CCMT

Center For Compressible Multiphase Turbulence Overview

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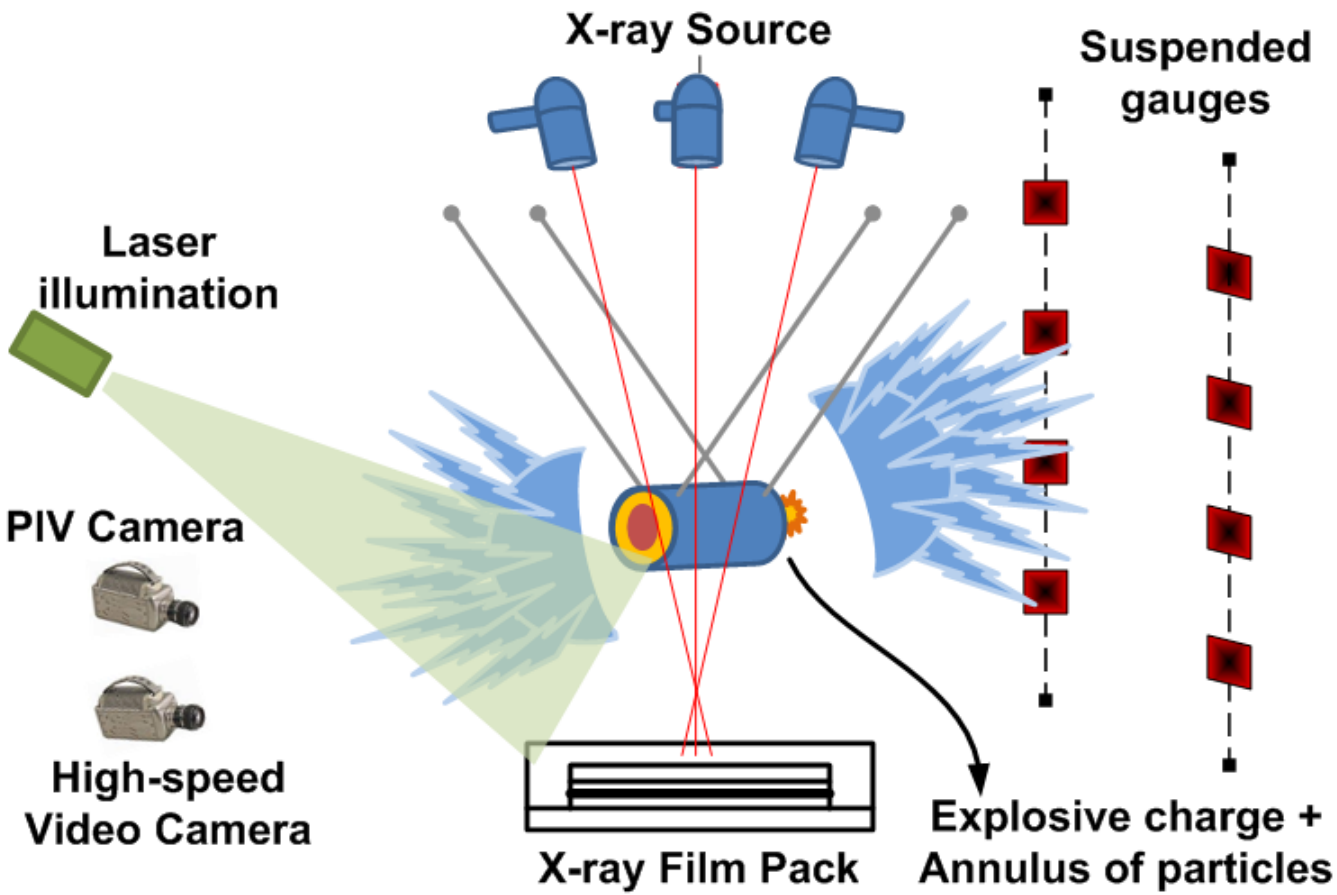
Center for Compressible Multiphase Turbulence

Purpose of the Center

- To radically advance the field of CMT
- To advance predictive simulation science on current and near-future platforms with uncertainty budget as backbone
- To advance a co-design strategy that combines exascale emulation, exascale algorithms, exascale CS
- To educate students and postdocs in exascale simulation science and place them at NNSA laboratories

