AST Review
April 12-13, 2018
Thursday April 12, 2018

7:45    Van pick up at University Hilton
8:00-9:00 Full Breakfast
         (Review Team and other NNSA personnel will meet in small conference room)
9:00-9:05 Introductions and opening remarks
9:05-10:15 Overview, Y5 Plans, Y4 Accomplishments (Jackson, Balachandar)
10:15-10:30 Coffee break
10:30-11:00 Integration of experiments and simulations (Rollin)
11:00-11:50 CMT-nek (Jason Hackl, David Zwick)
11:50-1:00 Lunch (RT will meet in small conference room)
1:00-1:50 Exascale (Lam, Stitt)
1:50-2:40 CS (Ranka, Banerjee)
2:45-3:00 Coffee break
3:00-3:50 V&V and UQ (Haftka, Park, Kim)
4:00-5:15 Lightning Round of Students’ Posters/ Poster Session (light refreshments served)
5:15-6:30 RT Caucus
6:30-8:00 Dinner (Faculty, Staff and Visitors; transportation will be provided for all visitors to the University Hilton)
Friday April 13, 2018

7:45 Van pickup at University Hilton
8:00-9:00 Full Breakfast
   (Review Team and other NNSA personnel will meet in small conference room)
9:00-10:30 Student Presentations – I
   Giselle Fernandez (15 mins)
   Chandler Moore (15 mins)
   Goran Marjanovic (15 mins)
   Kyle Hughes (15 mins)
   Heather Zunino (ASU; 30mins)
10:30-10:45 Coffee Break
10:45-11:15 Student Presentations – II
   Keke Zhai (15 mins)
   Sai Chenna (15 mins)
11:15-12:15 Y6 Plans and Center Response to RT Questions (PI Team)
12:15-4:00 Lunch (RT will meet in small conference room)
   Private RT deliberations (small conference room)
   Discussions between Center Management and AST as appropriate (large conference room)
4:00-4:30 RT Summary for Center Management (large conf. room)
4:30 Review ends
AST Review April 12-13, 2018 Attendee List

**Faculty**

- S. Balachandar “Bala” — University of Florida — bala1s@ufl.edu
- Rafi Haftka — University of Florida — haftka@ufl.edu
- Nam-Ho Kim — University of Florida — nkim@ufl.edu
- Herman Lam — University of Florida — hlam@ufl.edu
- Sanjay Ranka — University of Florida — ranka@cise.ufl.edu
- Greg Stitt — University of Florida — gstitt@ece.ufl.edu
- Tom Jackson — University of Florida — tlj@ufl.edu
- Siddharth Thakur “ST” — University of Florida — sst@ufl.edu
- Bertrand Rollin — Embry-Riddle — rollinb@erau.edu
- Ju Zhang — Florida Institute of Technology — jzhang@fit.edu

**Review Team**

- Sam Schofield (Chair) — LLNL — schofield5@llnl.gov
- Brian Carnes (V&V/UQ) — SNL — bcarnes@sandia.gov
- Robert Clay (CS) — SNL — rclay@sandia.gov
- Gabe Rockefeller (CS) — LANL — gaber@lanl.gov
- Kambiz Salari (Physics) — LLNL — salari1@llnl.gov
- Erik Vold (Physics) — LANL — elv@lanl.gov
- Jeremiah Wilke (CS) — SNL — jjwilke@sandia.gov

**Others**

- Tina Macaluso — Leidos/NESD — antoinette.macaluso@leidos.com
- Bob Voigt — Leidos/NESD — rvoigt@krellinst.org
- John Feddema — SNL — jtfedde@sandia.gov
- Fernando Grinstein — LANL — fgrinstein@lanl.gov
- Ana Kupresanin — LLNL — kupresanin1@llnl.gov
- Alan Kuhl — LLNL — kuhl2@llnl.gov
- Brian Taylor — Eglin AFB — brian.taylor.56@us.af.mil
- Greg Weirs — Sandia — vgweirs@sandia.gov

**Research Staff**

- Tania Banerjee — University of Florida — tmishra@cise.ufl.edu
- Kei Fujisawa — University of Florida — fujisawa_ocean_eng@yahoo.co.jp
- Jason Hackl — University of Florida — jason.hackl@ufl.edu
- Nguyen Tri Nguyen — University of Florida — tringuynett@gmail.com
- Chanyoung Park — University of Florida — cy.park@ufl.edu
**Center for Compressible Multiphase Turbulence**

**Students**
Ryan Blanchard  
Sai Chenna  
Paul Crittenden  
Brad Durant  
Giselle Fernandez  
Mohamed Gadou  
Joshua Gargo  
Trokon Johnson  
Tanner Jones  
Kyle Hughes  
Rahul Koneru  
Tadbhagya Kumar  
Adeesha Malavi  
Goran Marjanovic  
Yash Mehta  
Chandler Moore  
Aravind Neelakantan  
Samaun Nili  
Brandon Osborne  
Frederick Ouellet  
Carlo Pascoe  
Raj Rajagoplan  
Ben Reynolds  
Chad Saunders  
Shirly Spath  
Prashanth Sridharan  
Cameron Stewart  
Keke Zhai  
Yiming Zhang  
Heather Zunino  
David Zwick  

**Administration Staff**
Hollie Starr  

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epzbekwic@ufl.edu  

**University of Florida**  
hstarr@ufl.edu
Overview & Integration
Y4 Accomplishments
Y5 Plans

T.L. Jackson
S. Balachandar

AST Meeting Agenda

Thursday
- Overview, Integration, Y5 Plans, Y4 Accomplishments (Jackson, Balachandar)
- Integrated Simulations: Transitioning from RocFlu to CMT-nek (Rollin)
- CMT-nek (Hackl, Zwick)
- Lunch
- BE Results at Scale (Lam, Stitt)
- CMT-nek: CS Updates (Ranka)
- V&V and UQ (Park)
- Student Lightning Round
- Poster Session
- RT Caucus
- Dinner 6:30-8:00 (University Hilton; Dogwood Room)

Friday
- Student Presentations (7)
- Y6 Plans and Response to RT Questions (PI Team)
- Lunch
- RT Deliberations/Summary
Leadership

Phyics and Code Development

S. (Bala) Balachandar
Siddharth Thakur (ST)
Thomas Jackson
Paul Fischer
Ju Zhang
Bertrand Rollin
Stanley Ling

UQ and V&V

Raphael Haftka
Nam-Ho Kim

Experiments

Ronald Adrian
Charles Jenkins
Donald Littrell
Sanjay Ranka
Herman Lam
Gregory Stitt
Scott Parker

CS/Exascale

UF members in red

Research Staff & Senior PhD Students

Tania Banerjee
Angela Diggs
Kei Fujisawa
Jason Hackl

Nguyen T. Nguyen
Chanyoung Park
Carlo Pascoe
Current Students (Undergraduate & Graduate)

Heather Zunino
ASU
Prashanth Sridharan
Yash Mehta
Yiming Zhang
Frederick Ouellet
Brad Durant
Giselle Fernandez
Mohamed Godou
Joshua Gorna
Taokin Johnson
Kyle Hughes
Tanner Jones
Rahul Konuru
U/IU (Illinois)
Aderisha Malavi
Goran Marjanovic
Yash Mehta
Chandler Moore
Aravind Neelakantan
Samaun Nili
Brandon Osborne
Frederick Duquette
Raj Rajegopalan
Ben Reynolds (B.S.)
Chad Saunders
Shirly Spath (B.S.)
Prashanth Sridharan
Keke Zhai
Yiming Zhang
Heather Zunino (ASU)
David Zwick

Internship Program – Completed (16)

- Heather Zunino
  LANL
  May-Aug, 2014
  Dr. Kathy Prestridge
- Kevin Cheng
  LLNL
  May-Aug, 2014
  Dr. Maya Gokhale
- Nalini Kumar
  Sandia
  March-Aug, 2015
  Dr. James Ang
- Christopher Hajas
  LLNL
  May-Aug, 2015
  Dr. Maya Gokhale
- Christopher Neal
  LLNL
  June-Aug, 2015
  Dr. Kambiz Salari
- Carlo Pascoe
  LLNL
  June-Aug, 2015
  Dr. Maya Gokhale
- Giselle Fernandez
  Sandia
  Oct-Dec, 2015
  Drs. Gregory Weirs & Vincent Mousseau
- Justin Mathew
  LANL
  May-Aug, 2015
  Dr. Nick Hengartner
- David Zwick
  Sandia
  May-Aug, 2016
  Drs. John Pott & Kevin Ruggirello
### Internship Program – Completed (16)

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Duration</th>
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<tbody>
<tr>
<td>Goran Marjanovic</td>
<td>Sandia</td>
<td>Aug-Nov, 2016</td>
<td>Drs. Paul Crozier &amp; Stefan Domino</td>
</tr>
<tr>
<td>Georges Akiki</td>
<td>LANL</td>
<td>May-Aug, 2016</td>
<td>Dr. Marianne Francois</td>
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<tr>
<td>Paul Crittenden</td>
<td>LLNL</td>
<td>Spring, 2017</td>
<td>Drs. Kambiz Salari &amp; Sam Schofield</td>
</tr>
<tr>
<td>Mohamed Gadou</td>
<td>LANL</td>
<td>Summer, 2017</td>
<td>Dr. Galen Shipman</td>
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<tr>
<td>Trokon Johnson</td>
<td>LANL</td>
<td>Summer, 2017</td>
<td>Drs. Cristina Garcia-Cardona, Brenda Wohlgberg, Erik West</td>
</tr>
<tr>
<td>Yash Mehta</td>
<td>LLNL</td>
<td>Summer, 2017</td>
<td>Dr. Kambiz Salar</td>
</tr>
<tr>
<td>Kyle Hughes</td>
<td>LANL</td>
<td>Fall, 2017</td>
<td>Dr. Kathy Prestridge</td>
</tr>
</tbody>
</table>

### Internship Program – Not Completed

- Summer 2018
  - Prashanth Sridharan (MAE, Physics); LANL
  - Fred Ouellet, PhD (MAE, Physics and UQ); LANL

- Brad Durant, PhD (MAE, Physics and UQ)
- Joshua Garno, PhD (MAE, Physics and UQ)
- Chandler Moore, PhD (MAE, Physics) (NSF Fellowship)
Graduated Students & Postdocs

- Kevin Cheng, MS (2014), Dr. Alan George, ECE
- Hugh Miles, BS (2015), Dr. Greg Stitt, ECE
- Chris Hajas, MS (2015), Dr. Herman Lam, ECE
- Angela Diggs, PhD (2015), Dr. S. Balachandar, MAE
  - Currently employed at Eglin AFB and working with center
- 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
- Parth Shah, MS (2016), Drs. H. Lam and G. Stitt
  - 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
- Ajay Ramaswamy, MS (2017), Drs. H. Lam and G. Stitt
- Justin Matthew, MS (2017), Drs. Haftka and Kim, MAE
  - Proctor & Gamble, Cincinnati OH
- Yiming Zhang, PhD (2018), Drs. Haftka and Kim, MAE
  - GE Global Research, Niskayuna, NY
PhD Students Expected Graduation Dates

