Development of an Eulerian Polydisperse Multiphase Flow Model

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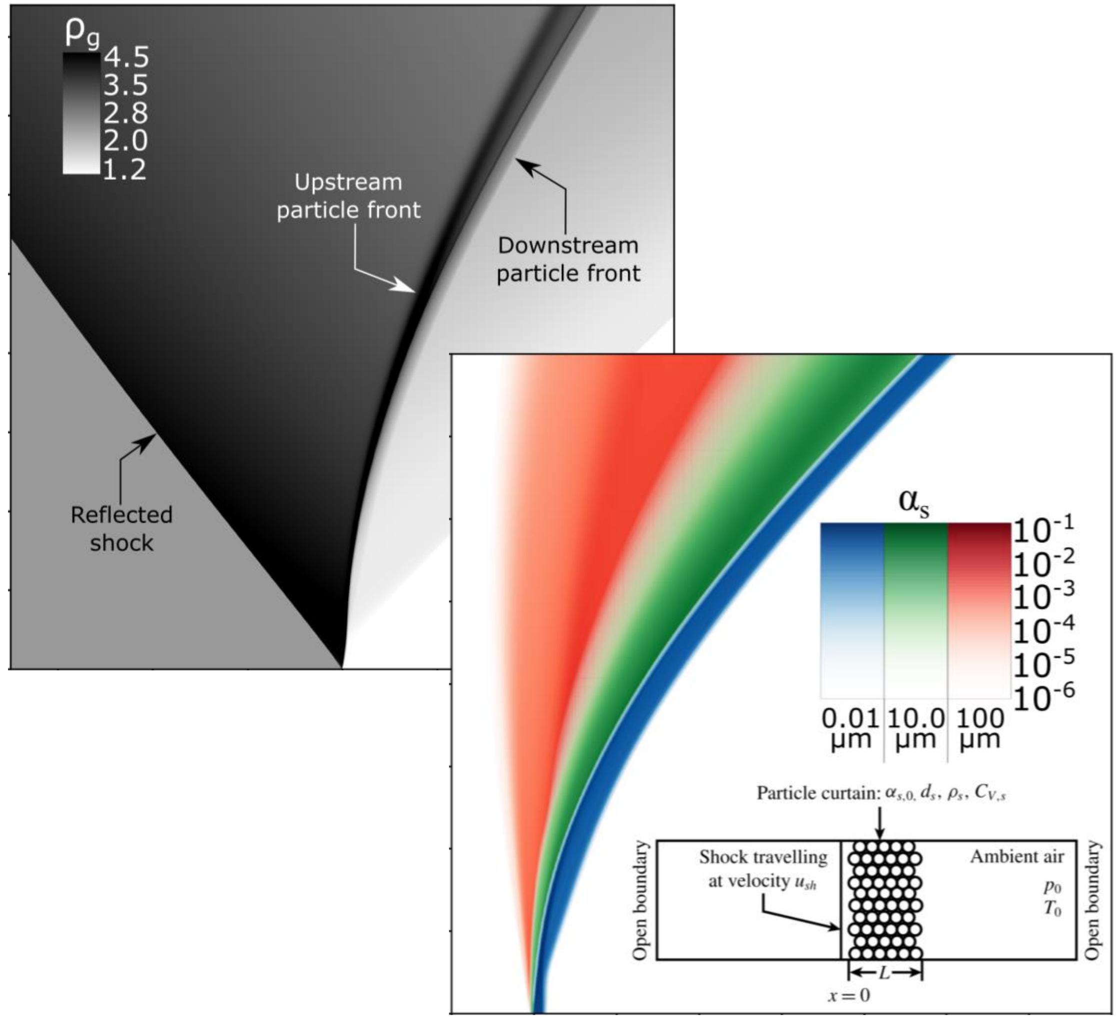

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Metal particles are used in explosive charges where the are dispersed, mix, and burn in the shock-heated air which enhances the blast.

- We model these systems numerically to avoid experimental complexities associated with measurement difficulty.
- Particle diameter can have great effect on the flow dynamics due to Stokes-number-dependent physics.