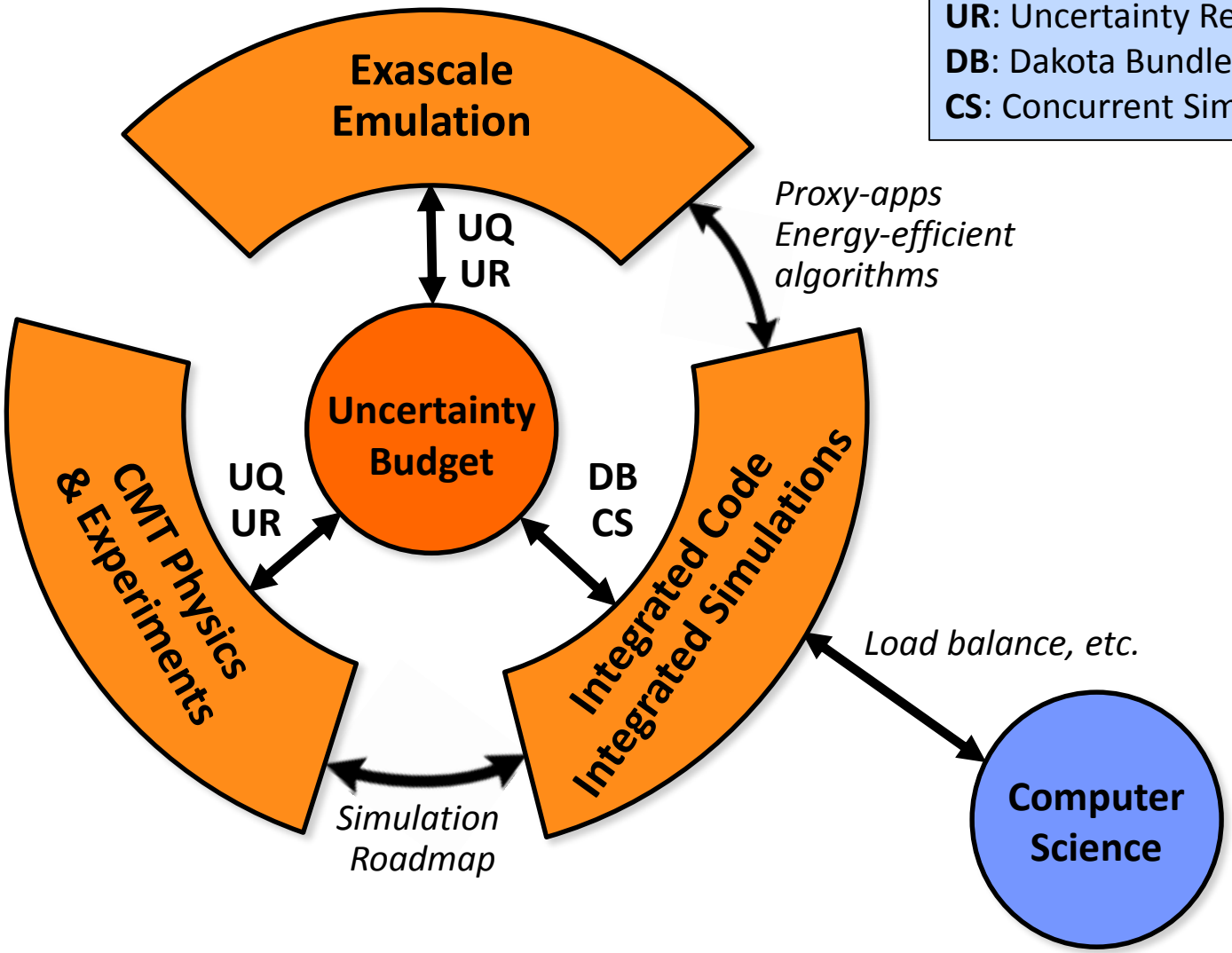
Demonstration Problem



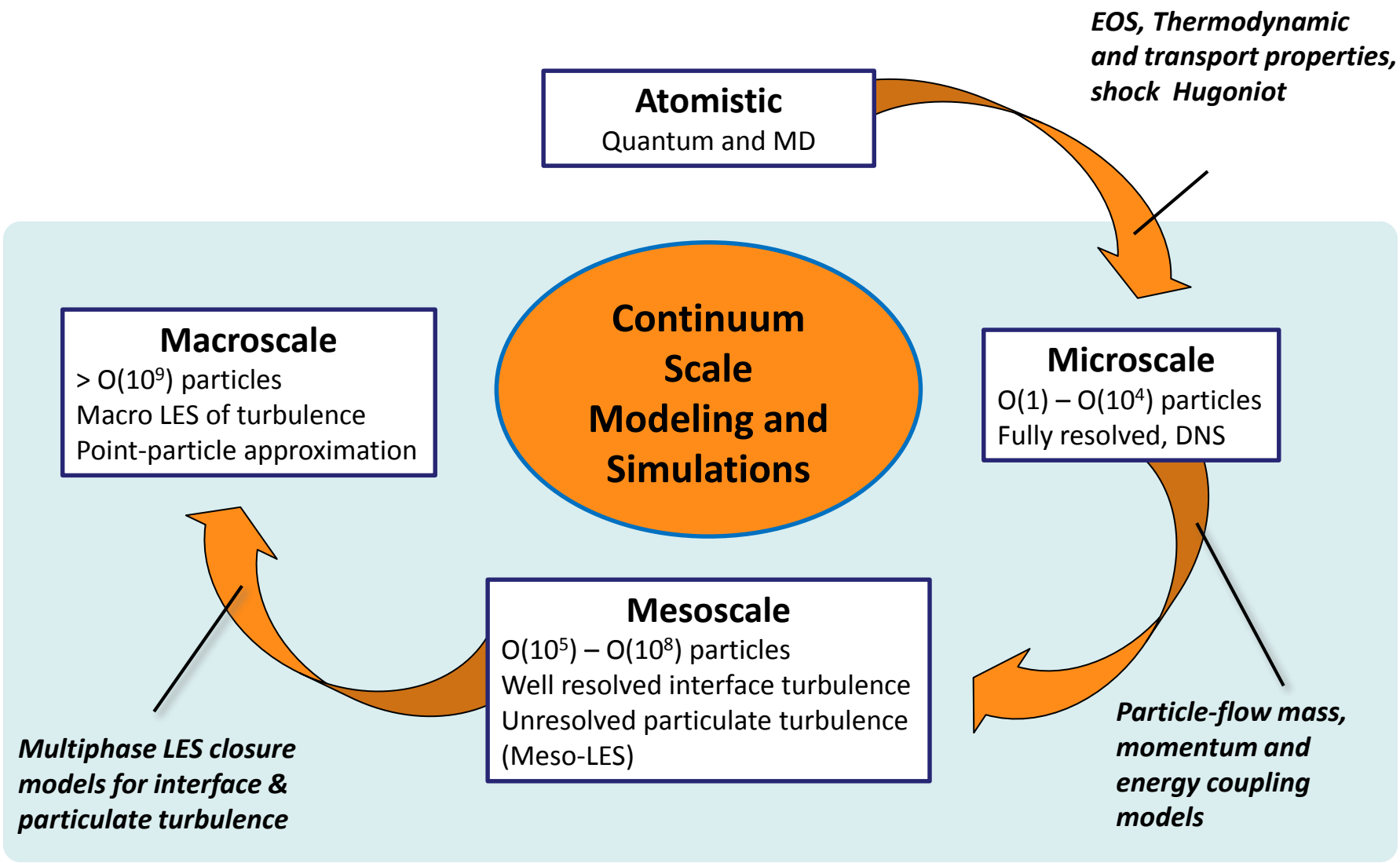
- Integrated simulations
- Experimental measurements for validation

How Different Pieces Fit

UQ: Uncertainty Quantification
UR: Uncertainty Reduction
DB: Dakota Bundles
CS: Concurrent Simulations



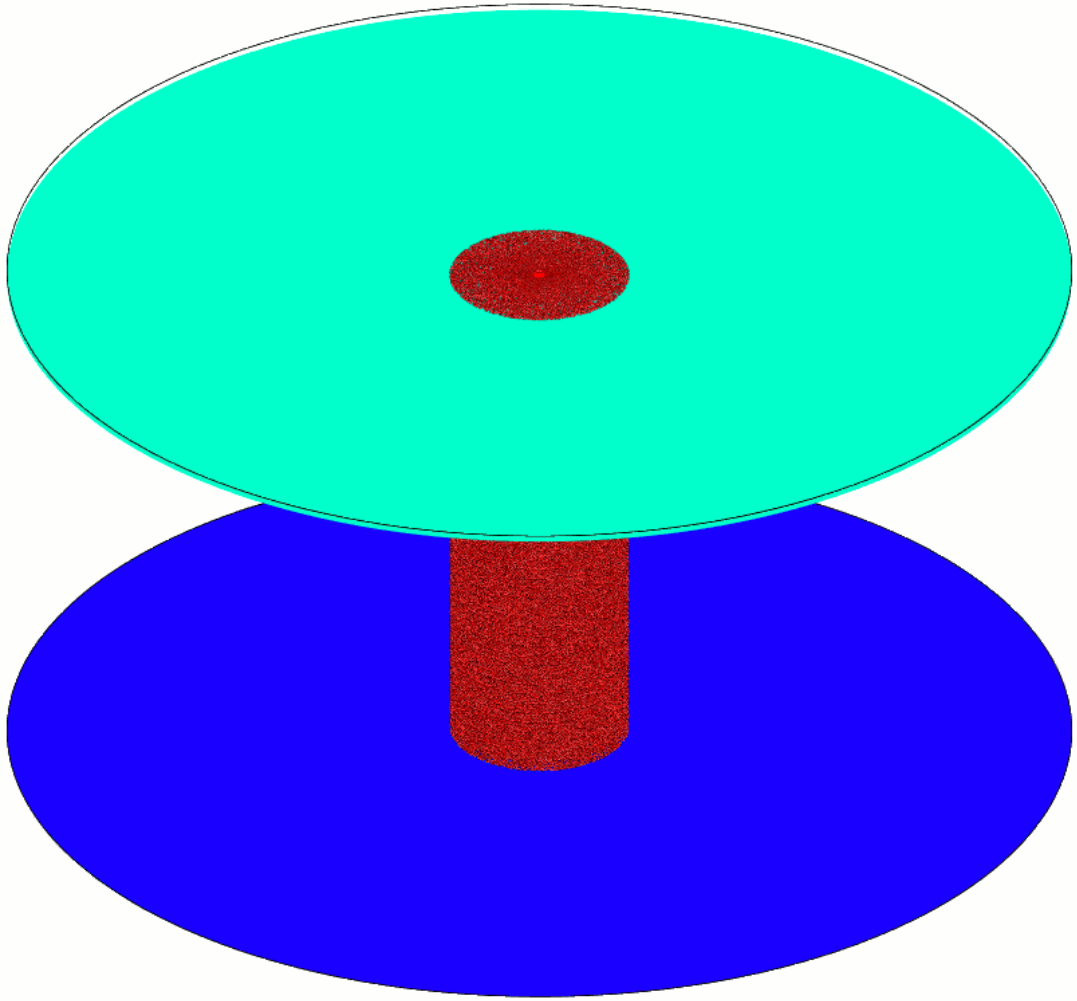
Multiscale Coupling Strategy



3D-Cylindrical Explosive Dispersal of Particles up to 200µs

Features:

