Center for Compressible Multiphase Turbulence (CCMT)
Updates

S. Balachandar
Demonstration Problem
Center for Compressible Multiphase Turbulence

Overarching Goals

- 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 behavioral emulation, exascale algorithms, exascale CS
- To educate students and postdocs in exascale simulation science and place them at NNSA laboratories
Prediction Metrics

PM-1: Blast Wave Location
PM-2: Particle Front Location
PM-3: Number of Instability Waves
PM-4: Amplitude of Instability Waves
Physical Models – Sources of Error

**Detonation phase**

- T1: Detonation model
- Explosive material
- Metal particles
- Hot, dense, high pr gas
- Shock wave

**Dispersion phase**

- T2: Multiphase turbulence model
- T3: Thermodynamic & transport model
- T4: Interaction model
- T5: Compaction model
- T6: Point particle force model
- T7: Point particle heat transfer model

**Compaction/collision phase**

- T8: Deformation model
Multiscale Integration Strategy

Atomistic
Quantum and MD

EOS, Thermodynamic and transport properties, shock Hugoniot

Continuum Scale Modeling and Simulations

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

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

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

CCMT
Uncertainty Budget – Overall Plan

- T2 – Turbulence modeling
- T5 – Compaction modeling
- T4 – Particle interaction modeling
- T6 – Force coupling modeling
Y1-Y4 Accomplishments

1. Uncertainty quantified experiments (Forensic UQ)
2. Co-design of CMT-nek – An Exascale code
3. Dynamic load balancing – A must for multiphase flow
4. Physics-driven & data-driven modeling
5. Design space exploration with Behavioral Emulation (BE)

Lab Interactions
## Validation Blastpad Experiments (@Eglin AFB)

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Explosive length [mm]</td>
<td>AFRL measurement</td>
</tr>
<tr>
<td>Explosive diameter [mm]</td>
<td>AFRL measurement at 5 locations</td>
</tr>
<tr>
<td>Explosive density [kg/m$^3$]</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Explosive quality</td>
<td>AFRL X-ray</td>
</tr>
<tr>
<td>Particle diameter [mm]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle density [kg/m$^3$]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle volume fraction</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Ambient pressure [kPa]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Ambient temperature [°C]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Probe locations [m]</td>
<td>CCMT measurement</td>
</tr>
</tbody>
</table>

**Poster:** Kyle Hughes, UF

SEM of single steel particle at 1000x zoom.

SEM of several steel particles at 100x zoom.

Camera 3 at 1.067 ms after detonation showing the differing results for shock position
Other Microscale & Mesoscale Experiments

Mesoscale P-rad experiments performed at LANL

Poster: Kyle Hughes, UF

60% volume fraction

40%

20%

\[ t = 4 \, \mu s \]
CMT-nek Development

Goals

- Co-design an exascale code (CMT-nek) for compressible multiphase turbulence
- Perform micro, meso and demonstration-scale simulations
- Develop & incorporate energy and thermal efficient exascale algorithms

Poster: David Zwick, UF

Mach 3

- 32.4 M Degrees of freedom
- 1 M computational particles
- 32768 MPI ranks
Nek5000 + CMT-nek = Powerful Tool

<table>
<thead>
<tr>
<th></th>
<th>Existed</th>
<th>New</th>
<th>nek5000</th>
<th>CMT-nek</th>
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<tbody>
<tr>
<td><strong>Fluid-Fluid</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Incompressible</td>
<td>✔️</td>
<td></td>
<td>✔️</td>
<td>✔️</td>
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<tr>
<td>Low-Mach-number</td>
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<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
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<tr>
<td>Shock waves</td>
<td></td>
<td></td>
<td>✔️</td>
<td>✔️</td>
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<tr>
<td><strong>Tracer Particles</strong></td>
<td></td>
<td></td>
<td>✔️</td>
<td>✔️</td>
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<tr>
<td><strong>Particle-Fluid</strong></td>
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<td></td>
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<tr>
<td>(1-way coupled)</td>
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<td>✔️</td>
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<tr>
<td>(2-way coupled)</td>
<td></td>
<td></td>
<td>✔️</td>
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<tr>
<td><strong>Particle-Particle</strong></td>
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<td></td>
<td>✔️</td>
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<tr>
<td>(4-way coupled)</td>
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<td>✔️</td>
<td>✔️</td>
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- Goal is to expand from current ~250 users to $O(10^3)$ worldwide users
- Last month UF hosted the nek5000/CMT-nek developer/user meeting
- Key features: higher-order accuracy and scalability to $O(10^6)$ MPI ranks
Expansion Fan – Particle Bed Interaction