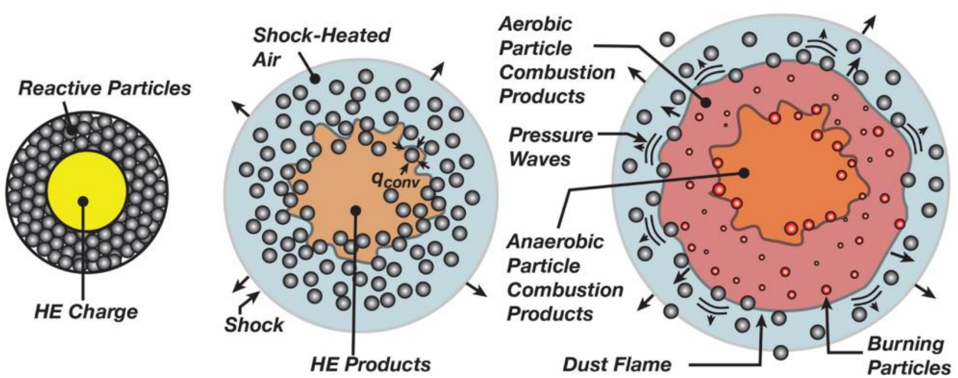
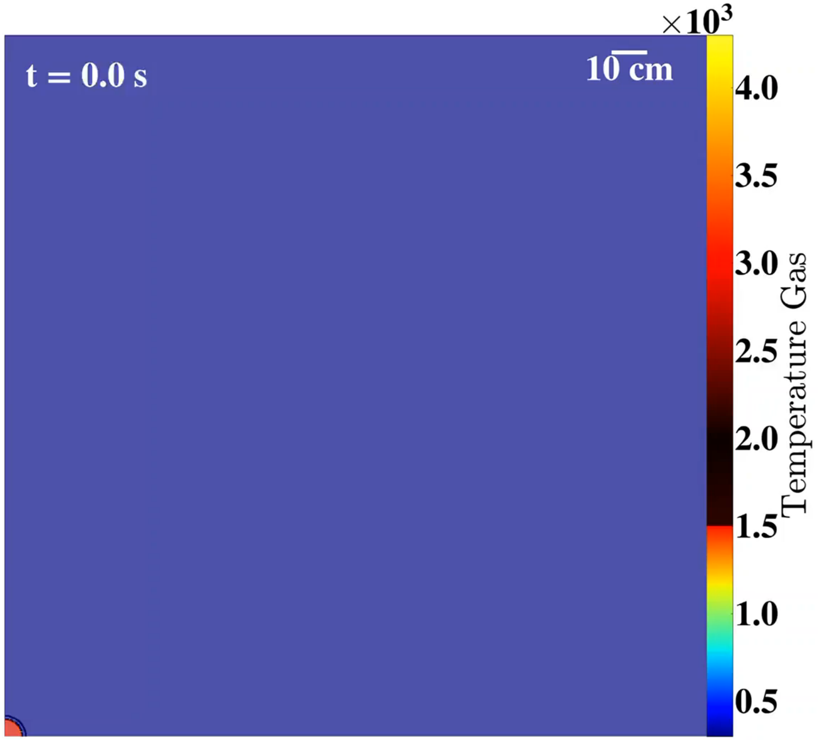


Diagram of afterburning process in metalized blast.

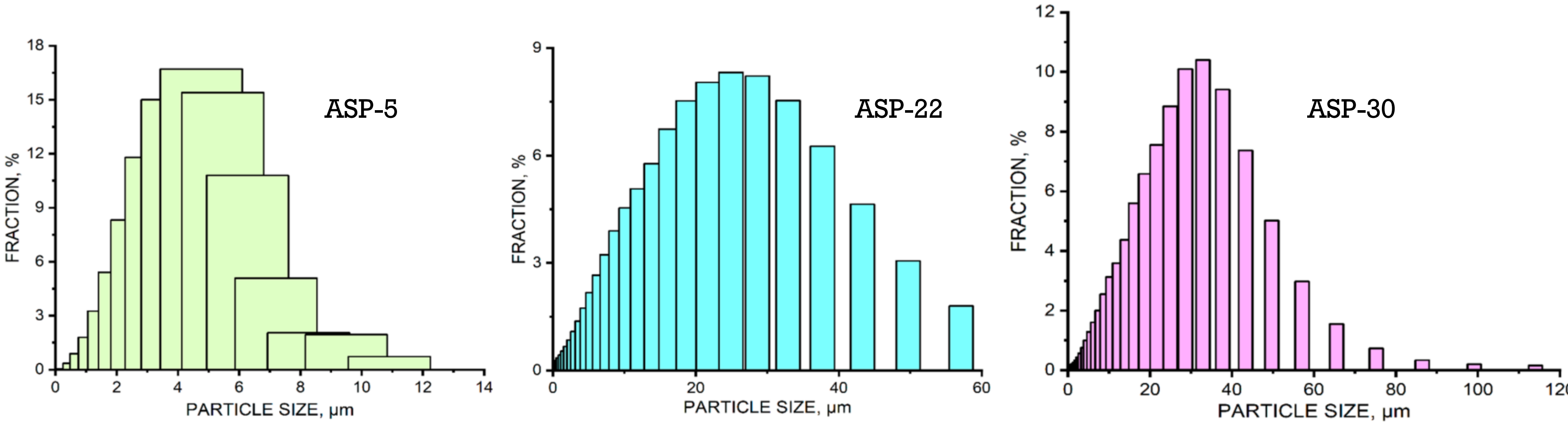


Prompt ignition of Al particles packed around a TNT charge.