- 30 Millions computational cells
- 5 Millions computational particles
- r_{max} = 0.30cm



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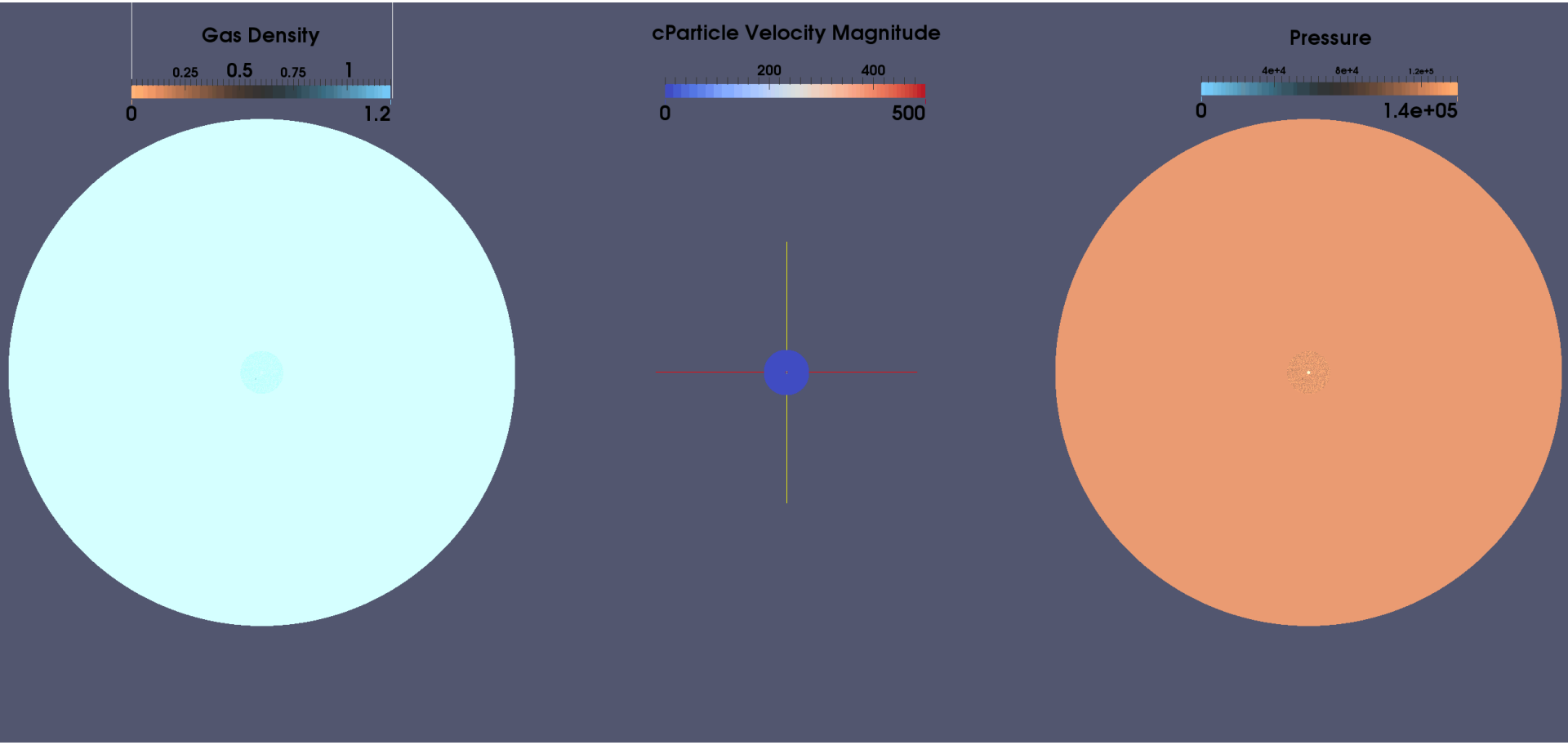
2D-Cylindrical Explosive Dispersal of Particles up to 1ms

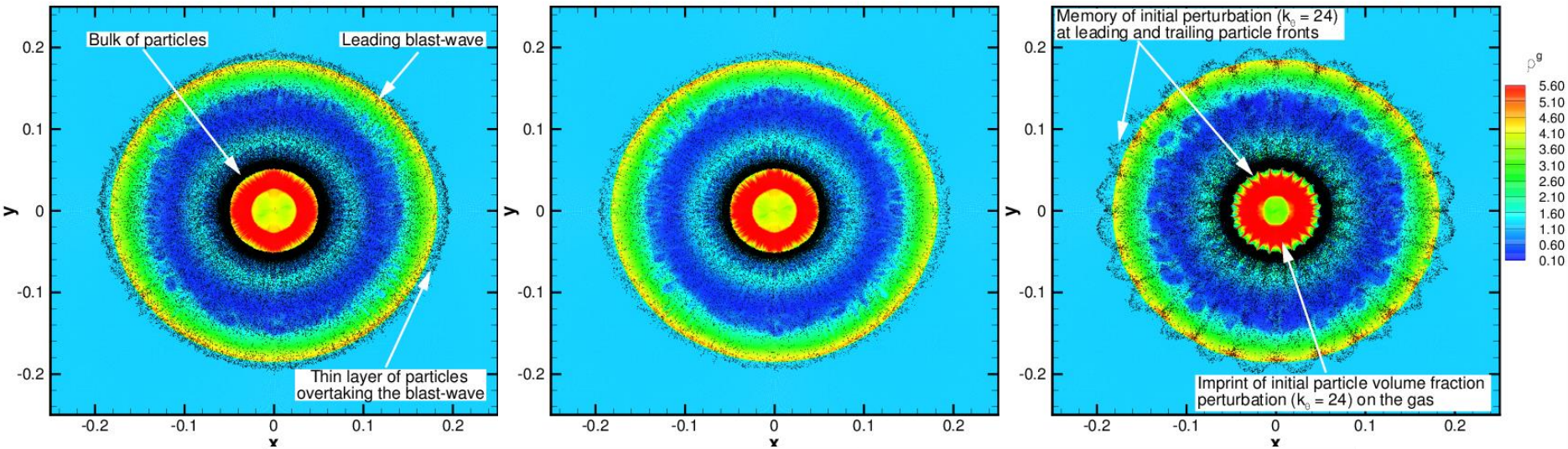
Features:

- **2.5 Millions computational cells**
- **1 Millions computational particles**
- **r_{max} = 0.60cm**



