Center For Compressible Multiphase Turbulence Overview

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Outline

- Demonstration Problem
- Unique Multiscale Approach
- Software Plan
- Exascale Emulation
- V&V, UQ Innovations
- UF Team & Partnership
- NNSA Interaction
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
Extreme Multiphase Flow

We desire to perform predictive simulation of these flows with as much multi-scale physics as possible.
Complex interactions require a unified approach

- Momentum, energy coupling
- Turbulence modulation
- Preferential accumulation

- Shock-turbulence interaction
- Shock-particle interaction
- Additional shocks and expansions
- Strong flow modification
Compressible Multiphase Turbulence

- Our focus will be on
  - Turbulence at the rapidly expanding material front
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities induced turbulence
  - Multiphase instability and particulate mixing at the front
  - Self-assemble of explosive-driven particles

- We will minimize the following complications
  - Free-shear and wall turbulence (stay away from boundaries)
  - Detonation physics (use simple, well-studied explosives)
  - Fragmentation or atomization physics (avoid casing, liquids)
  - Reactive physics (use non-reactive metal particles)
Multiscale Approach

Atomistic Scale

Microscale
Cluster of particles
$O(1) - O(10^4)$

Mesoscale
Instabilities
$O(10^5) - O(10^7)$

Macroscopic Scale
Experimental setup
$> O(10^9)$
Multiscale Coupling Strategy

**Macrocale**

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

**Continuum Scale Modeling and Simulations**

**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

**Atomistic**

- Quantum and MD

**EOS, Thermodynamic and transport properties, shock Hugoniot**

- Particle-flow mass, momentum and energy coupling models
Multiscale Coupling Strategy

- Our approach is similar in spirit to many ongoing multiscale efforts
  - “Divide, Bridge, and Conquer” strategy

- Unique aspects of present approach
  - Lagrangian particles preserve heterogeneity and anisotropy
  - Opportunities for concurrent macro, meso and microscale simulations
    - But there is no dimensionality reduction as in contact-line problems
Scientific Issues to be Addressed

At Micro to Mesoscale

- Mass, momentum and energy coupling at extreme conditions of pressure and temperature
- Understand and modeling of particle-particle, wake-particle and wake-wake interactions

At Meso to Macroscale

- Extend understanding of Rayleigh-Taylor and Richtmeyer-Meshkov instabilities to multiphase flows
- Establish the statistical properties of the interfacial multiphase turbulence
- Physics of particle self-assembly into focused jets
Master Plan

- **Problem Hierarchy:** to systematically validate our multiscale framework and establish uncertainties

- **Systems Engineering Plan:** to build on existing codes and simulation framework for current petascale and future exascale capability

- **Simulation Road Map:** that organizes the proposed integrated simulations and work towards exascale
Multi-scale Problem Hierarchy

Demonstration Problem
Explosive-driven
Cylindrical annulus of particles

(Macro) System-scale
Validation & UQ
of full physics

Shock-tube
Planar bed of particles

Explosive-driven
Planar bed of particles

Mesoscale
Validation & UQ
of coupled physics

Shock-tube
Cluster of particles

Explosive-driven
Cluster of particles

Microscale
Validation & UQ
of coupling modules

Explosive
characterization

Particles
characterization

Calibration
of EOS, etc.

Characterization
Calibration
Uncertainty Quantification
Multiscale Problem Hierarchy

Shock-tube
Planar bed of particles

Shock-tube
Cluster of particles

Explosive-driven
Planar bed of particles

Explosive-driven
Cluster of particles

Explosive due to
Cylindrical annulus of particles

Mesoscale
Validation & UQ of coupled physics

Characterization Calibration

Microscale
Validation & UQ of coupling modules

E of full physics
Multiscale Problem Hierarchy

- **Demonstration Problem**
  - Explosive-driven
  - Cylindrical annulus of particles

- **Shock-tube**
  - Planar bed of particles

- **Shock-tube**
  - Cluster of particles

- **Explosive-driven**
  - Planar bed of particles

- **Explosive-driven**
  - Cluster of particles

- **Explosive Track**
  - AFRL @ Eglin

- **(Macro) System-scale**
  - Validation & UQ of full physics

- **Mesoscale**
  - Validation & UQ of coupled physics

- **Microscale**
  - Validation & UQ of coupling modules

- **Characterization**
  - Calibration
Simulation Roadmap

Macro
1x500 5M
Characterized E&F; DEM at high vol frac;
highest resolution;
Reactive 2-phase LES;
Final coupling models