Posey et al., Physics of Fluids, 2021

We want to model realistic polydisperse powders to better study the effects of particle size on blast dynamics.

- Commercial powders are not monodisperse.



Particle size distributions of commercial powders, modified from Shinkaryov et al. (2021).

We will account for new granular physical processes not yet considered for aluminized blasts in our previous work.

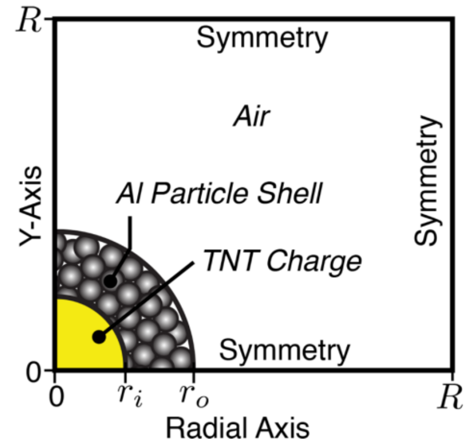
- **Forces arising from finite-size particles**
  - These terms arise from derivation from the Boltzmann equation for the fluid and particles (Fox 2019).
- **Long-range particle interaction**
  - Fluid-mediated particle interactions are important for dilute inhomogeneous flows.
- **Collisions using BGK closure**
  - This closure method assume that a collision source term relaxes particles to a Maxwellian distribution.

$$\boldsymbol{R} = \left(\Theta_p + \tfrac{1}{5}\left\|\boldsymbol{u}_{pf}\right\|^2\right)\boldsymbol{I} + \tfrac{2}{5}\boldsymbol{u}_{pf} \otimes \boldsymbol{u}_{pf} \qquad \boldsymbol{F}_{pf} = \boldsymbol{R} \cdot \nabla\rho_f + \frac{2}{3}\rho_f\left(\nabla \cdot \boldsymbol{u}_f\right)\boldsymbol{u}_{pf}$$

$$\boldsymbol{P}_{pfp} = \rho_f \alpha_p \left(B_1\left(\alpha_p, Re_p\right)\left\|\boldsymbol{u}_{pf}\right\|^2 \boldsymbol{I} - B_2\left(\alpha_p, Re_p\right)\boldsymbol{u}_{pf} \otimes \boldsymbol{u}_{pf}\right)$$

$$C = \left(\alpha_p \rho_p G - M\right)$$

The gas-phase equations describe conservation of mass, energy and momentum with coupling terms to the particles



- Mass:

$$\frac{\partial \alpha_f \rho_f}{\partial t} + \nabla \cdot \left(\alpha_f \rho_f \boldsymbol{u}_f\right) = 0$$

- Momentum:

$$\frac{\partial \alpha_f \rho_f \boldsymbol{u}_f}{\partial t} + \nabla \cdot \left(\alpha_f \rho_f \boldsymbol{u}_f \otimes \boldsymbol{u}_f + p_f \boldsymbol{I} + \boxed{\rho_f \alpha_p \boldsymbol{R}}\right) = \boldsymbol{D} + \alpha_p\left(\nabla p_f + \boxed{\boldsymbol{F}_{pf}}\right) + \boxed{\nabla \cdot \boldsymbol{P}_{pfp}}$$

- Total Energy:

$$\frac{\partial \alpha_f \rho_f E_f}{\partial t} + \nabla \cdot \left(\alpha_f \rho_f \boldsymbol{u}_f E_f + \alpha_f \boldsymbol{u}_f p_f + \alpha_p \boldsymbol{u}_p p_f + \boxed{\rho_f \alpha_p \boldsymbol{u}_p \cdot \boldsymbol{R}}\right) =$$
$$D_E + \alpha_p \boldsymbol{u}_{\boldsymbol{p}} \cdot \left(\nabla p_f + \boxed{\boldsymbol{F}_{pf}}\right) + \boxed{\boldsymbol{u}_{\boldsymbol{p}} \cdot \left(\nabla \cdot \boldsymbol{P}_{pfp}\right)} + H_{pf}$$

- Ideal gas equation of state used to find gas pressure.

We employ a quadrature-based moment method approach from kinetic theory to model a polydisperse powder.

- The particles obey a population balance equation (generalization of the Boltzmann equation):

$$\frac{\partial n}{\partial t} + \underbrace{\boxed{\nabla \cdot \left(\boldsymbol{u} n - p_p \frac{\partial n}{\partial \boldsymbol{u}} \right)}}_{\text{Real Space Flux}} + \overbrace{\boxed{\frac{\partial}{\partial \boldsymbol{u}} \cdot (\boldsymbol{A} n)}}^{\text{Velocity Space Flux}} + \underbrace{\boxed{\frac{\partial}{\partial e} (A_e n)}}_{\text{Phase Space Flux}} = C$$

- More internal coordinates (such as particles species mass fractions and particle electric charge) can be added to this equation to model more complex physical phenomena.

