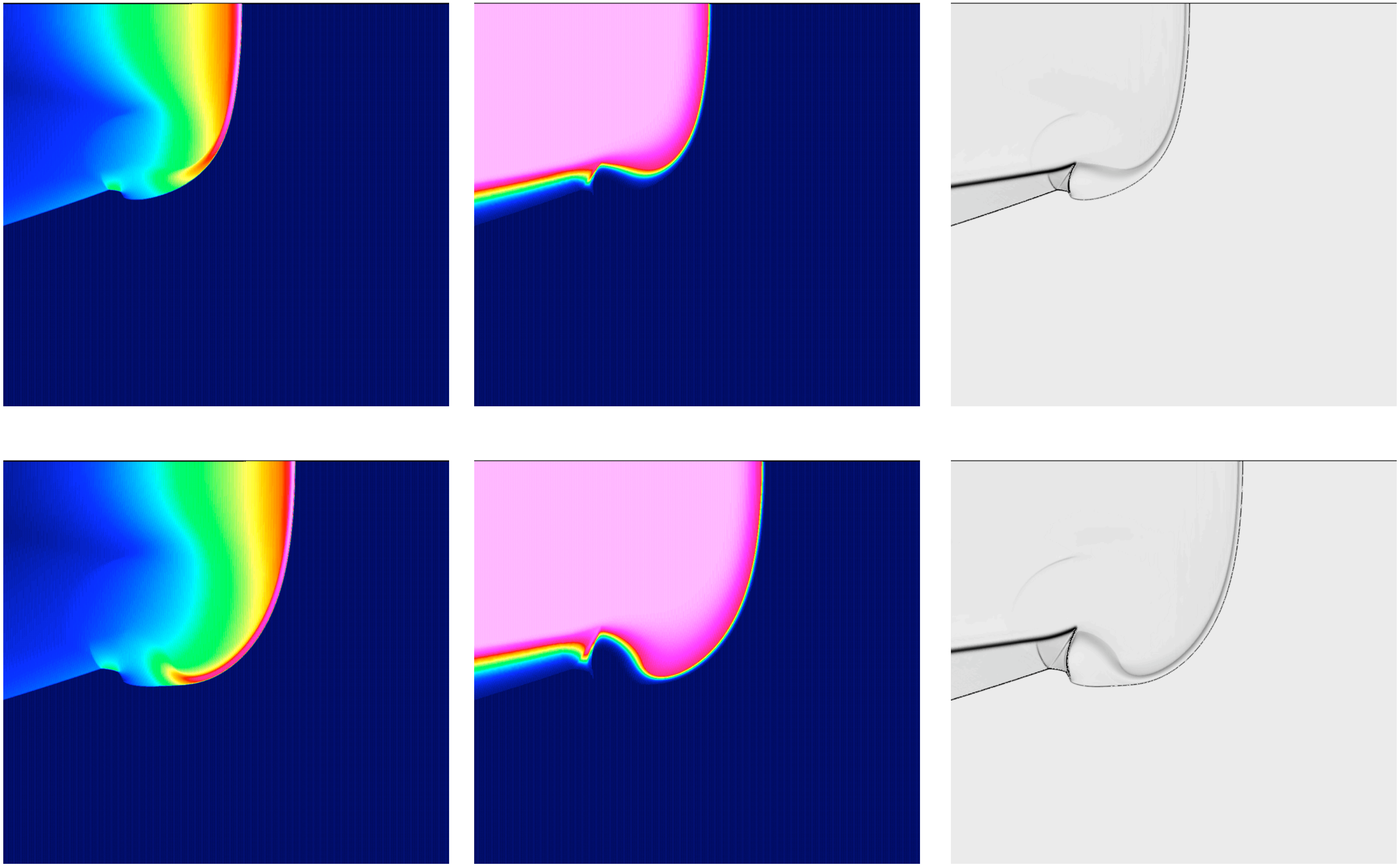
Steady pre-diffraction detonation...