Macro
3x100 2M
Characterized E&F; Collisonal model;
High resolution;
Reactive 2-phase LES;
Adv coupling models

Macro
5x20 1M
Characterized E&F; Multi-phase LES;
Inter coupling models

D1c
3x1
1M
Experimental geometry;
Multi-phase LES;
Prelim coupling models

D1b
5x10 500k
End effects ignored;
Low/modest vol frac;
Multi-phase LES;
Prelim coupling models

D1a
5x10 300k

D1e
3x1
5M

C2c
5x1
2M
PRS - Higher vol frac
O(10^{0.7}) particles
Explosive dispersal
Particle deformation

C2b
3x1
1M
PRS - Higher vol frac
O(10^{0.6}) particles
Explosive dispersal
Particle deformation

C2a
3x1
500k
Modest volume fraction
O(10^{5}) particles
Explosive dispersal
Inter coupling models

C1b
3x1
800k
PRS - Higher vol frac
O(10^{0.6}) particles
Planar shock, contact,
& fan interaction Planar curtain

C1c
3x1
1M

B2c
3x1
500k

B2b
2x1
2M

B1c
3x1
1M

B1b
2x1
1M

B1a
3x1
250k

B0a
10x10 50k

Micro
Explosive driver; O(10^{3}) particles;
Modest volume fraction
Advanced EOS/
Hugoniot

Micro
Explosive driver; O(10^{3}) particles;
Modest volume fraction
Advanced EOS/
Hugoniot

Micro
Explosive driver; O(10^{3}) particles;
Modest volume fraction
Advanced EOS/
Hugoniot

Micro
High volume fraction Planar shock tube;
O(10^{4}) particles;
Full resolution;
Shock/contact/fan

Micro
Explosive driver; O(10^{3}) particles;
Modest volume fraction
Advanced EOS/
Hugoniot

Micro
Explosive driver; O(10^{3}) particles;
Modest volume fraction
Advanced EOS/
Hugoniot

Micro
Explosive driver; O(10^{4}) particles;
Full resolution;
Shock/contact/fan

Key
Yr1: Yellow
Yr2: Cyan
Yr3: Orange
Yr4: Green
Yr5: Pink

Xyz/nxm Proc

Xy = As in Figure 6
a = # of bundles
m = Bundle size
Proc = Processors
PRS = Partially Resolved Simulations

Macroscale

Mesoscale

Microscale
Rocfun – Existing Integrated Code

- Developed under ASAP program & continued at University of Florida
- Mature code, used in several projects, demonstrated scalability
- Unified code for microscale, mesoscale and macroscale simulations
- Extensively verified, detailed documentation, rigorous validation
Co-design: Rocfun + Nek5000 = CMT-Nek

- **Rocfun**
  - Geometric flexibility
  - Compressible NS
  - Lagrangian particles
  - Shock + turbulence

- **Nek5000**
  - Geometric flexibility
  - High-order accuracy
  - Parallel performance

- **CMT-Nek**
  - Geometric Flexibility
  - High-order accuracy
  - Compressible NS
  - Lagrangian particles
  - Shock + turbulence
  - Parallel Performance

Stage I, II, III
Petascale code

Stage III, + Exascale code
Scalability to Million Processes

- Scales beyond 1 million MPI processes:
  - 524288 cores
    - 1 or 2 ranks/core
  - 60% parallel efficiency at 1 million processes
- Scalable multigrid solvers:
  - 15 iterations/step
- Scalable I/O: 72 GB/sec
Exascale Emulation with FPGAs

Multiscale approach to Exascale studies:

- Exploration of Exascale devices, nodes, and systems, represented by fabrics of interconnected Architecture BEOs (behavioral emulation objects)

  - MICRO: study and characterization of devices for Exascale
    - Fabric of BEOs representing key resources at device scale
    - Processor cores, memory hierarchy, chip-level interconnect, I/O

  - MESO: study and characterization of nodes for Exascale
    - Fabric of BEOs representing key resources at node scale
    - Processor devices, memory, server-level interconnect, storage

  - MACRO: study and characterization of systems for Exascale
    - Fabric of BEOs representing key resources at system scale
    - Processing nodes, system-level interconnect, storage

- Architecture BEOs stimulated by corresponding set of Application BEOs
Uncertainty Budget – Backbone of CCMT

