Center For Compressible Multiphase Turbulence Overview

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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

Exascale Emulation

Uncertainty Budget

Integrated Code
Integrated Simulations

CMT Physics & Experiments

Simulation Roadmap

Proxy-apps
Energy-efficient algorithms

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

Load balance, etc.

Computer Science
Multiscale Coupling Strategy

Continuum Scale Modeling and Simulations

Atomistic
Quantum and MD

Macroscale
> O(10^9) particles
Macro LES of turbulence
Point-particle approximation

Mesoscale
O(10^5) – O(10^8) particles
Well resolved interface turbulence
Unresolved particulate turbulence (Meso-LES)

Microscale
O(1) – O(10^4) particles
Fully resolved, DNS

EOS, Thermodynamic and transport properties, shock Hugoniot

Multiphase LES closure models for interface & particulate turbulence

Particle-flow mass, momentum and energy coupling models
3D-Cylindrical Explosive Dispersal of Particles up to 200μs

Features:
- 30 Millions computational cells
- 5 Millions computational particles
- $r_{\text{max}} = 0.30\text{cm}$
2D-Cylindrical Explosive Dispersal of Particles up to 1ms

Features:
- 2.5 Millions computational cells
- 1 Millions computational particles
- $r_{\text{max}} = 0.60\text{cm}$
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)

\[
F(t) = 6\pi \mu a (\overline{u}^S - u^P) + V \left( \rho \frac{D\overline{u}}{Dt}^V \right) + V \int_{\xi = -\infty}^{t} \left( K_{IU} \left( \frac{t - \xi}{a} \right) \left[ \frac{d\rho u}{dt} \right]^V \right) \frac{c_0}{a} d\xi \\
+ \int_{\xi = -\infty}^{t} \left( K_{IU} \left( \frac{t - \xi}{a} \right) \left[ \frac{d^2 \rho x}{dt^2} \right]^V \right) \frac{c_0}{a} d\xi
\]
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

FCC 40% Volume Fraction

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<th>Volume Fraction</th>
<th>Mach 1.22</th>
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<th>Mach 3.0</th>
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Decision Making with Uncertainty Budget

Decision making based on uncertainty of prediction metrics

Uncertainty Reduction
Validation & Uncertainty Quantification
Uncertainty Reduction

Macroscopic Experiments/Simulations
Validation UQ & Uncertainty Propagation

Mesoscale Experiments/Simulations
Validation UQ & Uncertainty Propagation

Microscopic Experiments/Simulations
Validation and UQ

Experiments → Validation → Numerical Simulation → Mimic → Surrogate Model

- Measured Input
- Measurement Uncertainty in Input
- Measured Prediction Metrics
- Measurement Uncertainty in PM

- Physical Model Error
- Numerical Model Error
- Numerical Solution Error
- Propagated Uncertainty

Prediction Metrics
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

Graph showing edge location over time with different colors representing percent of total uncertainty in different regions.
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?