CCMT

Particle Velocity (m/s)

Fluid Velocity (m/s)

Front Rise Velocity

ASU Experiment

Strong Scaling:
- 15 million grid points
- 8.4 million particles

Weak Scaling:
- 864 grid points/rank
- 1024 particles/rank

864,760 grid points
8.4 million particles

- Particle Total
- Interpolation
- Hydrodynamic Force
- Integration
- Send Ghost Particles
- Projection
- Collisional Force
- Other
Co-Design & Dynamic Load Balancing

- Ghost particle algorithm
- Crystal-tuple inter-node data transfer for particles
- Dynamic load balancing: Centralized, distributed and hybrid algorithms
- Adaptive automated triggering of load balance
- Novel trace-based performance predictor

Poster: David Zwick, UF
Fully-Resolved Microscale Simulations

Purpose

- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation
- Shock propagation over a structured array
- Shock propagation over a random array
- Shock + Contact + particles
- Shock over deformable particles

With Kambiz Salari (LLNL)
PIEP Modeling Through Machine learning

\[ \phi = 44\%, \ Re = 20, \ N = 459 \]

Nek5000 simulation with PIEP

Data-driven force map

R² Values:

<table>
<thead>
<tr>
<th>R²</th>
<th>( \phi )</th>
<th>( Re )</th>
<th>Drag</th>
<th>Lift</th>
<th>Torque</th>
<th>Drag</th>
<th>Lift</th>
<th>Torque</th>
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<td>0.70</td>
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<tr>
<td>0.1</td>
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<td>0.2</td>
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<td>0.48</td>
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<td>0.45</td>
<td>0.21</td>
<td>0.01</td>
<td>0.09</td>
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<td>0.45</td>
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<td>0.63</td>
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CCMT PIEP: Pairwise Interaction Extended Point-particle
FPGA-Accelerated Design Space Exploration (DSE)

- **BE Advantage:** significantly faster than existing simulators
- **BE Limitation:** still not fast enough for DSE of exascale systems
- **Approach:** Use FPGA acceleration to improve exploration
  - Sacrifice analysis capabilities to prune design space
  - Use BE-SST to analyze remaining candidates

**CMT-nek design space:**
- 20 values for \( l_{el}, l_{x1}, l_{part} \)
- 10 different numbers of cores
- 10 different core types
- 10 different memory configurations
- 4 different network topologies

32 million options to explore

**BE Simulator (SW)**

~Minutes per simulation
Collapsed Pipeline Multi-FPGA Performance

CMT-Bone-BE is the proxy app

Performance prediction & DSE on varies MPI ranks

Behavioral emulation: BE-SST (software) vs FPGA (hardware)

Main point: FPGAs achieve similar scalability as BE-SST, but orders of magnitude faster

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>Num. of Events</th>
<th>% LU</th>
<th>Latency (cycles)</th>
<th>Hardware MSPS</th>
<th>Hardware GEPS</th>
<th>BE-SST KEPS</th>
<th>Hardware Speedup</th>
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<td>44</td>
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<td>92,160</td>
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<td>482</td>
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<td>128</td>
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<td>498</td>
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<td>515</td>
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<tr>
<td>512</td>
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<td>531</td>
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<td>1K</td>
<td>32</td>
<td>1,646,592</td>
<td>84</td>
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<td>1M</td>
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<td>112,459,776</td>
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<td>1,148,056</td>
<td>3.19x10^4</td>
<td>36</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>