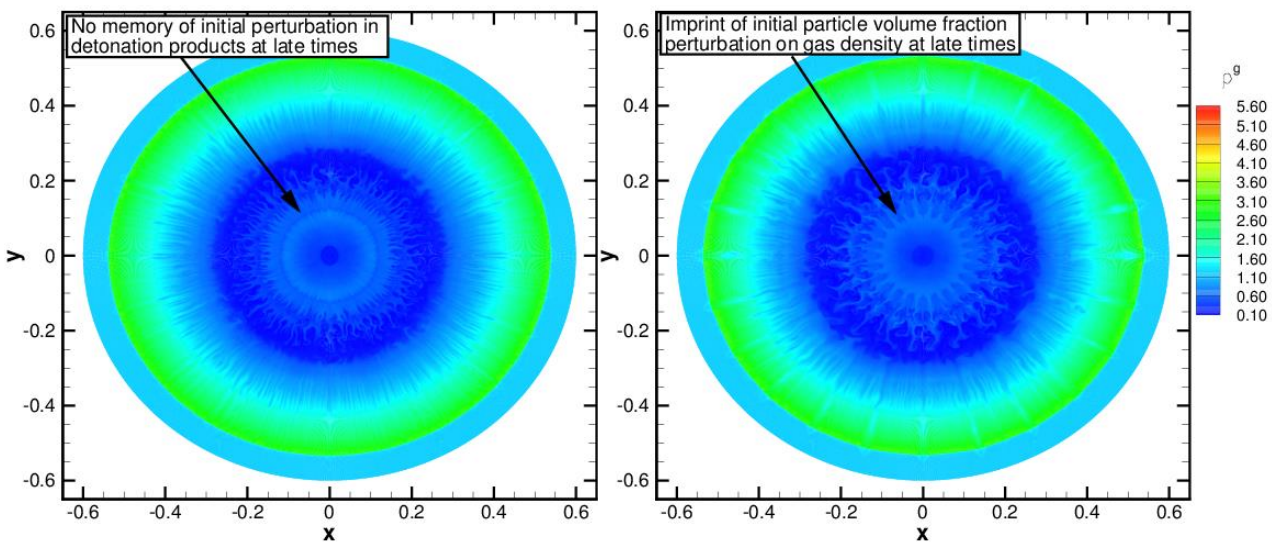
2D-Cylindrical Explosive Dispersal of Particles - IC study

No Perturbation | **Charge Perturbed** | **Particle Vol. Frac. Perturbed**



Later time, looking only at The gas phase

Charge Perturbed | **Particle Vol. Frac. Perturbed**



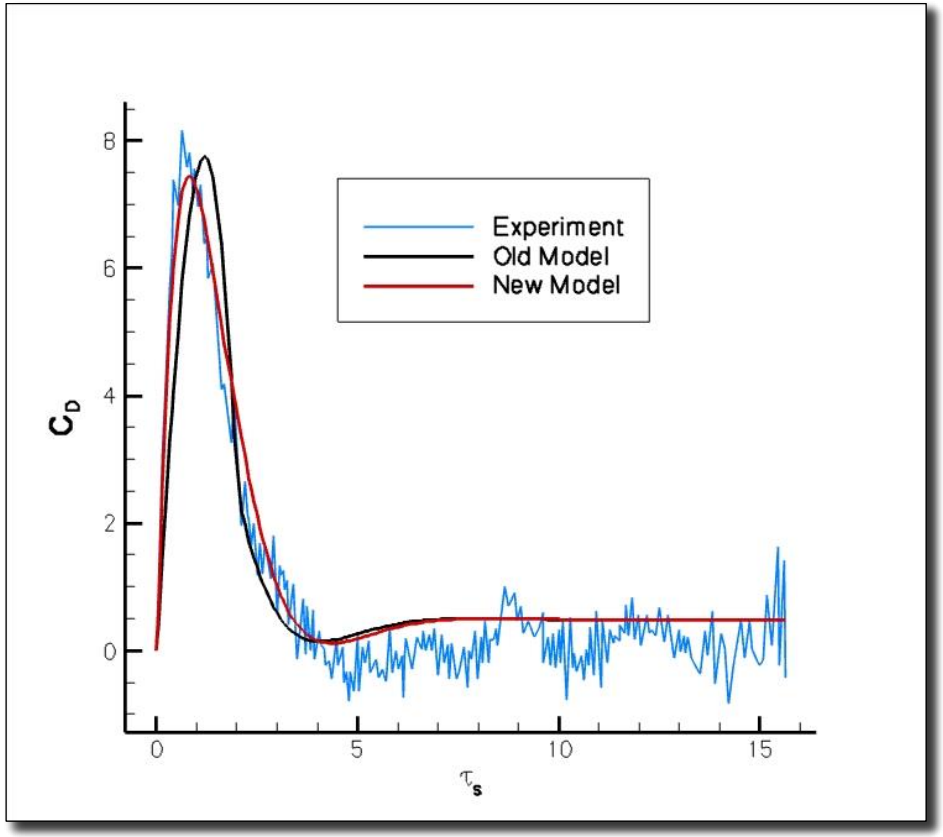
A small perturbation in the charge has no influence on the particle dispersal

Shock-Particle Modeling

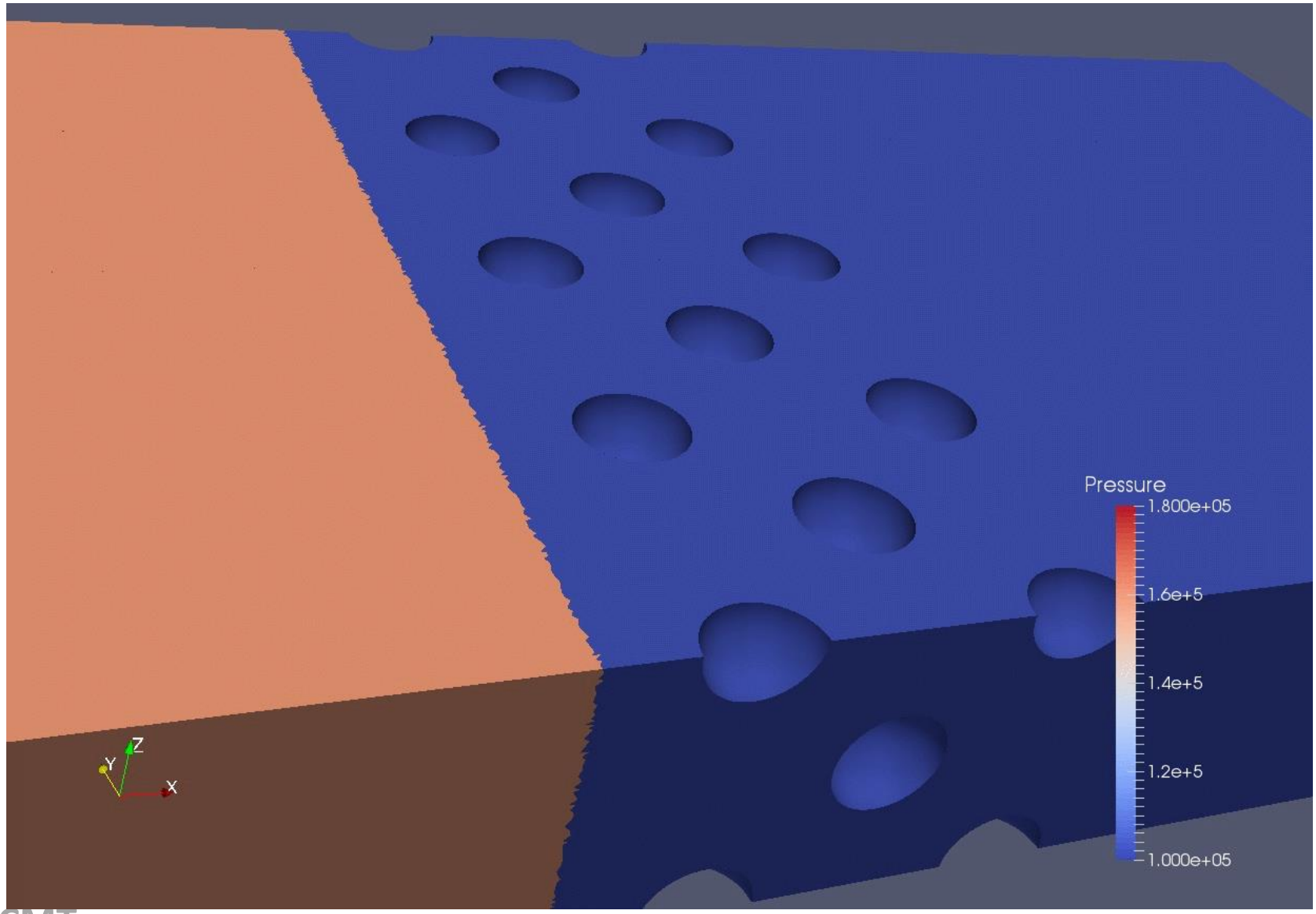
- Include the divergence term of F_{IU} (New Model)

$$F(t) = 6\pi\mu a(\overline{u}^S - u^P) + V\left(\overline{\rho\frac{Du}{Dt}}^V\right) + V\int_{\xi=-\infty}^{t}\left(K_{IU}\left((t-\xi)\frac{C_0}{a}\right)\left[\overline{\frac{d\rho u}{dt}}^V\right]\frac{C_0}{a}\right)d\xi$$

$$+\int_{\xi=-\infty}^{t}\left(K_{IU}\left((t-\xi)\frac{C_0}{a}\right)\left[\overline{\frac{d^2x\rho}{dt^2}}^V\right]\frac{C_0}{a}\right)d\xi$$