Taking statistical moments of the mesoscale model can be used to model macroscopic values.

- Mass-velocity moments are computed from the population balance equation to find transport equations for particle mass, momentum, and kinetic energy.

$$\alpha_p \rho_p = \int mn(t, \boldsymbol{x}, m) dm \qquad \alpha_p \rho_p \boldsymbol{u}_p = \iint \boldsymbol{u} mn(t, \boldsymbol{x}, m, \boldsymbol{u}) dm d\boldsymbol{u}$$

$$\alpha_p \rho_p K_p = \frac{1}{2} \iint \|\boldsymbol{u}\|^2 mn(t, \boldsymbol{x}, m, \boldsymbol{u}) dm d\boldsymbol{u}$$

- Mass-internal-energy moments are computed from the population balance equation to find transport equations for particle internal energy.

$$\alpha_p \rho_p e_p = \iint emn(t, \boldsymbol{x}, m, e) dm de$$

Size moments are used to track particle mass.

- Size moments are defined by:

$$\mathcal{M}_{r/3} = \int m^{r/3} n(t, \boldsymbol{x}, m) dm$$

- Size moments used rather than mass moments to avoid numerical roundoff error changing low-order moments.
  - This will be especially important when burning particles are considered.

- We need at least 2N+1 (where N = # of particle diameters) size moments for Gauss quadrature.
  - For 3 particle diameters, we need at least 7 size moments.

$$\frac{\partial \mathcal{M}_{r/3}}{\partial t} + \underbrace{\boxed{\nabla \cdot \boldsymbol{u}_{r/3}}}_{\text{Flux}} = 0$$

Momentum and kinetic energy moments can be similarly defined.

- Mass-velocity moments are defined by:

$$\boldsymbol{\mathcal{U}}_r = \iint m^r \boldsymbol{u} n(t, \boldsymbol{x}, m, \boldsymbol{u}) dm d\boldsymbol{u}$$

- Isotropic mass-kinetic-energy moments are defined by:

$$\mathcal{K}_r = tr\left(\iint m^r (\boldsymbol{u} \otimes \boldsymbol{u}) n(t, \boldsymbol{x}, m, \boldsymbol{u}) dm d\boldsymbol{u} \right)$$

- A full mass-kinetic-energy moment tensor can be defined if anisotropy is desired.

$$\boldsymbol{\mathcal{K}}_p = \alpha_p \rho_p \left(\boldsymbol{u}_p \otimes \boldsymbol{u}_p + \Theta_p \boldsymbol{I} \right)$$

Higher-order moments are used to track particle momentum and kinetic energy.

- To find the momentum and kinetic energy of each particle diameter, we need N transport equations.
  - For 3 particle diameters, we need 3 first-order velocity moments and 3 second-order velocity moments.

$$\frac{\partial \boldsymbol{\mathcal{U}}_r}{\partial t} + \underbrace{\boxed{\nabla \cdot \left(\boldsymbol{\mathcal{U}}_r \otimes \boldsymbol{\mathcal{U}}_r + p_p \mathcal{M}_r \boldsymbol{I}\right)}}_{\text{Flux}} = -\underbrace{\boxed{\frac{1}{\rho_p}\left(\nabla p_f + \boldsymbol{F}_{pf}\right)\mathcal{M}_r - \frac{\mathcal{M}_r}{\alpha_p \rho_p} \nabla \cdot \boldsymbol{P}_{pfp}}}_{\text{Interphase Coupling}} - \overbrace{\boxed{\boldsymbol{D}_r}}^{\text{Drag}} + \underbrace{\boxed{\boldsymbol{C}_r}}_{\text{Collisions}}$$

$$\frac{\partial \mathcal{K}_r}{\partial t} + \underbrace{\boxed{\nabla \cdot \left(\mathcal{K}_r \boldsymbol{u}_p + p_p \boldsymbol{\mathcal{U}}_r\right)}}_{\text{Flux}} = -\underbrace{\boxed{\frac{1}{\rho_p}\left(\nabla p_f + \boldsymbol{F}_{pf}\right) \cdot \boldsymbol{\mathcal{U}}_r - \frac{\boldsymbol{\mathcal{U}}_r}{\alpha_p \rho_p} \nabla \cdot \boldsymbol{P}_{pfp}}}_{\text{Interphase Coupling}} - \overbrace{\boxed{D_{r,E}}}^{\text{Drag}} + \underbrace{\boxed{\frac{1}{2} C_{r,E}}}_{\text{Collisions}}$$

Mass-internal-energy moments are used to track particle internal energy.