Novo-G#

- 64 GiDEL ProceV (Stratix V)
- 4x4x2 3D torus or 5D hypercube
- 6 Rx-Tx links per FPGA
- Measured 32 Gbps per link
- 150 ns latency across links
- Require 64bits/cycle between FPGAs
- 335MHz, 21.4 Gbps, 51 additional lat
- 450MHz, 28.8 Gbps, 68 additional lat
- 500 MHz before link BW saturation

NNSA Lab Interaction

Student Internship Completed (19)

- Heather Zunino, Mentor: Dr. Kathy Prestridge (LANL)
- Kevin Cheng, Mentors: Dr. Maya Gokhale, Dr. Scott Lloyd (LLNL)
- Nalini Kumar, Mentor: Dr. James Ang (SNL)
- Chris Hajas, Mentor Dr. Maya Gokhale (LLNL)
- Christopher Neal, Mentor Dr. Kambiz Salari (LLNL)
- Carlo Pascoe, Mentor Dr. Maya Gokhale (LLNL)
- Giselle Fernandez, Mentors: Dr. Greogy Weirs, Dr. Vincent Mousseau (SNL)
- Justin Mathew, Mentor: Dr. Nick Hengartner (LANL)
- Trokon Johnson, Mentors: Drs. Cristina Garcia-Cardona, Brendt Wohlberg, Erik West (LANL)
- David Zwick, Mentors: Dr. John Pott, Dr. Kevin Ruggirello (SNL)
- Mohamed Gadou, Mentor: Dr. Galen Shipman (LANL)
- Goran Marjanovic, Mentors: Dr. Paul Crozier, Dr. Stefan Domino (SNL)
- Georges Akiki, Mentor: Dr. Marianne Francois (LANL)
- Paul Crittenden, Mentor: Dr. Sam Schofield (LLNL)
- Yash Mehta, Mentor: Dr. Kambiz Salari (LLNL)
- Kyle Hughes, Mentor: Dr. Kathy Prestridge (LANL)
- Prashanth Sridharan, Mentor: Dr. Jonathan Regele (LANL)
- Brad Durant & Fred Ouellet, Will finish internship this fall
Graduated PhD Students & Postdocs

- Angela Diggs, PhD (2015), Dr. S. Balachandar, MAE
  - Eglin AFB (continuing)
- Bertrand Rollin, Postdoc in thru August 2014
  - Assistant Professor, Embry Riddle, Daytona Beach FL
- Mrugesh Shringarpure, Postdoc in thru January 2016
  - Research Engineer, ExxonMobil, Houston TX
- Subbu Annamalai, PhD (2015), Dr. S. Balachandar, MAE; Postdoc in thru March 2017
  - Senior Systems Engineer, Optym, Gainesville FL
- Georges Akiki, PhD (2016), Dr. S. Balachandar, MAE; Postdoc thru March 2017
  - Postdoctoral Associate, LANL
- Nalini Kumar, PhD (2017), Dr. H. Lam, ECE
  - Intel, Santa Clara CA
- Yiming Zhang, PhD (2018), Drs. Haftka and Kim, MAE
  - GE Global Research, Niskayuna, NY
- Mohammad Gadou, PhD (2018), Dr. S. Ranka, CISE
  - Bloomberg, New York, NY
- Cameron Stewart, PhD (2018), Dr. Balachandar, MAE
  - Naval Surface Warfare Center, Indian Head, MD

4 More PhDs graduating this summer
Additional Information

- Additional Graduate Program Announcements
  - David Zwick – NSF Fellowship Graduate Program (Aug 2016)
  - Georges Akiki - MAE Best Dissertation Award (TSFD; May 2017)
  - Chandler Moore – NSF Fellowship Graduate Program (Aug 2017)
  - 6 other PhD students – UF Graduate Student Fellowship

- Other metrics (Y1 – Y4)
  - Publications: 134
  - Presentations: 94

- Deep Dive Workshops
  - Exascale & CS Issues, Feb 3-4, 2015, University of Florida
  - Multiphase Physics, Oct 13-14, 2016, Tampa FL
  - CMT-nek/nek5000, April 17-18, 2018, Tampa FL

- Center Webpage
  - http://www.eng.ufl.edu/ccmt/
Do you have any questions?