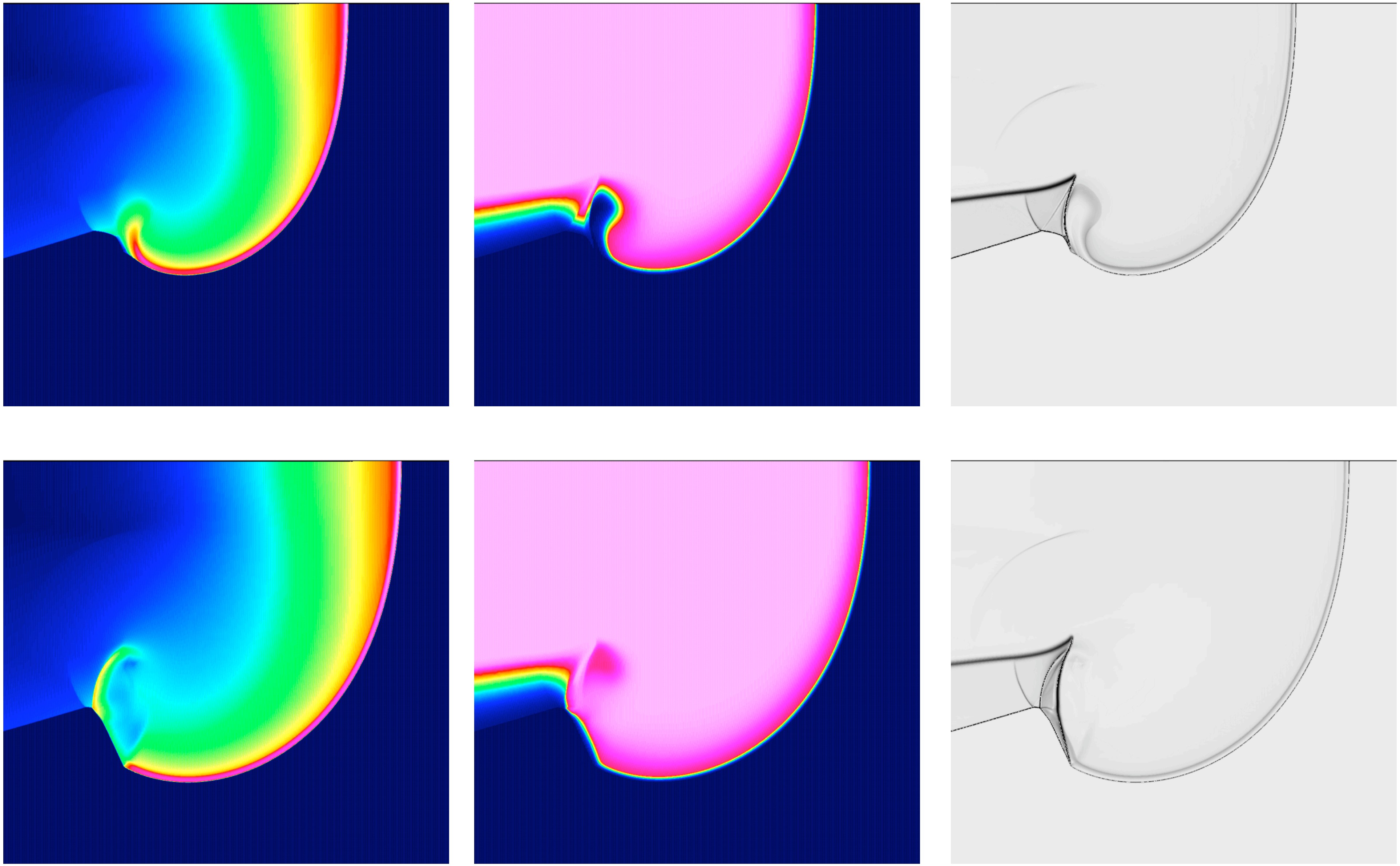
weak
confinement

strong
confinement

Post-diffraction detonation, weak confinement...



Post-diffraction detonation, weak confinement...



Concluding Remarks

- ☑ An accurate computational framework has been developed for the exploration of continuum models of high-speed reactive flow.
- ☑ Overlapping grid approach is used to handle complex geometries.
- ☑ Present computational study has illustrated the capability to handle multi-material flows and the associated material interface accurately.
- ☑ Ongoing work includes an analysis of multi-phase and multi-scale models of reactive flow and the development of parallel-AMR-overlapping grid techniques for their numerical solution.

Full details of the present work appear in...

J. Banks, D. Schwendeman, A. Kapila and W. Henshaw, *A high-resolution Godunov method for compressible multi-material flow on overlapping grids*, J. Comput. Phys.

J. Banks, et al., *A Study of Detonation Propagation and Diffraction with Compliant Confinement,* Combust. Theory and Modeling (preprint).