- Mass-internal-energy moments are defined by:

$$\mathcal{E}_r = \iint e m^r n(t, \boldsymbol{x}, m, e) dm de$$

- To find the internal energy of each particle diameter, we need N transport equations.
  - For 3 particle diameters, we need 3 mass-internal energy moments.

$$\frac{\partial \mathcal{E}_r}{\partial t} + \underbrace{\boxed{\nabla \cdot \left(\mathcal{E}_r \boldsymbol{u}_p\right)}}_{\text{Flux}} = \overbrace{\boxed{H_r}}^{\text{Convection}} - \underbrace{\boxed{\frac{1}{2} C_{r,E}}}_{\text{Collisions}}$$

- For $N = 3$, there are a total of 19 transport equations.
  - 3 equations for gas.
  - 5N+1=16 equations for particles.

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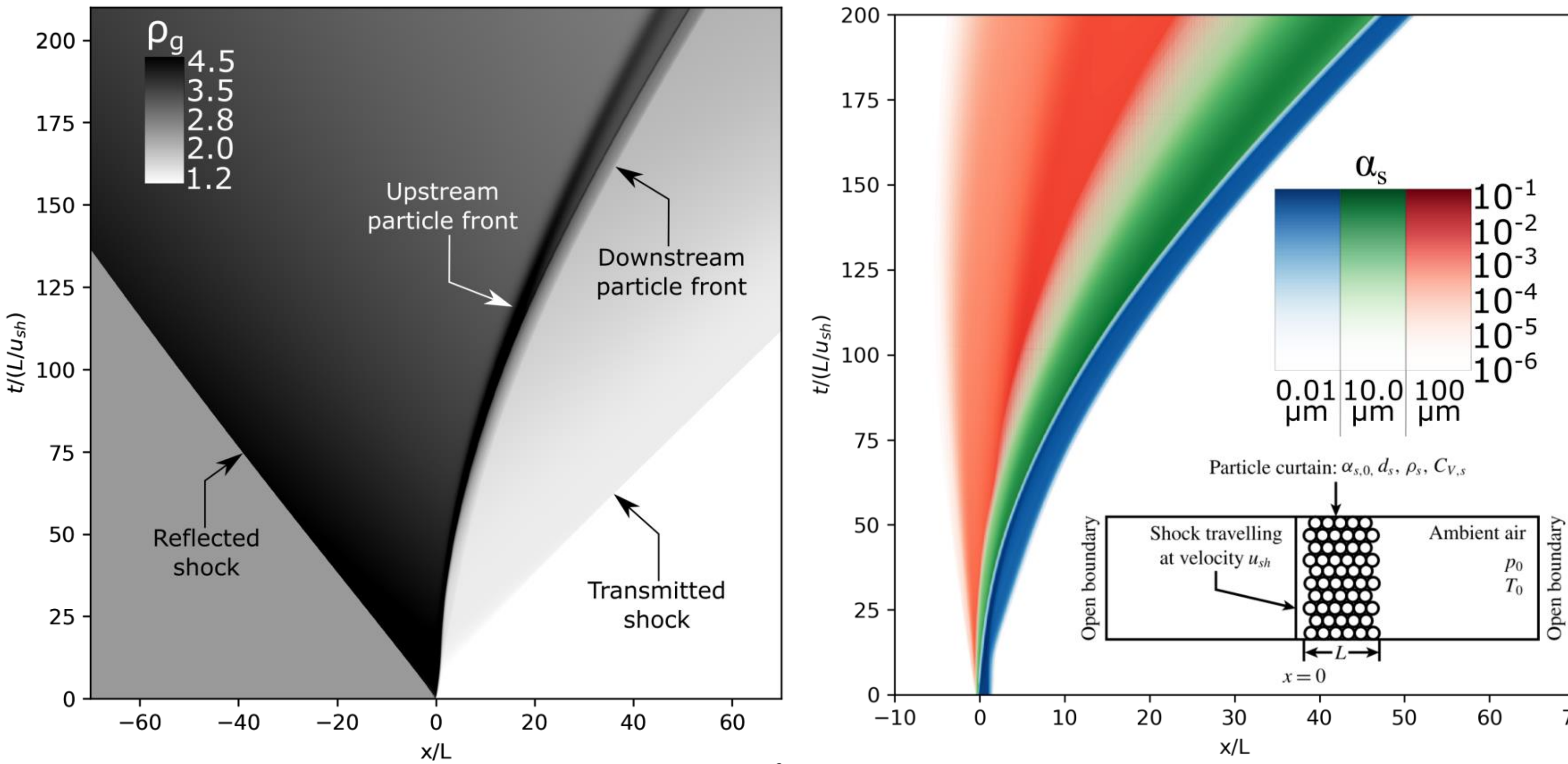
Particle collisions, drag, and convective heat transfer are treated analytically to ensure robustness and speed up already expensive computations.