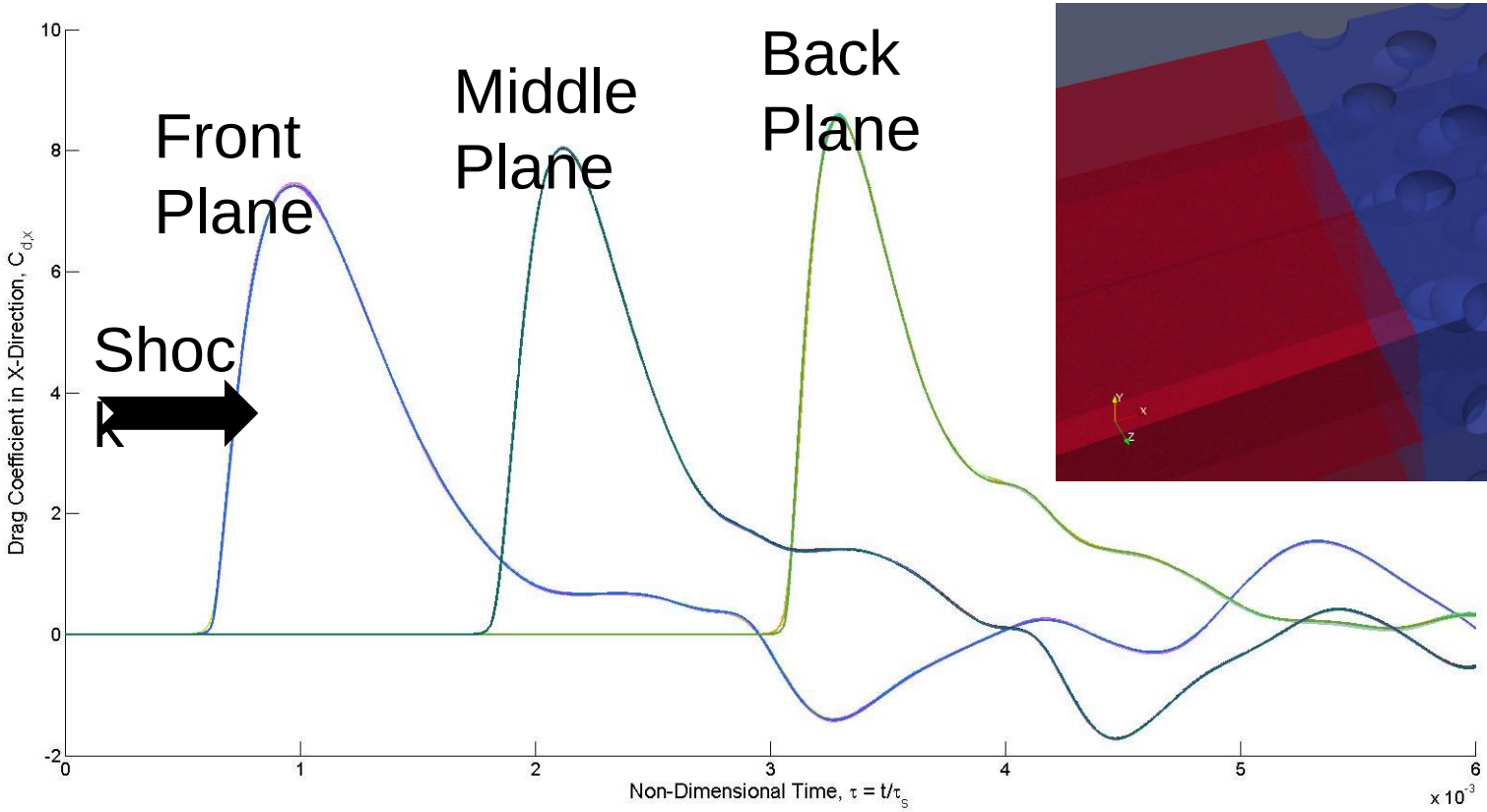


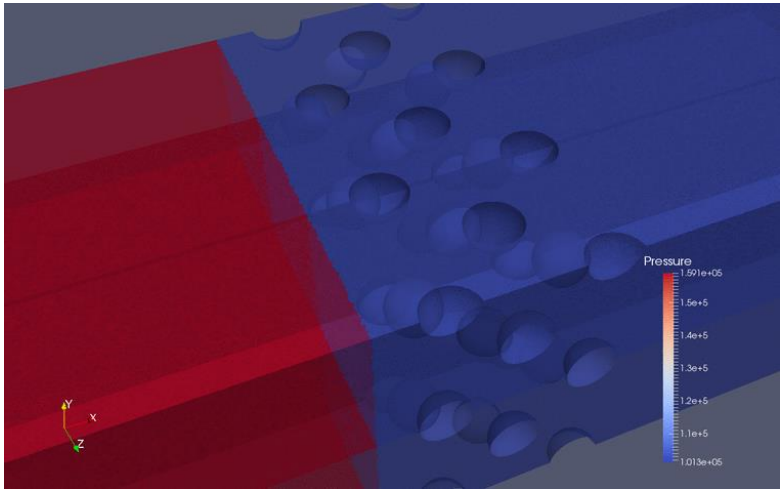
Multi-Particle (FCC) / Shock Interaction



Multi-Particle Force Analysis

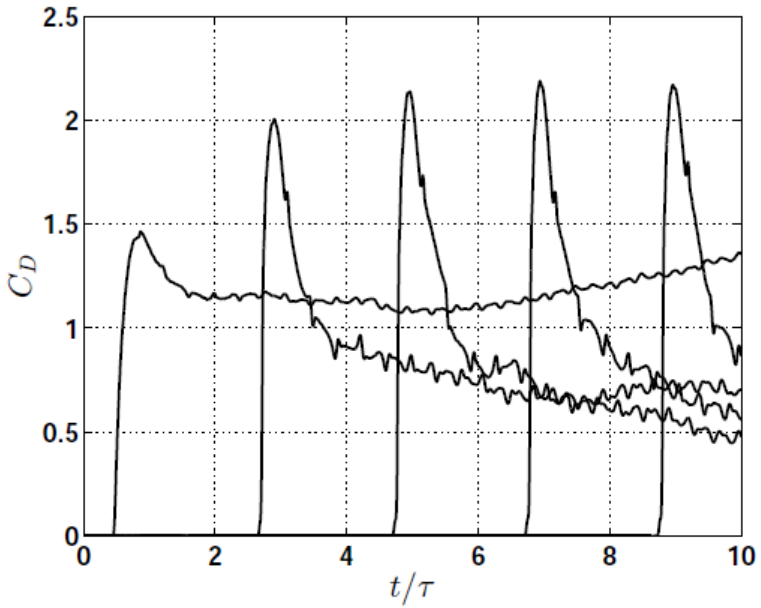
- Inviscid flow with a shock Mach number of 1.22
- 10% volume fraction (FCC arrangement)