- Periodic experiments and simulations of “Demonstration Problem” essential to establish uncertainty deficit
- We will determine contributions of models to uncertainty of demonstration problem
  - Multiscale uncertainty propagation with Bayesian updating and successive surrogates
  - Physics-inspired surrogate modeling for up-scaling
- Prioritize based on potential for reducing uncertainty
  - Improvements in physical models
  - Improvements in numerics and simulation roadmap
  - Improvements in experimental procedure/measurements
- Essential for achieving accuracy targets here and at NNSA
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

Mesoscopic Experiments/Simulations

Validation UQ & Uncertainty Propagation

Microscopic Experiments/Simulations
Uncertainty Budget – Implementation

- A dedicated research staff will be in charge of doing the overall uncertainty budget
- Will be assisted by a graduate student
- Will closely interact and obtain uncertainty information from other research staff and students
- Uncertainty budget will be used by Simulation/Experiments Planning & Review Team (SEPRT)
- Uncertainty budget will be used by Exascale Co-Design Team (ECT)
- Uncertainty budget will be used by Center Management Committee for resource allocation
Exascale Emulation Uncertainty Budget

Decision making for notional and Exascale platforms

Validation & Error Quantification

NGEE-Macro (System level)

Validation EQ & Error Propagation

NGEE-Meso (Node level)

Validation EQ & Error Propagation

NGEE-Micro (Device level)

Calibration of architecture and application BEOs

Same cycle for notional and exascale platforms but with uncertainty quantification and propagation
V&V UQ– Unique Aspects

- Uncertainty budget driven decision making
  - Validation that each change in models and experimental procedure improves prediction capabilities
- Pushing parallels between CMT multiscale modeling and multi-level exascale emulation
- Advanced techniques for reducing cost of uncertainty propagation
  - Hybrid surrogates and multiple surrogates.
- Novel techniques for extreme quantities and rare events
- Cross-cutting team-based approach to V&V and UQ
UF Team & Partnership

Explosive experiments, 7 Years, FIRE

Don Littrell
Mike Jenkins
AFRL-RW

Paul Fischer
ANL

Ron
Adrian
ASU

CMT
Physics

Exascale
Emulation

V&V
UQ

Integrated
Code
CS

Scott Parker
ANL

Petascale, 18 Years, 6 Joint publications

Subcontract only to ASU

Father of PIV
25 Years
23 Joint publications

Author of Nek
12 Years
9 Joint publications
The Center will be organized by physics-based tasks and cross-cutting teams, rather than by faculty and their research groups.
NNSA Interaction Goals

Research Exchange

- Maintain center’s focus on areas of relevance to NNSA and avoid duplication
- Leverage ongoing cutting-edge research at Labs
  - Experimental data for validation
  - Exascale emulation and simulation, proxy-apps

Relationships and Feedback

- Emphasize staff/student interaction with NNSA
  - Facilitate future employment at NNSA labs
  - Nurture existing and build new relationships

New Curriculum

- Graduate Certificate in “Scientific Computing”
  - PSAAP-II main beneficiary
Exascale Interactions

Proxy-apps from ExMatEx and Exact
SNL Structural Simulation Toolkit (SST)

NNSA

ANL
CESAR on Nek5000
And NekBone

Florida Team

Techniques for exascale emulation,
exascale UQ, load balancing,
multi-objective optimization
Experimental Interactions

SNL Multiphase shock tube experiments
LANL CoMuEx multiphase mixing experiments
LANL dynamic x-ray radiography technique

Input into Design of Experiments Techniques for extreme diagnostics
CMT Physics Interactions

LLNL Explosive dispersal and after-burn M&S
LLNL & LANL RT & RM instability simulations
ExaCT & LANL Compressible turbulence
SNL Heterogeneous detonation M&S, ...

Novel models and numerical methods for micro, meso & macroscale simulation

NNSA

Florida Team
Software Interactions

DAKOTA, SAMRAI, UQ Pipeline
Co-op, Hypre, OpenMPI, Zoltan, VisIt

NNSA

ALE3D, CALORE, CFDLib,
CTH, FUEGO, PREMO,
PRONTO, RAGE, SIERRA

CMT Codes and modules
Emulation (NGEE-micro, meso & macro)

Florida Team
Summary

- Compressible multiphase turbulence (CMT) is a science problem of strong relevance to NNSA
- We have developed a unique multiscale approach to answer important scientific questions
- Innovations in exascale emulation and UQ techniques will enable predictive exascale simulations of CMT
- We have assembled an outstanding team
- We look forward to close interaction with NNSA Labs
Do you have any questions?
We desire to perform predictive simulation of these flows with as much multi-scale physics as possible.
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