- Strang-splitting is used to separate these terms from the hydrodynamics.
- Mass and volume fraction are assumed to not change due to these processes.
- These source terms can be cast into a linear system of equations and solved using a matrix exponential method.

$$\begin{bmatrix} \frac{\partial u_{p,1}}{\partial t} \\ \frac{\partial u_{p,2}}{\partial t} \\ \vdots \\ \frac{\partial u_{p,N}}{\partial t} \\ \frac{\partial u_g}{\partial t} \end{bmatrix} = A \begin{bmatrix} u_{p,1} \\ u_{p,2} \\ \vdots \\ u_{p,N} \\ u_g \end{bmatrix} \qquad \begin{bmatrix} u_{p,1} \\ u_{p,2} \\ \vdots \\ u_{p,N} \\ u_g \end{bmatrix}_{t+\Delta t} = \begin{bmatrix} u_{p,1} \\ u_{p,2} \\ \vdots \\ u_{p,N} \\ u_g \end{bmatrix}_t e^{A\Delta t}$$

To begin characterizing our model, we study the interaction between a Mach 1.66 shock and a polydisperse particle curtain.

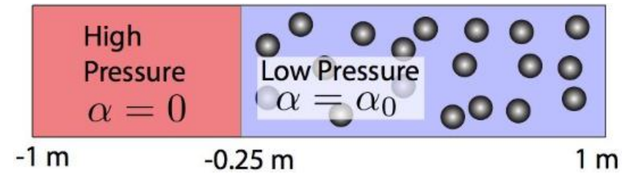
- Modified Godunov scheme using HLL approximate Riemann solver with 5th-order MUSCL spatial reconstruction.

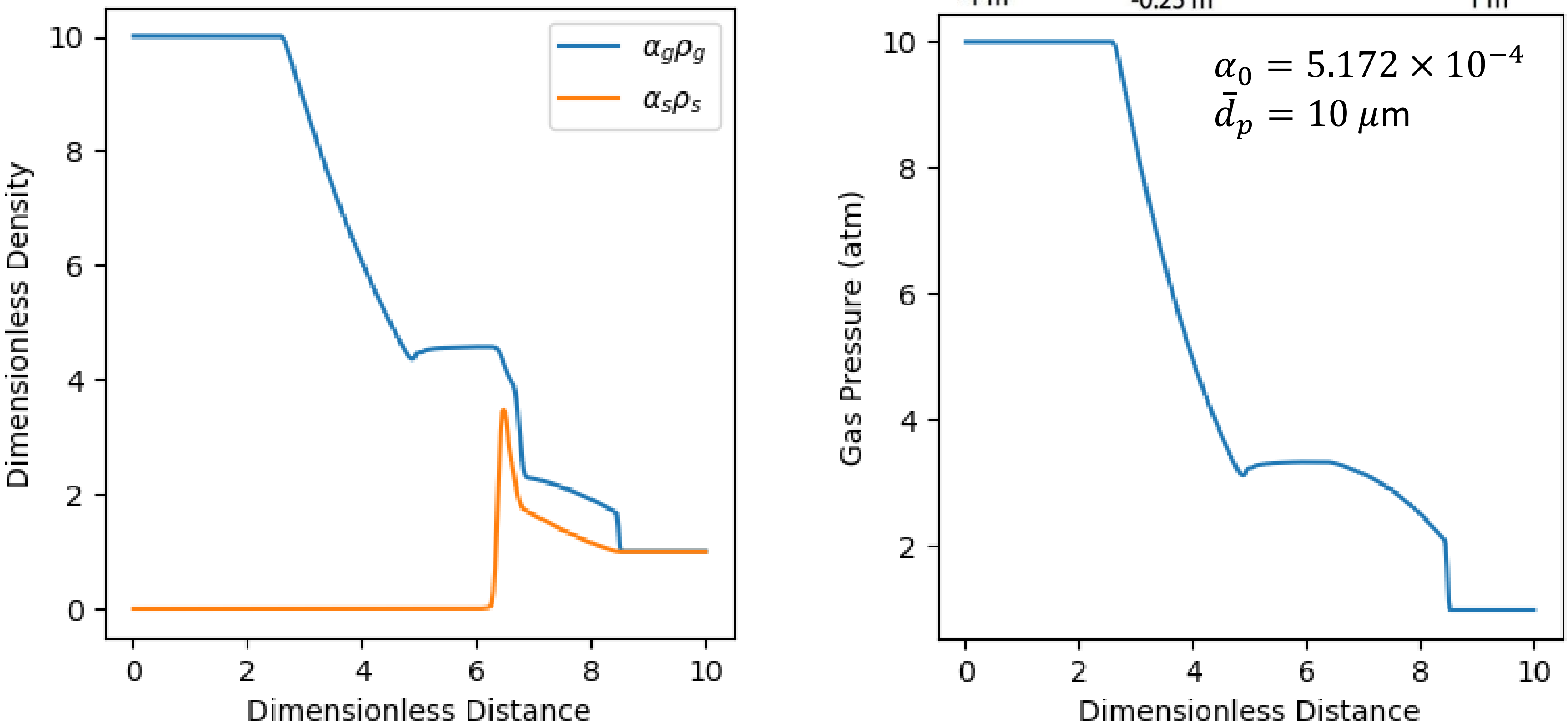


Position-time diagrams of gas density in units of kg m^{-3} (left) and volume fraction of each particle diameter (right).