- 2018
  - Paul Crittenden
  - Giselle Fernandez
  - Mohamed Gadou
  - Kyle Hughes
  - Goran Marjanovic
  - Yash Mehta
  - Carlo Pascoe
  - Prashanth Sridharan
  - Heather Zunino
- 2019
  - Rahul Koneru
  - Samaun Nili
  - Fred Ouellet
  - Keke Zhai
  - David Zwick
- 2020
  - Brad Durant
  - Josh Garno
- 2021
  - Sai Chenna
  - Trokon Johnson
  - Adeeja Malavir
  - Chandler Moore
  - Aravind Neelakantan
  - Raj Rajagopalan

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)
- 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
  - Multiphase Deep Dive 2; Stanford lead with Florida co-lead; Fall 2018
- Center Webpage
  - http://www.eng.ufl.edu/ccmt/
Additional Information

- CMT-nek/nek5000
  - April 17-18, 2018, Tampa FL
  - 24 talks
    - 4 from Florida – expanding nek5000
  - 33 participants
    - DOE laboratories represented
    - 3 Countries (US, Canada, Sweden)

Internal Workshops

- "Dakota - Tutorial" – organized by Chanyoung Park, February 19, 2015
- “A Boot Camp on CMT-nek” – organized by B. Rollin and J. Hackl, November 29, 2017
Educational Programs

- Institute for Computational Science (ICE)
- Course in Verification, Validation and Uncertainty Quantification taught every third semester (N. Kim, R. Haftka)
- Yearly a specialized course for HPC for computational scientists (as part of the Computational Engineering Certificate) (S. Ranka)
- Fall, 2016, 2018 – new graduate course on multiphase flows (S. Balachandar)
- Discusses exascale challenges and the NGEE work in the reconfigurable computing course (EEL5721/4720) and digital design (EEL4712) (H. Lam, G. Stitt)
- Uses the CCMT center as a motivational example in Introduction to Electrical and Computer Engineering (EEL3000) (H. Lam, G. Stitt)
- EEL6763 (Parallel Computer Architecture) (Ian Troxel)

Management: Tasks and Teams

The Center is organized by physics-based tasks and cross-cutting teams, rather than by faculty and their research groups

<table>
<thead>
<tr>
<th>Hour time slots</th>
<th>Exascale</th>
<th>CMT-nek</th>
<th>CS</th>
<th>Micro</th>
<th>Macro/Meso</th>
<th>UQ</th>
<th>Exp</th>
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<td>Macro/Meso</td>
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</table>

- Weekly interactions (black); Regular interactions (red)
- Teams include students, staff, and faculty
- All staff and large number of graduate students located on 2nd floor of PS&T Building
- Construction in PS&T Building to add 6 new office spaces for students
- All meetings held in PS&T Building
Outline

- Background
- Scope of the center
- Y4 accomplishments
- Y5 plans
- RocFlu to CMT-nek transition
- Integration and timeline
Demonstration Problem

PM-1: Blast Wave Location
PM-2: Particle Front Location
PM-3: Number of Instability Waves
PM-4: Amplitude of Instability Waves

Prediction Metrics
**Sequence of Events**

- **Dispersion phase**
  - Explosive material
  - Hot, dense, high pressure gas
  - Shock wave

- **Detonation phase**
  - Metal particles

- **Compaction/collision phase**

---

**Physical Models – Sources of Error**

- **T8**: Deformation model
- **T4**: Interaction model
- **T5**: Compaction model

- **T1**: Detonation model

- **T2**: Multiphase turbulence model
- **T3**: Thermodynamic & transport model
- **T6**: Point particle force model
- **T7**: Point particle heat transfer model
Updated Scope

- Our focus will be on
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities
  - Gas-particle coupling
  - Mixing at the rapidly expanding material front
  - Self-assembly of explosive-driven particles
  - Reduced emphasis on initial compaction

- Will avoid 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)
**Sources of Errors & Uncertainties**

- T1: Detonation modeling
- T2: Multiphase turbulence modeling
- T3: Thermodynamics & transport properties
- T4: Particle-particle interaction modeling
- T5: Compaction modeling
- T6: Force coupling modeling
- T7: Thermal coupling modeling
- T8: Particle deformation and other complex physics
- T9: Discretization and numerical approximation errors
- T10: Experimental and measurement errors & uncertainties

**Key Focus**
- Advance state-of-the-art
  - Multiphase turbulence
  - Force coupling model

**Uncertainty Budget – Overall Plan**

- **Macroscale**
  - T4: Discretization Errors
  - T2: T6
  - T5: Experimental Error & Uncertainty

- **Mesoscale**
  - ASU Mesoscale Experiments & Simulations
  - Sandia shock experiments & simulations
  - Eglin mesoscale Experiments & Simulations

- **Microscale**
  - Shock-Tube Track
  - Characterize Particle Bed
  - Characterize Particle Curtain
  - Characterize Particle Bed
  - Characterize Particles After Detonation
  - Calibration of Explosion

- **Explosive Track**
  - T8

- T2 – Turbulence modeling
- T5 – Compaction modeling
- T4 – Particle interaction modeling
- T6 – Force coupling modeling
4 Micro/Meso Campaigns & Target Models

- Sandia shock-tube
  - T6: Force coupling and T4: Particle-particle interaction
- ASU expansion fan
  - T2: Multiphase turbulence and T4: Particle-particle interaction
- Eglin microscale
  - T6: Force coupling
- Eglin mesoscale gas-gun
  - T5: Compaction
- Demonstration problem
  - Yearly hero run

Uncertainty Reduction Workflow

Experiments → Experimental input → Simulations
Experimental input → Input uncertainty → Target model error
Target model error → Measured Metrics → Computed Metrics

Large? → Target model improvement

Empty Success (Small error, but Large Uncertainty)
Useful Failure

Measurement / Prediction → Control Parameter

Experiments → Measurement / Prediction → Simulation

CCMT
Uncertainty Budget Workflow

- Experiments
- Experimental input
- Input uncertainty
- Simulations
- Forensic
- Measured Metrics
- Target model error
- Computed Metrics
- Error
- Uncertainty/error reduction
- Large?
- Target model improvement

- Uncertainty:
  - Sampling uncertainty
  - Measurement uncertainty
  - Measurement processing error

- Error:
  - Propagated uncertainty
  - Stochastic variability
  - Discretization error
  - Neglected feature/physics

- Large?
- Uncertainty/error reduction

UB Workflow - Experiment Worksheet

- Experimental input
  - Shock properties, particle properties, curtain properties, ...

- Input uncertainty
  - Quantified uncertainties in all the above

- Prediction metrics
  - PM1: Shock position, PM2: Upstream and downstream curtain

- Uncertainty & error quantification (UQ)
  - Error in PM1 and PM2 obtained from Schlieren
  - Error in X-ray image particle volume fraction

- Uncertainty & error reduction (UR)
  - Perform new experiments without spanwise gap
  - Improved measurement to reduce volume fraction uncertainty
### Hierarchical Error Estimation and UQ

- VVUU framework
- Target model
- Eglin Macroscale Simulations
- Eglin Macroscale Experiments
- Eglin Macroscale Simulations
- Eglin Macroscale Experiments
- Eglin Macroscale Simulations
- Eglin Macroscale Experiments

### Other Simulation Campaigns

- Microscale simulations of shock+contact over structured and random array of particles
  - Testing and improvement of force coupling (T6)
- Mesoscale simulations of turbulent multiphase jet/plume
  - Testing and improvement of multiphase LES (T2)
- Mesoscale simulations of sedimentation
  - Testing and improvement of particle-particle interaction model (T4)
- Mesoscale simulations of controlled instability
  - Evaluation of PM3 and PM4
**Key Accomplishments**

- Tight integration
- Empower students and staff
- PIEP model + Machine Learning
- CMT-nek a versatile multiphase flow code (scalable to >$O(10^6)$ core)
- Culture of UQ integration
- BE framework and FPGA
- Dynamic load balancing

**Y4 Highlights**

1. Macroscale – Hero Run
2. Blastpad & other validation experiments
3. CMT-nek development and transition
4. Mesoscale – CMT-nek simulation of expansion fan
5. Microscale – Shock + Contact
6. UQ workflow
7. Design space exploration with Behavioral Emulation
8. Dynamic load balancing of Euler-Lagrange
1: Demonstration Problem (Macroscale)

Goal
- Yearly perform the largest possible simulations of the demonstration problem and identify improvements to be made in predictive capability

Year 4
- Used existing code to perform large-scale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)
- Integrate additional capabilities for the hero runs: real gas EOS, reactive burn

Presentation
- Bertrand Rollin

CMT-Hero-1 demonstration simulation

- Features:
  - 32.4 M Degrees of freedom
  - 1 M computational particles
  - 0.3 x 0.3 x 0.0015 m
  - t_max = 0.3ms
  - 32768 MPI ranks
2: Blastpad Experiments

Goals

- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

Year 4

- Blast pad experiments at Eglin AFB
- Detailed instrumentation for validation
- Simulation informed experiments
- Integrated UQ

Presentation

- Bertrand Rollin, Kyle Hughes

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Source</th>
</tr>
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<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>
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<td>Explosive density [kg/m³]</td>
<td>AFRL calculation</td>
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<td>Explosive quality</td>
<td>AFRL X-ray</td>
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<td>Particle diameter [mm]</td>
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<td>Particle density [kg/m³]</td>
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<td>Particle volume fraction</td>
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<td>Ambient pressure [kPa]</td>
<td>AFRL weather station</td>
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<td>Ambient temperature [°C]</td>
<td>AFRL weather station</td>
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<tr>
<td>Probe locations [m]</td>
<td>CCMT measurement</td>
</tr>
</tbody>
</table>

SEM of single steel particle at 1000x zoom.
SEM of several steel particles at 100x zoom.

Tungsten Liner
Steel Liner
3: 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

Year 4
- Developed and released microscale version of CMT-nek for microscale simulations
- Developed and released mesoscale version of CMT-nek for mesoscale simulations
- Shock capturing with EVM
- CMT-nek in nek5000 repository

Presentation
- Jason Hackl and David Zwick
- Goran Marjanovic

Multiphase Capabilities

<table>
<thead>
<tr>
<th></th>
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<th>New</th>
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<td>Incompressible</td>
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<td>Low-Mach-number</td>
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<td>Shock waves</td>
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</tr>
<tr>
<td>Tracer Particles</td>
<td></td>
<td></td>
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<td>✓</td>
</tr>
<tr>
<td>Particle-Fluid</td>
<td></td>
<td>Dilute</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Dense</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Particle-Particle</td>
<td></td>
<td></td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

Multiphase exascale problems rely on efficient communication and computations to maintain both accuracy and scalability.
Algorithmic Scaling

**Ideal Setup:**
- Uniform flow in a periodic box
- N = 6 grid points in each direction

**Strong Scaling (s):**
- 15 million grid points
- 8.4 million particles

**Weak Scaling (w):**
- 864 grid points/rank
- 1,024 particles/rank

<table>
<thead>
<tr>
<th>Operation</th>
<th>Slope (s)</th>
<th>Slope (w)</th>
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<tbody>
<tr>
<td>Interpolation</td>
<td>-1.00</td>
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<td>Projection</td>
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<td>Sand Ghosts</td>
<td>-0.72</td>
<td>0.12</td>
</tr>
<tr>
<td>Collision Force</td>
<td>-1.95</td>
<td>-0.01</td>
</tr>
</tbody>
</table>

- Presentation
  - Keke Zhai

---

4: Mesoscale Simulations & Experiments

**Goal**
- Perform a hierarchy of mesoscale simulations to allow rigorous validation, uncertainty quantification and propagation to the demonstration problem

**Year 4**
- 4-way coupled simulation with CMT-nek
- Mesoscale simulations of expansion fan over a bed of particles
- 4-way coupled simulations with and without PIEP
- Bundled simulations for UQ

**Presentation**
- David Zwick

---
4: Mesoscale Simulations & Experiments

**Goals**
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

**Year 4**
- Expansion fan experiments at ASU
- Detailed instrumentation for validation
- Simulation informed experiments
- Integrated UQ

**Presentation**
- Heather Zunino (ASU)

---

5: Microscale Simulations

**Goals**
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation

**Year 4**
- Shock propagation over a structured array
- Shock propagation over a random array
- Shock + Contact + particles
- Shock over deformable particles

With Kambiz Salari (LLNL)
**5: Pairwise Interaction Extended Point-Particle Model**

Pairwise Interaction Extended Point-Particle Model (PIEP) is used to simulate high-speed compressible flows. The table shows comparison between PIEP-Physics and PIEP-Hybrid models for different conditions.

