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Dynamic Detonation Failure in Charges of High Explosive

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Overview

Compressible Multi-Material Flows:

Introduction

- Motivation/Goals

Mathematical Model

- Governing equations (Multi-material reactive Euler equations)
- Model reaction systems

Numerical Technique

- High-resolution Godunov method
- Adaptive mesh refinement (AMR) for sharp features
- Treatment of material interfaces
- Treatment of stiff reaction sources

Numerical Examples

- Algorithmic verification via simple rate stick
- Detonation dynamics for expanding geometry (“dead zones” and desensitization)
- Detonation dynamics for converging geometry

Summary

Questions

Introduction

Motivation:

- Attractive features of shock capturing methods
  - AMR
  - Smooth mapped geometries on logically rectangular structured meshes
  - Non-linearly stable high resolution numerical methods (e.g. TVD)
  - Direct discretization of integral conservation laws

- Shock capturing methods traditionally have difficulty with material interfaces
  - Numerical oscillations (particularly in the pressure)
  - Tightly coupled to stiff reaction sources causes unphysical results

Goals:

- Develop a multi-material numerical capability that allows an accurate treatment of interfaces within a shock-capturing, overlapping grid, AMR framework

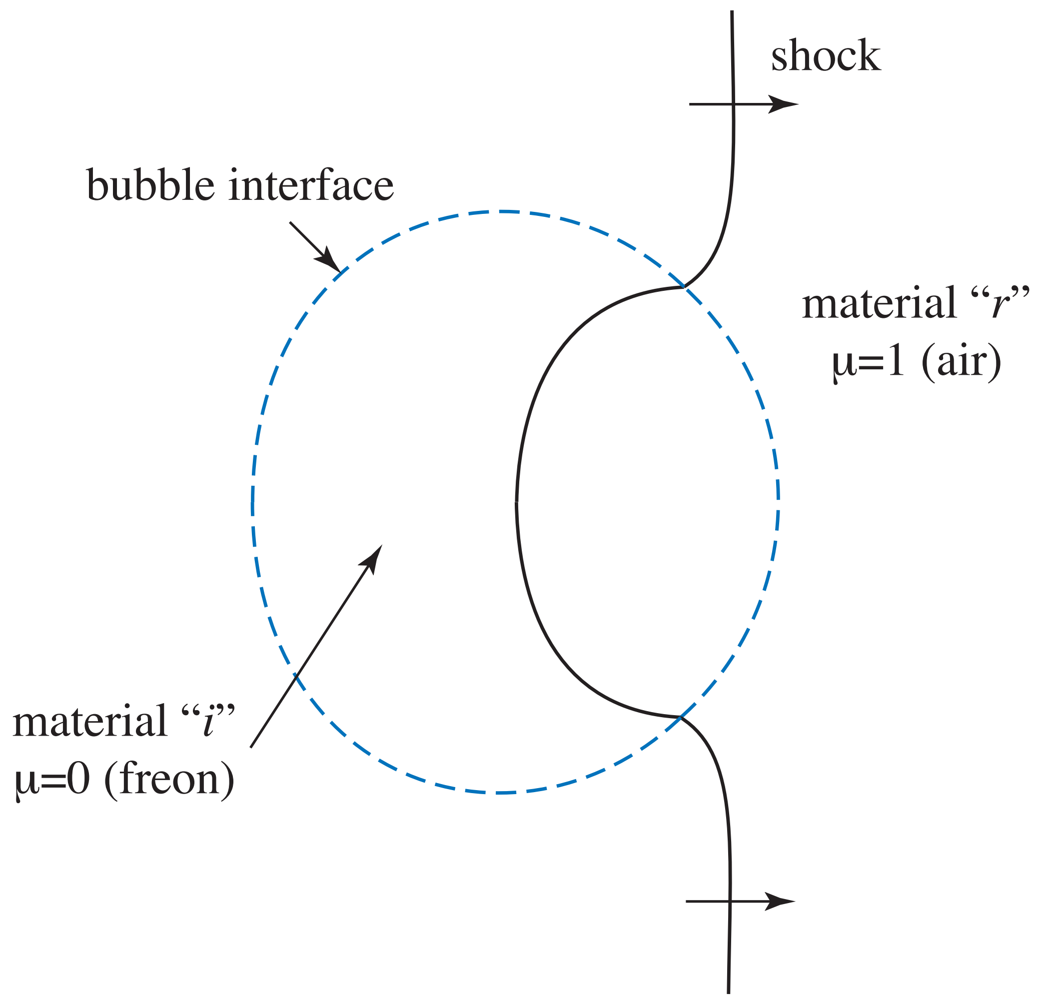
- Verify this method for reacting flows via a simple reacting rate stick and shock polar analysis

- Study detonation dynamics for diverging geometries (dead zone formation)
  - Standard ignition-and-growth (I&G) model
  - Extended I&G model to include shock desensitization

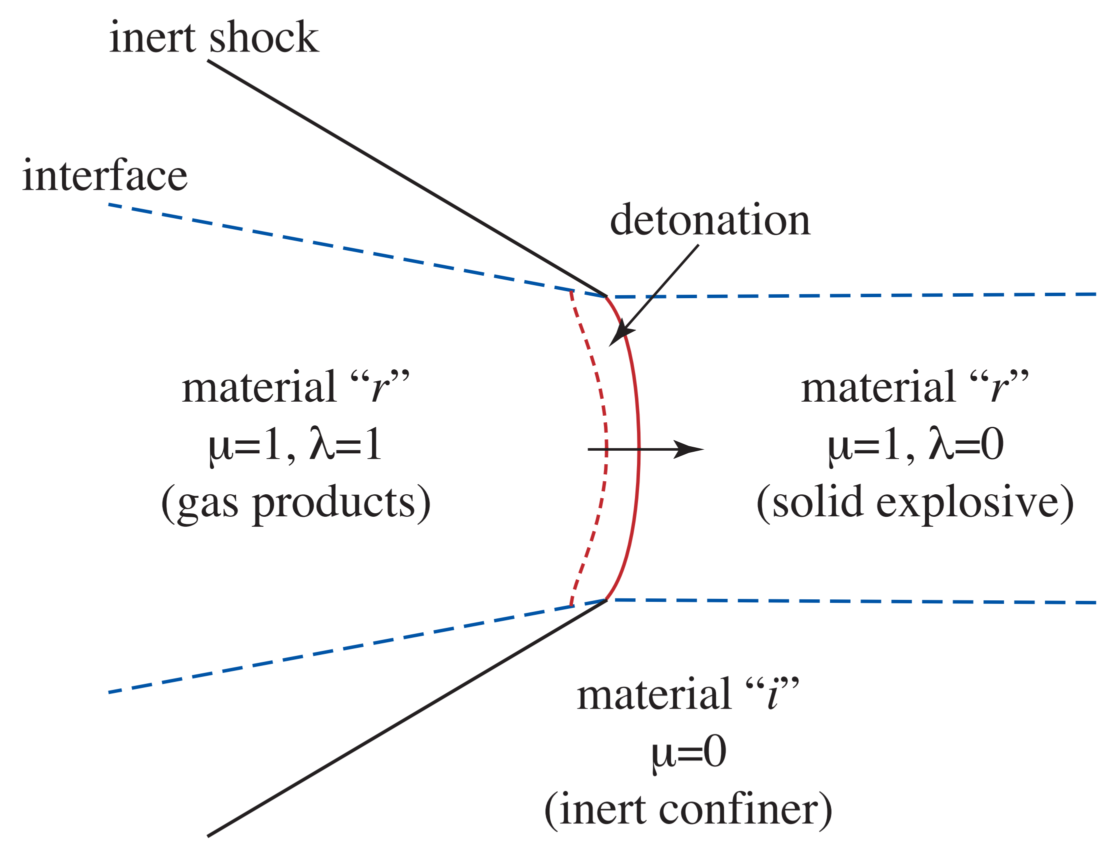
- Study detonation dynamics for converging geometries

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):

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\\ \rho\mu\\ \rho\lambda\\ \rho\phi\end{pmatrix}+\frac{\partial}{\partial x_1}\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ u(\rho E+p)\\ \rho u\mu\\ \rho u\lambda\\ \rho u\phi\end{pmatrix}+\frac{\partial}{\partial x_2}\begin{pmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ v(\rho E+p)\\ \rho v\mu\\ \rho v\lambda\\ \rho v\phi\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\ \rho\mathcal{R}\\ \rho\mathcal{S}\end{pmatrix}$$

where

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

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: Case 1

Pressure–dependent rate law:

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

where

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

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

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

No desensitization model:

Reaction/EOS Model: Case II

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

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

where

$$\mathcal{R}_I = \begin{cases} 0 & \text{if } \rho/\rho_0 < 1 + a(\phi) \\ I(1-\lambda)^b(\rho/\rho_0 - 1 - a(\phi))^x & \text{if } \rho/\rho_0 \geq 1 + a(\phi) \text{ and } \lambda \leq \lambda_{I,\max} \end{cases} \quad \text{(hot spot ignition)}$$

$$\mathcal{R}_{G_1} = \begin{cases} G_1(1-\lambda)^c\lambda^d p^y & \text{if } \lambda_{G_1,\min}(\phi) < \lambda \leq \lambda_{G_1,\max} \\ 0 & \text{if } \lambda > \lambda_{G_1,\max} \end{cases} \quad \text{(rapid growth)}$$

$$\mathcal{R}_{G_2} = \begin{cases} 0 & \text{if } \lambda < \lambda_{G_2,\min} \\ G_2(1-\lambda)^e\lambda^g p^z & \text{if } \lambda \geq \lambda_{G_2,\min}. \end{cases} \quad \text{(slow growth)}$$

Mixture JWL EOS:

$$\left.\begin{aligned} F_k(V) &= A_j\left(\frac{V}{\omega_k} - \frac{1}{R_{1,k}}\right)\exp\left(-R_{1,k}V\right) + B_j\left(\frac{V}{\omega_k} - \frac{1}{R_{2,k}}\right)\exp\left(-R_{2,k}V\right) \\ Z_k(V) &= A_j\left(\frac{V}{\omega_k}\right)\exp\left(-R_{1,k}V\right) + B_j\left(\frac{V}{\omega_k}\right)\exp\left(-R_{1,k}V\right) \end{aligned}\right\} k = i,s \text{ or } g$$

Desensitization model:

$$\mathcal{S} = A_r p(1-\phi)(\phi + e_r)$$

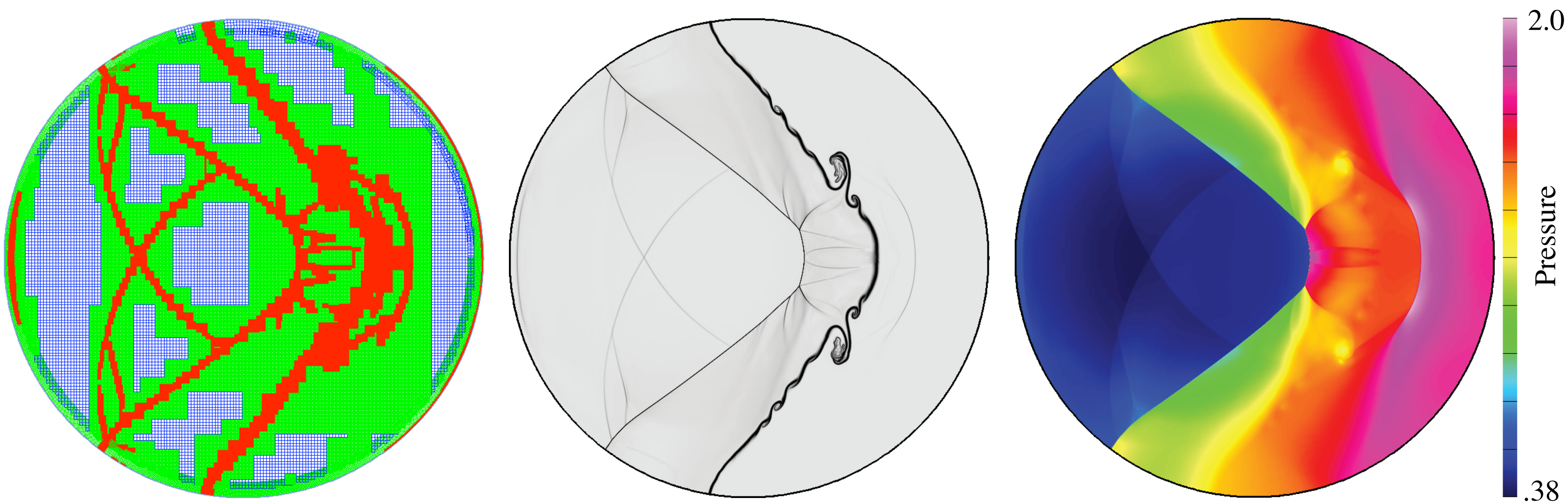
- Parameters for reactive material fit to experimental data (e.g. PBX-9502)
- Parameters for inert material chosen to mock “strong” or “weak” confinement

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$(\mathcal{G}, t_{\rm final})$
$\{$
$t := 0; \quad n := 0;$
$u^n :=$ **applyInitialCondition** $(\mathcal{G})$;
while $t < t_{\rm final}$
if $(n \bmod n_{\rm regrid} == 0)$ *// 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):