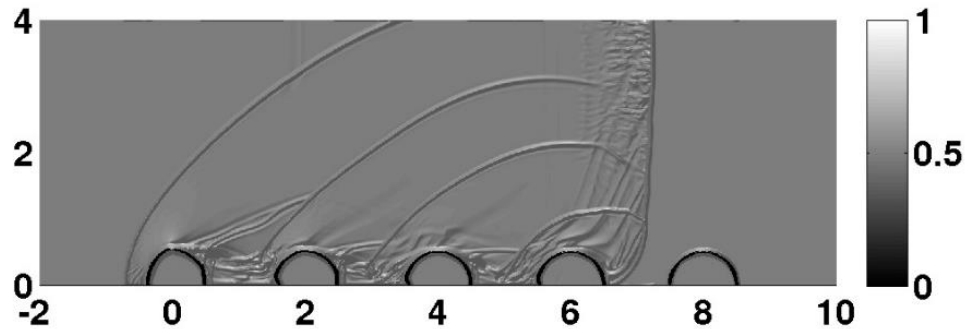




Force histories

Shock Interaction with Array of Particles



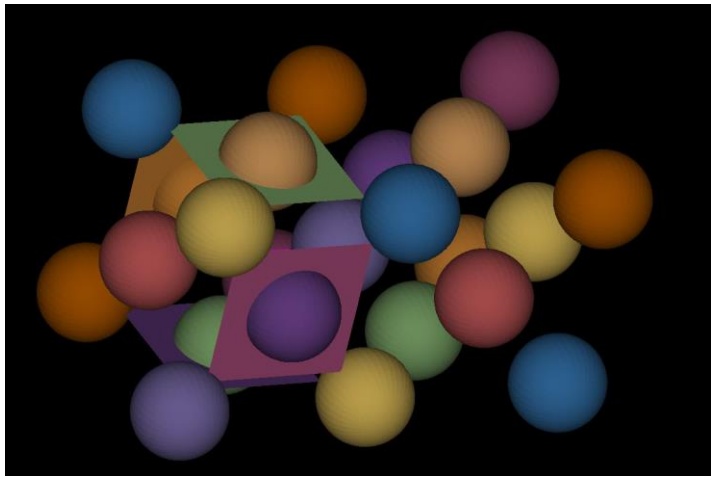


- Spacing one d_p
- $C_{D,max}$ for 5th particle:
  - 15% increase at M = 1.22
  - 48% increase at M = 2.0

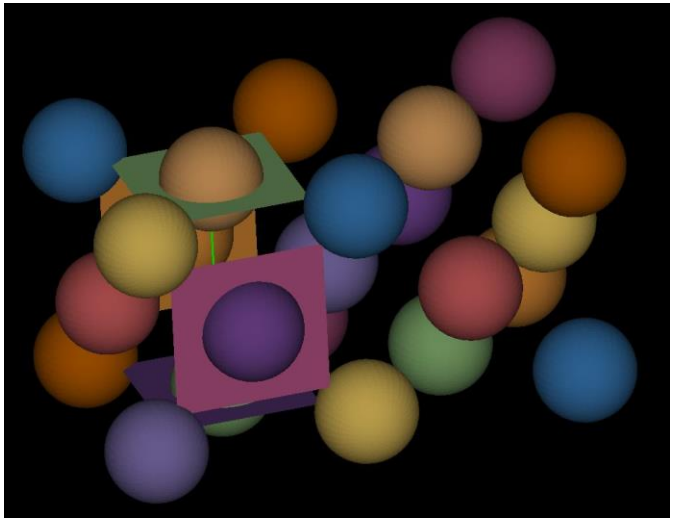
- Spacing one d_p / 2
- $C_{D,max}$ for 5th particle:
  - 8% increase at M = 1.22
  - 20% increase at M = 2.0