<table>
<thead>
<tr>
<th>Re Values</th>
<th>PIEP-Physics</th>
<th>PIEP-Hybrid</th>
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</thead>
<tbody>
<tr>
<td>( \phi = 44% , Re = 20, N = 459 )</td>
<td>Drag, Lift, Torque</td>
<td>Drag, Lift, Torque</td>
</tr>
<tr>
<td>0.1 46</td>
<td>0.70, 0.88, 0.75</td>
<td>0.72, 0.75, 0.79</td>
</tr>
<tr>
<td>0.1 78</td>
<td>0.65, 0.88, 0.66</td>
<td>0.67, 0.72, 0.72</td>
</tr>
<tr>
<td>0.1 179</td>
<td>0.35, 0.59, 0.44</td>
<td>0.44, 0.69, 0.52</td>
</tr>
<tr>
<td>0.2 18</td>
<td>0.38, 0.34, 0.44</td>
<td>0.46, 0.74, 0.71</td>
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<tr>
<td>0.2 88</td>
<td>0.30, 0.48, 0.72</td>
<td>0.63, 0.63, 0.77</td>
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<tr>
<td>0.46 21</td>
<td>0.91, 0.09, 0.47</td>
<td>0.55, 0.59, 0.76</td>
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<tr>
<td>0.46 118</td>
<td>0.21, 0.19, 0.51</td>
<td>0.03, 0.57, 0.65</td>
</tr>
</tbody>
</table>

**Presentation:** Chandler Moore

---

**6: UQ Workflow**

**Goals**
- Develop UB as the backbone of the Center
- Unified application of UB for both physics and exascale emulation

**Year 4**
- Identify main uncertainty sources and quantify their contributions to the model uncertainty of the shock tube simulation
- Reduce uncertainty to focus on model error
- UQ and propagation in the context of exascale emulation
- JWL mixture-EOS surrogate for efficient computation

**Presentation**
- Nam-Ho Kim, Giselle Fernandez, Kyle Hughes

**Sandia shock tube**

**UQ Workflow**

**Pseudo-turbulence**
**UQ of Eglin Microscale**

- U in Density with CI 95%
- U in Diameter with CI 95%
- U in Explosive Density with CI 95%

- Feb 15 #1
- Feb 15 #2
- Oct 14 #1

**7: Exascale Emulation**

**Goal**
- Develop behavioral emulation (BE) methods and tools to support co-design for algorithmic design-space exploration and optimization of key CMT-bone kernels & applications on future Exascale architectures

**Year 4**
- Enhanced BE methods with network models, interpolation schemes, and benchmarking for CMT-bone AppBEOS
- Performed large-scale experiments on DOE platforms with BE-SST simulator
- Started design space exploration
- Improved throughput and scalability for FPGAs

**Presentation**
- Herman Lam, Greg Stitt, Sai Chenna
**Design Space Exploration: Results**

- **Application**: CMT-nek particle solver
- **Architecture**: Vulcan (512k cores)
- 1 design candidate** – BE-SST** - 12000 minutes
- Entire space (270K candidates) – BE-FPGA - 100 minutes

**BE-FPGA Simulations of Vulcan (512k cores)**

- **BE-FPGA Simulation**
- **BE-SST Simulation (32k cores)**
- **CMT-nek Particle-Solver Execution (4k cores)**

**Goal**

- Derive computationally intensive portions of the CMT-nek code and understand its performance, thermal and energy issues

**Year 4**

- Carried out extensive investigation of performance and energy issues for CMT-bone
- Hybrid CPU-GPU implementation of CMT-bone and optimization
- Thermal aware optimization
- Dynamic load balancing with particles

**Presentation**

- Sanjay Ranka, Keke Zhai

**8: Dynamic Load Balancing**

**67,206 MPI ranks**
1,867 nodes, 36 cores/node
900,000 elements
1,125,000,000 particles
Grid size: 5x5x5
Rarefaction test
9.97x improvement in performance
CMT-nek Transition Workshop

A Boot Camp on CMT-nek
November 29, 2017
Organizers: Bertrand Rollin and Jason Hackl

**Agenda**

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  Speaker: Jason Hackl | 1:30 pm – 2:15 pm

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  Speaker: David Zwick | 2:15 pm – 2:45 pm
  
  Break

- **Running CMT-nek**
  Speakers: Goran Marjanovic and Brad Durant | 3:00 pm – 3:45 pm

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- **Lesson Learnt from CCMT’s Simulations**
  Speakers: Fred Ouellet and Yash Mehta | 4:15 pm – 4:45 pm

---

**CMT-Hero Timeline**

<table>
<thead>
<tr>
<th>Y4-Q1</th>
<th>Y4-Q2</th>
<th>Y4-Q3</th>
<th>Y4-Q4</th>
<th>Y5-Q1</th>
<th>Y5-Q2</th>
<th>Y5-Q3</th>
<th>Y5-Q4</th>
</tr>
</thead>
<tbody>
<tr>
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</tbody>
</table>

- **S4a CMT-Hero 1**
  - EVM tuning
  - 4-way Coupling
  - Compaction

- **S4b CMT-Hero 2**
  - 4-way coupling

- **S4c CMT-Hero 3**
  - Real gas EOS
  - Outflow BC
  - Load Balancing

- **S4d CMT-Hero 4**
  - Reactive burn
  - Smart start
  - Improved models
Demonstration Problem Roadmap

<table>
<thead>
<tr>
<th>Year 1</th>
<th>Year 2</th>
<th>Year 3</th>
<th>Year 4</th>
<th>Year 5</th>
<th>Year 6</th>
<th>Year 7</th>
<th>Year 8</th>
<th>Year 9</th>
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<tbody>
<tr>
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<tr>
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<tr>
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<tr>
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<td>Initial Particle Number fractions</td>
<td>Initial Particle Number fractions</td>
<td>Initial Particle Number fractions</td>
<td>Initial Particle Number fractions</td>
<td>Initial Particle Number fractions</td>
</tr>
<tr>
<td>Gas-Particle Coupling</td>
<td>Gas-Particle Coupling</td>
<td>Gas-Particle Coupling</td>
<td>Gas-Particle Coupling</td>
<td>Gas-Particle Coupling</td>
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<td>Particles in cold perturbation</td>
</tr>
<tr>
<td>Reactive burn</td>
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<td>Reactive burn</td>
<td>Reactive burn</td>
<td>Reactive burn</td>
<td>Reactive burn</td>
</tr>
</tbody>
</table>

Transition to CMT-nek – Simulation Plan

- CMT-nek support
  - Benjamin Buick
  - Breden Durante
  - Byoung T. Lim

- Blastpipe (3D)
  - UA/UQ on Prediction Targets
  - Complex Flows

- Sudden Shock Tube
  - Shock-Particle Interaction
  - Multiphase Turbulence

- Spin Microscope
  - Real gas EOS
  - Reactive Burn
  - Black-Particle Interaction
  - Outflow Boundary Conditions

- Continuous Modeling Effort
  - PEP model Extension
  - EOS/thermodynamics
  - Expansion Finiti
  - Particle Interaction
  - Gas/Phase Interaction
**CMT-nek Micro-Meso-Hero Timeline**

<table>
<thead>
<tr>
<th>S3 Micro Sims</th>
<th>S2 ASU Meso</th>
<th>S3 Eglin Meso</th>
<th>S4 CMT-Hero</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y4-Q1</td>
<td>Y4-Q2</td>
<td>Y4-Q3</td>
<td>Y4-Q4</td>
</tr>
<tr>
<td>4-way coupling</td>
<td>Load Balancing</td>
<td>Compaction</td>
<td>ASU Meso</td>
</tr>
<tr>
<td>Goran Marjanovic</td>
<td>David Zwick</td>
<td>Josh Garno</td>
<td>Rahul Koneru</td>
</tr>
</tbody>
</table>

**Major Plans for Y5**

- Complete CMT-Hero2, CMT-Hero3, and CMT-Hero4
- Complete a UB cycle for ASU expansion fan, Eglin mesoscale
- Propagate uncertainties and perform the UB cycle for the Eglin blastpad experiment
- Complete ASU simulation at an unprecedented resolution and detailed comparison with experimental measurements
- Finalize load balancing and release it for wide external use
- Complete the implementation of CMT-nek on CPU-GPU
- Predict and later test the performance of CMT-nek on “Summit”
- End-to-end design space exploration of CMT-nek using multiple FPGA
Risks & Mitigation

- Comprehensive risk assessment and backup plans from each team
- We have successfully crossed some fundamental risks we started with: Will DGSEM work for compressible flows with shocks? Will Eglin carry out macroscale experiments?
- Optimal tuning of EVM for extreme blast conditions
  - Stay with first order wave-speed viscosity, etc.
- Particle compaction is too hard at explosive condition
  - Solve very early time using 2-fluid model
- Building even a surrogate of the macroscale problem may be too expensive
  - Limit to one or two high fidelity & several lower fidelity simulations
- Current load balancing strategy may face memory limitation
  - Experiment domain partitioning strategies that loosely maintain spatial locality
- BE-SST simulation of beyond 1M MPI ranks
  - Limit to 1M MPI ranks

Do you have any questions?
Integrated Simulations:
Transitioning from Rocflu To CMT-nek

Bertrand Rollin
### From Rocflu to CMT-nek

<table>
<thead>
<tr>
<th>Method</th>
<th>Rocflu</th>
<th>CMT-nek</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh</td>
<td>Mixed cells (tetrahedra, hex)</td>
<td>Spectral elements (hex)</td>
</tr>
<tr>
<td>Shock capturing</td>
<td>WENO gradient reconstruction</td>
<td>Artificial viscosity</td>
</tr>
<tr>
<td>Time marching</td>
<td>RK3, RK4</td>
<td>TVDRK3</td>
</tr>
<tr>
<td>Point particle modeling</td>
<td>2-way coupled</td>
<td>4-way coupled</td>
</tr>
<tr>
<td>Parallel capability</td>
<td>O(10^6) MPI ranks, No load-balancing</td>
<td>O(10^6) MPI ranks, load-balanced</td>
</tr>
</tbody>
</table>

- Jason Hackl and David Zwick, 11:00 am

---

### CMT-nek Transition Workshop

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- **Lesson Learnt from CCMT's Simulations**  
  Speakers: Fred Ouellet and Yash Mehta | 4:15 pm – 4:45 pm
Bring predictive capabilities to particle-laden flow simulations under extreme conditions.