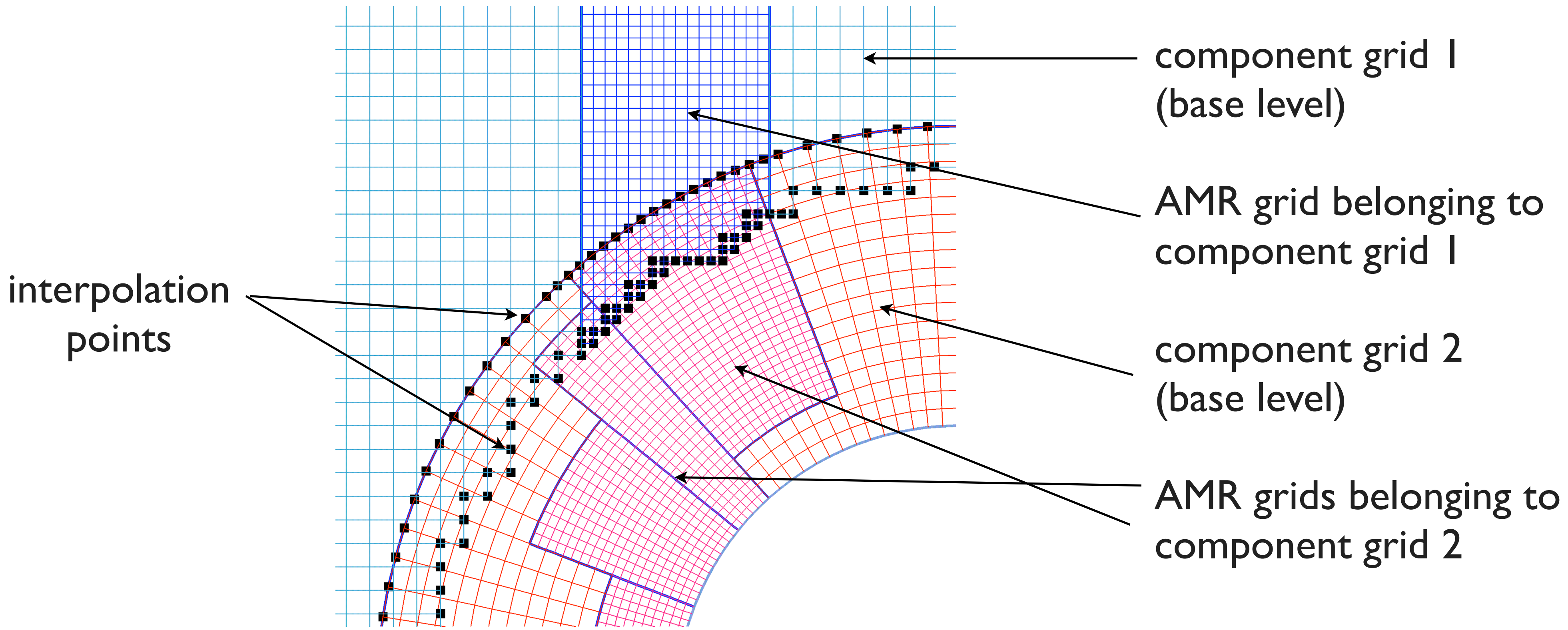
For each component grid at a fixed time...

- 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...

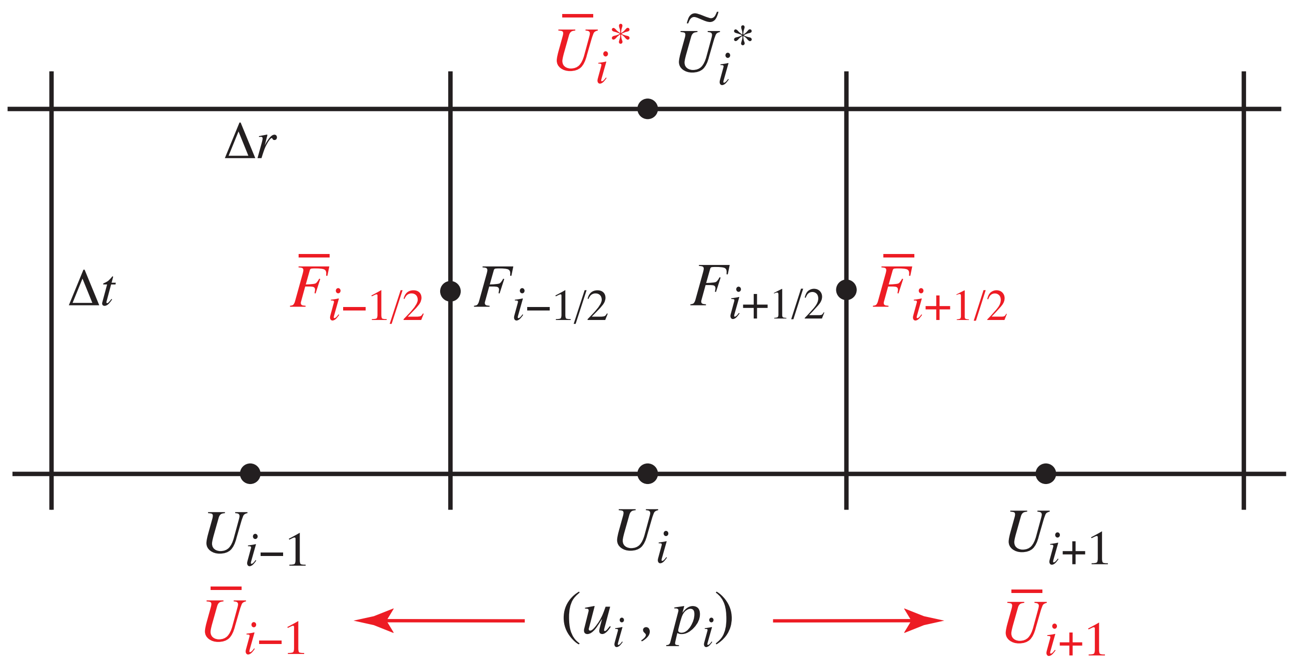
$$U_{\mathbf{i}}^{n+1} = \mathcal{S}_h(\Delta t/2)\,\mathcal{S}_f(\Delta t)\,\mathcal{S}_h(\Delta t/2)\,U_{\mathbf{i}}^n, \qquad U_{\mathbf{i}}^n = \text{cell average of } \mathbf{u} \text{ at } \mathbf{r}_{\mathbf{i}},\ t_n$$

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

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

$$\tilde{U}_i^{*} = U_i - \frac{\Delta t}{J \Delta r}\left(F_{i+1/2} - F_{i-1/2}\right) \qquad \bar{U}_i^{*} = U_i - \frac{\Delta t}{J \Delta r}\left(\bar{F}_{i+1/2} - \bar{F}_{i-1/2}\right)$$

(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...

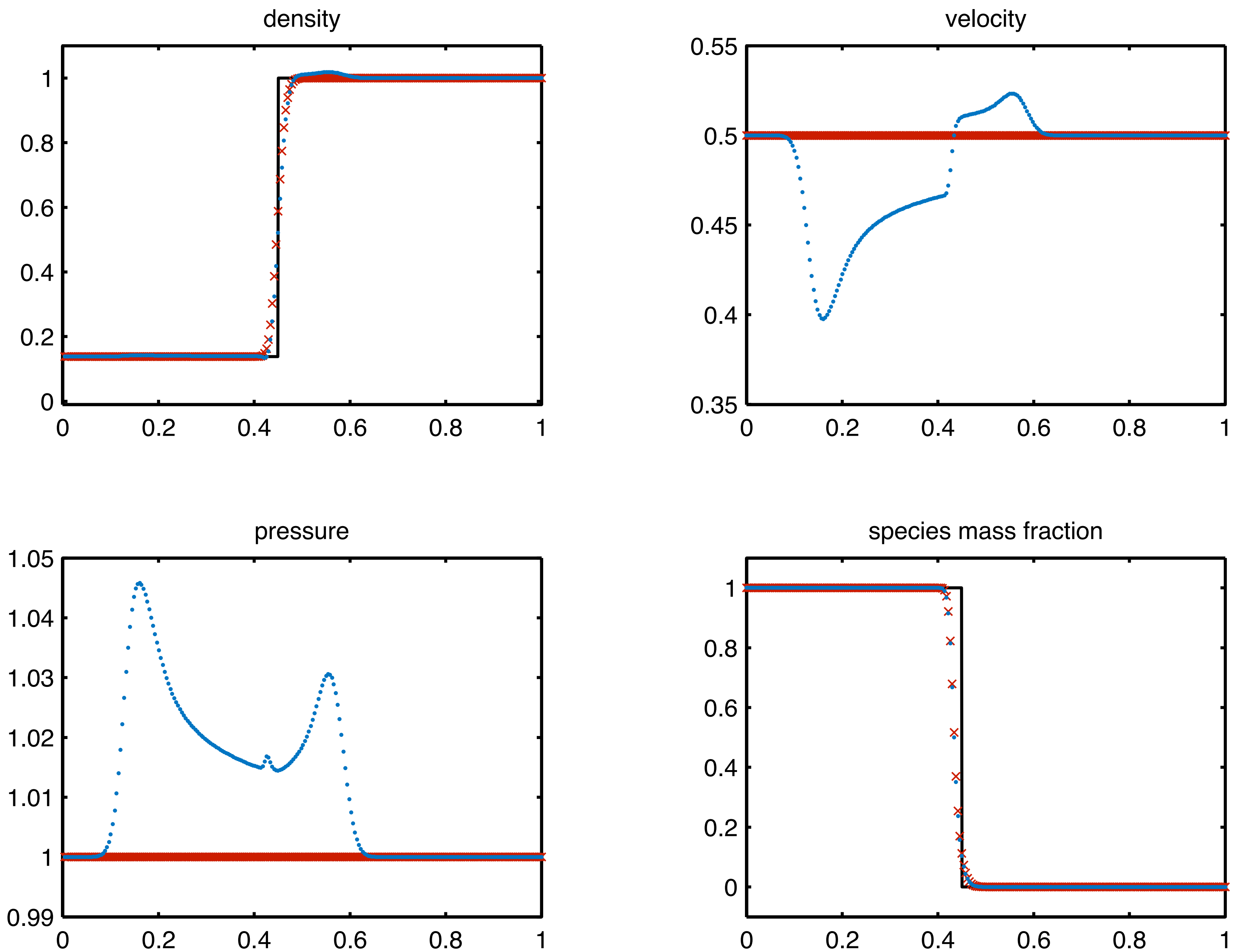
$$U_i^{*} = \tilde{U}_i^{*} + \Delta G_i^{*}\ , \qquad \text{where} \quad \Delta G_i^{*} = \left[0,\ 0,\ \Delta E_i^{*},\ 0, 0\right]^T$$

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)

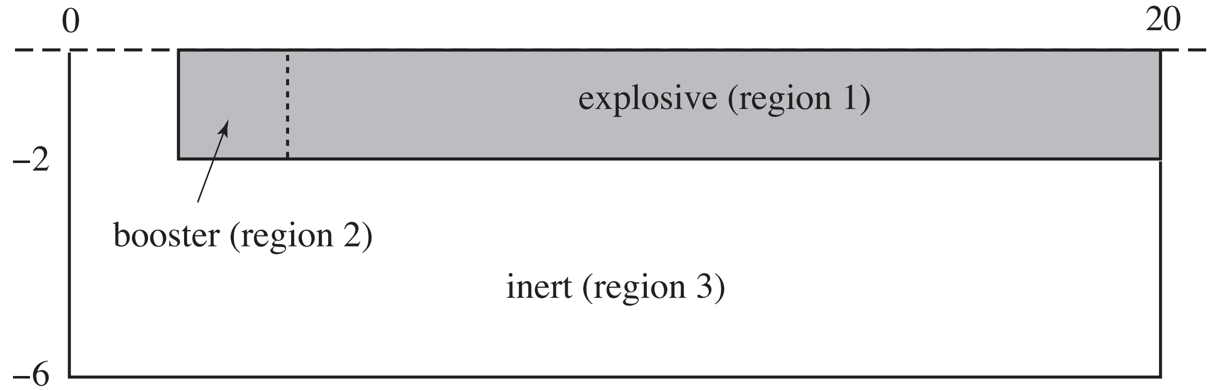
$(\rho_R, u_R, p_R, \mu_R) = (1.0, 0.5, 1.0, 0.0)$ for $x \geq 0.4$ at $t = 0$ (air on the right)