Shock/Multi-Particle Simulations

FCC 20% Volume Fraction



FCC 30% Volume Fraction

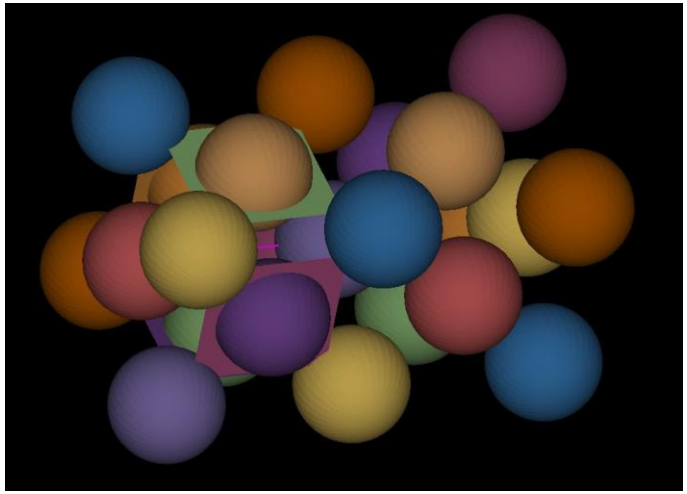


Mach

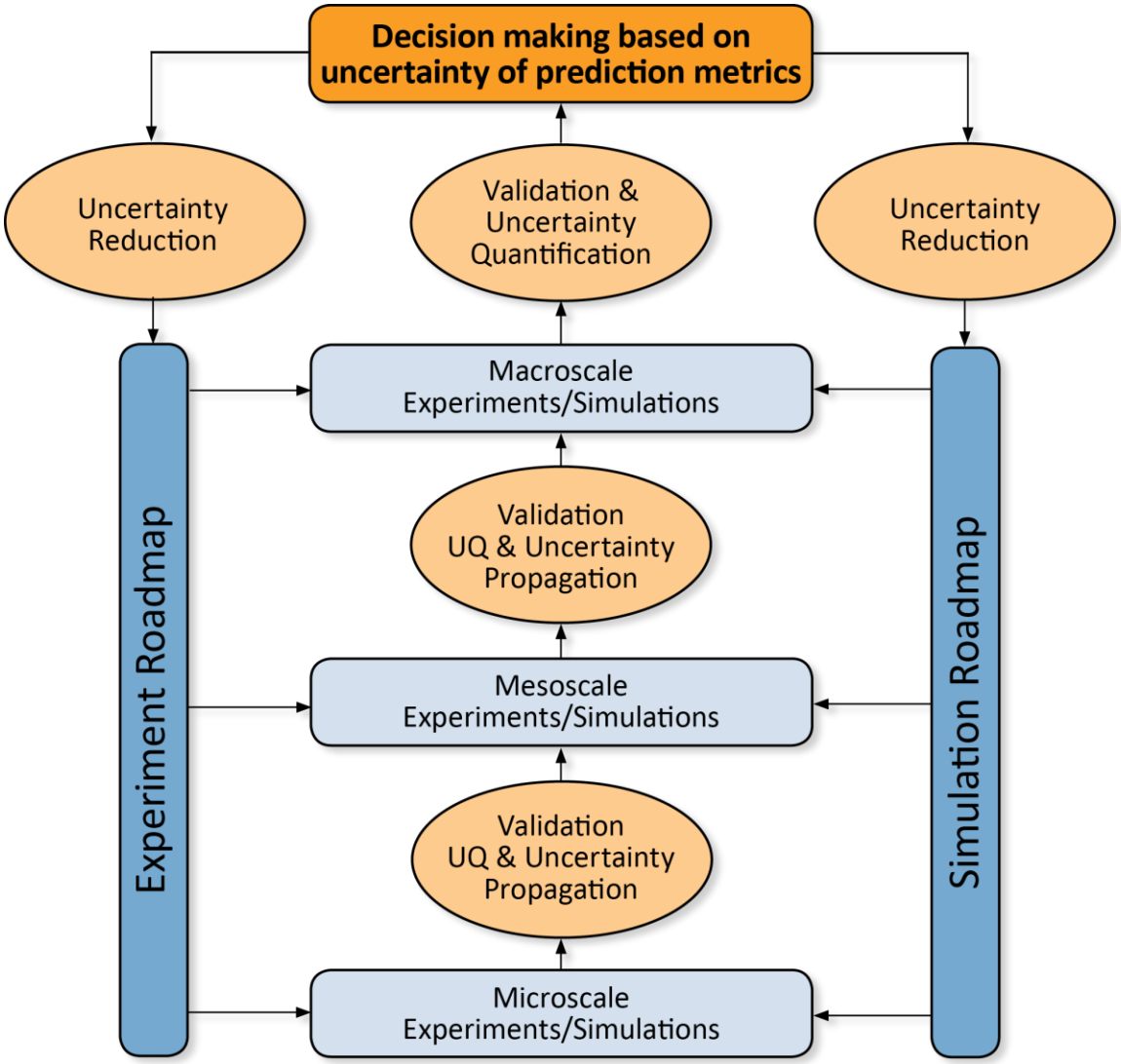
Volume Fraction φ

	1.22	2.0	3.0	6.0
0.10				
0.20				
0.30				
0.40				

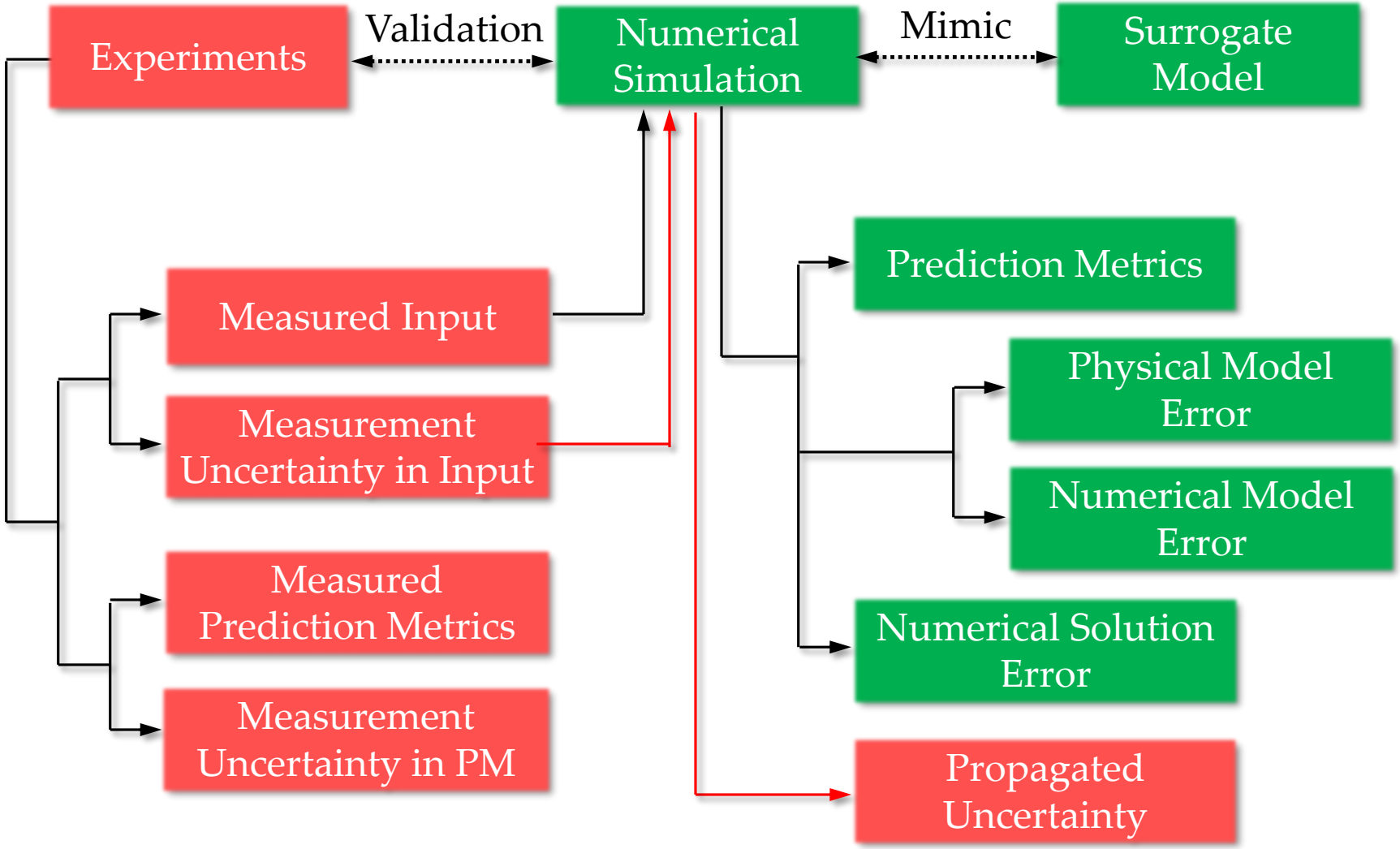
FCC 40% Volume Fraction



Decision Making with Uncertainty Budget

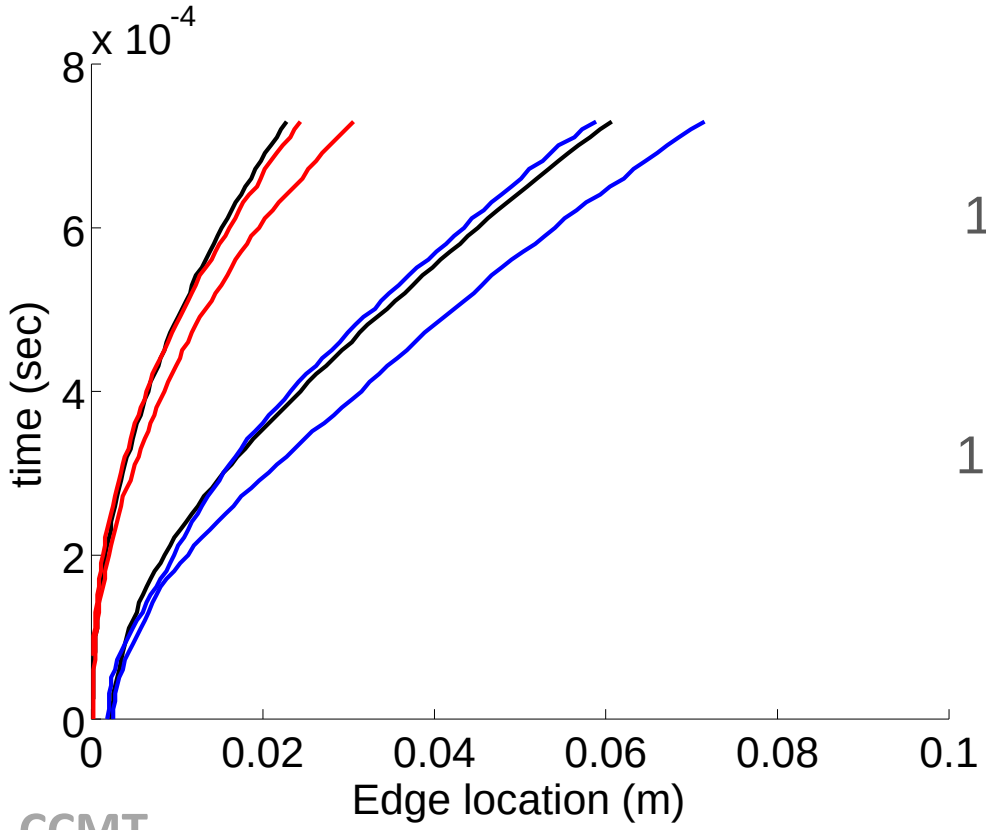


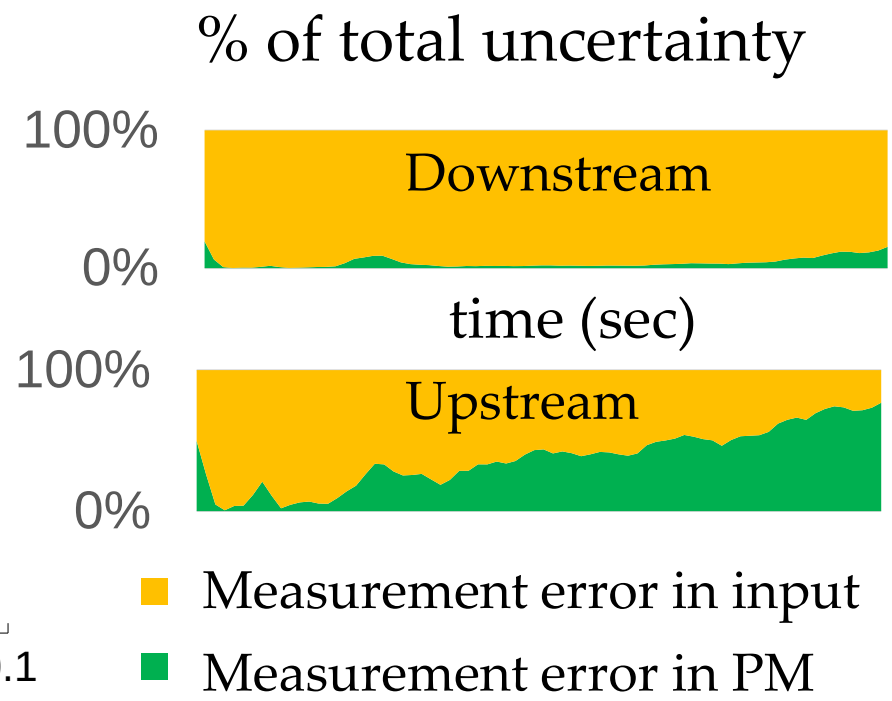
Validation and UQ



Model Error of Shock-Tube Simulation

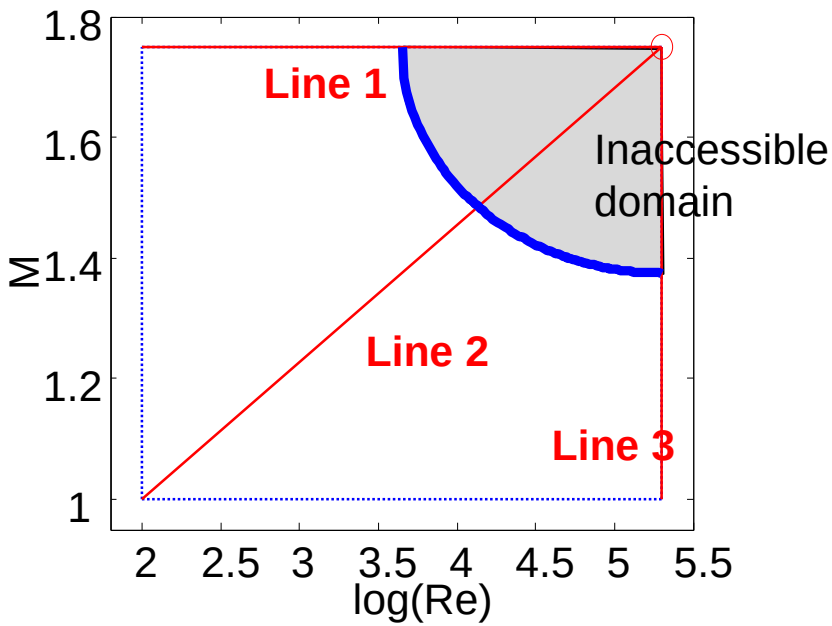
- Model error = Physical model error + Numerical model error
- 95% confidence interval of particle curtain edge location due to model error for the nominal input
- Reducing uncertainty in the model error