Sequence of Events and Physical Modeling

- **Detonation phase**
  - T1: Detonation model
  - Explosive material
  - Hot, dense, high pr gas
  - Shock wave

- **Compaction/collision phase**
  - T2: Multiphase turbulence model
  - T4: Collision model
  - T5: Compaction model
  - T6: Point particle force model

- **Deformation model**
  - T8: Deformation model
  - Metal particles

- **Dispersion phase**
  - T3: Thermodynamic & transport model
  - T7: Point particle heat transfer model

Key physics models:
- Red: T1, T2, T3, T4, T5, T6

Other physics models:
- Black: T7
## Demonstration Problem Roadmap

<table>
<thead>
<tr>
<th>Case</th>
<th>Simulation Time</th>
<th>Degrees of Freedom</th>
<th>MPI ranks</th>
<th>No. computational particles</th>
<th>Initial Particle volume fraction</th>
<th>Gas-Particle Coupling</th>
<th>Particle bed perturbation</th>
<th>Reactive burn</th>
<th>Equation of state</th>
<th>Year 1 - 4</th>
<th>Year 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hero 1</td>
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<tr>
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<tr>
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<tr>
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</tr>
</tbody>
</table>

- CCMT
- Demonstration Problem Roadmap

### CMT-nek Development

- EVM parameter tuning
- Equation of State/Multi-species formulation
- Reactive Burn Initial Conditions
- Boundary Conditions
- 4-way coupling
- Particles Compaction
- Particles Load Balancing
- Intelligent Starting Condition
- Integration of improved coupling models

- Jason Hackl and David Zwick, 11:00 am
CMT-Hero Timeline

CMT-Hero 1
- EVM tuning
- 4-way coupling

CMT-Hero 2
- Compaction
- Outflow BC

CMT-Hero 3
- Real gas EOS
- Load Balancing

CMT-Hero 4
- Reactive burn
- Smart start
- Improved models

CMT-HERO 1 – Initial Conditions

Mesh Parameters

- Domain size ($L_x \times L_y \times L_z$): 0.3m x 0.3m x 0.015m
- Number of elements ($N_x \times N_y \times N_z$): 1.2 M (636 x 636 x 3)
- Order of polynomial (p): 3
- Number of Degree of Freedom: 32.4 M

Initial Conditions

- Pressure: 100 atm
- Density: 23,536.8 kg/m³
- Temperature: 1500 K
- Charge radius: 3.8 mm
- Particle bed thickness: 2 cm
- No. of particles: 1 M
- Particle Volume Fraction: 5%

Parameters in Entropy Viscosity Method

- $C_{max}$ (Constant in wave speed based viscosity): 1.0
- $C_e$ (Constant in entropy residual based viscosity): 40
CCMT

CMT-Hero 1

- Features:
  - 32.4 M Degrees of freedom
  - 1 M computational particles
  - 0.3 x 0.3 x 0.0015 m
  - $t_{\text{max}} = 0.3$ ms
  - 32768 MPI ranks

➡️ Chanyoung Park, 3:00 pm

CMT-Hero 1 – Profiles

- Gas Density (kg/m$^3$)
- Particle Volume Fraction
CMT-Hero 1 – Prediction Metrics

- Time (s)
  - 0
  - 50
  - 100
  - 150
  - 200
  - 250

Blast Wave Location (m)
- 0
- 0.05
- 0.1
- 0.15
- 0.2

Outer Front Location (m)
- 0
- 0.05
- 0.1

CMT-Hero 1

Hero Run 3

- Features:
  - 60 Million computational cells
  - 15 Million computational particles
  - r_{max} = 4.00 m
  - t_{max} = 2.50 ms
  - 5760 cores
  - 1 mode perturbation in the initial particle distribution
Demonstration Problem: Predictions

Blast Wave Location (PM-1)

Particle Front Location (PM-2)
The initial volume fraction distribution leaves an imprint in the fluid flow field.

The initial volume fraction distribution creates a channeling effect.

Amplification of Departure From Axisymmetry

1. Initial multi-modal perturbation in the particles
2. Metric of departure from axisymmetry
3. Which initial disturbances amplify most the departure?
4. High number of simulations (2500)
5. Surrogate Models
6. Optimization

Giselle Fernandez, tomorrow 10:30 am
Eglin Blastpad Experimental Setup

- Six shots
  - 2 bare charges
  - 1 charge w/tungsten (n)
  - 2 charges w/steel (n)
  - 1 charge w/steel (u-n) (Barreto et al. 2015)

- Instrumentation:
  - 54 pressure probes
  - 8 Momentum traps
  - 4 high speed video cameras
  - 6 Linear optical transducers
Eglin Blastpad Simulation Setup

Note: Bare charge setup is shown, particles will be included in parallel runs

Preliminary Simulation Details:

- 1 million cells in two dimensions
- To be run on 256 cores using LLNL’s Quartz machine
- Exhaust boundary is an outflow
- Other bottom boundaries are slipwalls
- 4 probes set in locations of experimental sensors
- 40 other probes set in near-charge region

Demonstration Problem – A Summary

- Last Rocflu Hero Run completed
- UQ analysis continues
- Study of Physics of the Demonstration problem continues
- CMT-Hero 1 completed
- CMT-Hero 2 in progress
- Blastpad tests in progress

David Zwick, 11:00 am
4 Micro/Meso Campaigns & Target Models

- Sandia shock-tube
  - T6: Force coupling and T4: Particle-particle interaction
- ASU expansion fan
  - T2: Multiphase turbulence and T4: Particle-particle interaction
- Eglin microscale
  - T6: Force coupling
- Eglin mesoscale gas-gun
  - T5: Compaction
- Demonstration problem
  - Yearly hero run

Eglin Microscale/Mesoscale Experiments
Simulations implement the JWL equation of state and reactive burn initial condition for the explosive.

Plan for Uncertainty Quantification Analysis
- Vary input parameters of particle density, particle diameter, and explosive mass for batch run (5 x 5 x 5 x 3 simulations) to construct surrogate model
- Done for all variations of particle configuration

Experiment has a vent in the back of the explosive where the detonator attaches
- Simulations will account for the effects of this vent

Mesoscale Simulation of Microscale Experiment

Geometric Features
- Straight Barrel
- Parabolic Explosive Front
- Deformed Barrel
- Deformed Barrel AND "Parabolic" Explosive Front

Explosive Initial Conditions
- Lumped detonation
- Two Material Reactive Burn

\[ t_{\text{SIM}} = 22.46 \, \mu s \]
\[ t_{\text{EXP}} = 22.50 \, \mu s \]
Validation Data Details:
- Drag models same as for Sandia’s shock-tube simulation campaign
- Crosshairs show experimental data points with uncertainty
- The filled band outlines the max and min trajectories of the 25 particle
- Simulation results are time shifted based on Reactive Burn detonation times

Simulation Details:
- Real gas equation of state (JWL)
- Point-particle model
- Explosive modeled with a reactive burn initial profile
### CMT-nek Micro-Meso-Hero Timeline

<table>
<thead>
<tr>
<th></th>
<th>Y4-Q1</th>
<th>Y4-Q2</th>
<th>Y4-Q3</th>
<th>Y4-Q4</th>
<th>Y5-Q1</th>
<th>Y5-Q2</th>
<th>Y5-Q3</th>
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<td><strong>S2 ASU Meso</strong></td>
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<td>Improved models</td>
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<td><strong>S4 CMT-Hero</strong></td>
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</tbody>
</table>

- Goran Marjanovic
- David Zwick
- Josh Ganno
- Rahul Koneru
- Fred Ouellet

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**Do you have any questions?**
CMT-nek: A compressible multiphase DGSEM extension to nek5000

Jason F. Hackl
David Zwick
Accomplishments in Year 4

- Discontinuous Galerkin SEM of 2nd derivatives
  - Entropy viscosity for stabilizing shocked flow
- Particle 4-way coupling
- Compressible multiphase flows with shocks
- Transition to CMT-nek
  - Microscale: shock-sphere interactions
  - Mesoscale: ASU expansion
  - Macroscale: CMT-Hero 1: blast with particles
  - Detonation conditions (gas only)

Outline

1. CMT-nek gas dynamics
   a. Discontinuous Galerkin method for gas flow solver
   b. Entropy viscosity method
   c. V&V of shock-capturing and microscale flow
2. CMT-nek multiphase
   a. Lagrangian particles and scaling
   b. Path to demonstration problem
3. Code development and future work
   a. Transition and timeline
   b. Risk mitigation
   c. Future work
Discontinuous Galerkin Spectral Elements

\[ \frac{\partial U}{\partial t} + \nabla \cdot H (U, \nabla U) = R \]

flux = convective + diffusive
\[ H_i = H_i^c (U) + H_i^d (U, \nabla U) \]

Right-hand-side for fully explicit TVDRK3
\[ \left[ \frac{\partial U}{\partial t} \right] = B^{-1} \left( I_{vol}^{(c)} - I_{sfc}^{(c)} \right) \]
\[ \text{Inviscid Euler equation fluxes } H^c \]
\[ - B^{-1} (I_{GU} - I_{G^+U} - I_{KU} - R) \]
Artificial viscosity \( H^d \) + source terms

Gauss-Lobatto-Legendre quadrature on tensor product of \( N \) points

- Mass matrix \( B \)
\[ \int_{-1}^{1} \int_{-1}^{1} f(\mathbf{r}) J d\mathbf{r} \approx B \mathbf{f}, \quad B_{ij} = \omega_i f(r_i) J \delta_{ij} \]

Numerical flux \( H^e(U-,U^+) \)
- restriction \( E \)
- nek5000 gather-scatter operation \( QQ^T \)

\[ \{ \{ u \} \} = \frac{1}{2} (u^- + u^+) = \frac{1}{2} QQ^T [E u] \quad u^+ = (QQ^T - I) [E u] \]

Volume: \( O(N_{elem} M^4) \)
Surface: \( O(N_{elem} M^2) \)

Interpolation to \( M=3(N-1)/2 \) GL points via matrix \( I \) for polynomial dealiasing

Finite difference op \( D \)
\[ \frac{\partial}{\partial x_i} \approx \frac{\partial r_k}{\partial x_i} \frac{\partial f}{\partial r_k} \]

isoparametric transformation metrics

**DGSEM: diffusive flux integrals**

Quasi-linear flux Jacobian $A$

$$ H^d_{ij} = \mathcal{A}_{ijkl} \frac{\partial (U_k / \phi_g)}{\partial x_l} $$

\( \phi \) equation, flux in \( x_i \)

Weighted residual, integrate by parts → primal form → DGSEM ops

$$ \int_{\Omega_x} \nu \nabla \cdot H^d_{ij} \, dV \rightarrow I_{KU} - I_{GU} + I_{GTV} $$

$$ I_{GU} = \int_{\Gamma} \left\{ \langle \mathcal{A} \nabla U \rangle \cdot [v] \, dA \rightarrow v^T \mathbf{E}^T \mathbf{B}_A \left[ (H^d_{ij} \cdot n) - \langle (H^d_{ij} \cdot n) \rangle \right] \right\} $$

$$ I_{GTV} = \int_{\Gamma} \left\{ \langle \mathcal{A} \nabla U \rangle \cdot [U] \, dA \rightarrow v^T \mathbf{D}_{ij} \mathcal{A}_{ijkl} \mathbf{E}^T \mathbf{B}_A \left[ U^2 - \langle U \rangle \right] [n_i] \right\} $$

$$ I_{KU} = \int_{\Omega_x} (\nabla u) \cdot H^d_{ij} \, dV \rightarrow v^T \mathbf{D}_{ij} \mathbf{B} [r_{k.x_i}] H^d_{ij} $$


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**Entropy viscosity method**

Artificial stress tensor\(^1\) (NOT Navier-Stokes) with AV that tracks the entropy residual

NOT weighted by volume fraction \( \phi_g \)

Diffusive flux of...