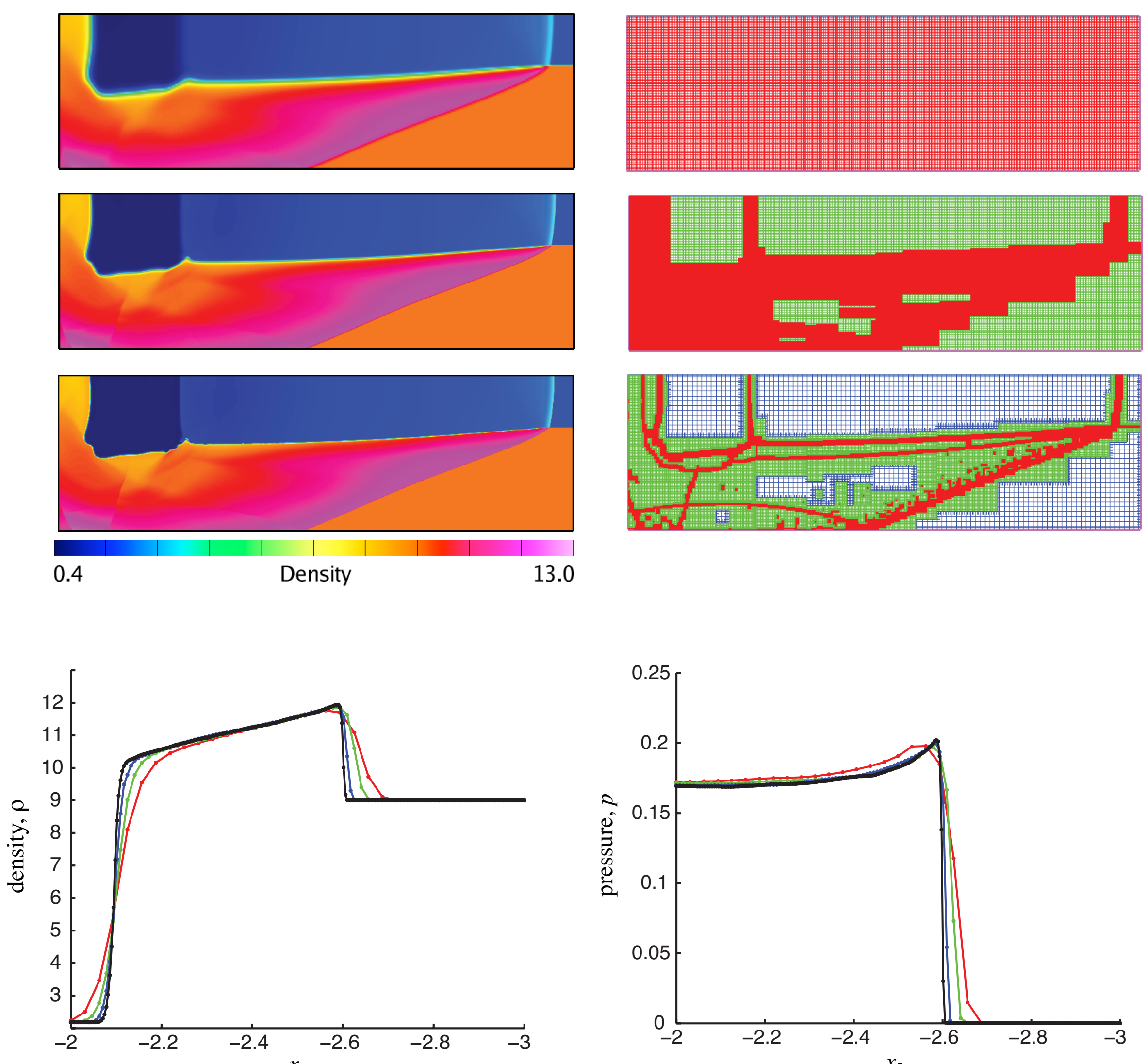
Solution at t=0.1: black = exact, blue = Godunov w/out correction, red = Godunov w/ correction

Simple reacting flow test case:

Simple rate stick with ideal gas EOS and pressure dependent rate law:

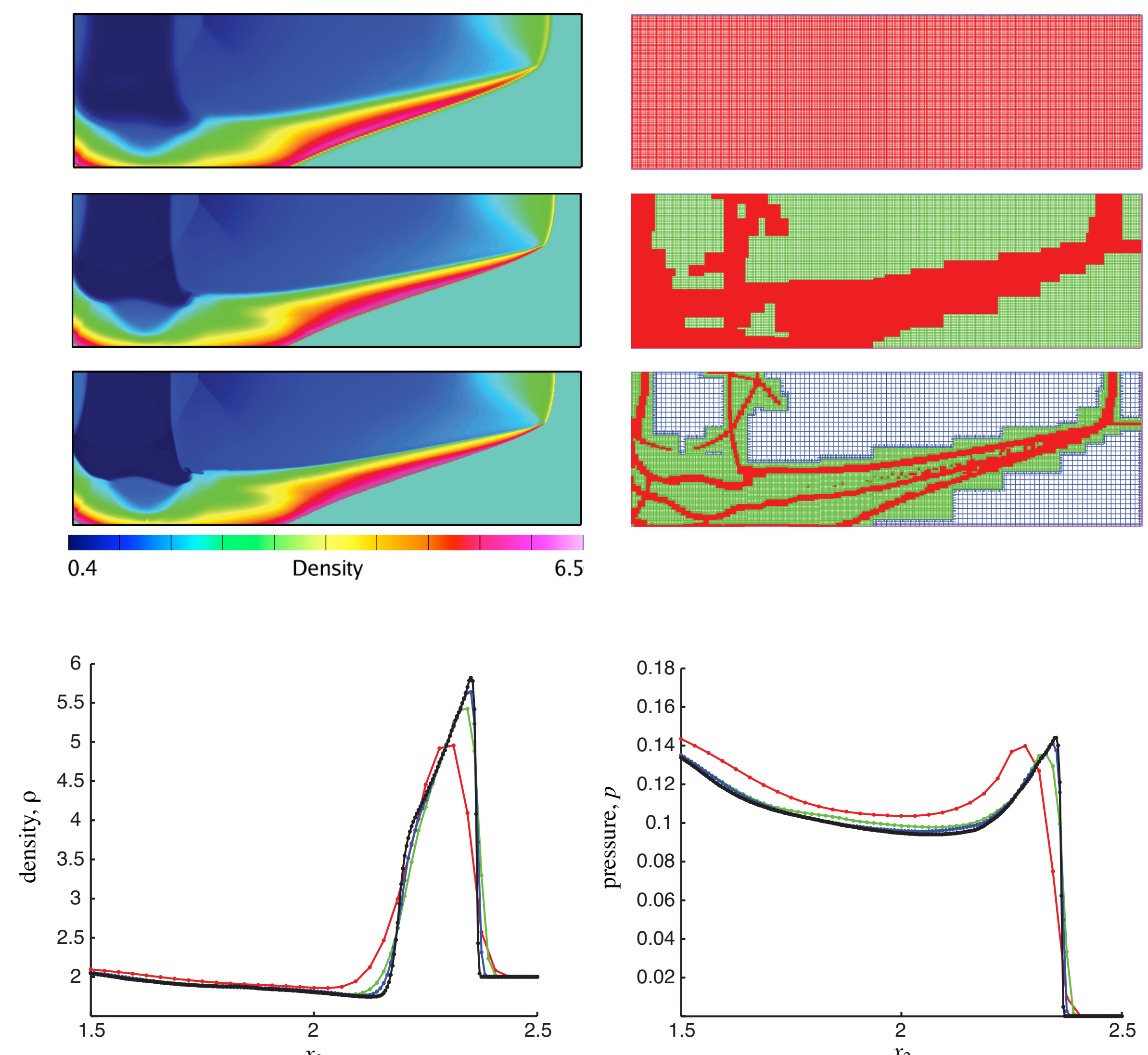


Strong Confinement



$x_2 = 18$

Weak Confinement

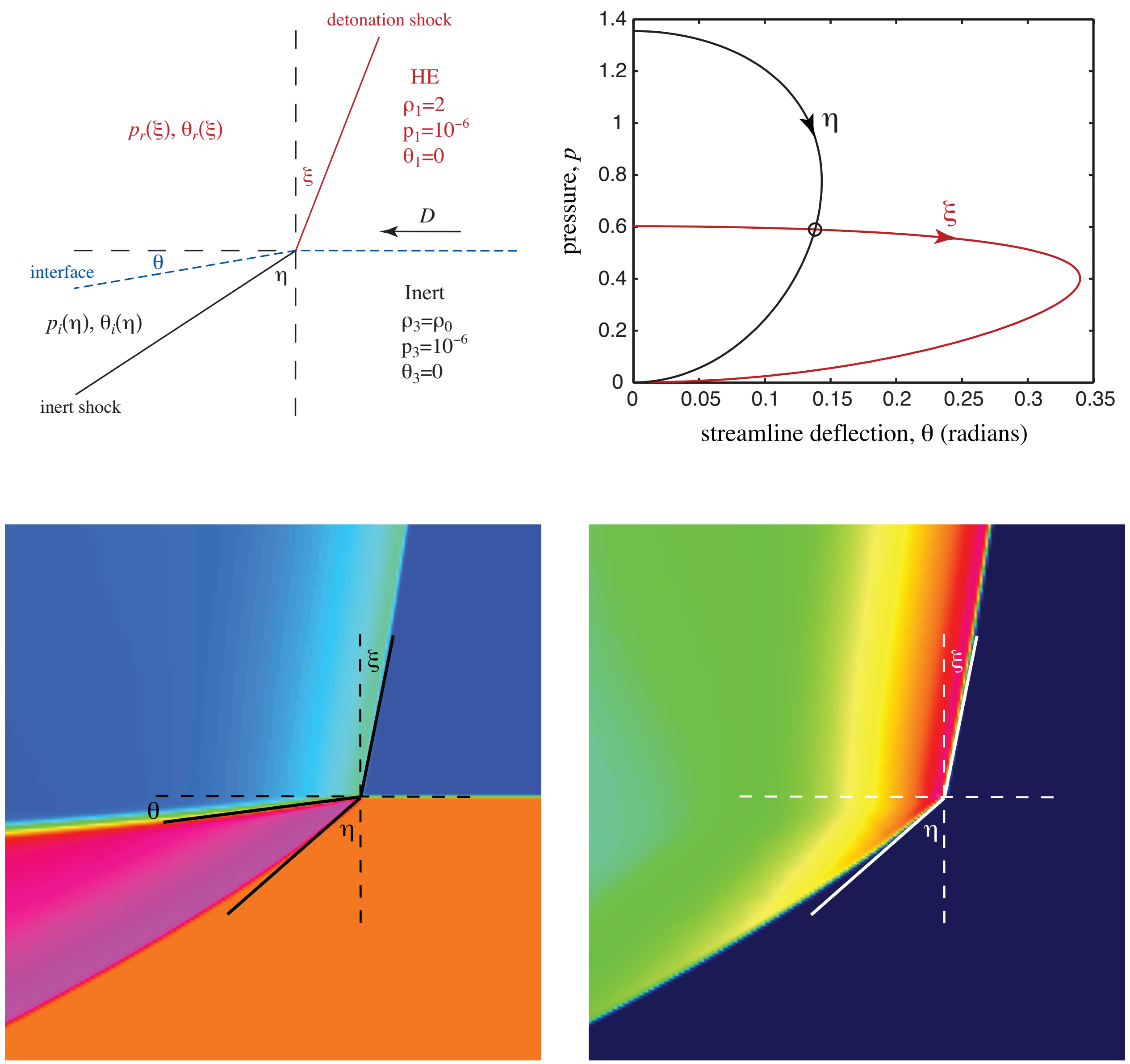


$x_2 = 18$

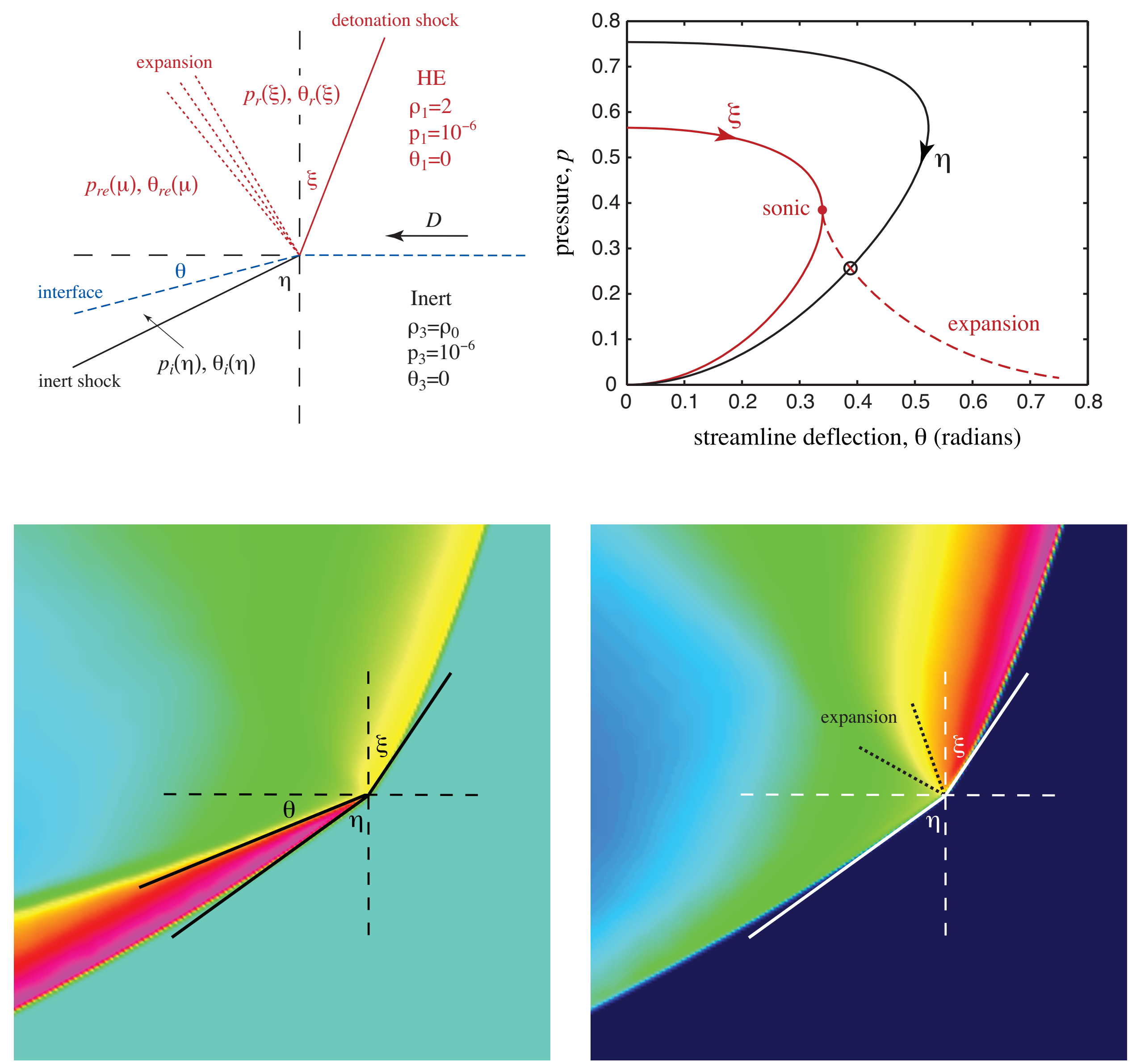
Simple reacting flow test case:

Shock polar analysis:

Strong Confinement



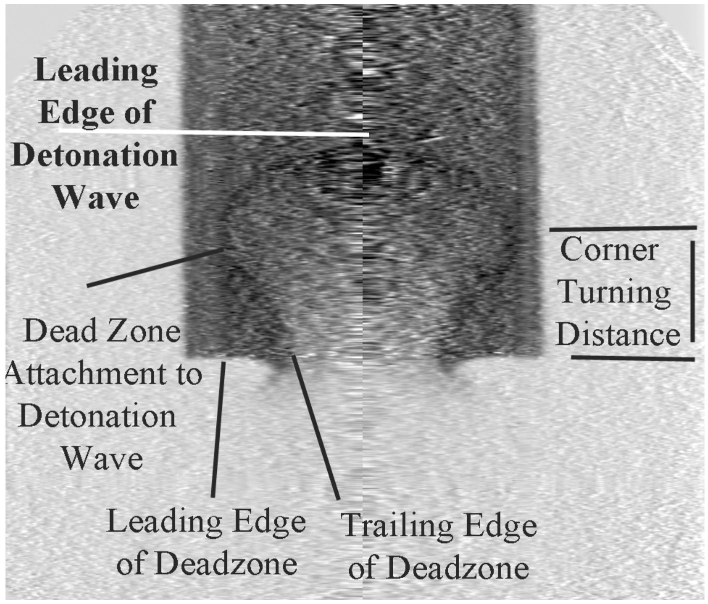
Weak Confinement



Detonation diffraction at a 90-degree corner:

Motivation: Corner-turning experiments...

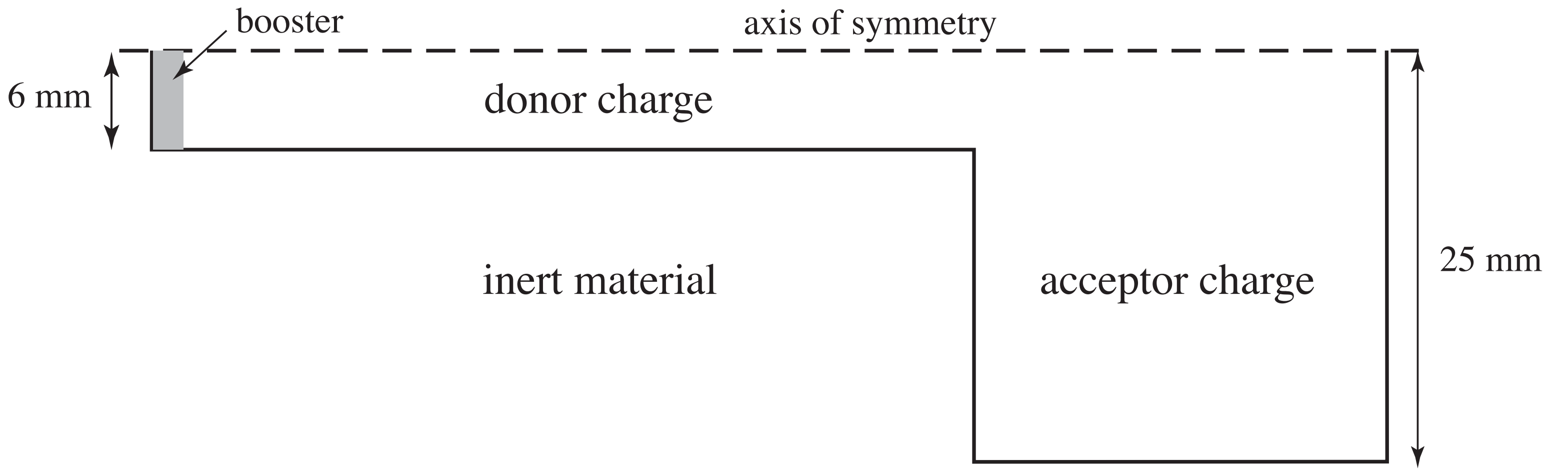
rate-stick charges.



Volume density image.

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

Model geometry...



Reaction/EOS

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

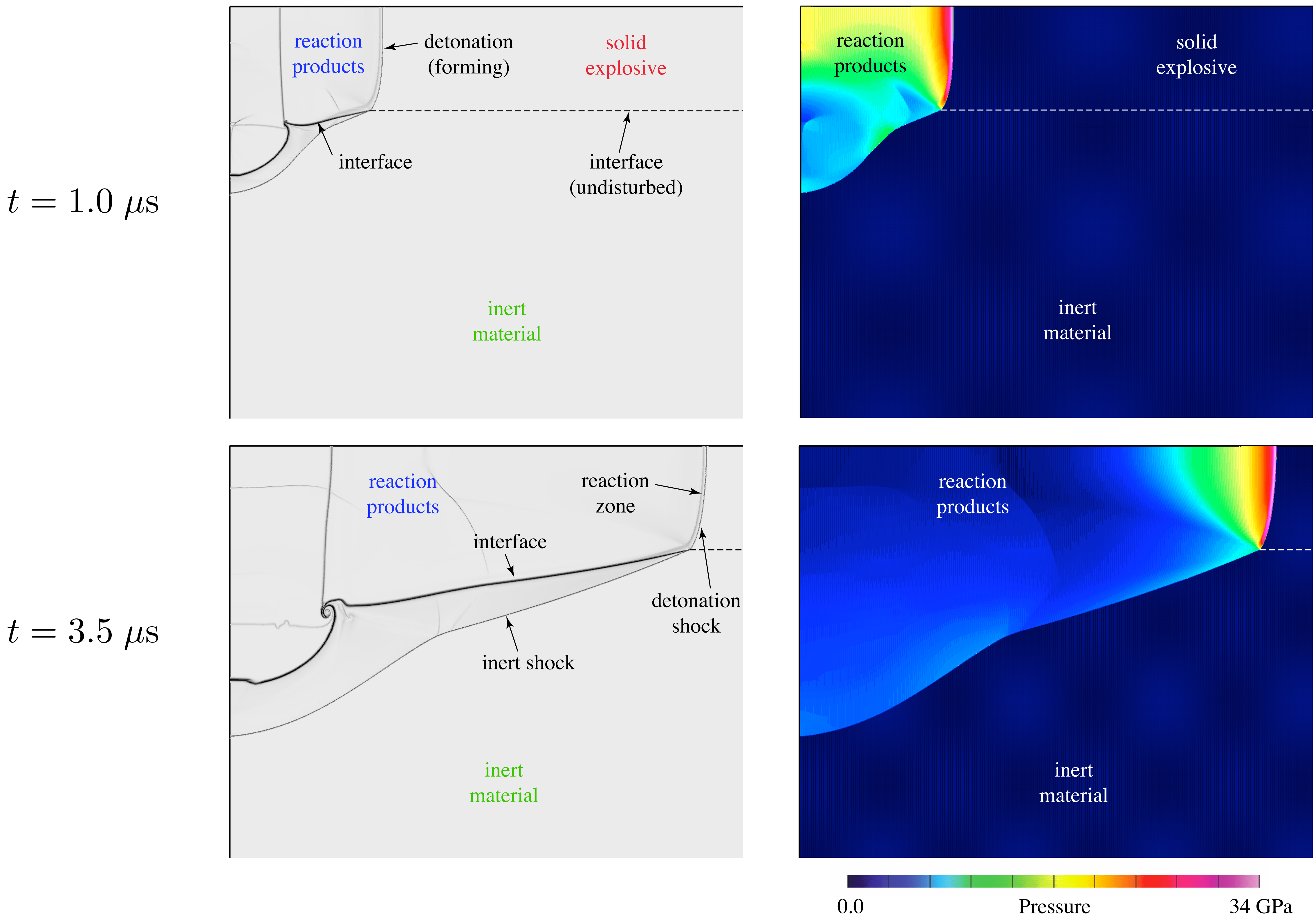
(Tarver & McGuire, 2002)

Base grid + AMR...

$$h_{\text{base}} = 0.1 \text{ mm} + 2 \text{ AMR grid levels} \quad \Rightarrow \quad h_{\text{eff}} = 0.00625 \text{ mm}$$

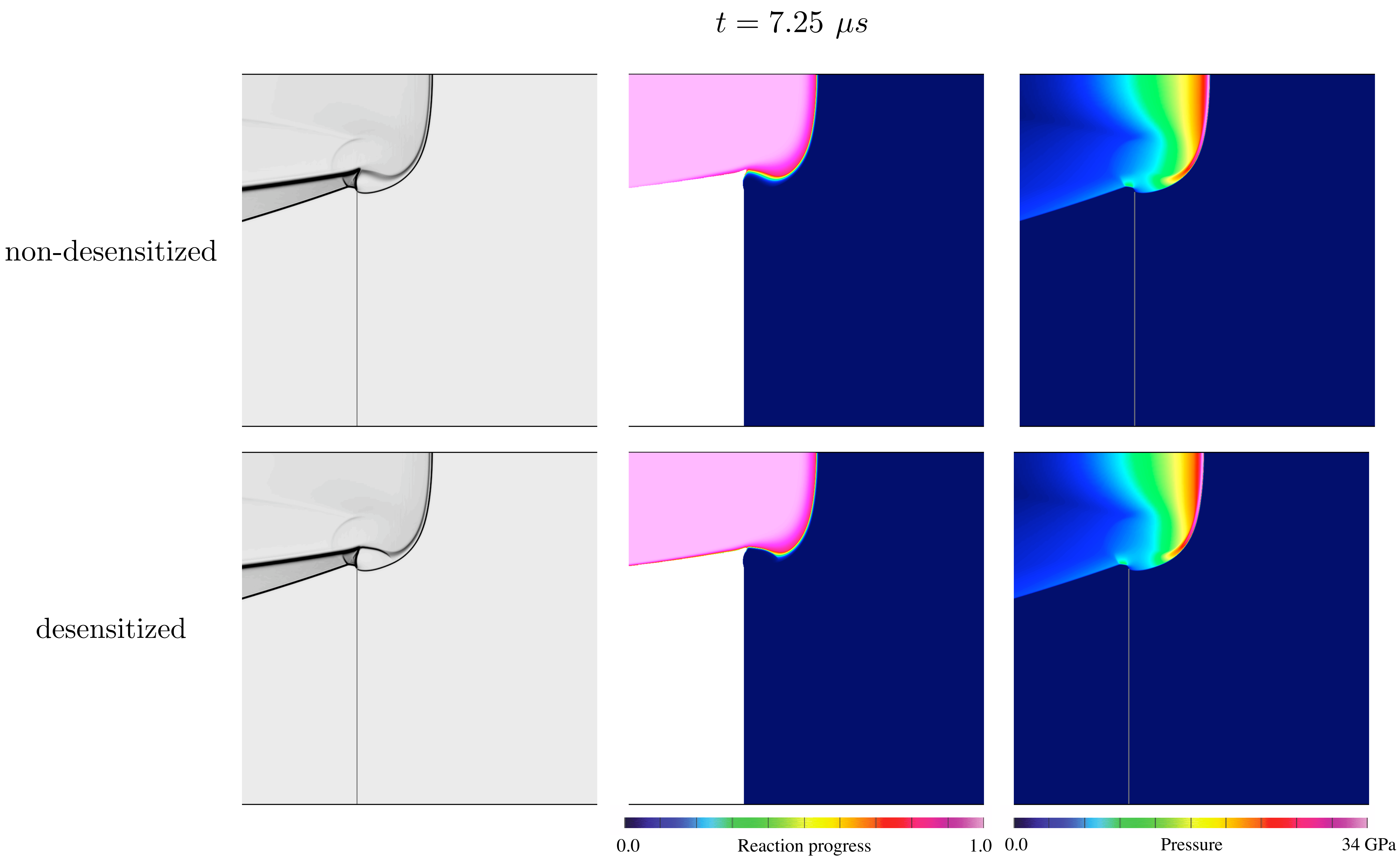
(approximately 75 grids cells across the reaction zone)

Stage 1: ignition and run to steady state in the donor charge...