To compare to experiments, we can model a dilute two-phase granular shock tube.

- We see good agreement with the results of Saito et al. (2003), Federov et al. (2007), and Houim et al. (2016).





Dimensionless density of both phases (left) and gas pressure (right) as a function of dimensionless distance.

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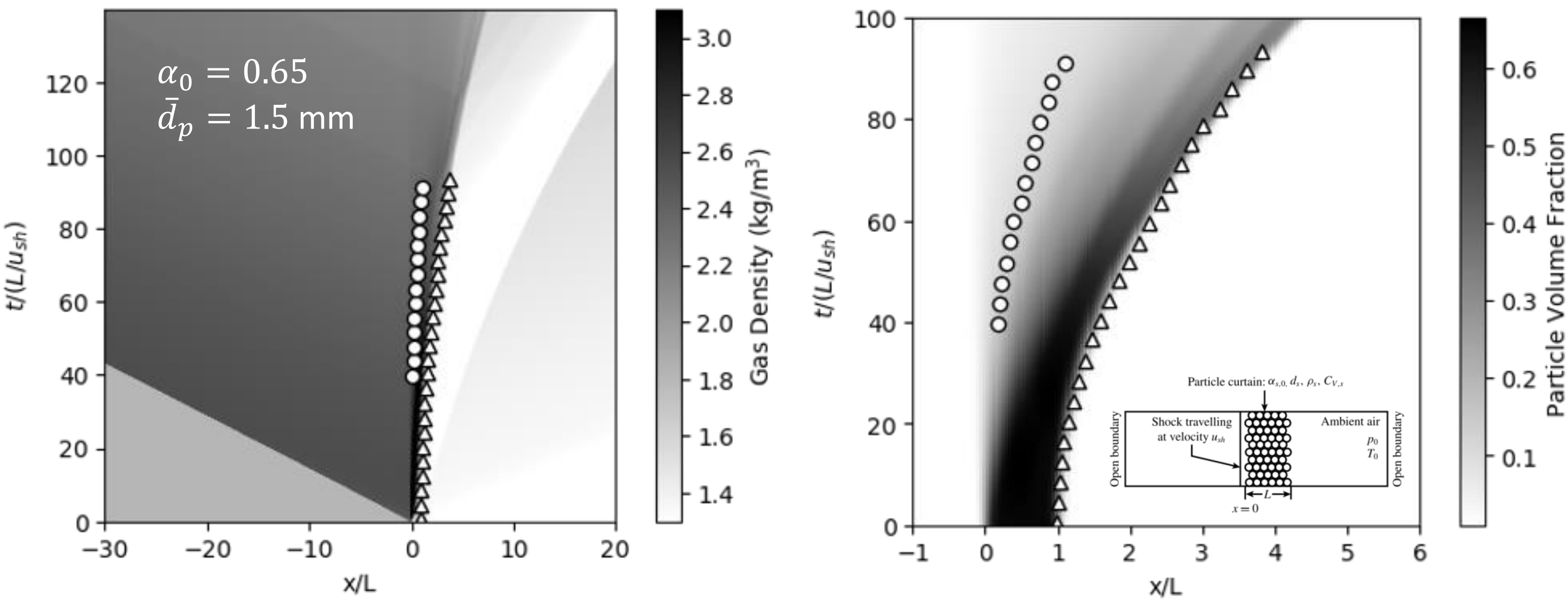
We can also compare to experiments of a monodisperse dense particle curtain-shock interaction.

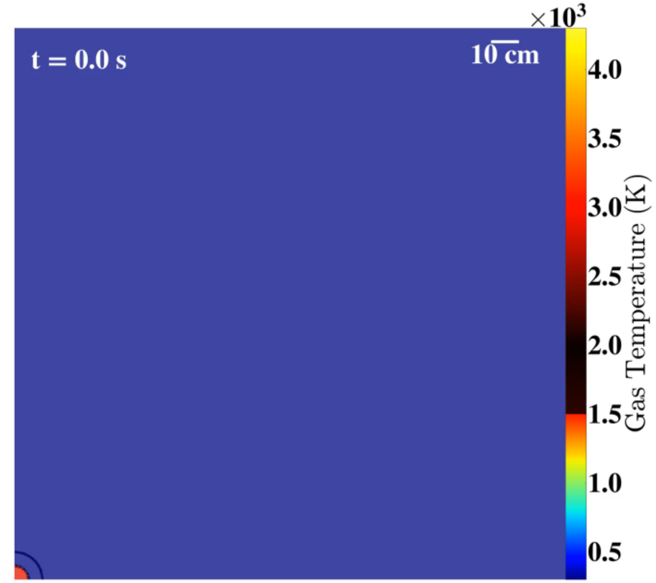
- We see good agreement with the experimental results of Ling et al. (2012) and Wagner et al. (2012).