**Mass**

$$ H^d_1 = -\kappa_s \nabla \rho $$

**Momentum**

$$ H^d_{i+1,j} = - \left( \rho \nu_s \sigma_{ij} + \kappa_s u_j \frac{\partial \rho}{\partial x_i} \right) $$

$$ \sigma_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} $$

**Energy**

$$ H^d_5 = - \left[ \rho \nu_s \mathbf{u} : \mathbf{e} + \kappa_s \mathbf{X} \left( \nabla (\rho c) + \frac{1}{2} |\mathbf{u}|^2 \mathbf{e} \right) \right] $$

Due to entropy viscosity

$$ \nu_s = c_g h \frac{|R_s|}{||s - \langle s \rangle||_\infty} $$

$$ \nu_{\text{max}} = c_{\text{max}} h \max \left( |\mathbf{u}| + c \right) $$

$$ \kappa_s = S \left( \min(\nu_s, \nu_{\text{max}}) \right) $$

$$ R_s \equiv \partial s / \partial t + \nabla : (\mathbf{u} \cdot s) $$

\( R_s \) approx by finite diff between RK3 stages\(^1\) $ s = \rho c_v \log \left( \frac{\rho}{\rho_0} \right) $\

\( C^0 \) by average \( R_s \) at face points. Smooth via

$$ S(R) = \frac{1}{12} (6 R_{i,j,k} + R_{i+1,j,k} + R_{i-1,j,k} + \ldots) $$


---

Convergence and validation

- Mass diffusivity $\kappa = P \nu$ regularizes solution

- $\nu$ reaches $\nu_{\text{max}}$ at shock wave

Calibrated $P$, $c_E$, $c_{\text{max}}$

<table>
<thead>
<tr>
<th>Sod (1978) 2-shock collision</th>
<th>Sod (1978)</th>
<th>2-shock</th>
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<tbody>
<tr>
<td>$c_{\text{max}}$</td>
<td>0.3</td>
<td>1.0</td>
</tr>
<tr>
<td>$c_E$</td>
<td>40</td>
<td>85</td>
</tr>
<tr>
<td>$P$</td>
<td>0.75</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Toro (2001) two-shock collision

Shock-sphere drag coefficient

- Mach 3 shock-sphere interaction, $N = 5$

- Mach 1.22 shock-sphere, two resolutions

<table>
<thead>
<tr>
<th>Mach 1.22</th>
<th>Mach 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{\text{max}}$</td>
<td>0.3</td>
</tr>
<tr>
<td>$c_E$</td>
<td>40</td>
</tr>
<tr>
<td>$P$</td>
<td>0.75</td>
</tr>
</tbody>
</table>


Shock-sphere interaction

Mach 1.22

Mach 3

Captured features identified in experiments & simulations:

Microscale: Potential flow over spheres

Tests generalized Faxen theorem:

\[ F^G = \frac{4}{3} \pi R^3 \rho \frac{Du}{Dt} v^2 + A \pi R^3 \int_{-\infty}^{\infty} K_{vo}(\xi) M \left[ \frac{D}{Dt} \right] \left[ \frac{\partial p}{\partial x} \right] \, d\xi \]

Mach

FCC 10% Volume fraction

FCC 15% Volume fraction

Ideal-gas Demonstration problem

Charge and Particles

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Charge</th>
<th>Ambient</th>
<th>EVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg m⁻³)</td>
<td>23.536</td>
<td>1.204</td>
<td>C₁₀</td>
</tr>
<tr>
<td>Pressure (atm)</td>
<td>100</td>
<td>1</td>
<td>C₂₄</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>1500</td>
<td>293.15</td>
<td>P</td>
</tr>
</tbody>
</table>

EVM:
- $C_{\text{max}} = 1.0$
- $C_{\text{ref}} = 40$
- $P = 0.75$

2D Verification-Gas only
- Rocflu: 2D, ~ 2.5E6 cells, dr=154 μm
- CMT-nek: 2D, ~ 1.6E6 dof,
  Element spacing = 235 μm

Charge and Particles

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Charge radius</td>
<td>3.8 mm</td>
</tr>
<tr>
<td>Particle bed thickness</td>
<td>2 cm</td>
</tr>
<tr>
<td>No. of particles</td>
<td>1E+6</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>5%</td>
</tr>
</tbody>
</table>
Multiphase nek5000 and CMT-nek

- CMT-nek is built on single-phase nek5000
- While not fully resolved, Eulerian-Lagrangian method can simulate a more realistic number of particles
- Challenges related to particle-fluid coupling
  - Physics, numerics, computer science
- Outline:
  - Particle implementation in CMT-nek/nek5000
  - Current validation efforts
  - Multiphase summary

### Multiphase Capabilities

<table>
<thead>
<tr>
<th></th>
<th>Existing</th>
<th>New</th>
<th>nek5000</th>
<th>CMT-nek</th>
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<tr>
<td><strong>Fluid-Fluid</strong></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>
<td>✓</td>
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<td>✓</td>
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<td>Shock waves</td>
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<td><strong>Tracer Particles</strong></td>
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<td><strong>Particle-Fluid</strong></td>
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<tr>
<td>Dilute</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Dense</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Particle-Particle</strong></td>
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</tbody>
</table>

Multiphase exascale problems rely on efficient communication and computations to maintain both accuracy and scalability.
### Multiphase Source Terms

**Projection: Particles Effect Surrounding Grid**

\[
R = \begin{bmatrix}
0 \\
\sigma_g : \nabla (\phi_p \mathbf{v}) + q_{pg} + q_{fg}
\end{bmatrix}
\]

**Particle-fluid force coupling and energy contribution**

**Particle-fluid energy coupling**

**Eulerian particle velocity**

### Governing Equations

For a single particle:

**Position:**

\[
\frac{dX}{dt} = \mathbf{V}
\]

**Momentum:**

\[
M_p \frac{d\mathbf{V}}{dt} = \mathbf{F}_{pg} + \mathbf{F}_{un} + \mathbf{F}_c + \mathbf{F}_b
\]

**Energy:**

\[
M_p C_{p,p} \frac{dT_p}{dt} = Q_h
\]

**Hydrodynamic force**

**Collisional force**

**Body force**

**Hydrodynamic heat transfer**
Inter-Particle Collision Model

Normal spring-damper soft-sphere collision model:

\[ F_{c,i} = \sum_{j=1}^{n} F_{c,i,j}^S + F_{c,i,j}^D \]

Spring force:
- Overlapping particles repel each other

Damping force:
- Colliding particles dissipate energy

From thousands of particles…
… to millions of particles…
… and even billions…

Ghost Particles

If a particle is near a MPI rank edge, it will create a copy of itself called a ghost particle

Used for:
1. Particle-fluid projection
2. Particle-particle collisions
Algorithmic Scaling

Ideal Setup:
- Uniform flow in a periodic box
- \( N = 6 \) grid points in each direction

Strong Scaling (s):
- 15 million grid points
- 8.4 million particles

Weak Scaling (w):
- 864 grid points/rank
- 1,024 particles/rank

<table>
<thead>
<tr>
<th>Operation</th>
<th>Slope (s)</th>
<th>Slope (w)</th>
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<tr>
<td>Interpolation</td>
<td>-1.00</td>
<td>0.00</td>
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<tr>
<td>Projection</td>
<td>-1.07</td>
<td>0.00</td>
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<tr>
<td>Send Ghosts</td>
<td>-0.72</td>
<td>0.12</td>
</tr>
<tr>
<td>Collision Force</td>
<td>-1.95</td>
<td>-0.01</td>
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Load Balancing on CMT-nek

- Time per time step:
  - 20.00 s for the original code
  - 2.52 s for the load balanced code
- There was no need to load balance during the simulation since the time per time step didn't increase over the threshold set to trigger load balancing

Vulcan
- 65,536 MPI ranks
- 16,384 nodes
- 4 cores per node
- 900,000 elements
- 1.125x10^9 particles
- Grid size: 5x5x5
- Rarefaction test
- 7.9x improvement in performance
Particle Verification

Coupling hierarchy:
- Fluid-particle (one-way)
  - One particle settling
- Particle-fluid (two-way)
  - Ghost particle creation
  - Eulerian vs. Lagrangian integration
- Particle-particle (four-way)
  - Single particle-wall collision
  - Nearest-neighbor count
  - Packed bed Voronoi volume distribution

Fluidized Bed

- Particle bed initially at ~ ¼ of height
- Particles initially randomly distributed in entire domain and allowed to settle

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>$N_p$</td>
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</tr>
<tr>
<td>$D_p$ (m)</td>
<td>1.200E-6</td>
</tr>
<tr>
<td>$\rho_p$ (kg/m$^3$)</td>
<td>1000</td>
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<tr>
<td>$L_x$ (m)</td>
<td>0.044</td>
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<tr>
<td>$L_y$ (m)</td>
<td>0.120</td>
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<tr>
<td>$L_z$ (m)</td>
<td>0.010</td>
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<td>$\rho_f$ (kg/m$^3$)</td>
<td>1.205</td>
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<tr>
<td>$\nu_f$ (Pa s)</td>
<td>1.8E-5</td>
</tr>
</tbody>
</table>

Simulations are performed with nek5000
Fluidized Bed Results

Particle volume fraction (Run 6)

Average pressure drop vs. inlet velocity

Particles in Expansion Waves

Background:
- Problem consists of a vertical shock tube with particle bed in driver section
- Particle bed swells upwards due to rapid decompression when diaphragm bursts
- Results are compared with Cagnoli et al. (2002) experiments, which provide first version of ASU simulations at reduced scale
- Simulation is a smaller periodic slice of entire domain

Experimental Setup:
Multiphase Refinement

- Grid refinement in multiphase flow is not well defined.
- We consider two types of refinement:
  1. Fluid refinement (grid resolution)
  2. Particle refinement (coarse graining)
- Three cases of increased refinement:

<table>
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<th>Coarse Graining</th>
<th>64</th>
<th>8</th>
<th>1</th>
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<td>Particles</td>
<td>89,081</td>
<td>712,647</td>
<td>5,701,176</td>
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<tr>
<td>Grid Points</td>
<td>776,250</td>
<td>6,210,000</td>
<td>49,680,000</td>
</tr>
<tr>
<td>MPI Ranks</td>
<td>8k</td>
<td>65k</td>
<td>524k</td>
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</table>

Coarse Graining: The number of real particles that each computational particle represents.