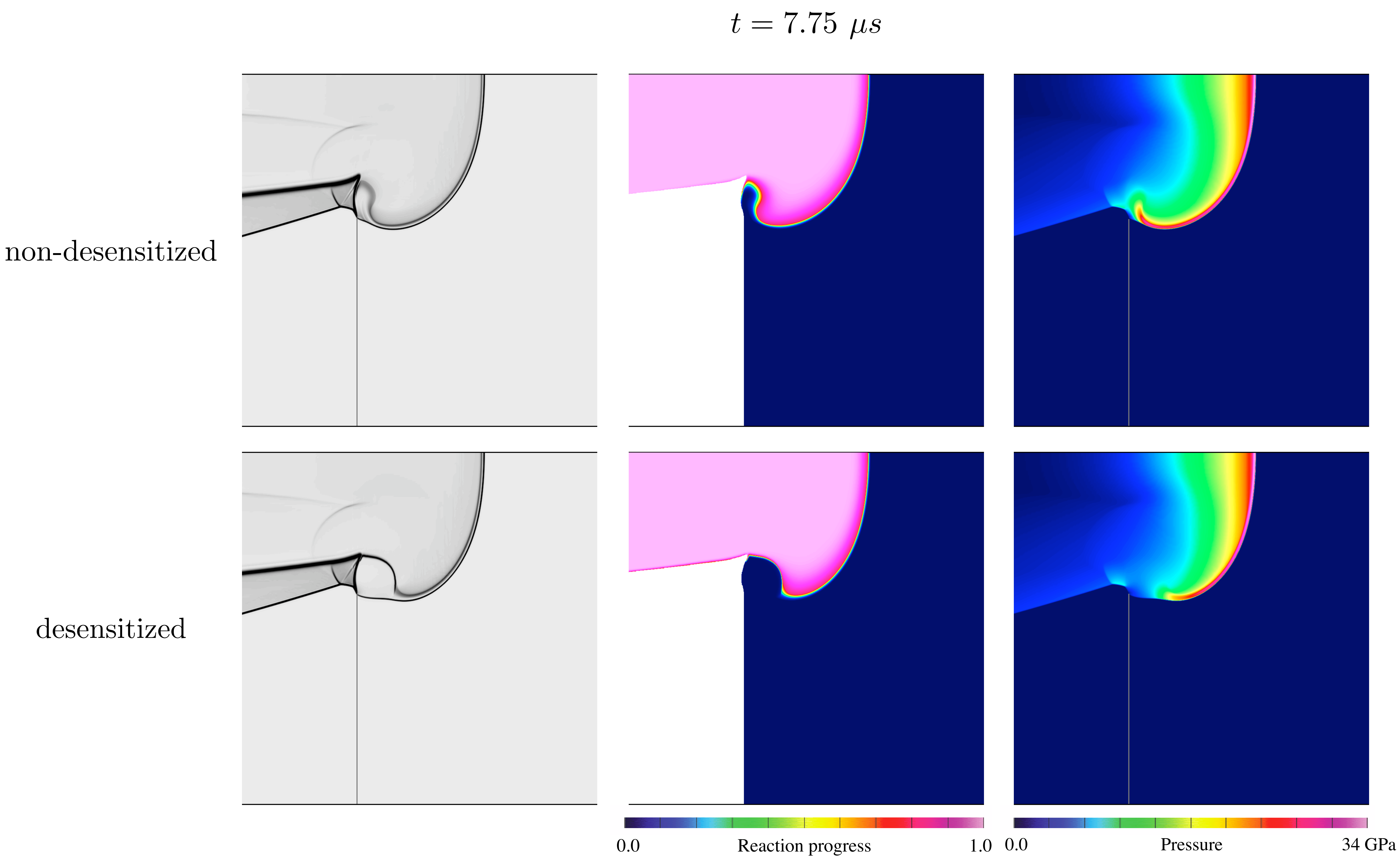


Detonation forms from the high-pressure "booster" state and runs to steady state in the donor charge.

Stage 2: detonation diffraction in the acceptor charge...



Stage 2: detonation diffraction in the acceptor charge...



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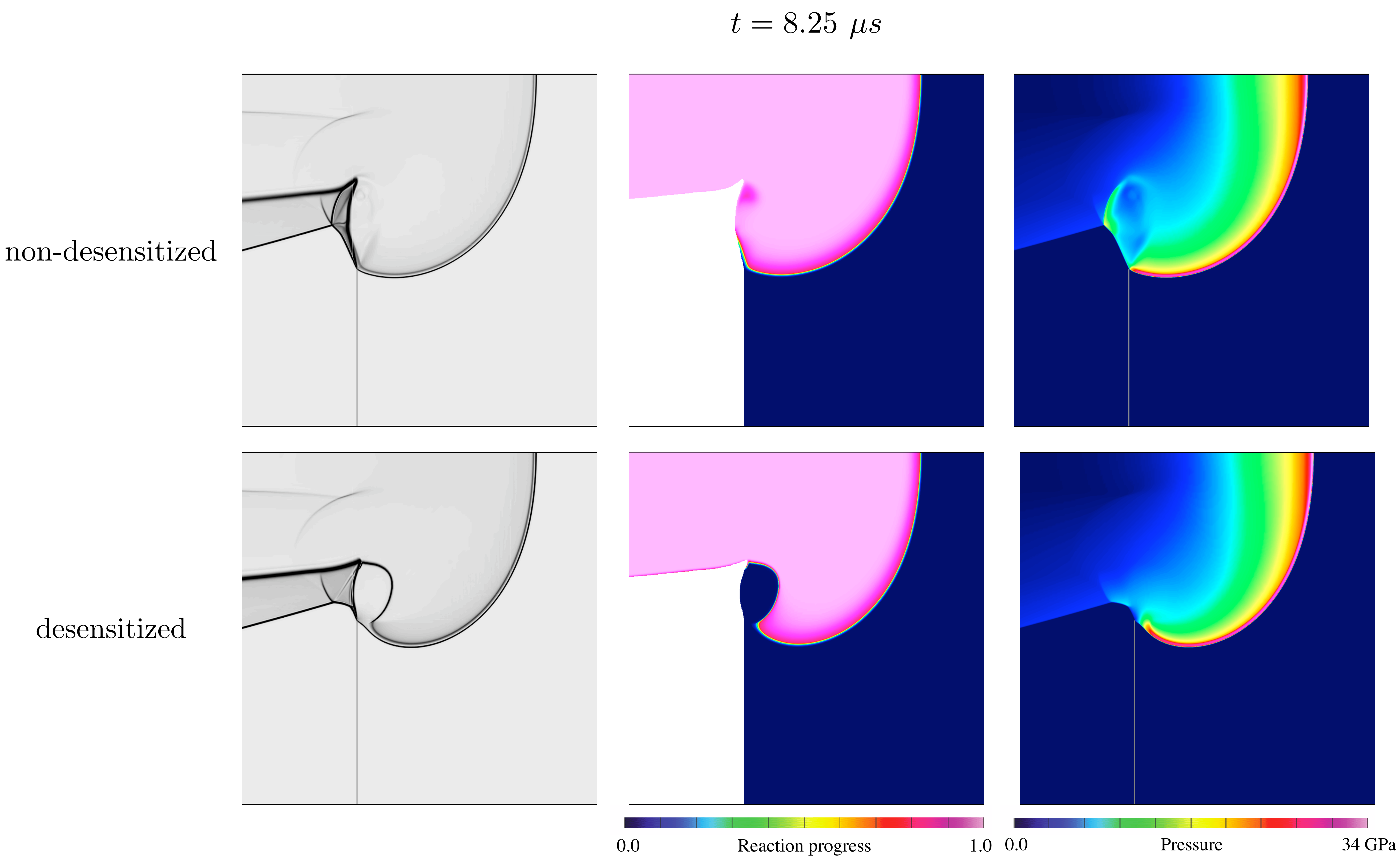
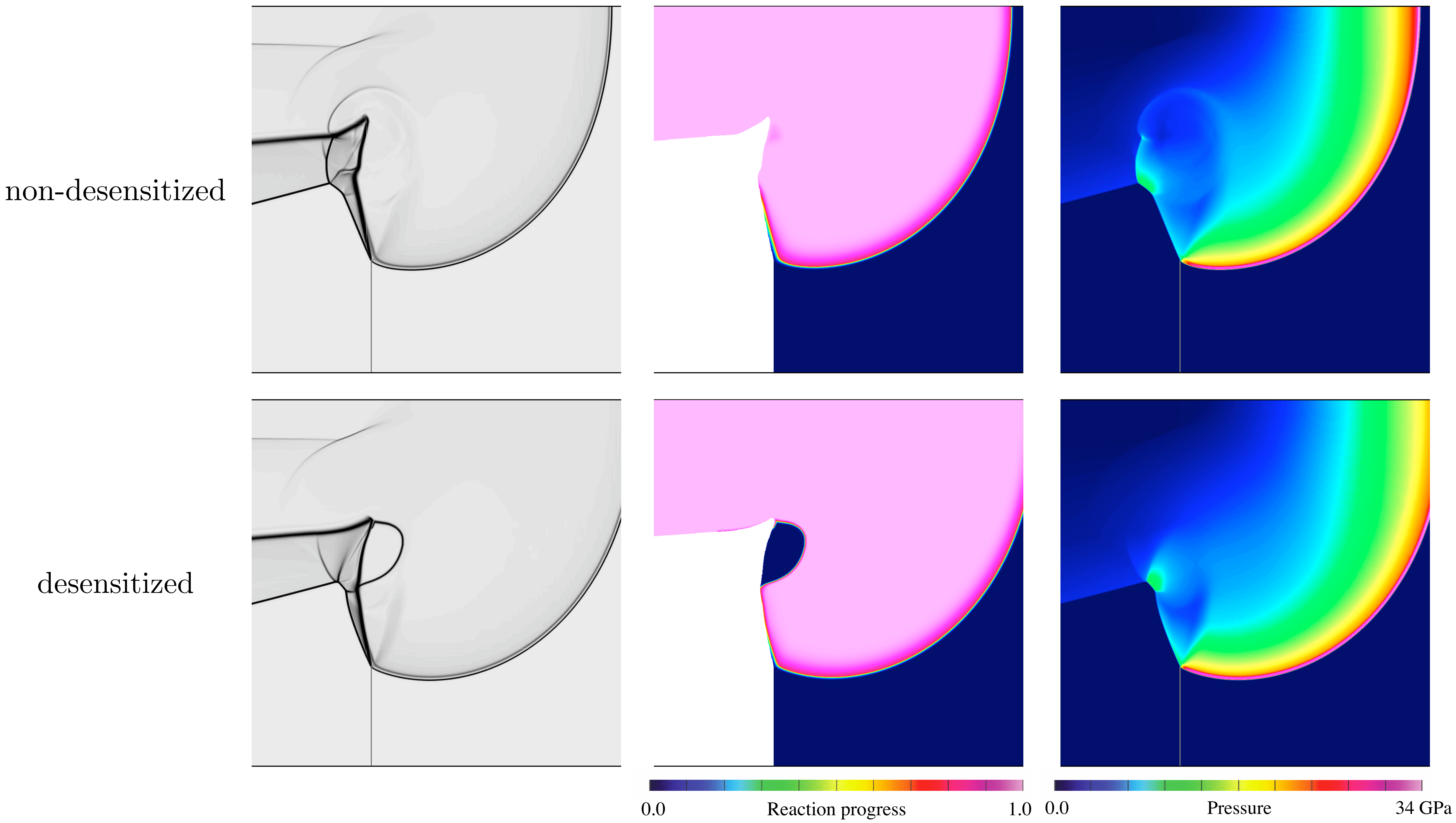


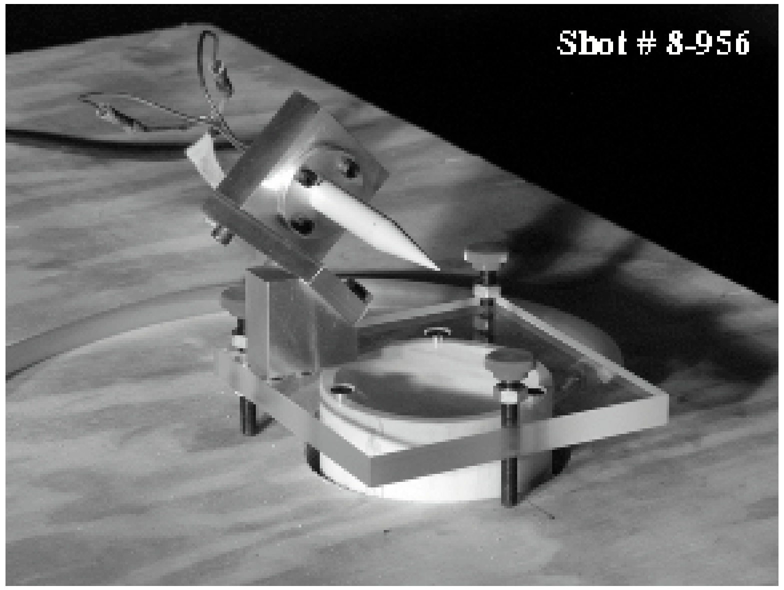
Stage 2: detonation diffraction in the acceptor charge...