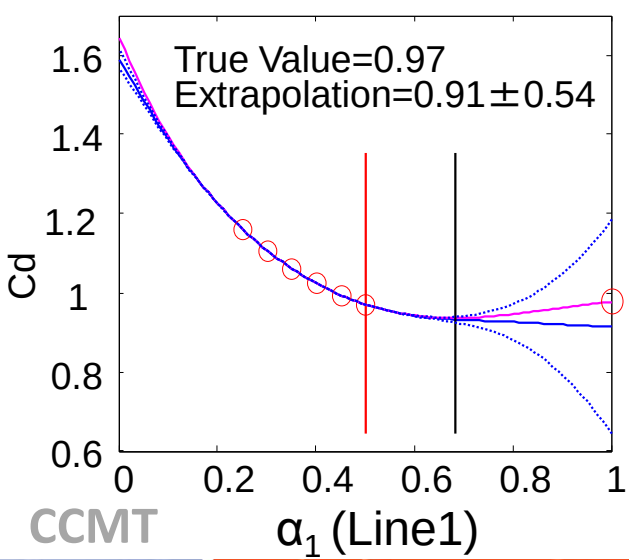


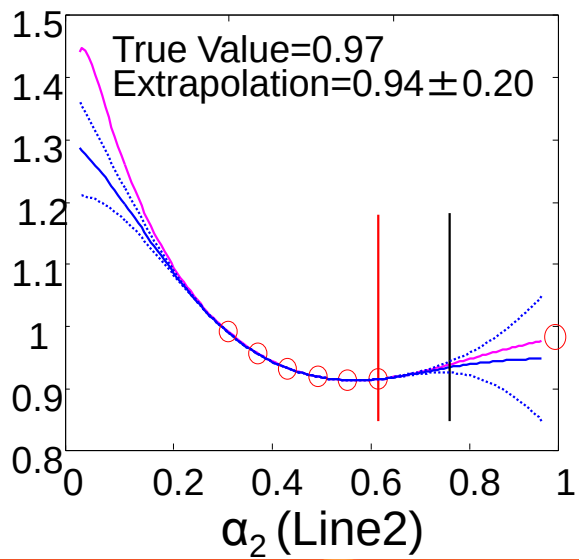


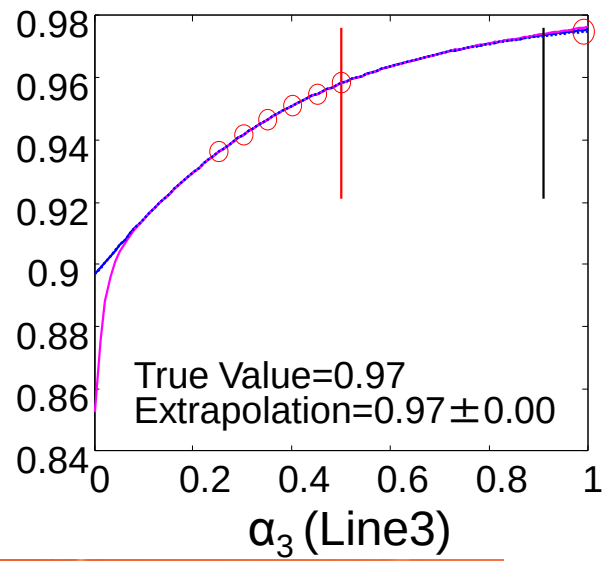
Extrapolation with the Method of Lines

- Drag force for Mach number and Reynolds number
- Extrapolation drag in high Mach number and high Reynolds number range









Overview of Year 1

Achievements:

- Code run on all DoE platforms available
- Code has been tested with 16k cores
- Signature problem has been run (2D & 3D)
- Study of the physics of the signature problem has started

Upcoming:

- Test with larger core count in preparation
- Mesoscale problems to start running shortly
- CoProcessing capability being implemented
- Improved models being implemented

Do you have any questions?