Simulation Setup

<table>
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<tr>
<th>Geometry</th>
<th>Simulation</th>
<th>Experiment</th>
<th>Simulation</th>
<th>Experiment</th>
<th>Simulation</th>
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<tr>
<td>$L$(cm)</td>
<td>23</td>
<td>23</td>
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<tr>
<td>$D_p$(cm)</td>
<td>0.2</td>
<td>3.8</td>
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<tr>
<td>$h_0$(cm)</td>
<td>6.5</td>
<td>6.5</td>
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<table>
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<th>Experiment</th>
<th>Simulation</th>
<th>Experiment</th>
<th>Simulation</th>
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<tbody>
<tr>
<td>$D_p$(µm)</td>
<td>38</td>
<td>38</td>
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<td></td>
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</tr>
<tr>
<td>$ρ_f$(kg/m³)</td>
<td>2,500</td>
<td>2,500</td>
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<td></td>
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<tr>
<td>$N_f$</td>
<td>$\sim2\times10^5$</td>
<td>89k, 713k, 5701k</td>
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<tr>
<td>$k_c$(kg/s²)</td>
<td>-</td>
<td>80, 40, 20</td>
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<tr>
<td>$ε_a$</td>
<td>-</td>
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Grid

<table>
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<tr>
<th>Simulations</th>
<th>Simulation</th>
<th>Experiment</th>
<th>Simulation</th>
<th>Experiment</th>
<th>Simulation</th>
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<tbody>
<tr>
<td>$N_e$</td>
<td>6k, 50k, 400k</td>
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</tr>
<tr>
<td>$N$</td>
<td>5</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>$Δx$(μm)</td>
<td>167, 83, 42</td>
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<tr>
<td>$δ_f/D_p$</td>
<td>2.85</td>
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<tr>
<td>$δ_f/Δx$</td>
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Initial Conditions

<table>
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<th>Conditions</th>
<th>Simulation</th>
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<td>$p_i$(kPa)</td>
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Simulations are performed with CMT-nek
Particle Front Movement

- Varying pressure difference across diaphragm
- Gidaspow drag force from fluidized bed community
- Measure initial velocities of bed height

<table>
<thead>
<tr>
<th>Case</th>
<th>Particle Velocity (m/s)</th>
<th>Fluid Velocity (m/s)</th>
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<tbody>
<tr>
<td>1</td>
<td>10.00</td>
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<tr>
<td>2</td>
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Front Rise Velocity

Multiphase Summary

- Particles have been simulated across a wide range of physics
- Necessary features:
  - Efficiency (exascale systems)
  - Accuracy (physics)
  - Load-balancing (multiphase)
- Particles are capable of reproducing multiphase physics:
  - Fluidized bed
  - Particles in expansion waves
Transition and code management

- CMT-nek workshop November 29, 2017
  - Training and introduction for CS, macroscale
- Host nek5000 User/Developer Meeting
  - Tampa, Florida April 17-18, 2018
- CMT-nek developer documentation
  - Doxygen driven
- Load balancing accepted to ICS’18
- Automated regression testing via travis.cl
- Macroscale group in transition

Demonstration problem roadmap

<table>
<thead>
<tr>
<th>CMT-Hero 1</th>
<th>CMT-Hero 2</th>
<th>CMT-Hero 3</th>
<th>CMT-Hero 4</th>
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### Transition plan: timeline

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### Transition plan: Risk Mitigation

<table>
<thead>
<tr>
<th>Capability</th>
<th>Risk</th>
<th>Remediation / alternative</th>
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<tbody>
<tr>
<td>Artificial viscosity</td>
<td>$c_p, c_v$ may not suffice for full duration of blast propagation</td>
<td>Alternative AV to EVM</td>
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<tr>
<td></td>
<td></td>
<td>Lv&amp;Ihme (2015) EBDG solution limiter</td>
</tr>
<tr>
<td>Particle compaction</td>
<td>No compaction model. Post-shock oscillation at low $A_p$ may violate positivity</td>
<td>Harris &amp; Crighton</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2-fluid model at small $t$</td>
</tr>
<tr>
<td>Initialization and small time</td>
<td>$\Delta t$ must start small, how should it grow with $t$?</td>
<td>2-fluid model at small $t$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Fluxes, RK scheme</td>
</tr>
<tr>
<td>Load balancing</td>
<td>Version control difficulties. $\sim 1$ element/task at $t=0$ for balanced particles</td>
<td>2-fluid $\rightarrow$ Lagr. PP.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Manual rebalancing at restarts</td>
</tr>
<tr>
<td>Boundary conditions</td>
<td>Need outflow BC allowing the blast wave to exit the domain.</td>
<td>Sponge layers</td>
</tr>
<tr>
<td></td>
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<td>Characteristic BC</td>
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<tr>
<td></td>
<td></td>
<td>Mesh stretching</td>
</tr>
<tr>
<td>Multi-species</td>
<td>Adding species for detonation products should be straightforward, but mixed EOS and artificial mass diffusion may interfere with multicomponent formulation.</td>
<td>Replace GP14 with Navier-Stokes</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1-equation JWL-ideal-gas mixture</td>
</tr>
<tr>
<td></td>
<td></td>
<td>See “Artificial viscosity”</td>
</tr>
<tr>
<td>Reactive burn</td>
<td>Replace IC with prescribed field for elements initially lying in the explosive.</td>
<td>Anticipate more severe small-time</td>
</tr>
</tbody>
</table>

AV: artificial viscosity  
BC: boundary conditions  
EBDG: Entropy bounded DG (*JCP* 295:715-739)  
JWL: Jones-Wilkins-Lee (1968) state equation  
PP: point-particle approach  
IC: initial conditions  
EOS: equation of state  
EVM: entropy viscosity method  
GP14: Guermond-Popov (2014)
Summary and Future Work

- CMT-nek is filling RocFlu’s shoes and beyond
  - Compressible multiphase flow, scalable
  - Microscale, mesoscale and macroscale transition underway
- Plan to fill capability gaps
  - Risk mitigation plan identifies alternatives
  - Computer science integration
  - Load-balancing (multiphase)
- Future work (new capability)
  - Entropy stability
  - Entropy-stable multiphase source terms
  - Mesh generation

Do you have any questions?
Exascale Behavioral Emulation

Principal Investigators:

Herman Lam, Greg Stitt

Center for Compressible Multiphase Turbulence (CCMT)
NSF Center for High-Performance Reconfigurable Computing (CHREC)
ECE Department, University of Florida

Exascale Behavioral Emulation (BE) Team

- Ryan Blanchard
  FPGA Acceleration

- Sai Chenna
  BE Design Space Exp.

- Trokon Johnson
  BE Tools

- Aravind Neelakantan
  BE Methods

- Carlo Pascoe
  FPGA Acceleration

- Raj Rajagopalan
  BE-SSY

- Ben Reynolds
  Thermal Modeling

- Chad Saunders
  Symbolic Regression
Overview & Goal of Behavioral Emulation (BE)

- **Code Development Team**
  - CMT-nek
  - Rocflu
  - nek5000

- **Exascale BE Team**
  - CMT-bone-BE

- **UQ Team**
  - Simulation Platforms
    - BE SST
    - FPGA Acceleration

**Behavioral Emulation (BE)**

- **Coarse-grained simulation**
- **BE methods & tools**

- **Model development & validation**
  - On existing archs for CMT-bone-BE kernels & comm. patterns: benchmarking & modeling: interpolation, symbolic regression

- **Prediction & DSE**
  - Extend validated models to explore near-future & notional architectures
  - Algorithmic DSE & optimization for CMT-nek kernels & apps on future arch.

**HW/SW co-design**

- Algorithmic & architectural design-space exploration (DSE)
- Coarse-grained BE simulation
  - Balance of simulation speed & accuracy for rapid design-space evaluation
Outline

- Review & overview:
  - Behavioral Emulation (BE)

  Research thrusts & achievements
  
  - BE-SST simulator & tools, experimental results
  - BE method enhancements
    - Multi-fidelity surrogate model for performance prediction
    - Symbolic regression for performance modeling
    - Thermal experiments & modeling
  - Acceleration using FPGAs
    - Speedup vs BE-SST
    - Scalability on multiple FPGAs
  - End-to-end case study - CMT-nek DSE using FPGAs
    - Design space exploration of CMT-nek

- Summary, conclusions, & future work

---

Key Achievements (Year 4)

- Large-scale experiments using BE-SST
  - Validation (100k+ MPI ranks) on Titan & Vulcan (< 9% error)
  - Predictive simulations approaching a million MPI ranks (Vulcan+ & Titan+)
  - Notional/near-future architecture - SUMMIT performance prediction

- Innovations in BE methods
  - UQ | Symbolic regression | Thermal modeling

- FPGA acceleration of BE simulation
  - Validation of dataflow, pipelined approaches (FEP, CP)
  - Scalability via multiple FPGAs

- End-to-end case study: CMT-nek DSE using FPGA
  - Algorithmic and parametric design space exploration
  - Achieved $10^6$ times speedup over BE-SST
Outline

- Review & overview:
  - Behavioral Emulation (BE)

Research thrusts & achievements

- BE-SST simulator & tools, experimental results
- BE methods
  - Multi-functional simulation tooling
  - Symbolic regression
    - Performance modeling
  - Thermal management
  - Acceleration using FPGAs
  - Speedup
  - Scalability
- End-to-end case study
  - Design space exploration of CMT-nek

Summary, conclusions, & future work

**BE-SST Simulator**

- **Motivation:** In-house BE simulator used to explore functionalities, but not very scalable or maintainable
- **BE-SST:** Developed by extending Structural Simulation Toolkit (SST)**
  - Framework for parallel simulations
  - Supported by developers & vendors
  - Flexibility in designing custom components

---


** From Sandia National Labs

---

**SST Capabilities**
- Parallel simulations
- Discrete event simulations
- Clock and event queries
- Network models
- Component models

**BE Influences**
- Software definitions
- Probabilistic simulation
- Abstract network definitions
- Abstract hardware definitions

**BE-SST**
- Parallel discrete event simulation environment
- Distributed component queues
- Software definition
- Probabilistic simulation
- Abstract network models
- Abstract component models
BE-SST Enhancements

- Communication model
  - Replaced static routing method with dynamic routing*
  - Inclusion of collectives such as MPI_Isend, MPI_Irecv, MPI_Waitall
- Performance model
  - Support for symbolic regression (in addition to interpolation API)
    - Symbolic regression with stochastic model
    - Improve accuracy (More details later)
- Leverage parallel capabilities of SST for BE-SST*
- Able to support trace-driven simulation**
  - For time-dependent simulations
  - To mimic CMT-nek with particles more accurately

* Details in Appendix
** Details in Sai Chenna’s presentation on Friday

Outline

- Review & overview:
  - Behavioral Emulation (BE)
- Research thrusts & achievements
  - BE-SST simulator & tools, experimental results
  - BE methods
    - Multi-fidelity surrogates
    - Symbolic regression
    - Thermal experiments
    - Acceleration on FPGAs
    - Scheduling & optimization
    - Scalability
    - End-to-end
      - Design space exploration of CMT-nek
- Summary, conclusions, & future work
BE simulations of HPC systems