$t = 8.75\ \mu s$



Detonation failure in converging geometry:

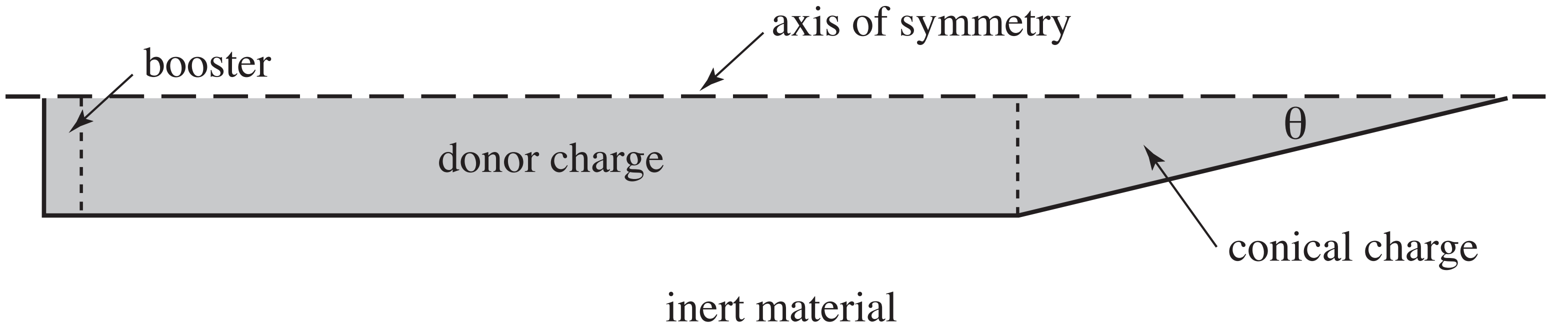
Motivation: "pencil" experiments...



experimental setup

T. R. Salyer and L. G. Hill
The Dynamics of Detonation Failure in Conical PBX 9502 Charges

Model geometry...



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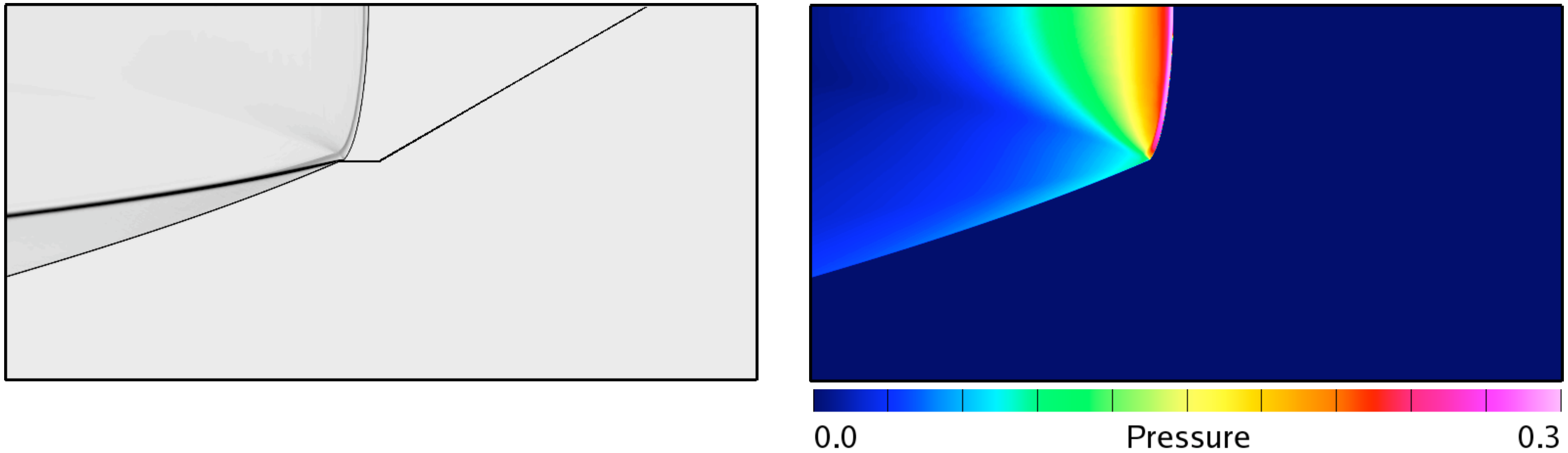
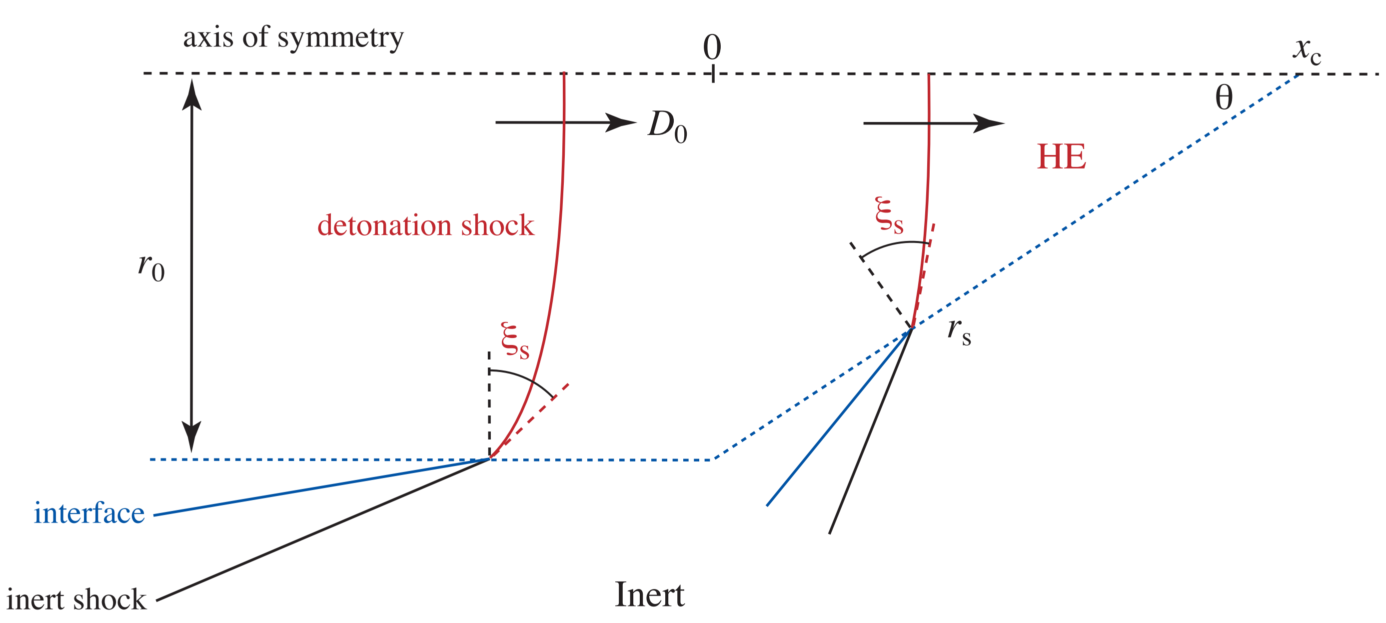
(approximately 75 grids cells across the reaction zone)

"Initial Conditions": quasi-steady state prior to cone ...

$$\theta = 30^\circ, \quad t = 0$$



Analysis of "subcritical" cones (a la Salyer and Hill)



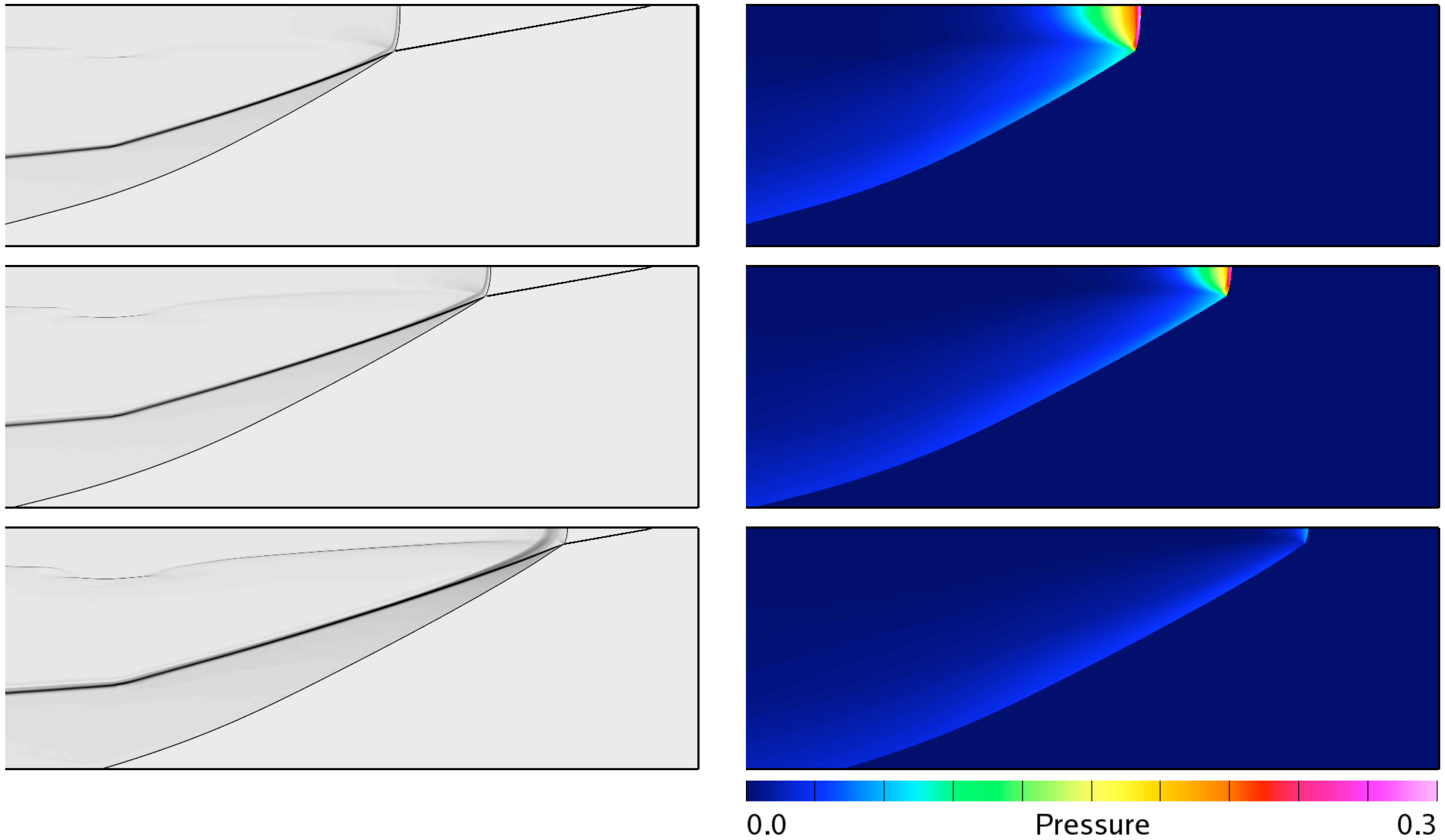
Detonation Dynamics: shallow cone angle ...