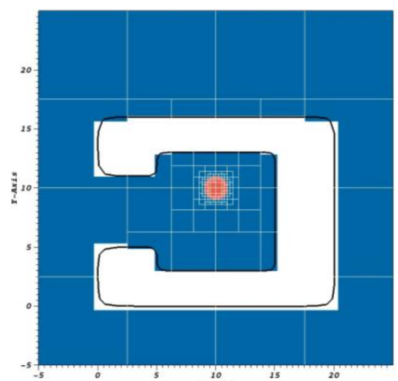
Position-time diagrams of gas density in units of kg m^{-3} (left) and particle volume fraction (right).

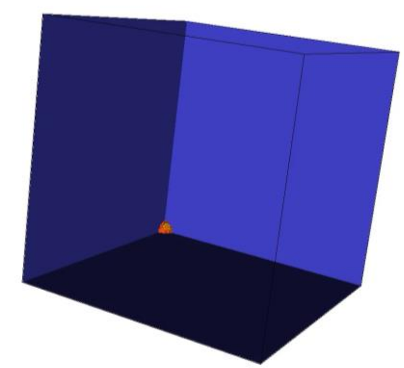
This new model will be added to our in-house code HyBurn to model metalized blasts, dust flames, and droplet sprays.

- Fully couples compressible reactive gases to granular flow
  - Eulerian and Lagrangian particles
- Combustion with detailed and simplified chemical kinetics
- Ideal and non-ideal (JWL, BKW) EoS models
- Massively parallel with adaptive meshing using the AMReX library
- High-order numerical methods – Up to 7th order
- Complex geometry using Immersed Boundary Methods
- Thermal radiation using filtered spherical harmonics



Combustion of TNT-dispersed Al particles.


Blast in an open room.


Explosive Al particle dispersal.

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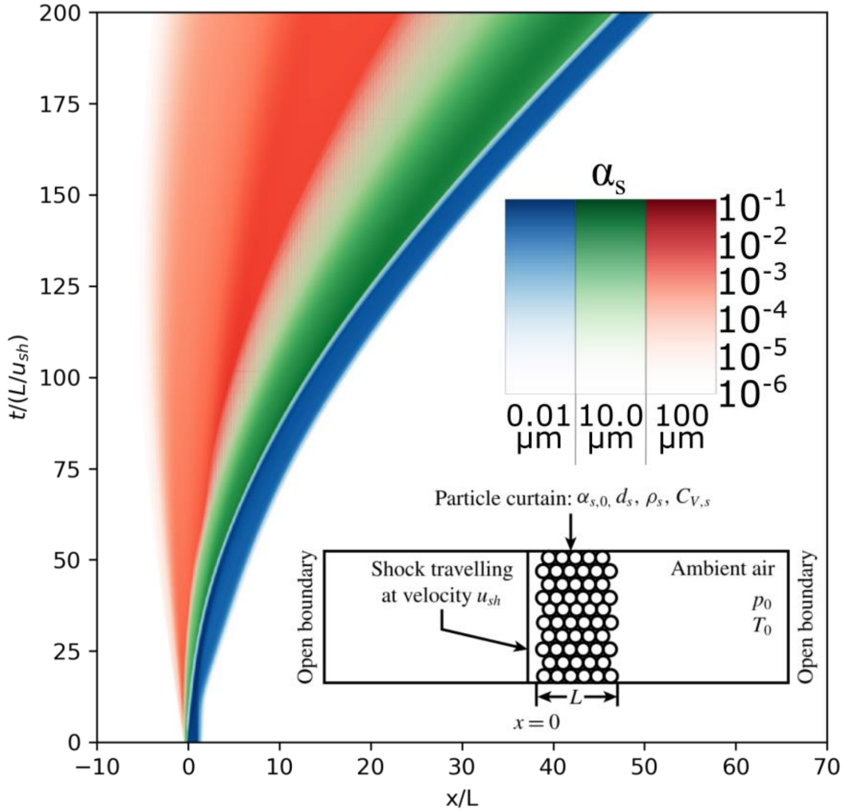
We have presented a new polydisperse Eulerian model in development, and plan to employ it in studying the physics of aluminized blasts and other complex multiphase systems.

- Future work includes:
  - Extending our flux schemes to HLLC/AUSM$^+$-up.
  - Adding chemical reactions between gases and particles.
  - Adding more transport equations to include higher-order physics (such as particle trajectory crossing).

Questions???



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