- **Titan @ ORNL**
  - Cray XK7 architecture with Cray Gemini interconnect
  - 16-core AMD opterons; 18k nodes; 300k cores
  - 18k K20X Kepler GPUs
  - 32GB + 6GB memory/node

- **Vulcan @ LLNL**
  - IBM BG/Q architecture
  - 16 cores/node, 24k nodes, 390k cores
  - 16GB memory/node

**Application Case Study: CMT-bone-BE**

- CMT-nek & CMT-bone (mini-app) both are large codes
- To support extensive DSE*, we need:
  - Key compute kernels & comm. patterns that affect performance
  - Abstract, modular, easy to modify and instrument for algorithmic DSE

- Computation- & communication-intensive portions of CMT-nek workflow in C & MPI
  - Volume-to-surface data extraction
  - Face data exchange (with neighbors)
  - Derivative computation volume points

- Easier to modify for algorithmic DSE
- 1000 vs 10s of thousands lines of code

* design-space exploration
Experiment Setup

- Application case study: CMT-bone-BE (gas solver)
- Application parameters
  - Calibration
    - element size: 5, 9, 13, 17, 21
    - elements/core: 8, 32, 64, 128, 256
  - Validation
    - element size: 5, 6, 9, 11, 16, 17
    - 64 elements/core
- Machine parameters
  - Validation up to 128k MPI ranks
  - Predictions up to 1M MPI ranks
  - Can perform both predictions and validations for larger systems
- Monte-Carlo Simulations

BE Simulations of Titan+

- Simulating bigger system than Titan (approaching 1 Million cores)
- Average % error between CMT-bone-BE simulation and execution time is 4%
- Maximum error is 17%

\[
\text{% error} = \frac{\sum (\text{Execution Time}) - \sum \text{Execution Time}}{\sum \text{Execution Time}} \times 100
\]
BE-SST Scalability

- Aiming for 1M+ cores; able to simulate 800K+
  - Memory bottleneck
- Uneven memory distribution across ranks while simulating
  - Bigger systems (e.g., 1 Million+ cores)
  - With more complex interconnects (e.g., 5D Torus of Vulcan)

* GCM
Graph Construction Memory: initial memory allocation before simulation

- Working with Sandia National Labs (Jeremy Wilke) to solve this issue

BE Simulations of Vulcans+

- Simulating a bigger system than Vulcans (512k cores)
- Average % error between CMT-bone-BE simulation and execution time is 4%
- Maximum error is 9%
BE Simulations of **Notional Architecture**

- **SUMMIT-like architecture**
  - IBM POWER compute nodes
  - 44 cores/node
  - Non-blocking fat-tree n/w topology

- **Initial methodology**
  - Compute models of **Vulcan (POWER architecture)**
  - Fat tree architectural details and latency numbers obtained from **Dr. Atchley Scott, ORNL**
  - Predictions up to 4k nodes (180224 cores)

- **Future work for notational exploration**
  - Abstract Machine Modeling (AMM)*

---

**SUMMIT-like Architecture**

- **System Performance**: 5 to 10x Titan
- **Number of nodes**: ~4600
- **Processor**: IBM Power9
- **Interconnect**: Non-Blocking fat tree
  - (dual-rail, single-plane)**
    - **Eighteen (18) 640-port Director Switches**
    - **256** Compute racks with **18** compute nodes/rack
    - Each rack has **two 36-port** Top-of-Rack (TOR) switches
    - Each node has **2 processors**; each processor has **22 cores** (44 cores/node)
    - **Within rack**: inter-node latency is ~ **0.7us** per hop
    - **Outside of rack**: additional **100us** per hop

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** Re-designed based on unpublished information obtained from Dr. Atchley Scott, ORNL
**BE Simulations of SUMMIT-like Arch**

- Showcases capability of BE to perform simulations on notional architecture
- Cannot validate the result at this point
- Going forward
  - Refine models as new information is available (e.g., IBM Power 9 data)
  - Validate when access to SUMMIT is available

**BE-SST Performance on Fat-tree Arch**

Comparison GCM* between 5-D torus and non-blocking fat tree archs in BE-SST (Build-time)

- In simulating equal # of nodes in BE-SST, GCM* for fat-tree configuration is approx. the same as the GCM* of 5-D torus
- In simulating equal # of cores in BE-SST, fat-tree configuration consumes only ~40% of GCM* consumed by 5-D torus configuration
Summary: BE Methods, Simulator, & Experiments

- **Large-scale experiments** using BE-SST
  - Validation (100k+ MPI ranks) on Titan & Vulcan (< 9%) error
  - **Predictive** simulations approaching a million MPI ranks
    (Vulcan+ & Titan+)
  - Near-future architecture - SUMMIT performance prediction

- **Going forward**
  - BE-SST enhancements (e.g., scaling toward exascale)
  - BE-SST studies on new-existing, near-future, or abstract archs

- **BE & BE-SST general accessibility & usability**
  - Continual documentation:
    - BE-SST: architecture, code, configuration, usage
  - Planned availability
    - BE-SST code
    - Use cases: with complete build & execution walkthrough, expected results, assumptions/restrictions

Outline

- **Review & overview:**
  - Behavioral Emulation (BE)

Research thrusts & achievements

- BE-SST simulator & tools, experimental results
- BE method enhancements
  - **Multi-fidelity surrogate model** for performance prediction
  - Symbolic regression
  - Thermal modeling
  - Acceleration
  - Speedups
  - Scalability
- End-to-end case study - CMT-nekDSE using FPGAs
- Design space exploration of CMT-nek

Summary, conclusions, & future work
Behavioral Emulation with UQ*

Goal: Improve BE models via validation and uncertainty estimation
- Reduce computational budget by fitting BE simulation to CMT-nek using Multi-Fidelity Surrogate (MFS)
- Extrapolation of CMT-nek towards large-scale runs using BE and MFS

Accuracy of corrected BE sim.
- At 10 left-out CMT-nek test points
- Overall RMSE < 10%
  with 7 or more CMT-nek data
- Reducing computation budget
  - Supplemen ting high-fidelity (CMT-nek) with low-fid. (BE simulation) runs


*See Aravind’s poster for more details

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    - Symbolic regression for performance modeling
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Symbolic Regression: Motivation

- **Motivation:**
  - Multi-parameter performance modeling is challenging
  - Requires accuracy, computational efficiency, simple implementation

- **Our previous approaches:**
  - N-dimensional interpolation:
    - Computationally expensive
    - Difficult to implement, needs customization for each example
    - Insufficient accuracy
  - Multi-variate linear regression:
    - Faster than interpolation, relatively simple to implement
    - Need thorough understanding of code to generate performance models
    - May not capture machine-specific behaviors that deviate from basic model

Symbolic Regression

- **Advantages:**
  - Captures machine-specific performance behaviors
  - Enables tradeoffs between accuracy and computational complexity
    - Can maximize performance for a given error constraint
  - Requires no prior knowledge of the kernel

- **Approach:** custom genetic-programming tool
  - Evolves “trees” from mathematical primitives
  - Multiple optimization goals: minimize error, minimize error given tree size constraint, minimize tree size given error constraint, etc.
Symbolic Regression: Results

<table>
<thead>
<tr>
<th>CMT-nek particle solver kernel</th>
<th>Linear Regression</th>
<th>Symbolic Regression</th>
<th>Error Improvement</th>
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<td>4.3%</td>
<td>1.1x</td>
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<tr>
<td>Average</td>
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<td>7.4%</td>
<td>14.8x</td>
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</tbody>
</table>

Problem: symbolic regression provides deterministic value
Corresponding performance models do not include variance

Solution: create separate models for minimum time and overhead
Execution time = minimum time + overhead time
Variation in overhead samples is modelled by a new parameter “rank”

Total Execution time = f(nx1,nelt,α) + g(nx1,nelt,α,rank)

3.68nx1⁴α + 1.71E⁻⁵ 3.54E⁻⁶(ern\_rank\_an\_elt) + 2.871E⁻⁶

nx1 = element-size; a = particles/gridpoint; nelt = elements-per-processor; rank = randomized parameter
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Summary, conclusions, & future work

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Thermal Benchmarking & Modeling

- Previously modeled energy/power using physical and simulation measurements
- Current focus: thermal modeling with IR images of KNL
  - Goal: minimize maximum temperature via load balancing
- More challenging than anticipated
  - CPU fans block thermal information of CPU
  - Tried custom fan setup, destroyed several processors
- Modified KNL for IR by cutting hole in case:
Thermal Benchmarking & Modeling

- Observations:
  - Different regions of the heat sink show widely different temperatures
  - Several columns show higher temperatures than others
    - Does not necessarily mean that processor is hotter at these points
  - Minimizing the maximum temperature in the image may not be most appropriate optimization goal
    - Need to weigh each region of the heat sink differently

Thermal Benchmarking Methodology

- Map functionality onto specific cores using OpenMPI
- Identity layout of cores from patterns in IR images
- For different core mappings, evaluate distribution of heat over time for different workloads
  - Example shows two different arrangements of 32 cores
  - Mapping to even cores shows cooler regions
- **Eventual goal**: use patterns to build models to assist with load balancing
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- **Summary, conclusions, & future work**

### FPGA-Accelerated Design-Space Exploration

**Example design space:**
- 20 values for lelt, lx1, lpart
- 10 different numbers of cores
- 10 different core types
- 10 different memory configurations
- 4 different network topologies

**32 million options to explore**

**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

See Carlo Pascoe’s poster: FPGA-pipelined Simulations for CMT-nek
Fully-expanded Pipeline (FEP)

1. Construct Data Flow Graph (DFG) from simulation configuration
   - AppBEO+ArchBEO define instructions and operand/output dependencies
   - Instructions map to vertices and dependencies map to edges in DFG
   - Various opportunities for graph-level optimizations

2. Mapping DFG to FPGA Pipeline

1. Extracting DFG from BE simulation configuration

2. Map DFG to pipeline circuit
   - Vertex attributes define operations and instantiate dedicated HW
   - Edge attributes (e.g., src/dst) instantiate pipeline register between src/dst pair
   - Various opportunities for circuit-level optimizations

Because each instruction (from sim) mapped to independent HW (no resource sharing), each vertex able to start next sim 1 cycle after current sim.