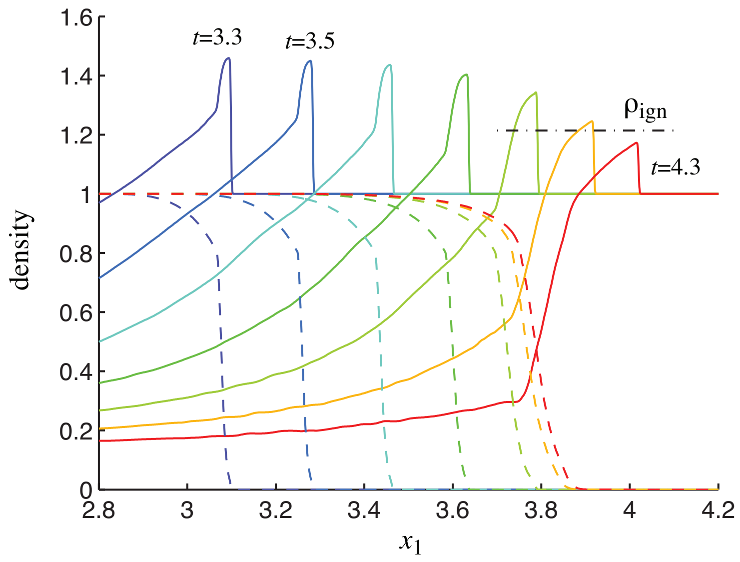
$\theta = 10^\circ$

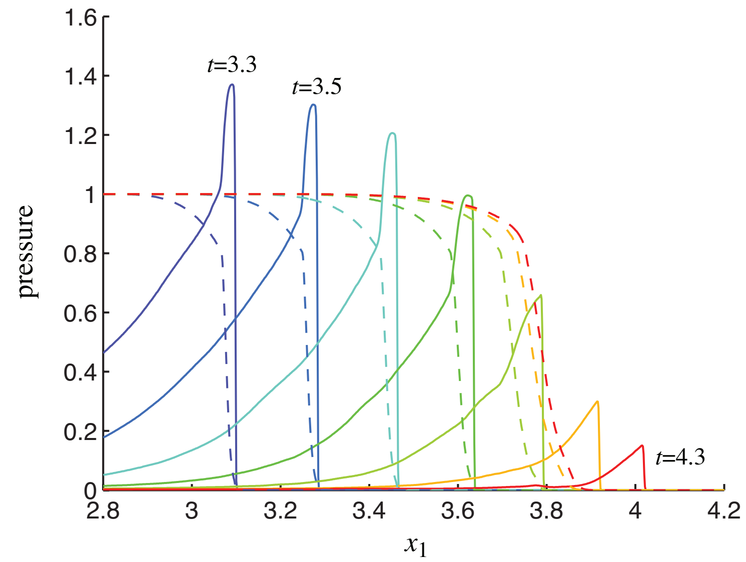
$t = 2.7$

$t = 3.5$

$t = 4.3$







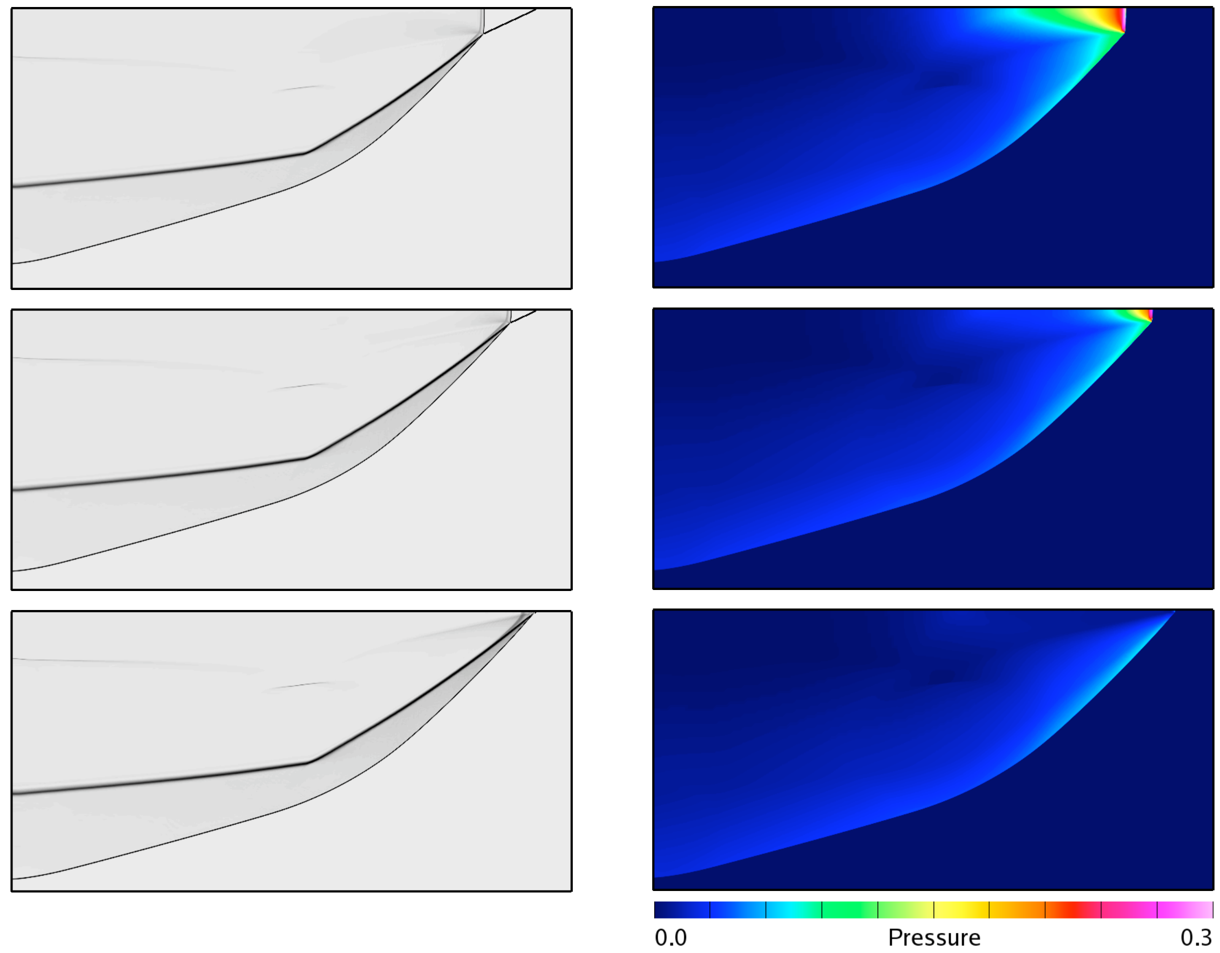
Detonation Dynamics: moderate cone angle ...

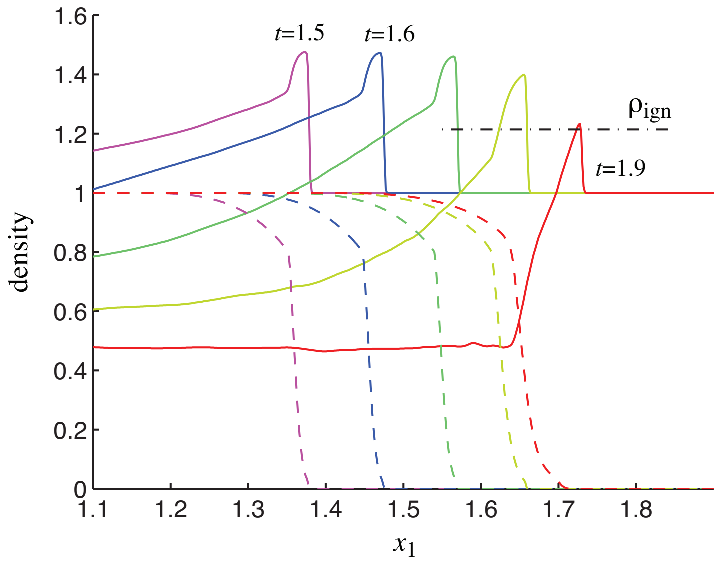
$$\theta = 25^\circ$$

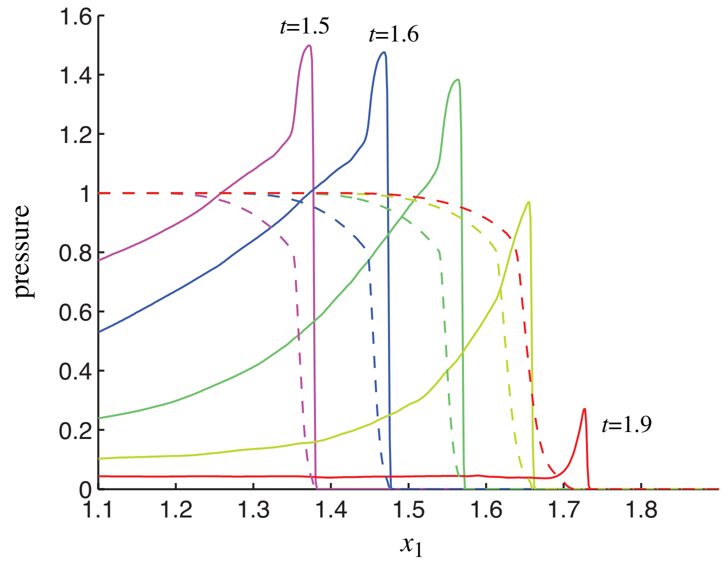
$t = 1.5$

$t = 1.7$

$t = 1.9$





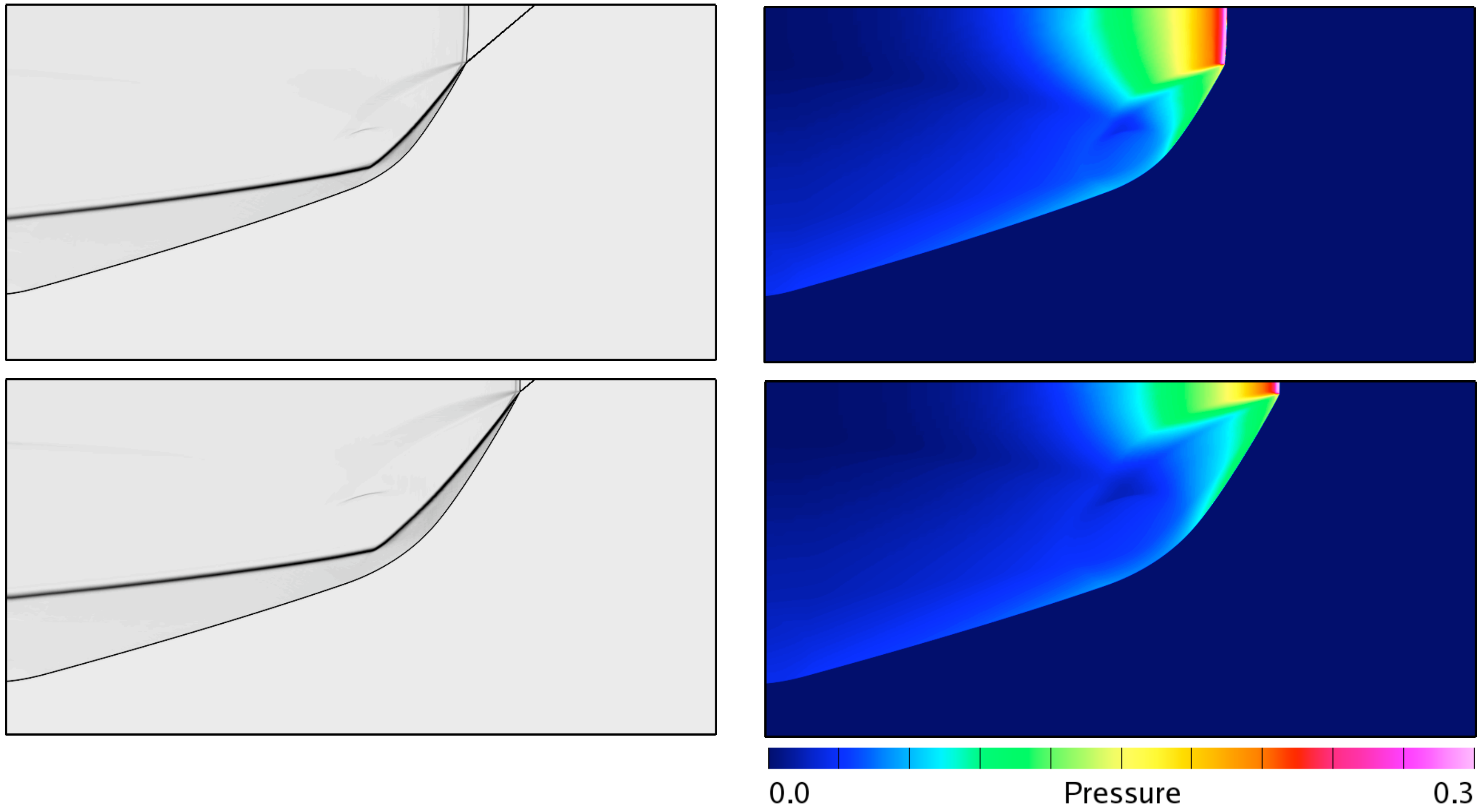


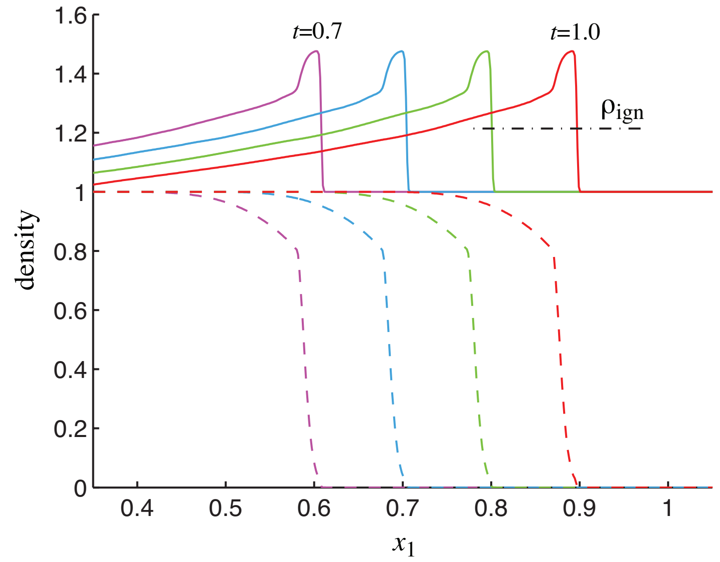
Detonation Dynamics: sharp cone angle ...

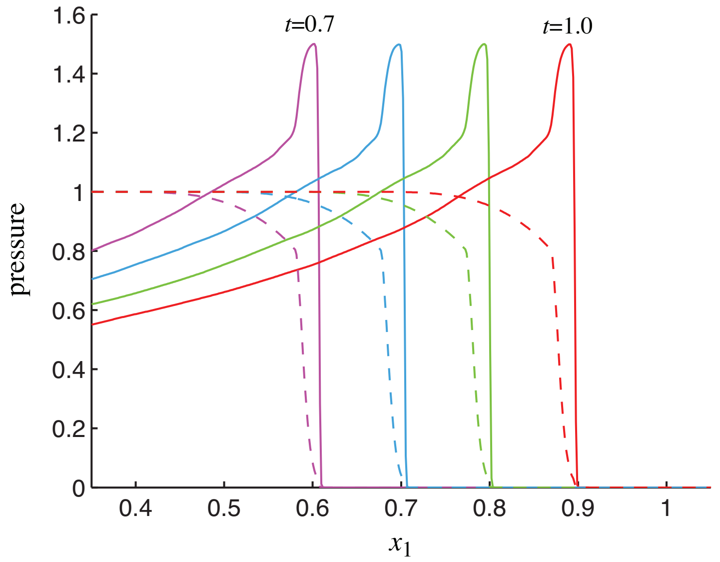
$$\theta = 40^\circ$$

$t = 0.7$

$t = 1.0$

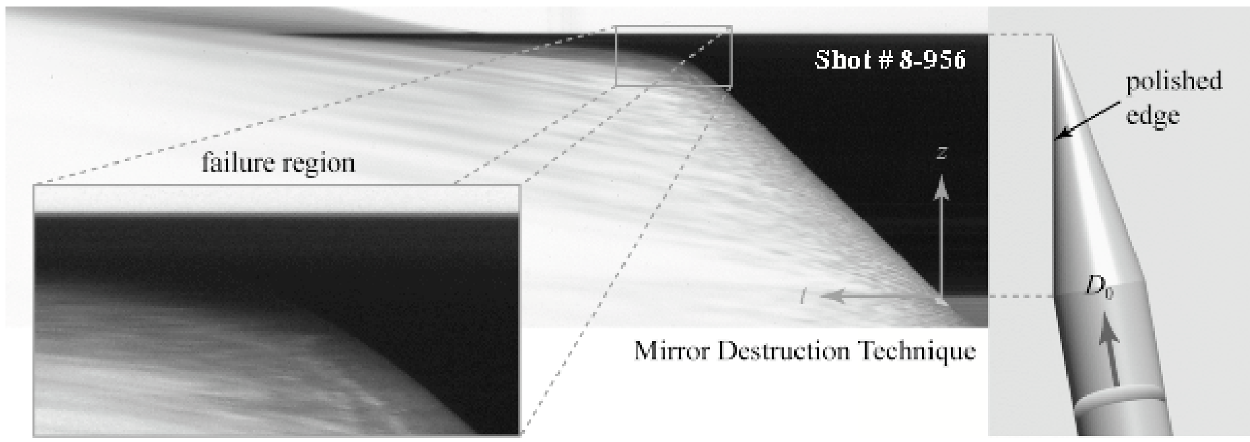


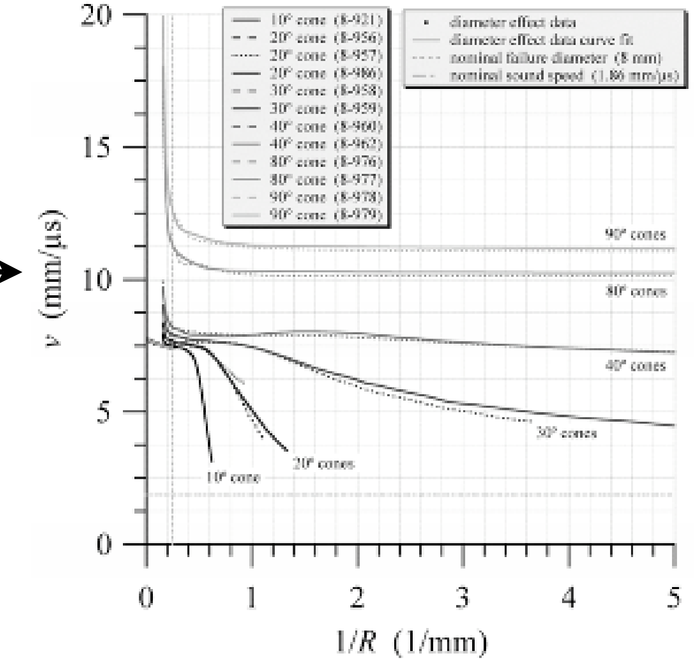




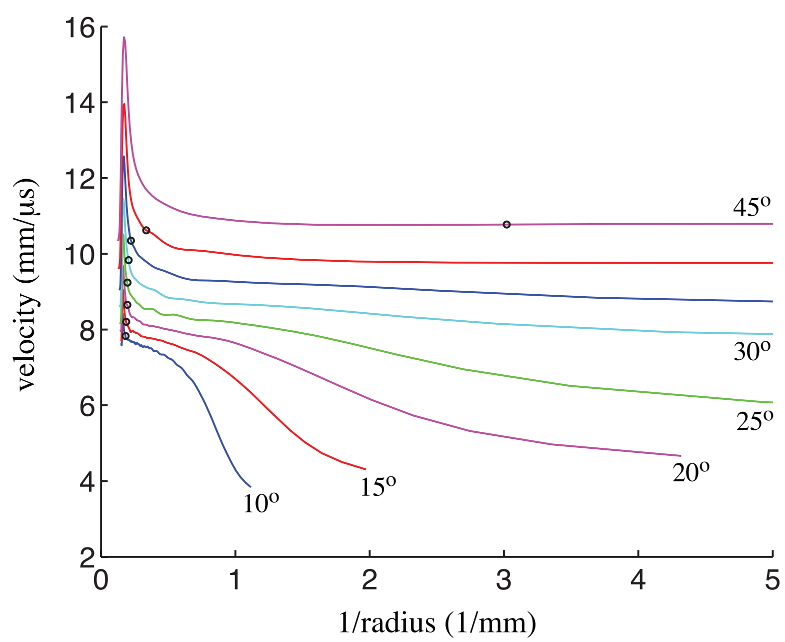
Detonation Dynamics: interface destruction ...

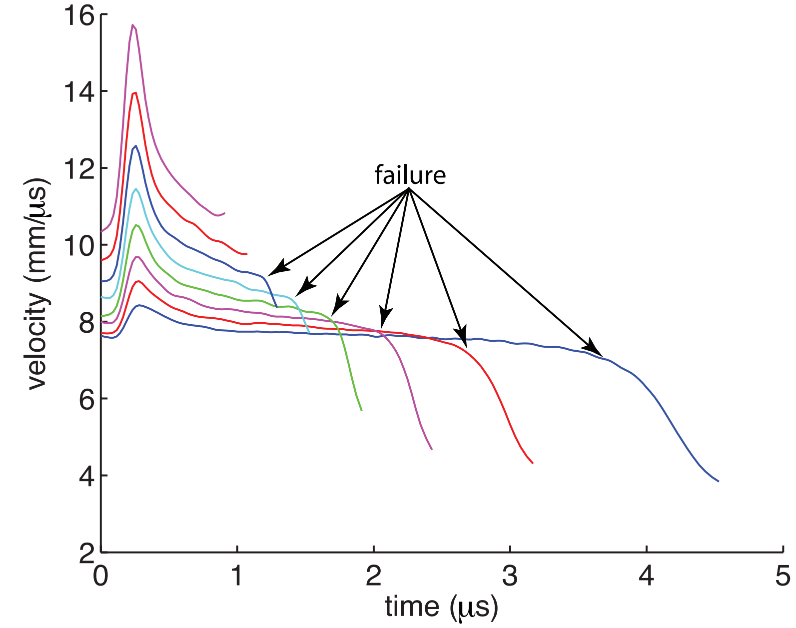
Results from Salyer and Hill





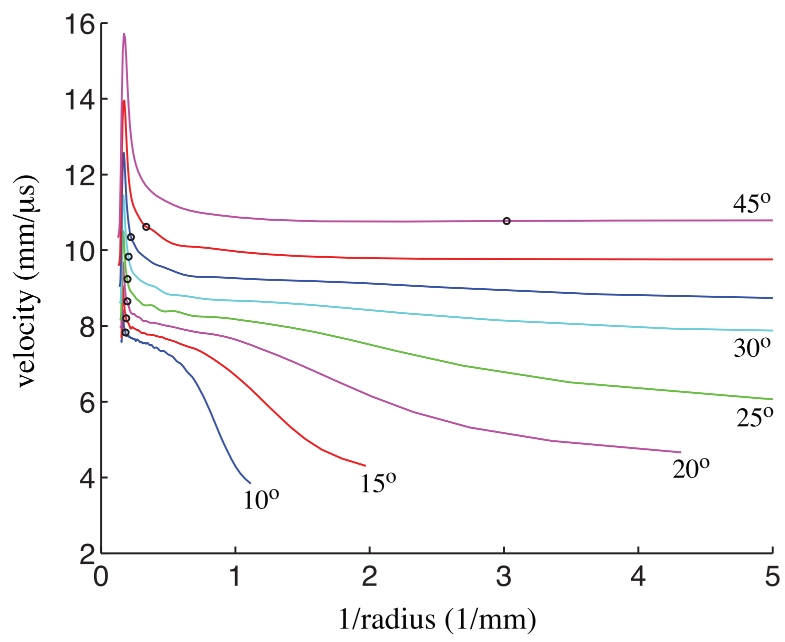
Simulation results

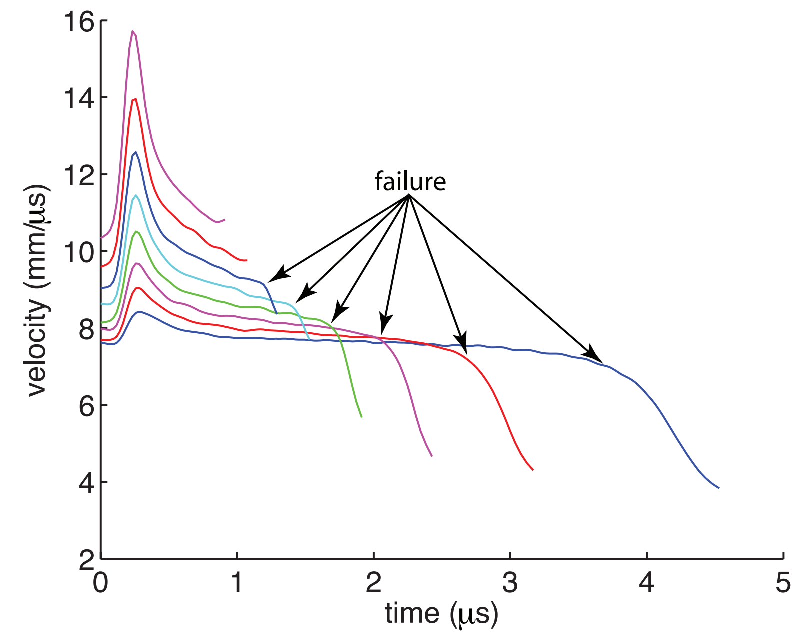




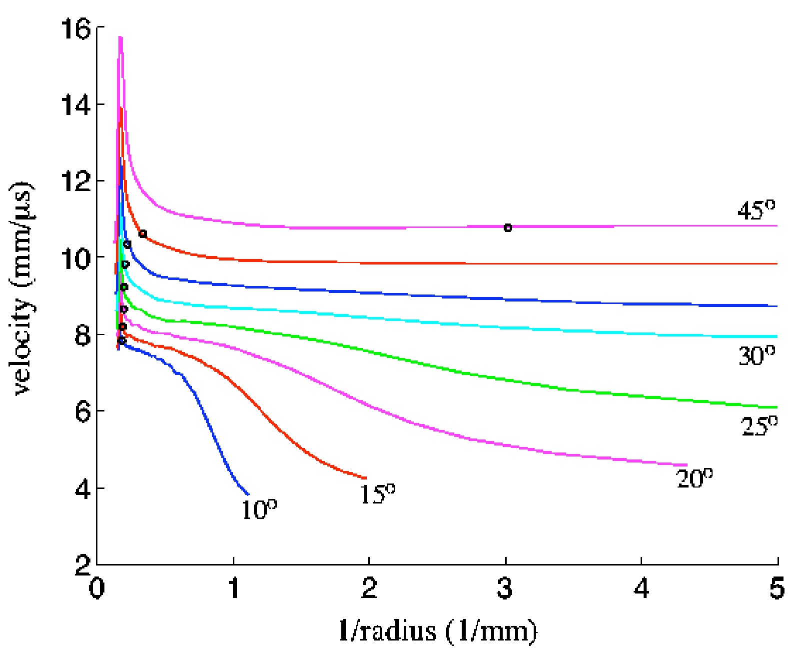
Detonation Dynamics: interface destruction ...

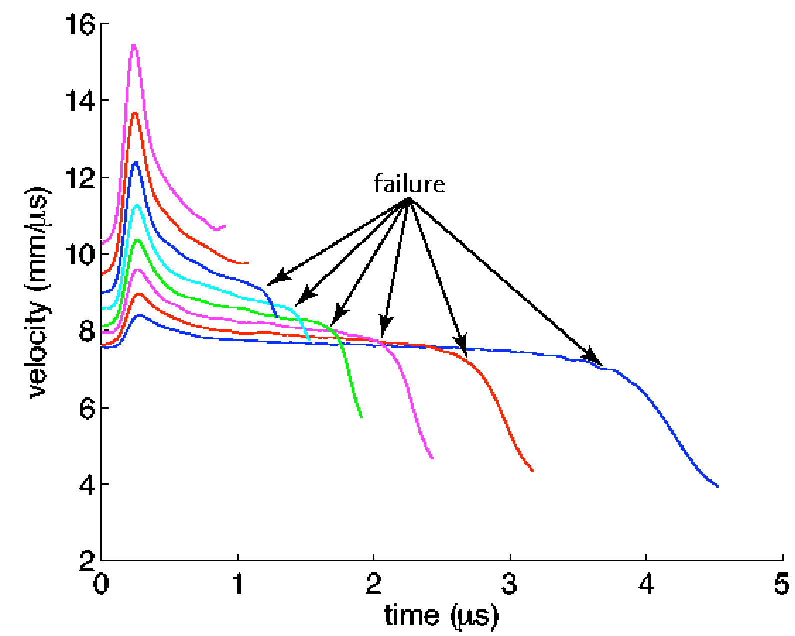
Results with no desensitization model





Results using desensitization model





Results are nearly identical for desensitized and non-desensitized models

Conclusions:

- An accurate and efficient numerical treatment of material interfaces for shock capturing schemes

- Overlapping grids used to capture complex geometry

- Validation on simple rate stick (shock polar analysis)

- Studies of detonation diffraction in shock desensitized high explosives

- Studies of detonation dynamics in converging rate sticks

Full details 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).

Thank you!!

Questions??