Collapsed Pipeline (CP)

1. Construct Data Flow Graph (DFG) from simulation configuration
   - AppBEO+ArchBEO define instructions and operand/output dependencies
   - Instructions map to vertices and dependencies map to edges in DFG
   - Partition into linear subgraphs and generate dependency lists

2. Mapping DFG to FPGA Pipeline

1. Extracting DFG, then identify subgraphs & dependencies

2. Map DFG to pipeline circuit
   - Vertex attributes define operations and Edge attributes instantiate pipeline register between src/dst pairs
   - Align subgraph traces such that cost is minimized and no dependencies are violated

Because each subgraph instruction mapped to independent HW, each vertex able to start next subgraph 1 cycle after current subgraph. All subgraphs must complete before sim can complete.
## Fully-Expanded & Collapsed Pipeline Tradeoffs

### Fully-Expanded Pipeline

**Advantages:**
- Superior performance in terms of simulation throughput and latency
- 280 - 320 MHz implies 280 - 320 million simulations per second independent of simulated MPI ranks

**Limitations:**
- Resources scale linearly with both MPI Ranks and number of timesteps
- Scaling across multiple FPGAs expected to be ineffective when considering exascale simulations

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<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>
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</table>

†Mega-Simulations-Per-Second, ‡Giga/Kila-Events-Per-Second, '–' indicates configuration unable to fit on a single FPGA

### Collapsed Pipeline

**Advantages:**
- Resources scale linearly with timesteps, but sublinearly with MPI Ranks
- Allows for significantly more timesteps due to its much lower base utilization
- Better scaling on single and multiple FPGAs

**Limitations:**
- Lower simulation throughput and longer initial latency, but still more than sufficient for rapid design-space exploration
CCMT

Collapsed Pipeline: Single-FPGA Performance/Scalability

As number of ranks increase:
- additional logic per rank approaches zero
- simulation throughput reduced by a factor of “ranks”
- event throughput remains proportional to instantiated event hardware

Pipelines scale linearly with length of simulation, however blockram eventually becomes limiting resource
- e.g., only fit 2 TS for 1 million ranks on Stratix V
- Motivation to explore partially-collapsed pipeline approach

Increased performance expected with Stratix 10
- Collapsed hardware specifically designed to exploit new Stratix 10 architecture

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>Num. of Events</th>
<th>% LU Latency (cycles)</th>
<th>Hardware MSPS</th>
<th>Hardware GFLOPs</th>
<th>BE-SST KEPS</th>
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</table>

Now able to reach million+ rank simulations in hardware

Rank limit due to insufficient blockram not logic

Expect greater performance when Stratix 10 becomes available

Throughput > 10Mx higher than BE-SST

Collapsed Pipeline: Multi-FPGA Performance/Scalability

Pipelines scale linearly with the length of simulation, but as a single, unidirectional pipe
- Partitioned easily/predictably across any number of connected FPGAs

Given a desired # of simulated ranks, timesteps, granularity (events per timestep), we can predict performance & # of FPGAs

Main point: FPGAs achieve similar scale as BE-SST, but orders of magnitude faster
- 1M ranks, 300+ of sims/second

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS FPGAs</th>
<th>Num. of Events</th>
<th>Lat to First Out (cycle³)</th>
<th>Mega Sims /second</th>
<th>Giga Events /second</th>
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</thead>
<tbody>
<tr>
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<td>1,646,592</td>
<td>21,196</td>
<td>0.33</td>
<td>539</td>
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<td>2.56e⁻³</td>
<td>1,142</td>
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<tr>
<td>128K</td>
<td>128</td>
<td>893,386,752</td>
<td>1,754,449</td>
<td>2.56e⁻³</td>
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<tr>
<td>1M</td>
<td>32</td>
<td>1,799,356,416</td>
<td>2,641,321</td>
<td>3.19e⁻⁴</td>
<td>575</td>
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<td>1M</td>
<td>64</td>
<td>3,598,712,832</td>
<td>4,234,337</td>
<td>3.19e⁻⁴</td>
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<tr>
<td>1M</td>
<td>128</td>
<td>7,197,425,664</td>
<td>7,414,540</td>
<td>3.19e⁻⁴</td>
<td>2,299</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

FPGA-Acceleration Summary

- Introduced two approaches for accelerating BE simulations:
  - Fully expanded pipeline: 7-9 orders of magnitude faster than BE-SST, but doesn’t scale well
  - Collapsed pipeline: 6 orders of magnitude faster than BE-SST, and scales well across multiple FPGAs
- Demonstrated simulations of 1M ranks
  - Larger than what BE-SST can currently handle
- Integrated symbolic regression into FPGA accelerator performance models
  - Determining attractive tradeoffs between accuracy and scalability is important for FPGA

Outline

- Review & overview:
  - Behavioral Emulation (BE)
- Research thrusts & achievements
  - BE-SST simulation
  - BE methods
    - Multi-fidelity
    - Symbolic regression
    - Thermal
  - Acceleration
    - Speedup
    - Scalability
  - End-to-end case study - CMT-nek use of FPGAs
    - Design space exploration of CMT-nek
- Summary, conclusions, & future work
**Design Space Exploration**

- **Goal:** Use FPGA to explore enormous design space
- **Application:** CMT-nek particle solver kernel
- **Performance parameters:**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Element-size</strong></td>
<td>5-25 (21)</td>
</tr>
<tr>
<td><strong>Element-count</strong></td>
<td>4-512 (8)</td>
</tr>
<tr>
<td><strong>particles/gridpoint (α)</strong></td>
<td>0.1-10 (19)</td>
</tr>
<tr>
<td><strong># of ranks</strong></td>
<td>16-1M (17)</td>
</tr>
</tbody>
</table>

**Algorithmic options:**
- **Time Integration:** Rk3,bdf
- **Interpolation:** Barycentric, Reduced Barycentric, Trilinear interpolation

Design space = **273,904** candidates
Design Space Exploration: Results

<table>
<thead>
<tr>
<th>Ranks</th>
<th>No of events</th>
<th>FPGA Avg. Simulation time (microseconds)</th>
<th>BE-SST* Avg. Simulation time (seconds)</th>
<th>FPGA speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1024</td>
<td>24,576</td>
<td>3.53</td>
<td>8.234</td>
<td>2.33x10^6</td>
</tr>
<tr>
<td>2048</td>
<td>49,152</td>
<td>7.06</td>
<td>6.5</td>
<td>9.21x10^3</td>
</tr>
<tr>
<td>4096</td>
<td>98,304</td>
<td>14.12</td>
<td>17.3</td>
<td>1.22x10^3</td>
</tr>
<tr>
<td>8192</td>
<td>196,608</td>
<td>28.24</td>
<td>31</td>
<td>1.10x10^3</td>
</tr>
<tr>
<td>16k</td>
<td>393,216</td>
<td>56.48</td>
<td>120</td>
<td>2.12x10^3</td>
</tr>
<tr>
<td>32k</td>
<td>786,432</td>
<td>112.96</td>
<td>145</td>
<td>1.28x10^3</td>
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<tr>
<td>64k</td>
<td>1,572,864</td>
<td>225.92</td>
<td>405</td>
<td>1.79x10^3</td>
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<tr>
<td>128k</td>
<td>3,145,728</td>
<td>451.84</td>
<td>531</td>
<td>1.17x10^3</td>
</tr>
<tr>
<td>256K</td>
<td>6,291,456</td>
<td>903.68</td>
<td>1569</td>
<td>1.74x10^3</td>
</tr>
<tr>
<td>512K</td>
<td>12,582,912</td>
<td>1807.36</td>
<td>7416</td>
<td>4.10x10^3</td>
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<tr>
<td>1M</td>
<td>25,165,824</td>
<td>3614.72</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>

- Each configuration (row) has **16,112** design candidates
- BE-SST takes **5.5 years** to explore the design space – **FPGA takes 61 seconds**
  - **550 years** including 100 Monte Carlo simulations for each design candidate vs **100 minutes**
  - FPGA sacrifices analysis capabilities of BE-SST to achieve this speedup

BE-FPGA Simulations of Vulcan (512k cores)

**BE-FPGA Simulation**

**BE-SST Simulation (32k cores)**

100 runs & 100 simulations

CMT-nek Particle-Solver Execution (4k cores)

**CMT-nek Particle-Solver Execution**

Application: CMT-nek particle solver
Architecture: Vulcan (512k cores)
1 design candidate** – **BE-SST** - **12000 minutes**
Entire space (270K candidates) – **BE-FPGA** - **100 minutes**

*ran on HiPerGator - 64 cores
*100 Monte-Carlo simulations/candidate
Design Space Exploration: Results

BE-FPGA Simulation predictions on Vulcan

- Algorithms vary
  - non-linearly w.r.t. element-size(N)
  - linearly w.r.t. particles/gridpoint(α) and elements-per-processor(nelt)
- BDF time-integration provides an average 3x speedup over baseline implementation
- Reduced barycentric interpolation provides an average 4.6x speedup
- Tri-linear interpolation provides an average 2457x speedup ($N^6$ vs $N^3$)

Key Achievements (Year 4)

- Large-scale experiments using BE-SST
  - Validation (100k+ MPI ranks) on Titan & Vulcan (< 9% error)
  - Predictive simulations approaching a million MPI ranks (Vulcan+ & Titan+)
  - Notional/near-future architecture - SUMMIT performance prediction
- Innovations in BE methods
  - UQ | Symbolic regression | Thermal modeling
- FPGA acceleration of BE simulation
  - Validation of dataflow, pipelined approaches (FEP, CP)
  - Scalability via multiple FPGAs
- End-to-end case study: CMT-nek DSE using FPGA
  - Algorithmic and parametric design space exploration
  - Achieved $10^6$ times speedup over BE-SST
Outline

- Review & Overview:
  - Behavioral Emulation (BE)
- Research thrusts & achievements:
  - BE-SST simulator & tools, experimental results
  - BE method enhancements
  - Multi-fidelity surrogate model for performance prediction
  - Symbolic regression for performance modeling
  - Thermal experiments & modeling
  - CMT-nek design space exploration using BE simulation
  - Acceleration using FPGAs
    - Of BE: speedup vs BE-SST, scale up on multiple FPGAs
    - Of CMT-nek kernels: approach & preliminary results
- Summary, conclusions, & future work

FPGA Acceleration Trends

- FPGAs growing trend in data centers
  - Microsoft Catapult, Amazon F1, Intel Broadwell+FPGA
  - National lab interest
- Recently performed case study on Intel Broadwell+Arria 10 (BDW+A10) for 2D convolution
  - 96x less energy than Broadwell
  - 15.7x less energy than P6000 GPU
- Future research?
  - FPGA acceleration of CMT-nek functions
  - Faculty part of NSF CHREC/SHREC

<table>
<thead>
<tr>
<th>Precision</th>
<th>Kernel Size</th>
<th>256x256</th>
<th>512x512</th>
<th>1024x1024</th>
<th>2048x2048</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>16-bit Fixed</td>
<td>3x3</td>
<td>55x</td>
<td>148x</td>
<td>191x</td>
<td>181x</td>
<td>167x</td>
</tr>
<tr>
<td>5x5</td>
<td>62x</td>
<td>170x</td>
<td>175x</td>
<td>173x</td>
<td>173x</td>
<td></td>
</tr>
<tr>
<td>7x7</td>
<td>58x</td>
<td>165x</td>
<td>171x</td>
<td>170x</td>
<td>170x</td>
<td></td>
</tr>
<tr>
<td>9x9</td>
<td>45x</td>
<td>152x</td>
<td>143x</td>
<td>144x</td>
<td>144x</td>
<td></td>
</tr>
<tr>
<td>Avg</td>
<td>53x</td>
<td>167x</td>
<td>169x</td>
<td>168x</td>
<td>168x</td>
<td></td>
</tr>
</tbody>
</table>

| Energy Comparison of BDW+A10 vs. Broadwell |
| Image Size |
| 256x256 | 512x512 | 1024x1024 | 2048x2048 | Avg |
| 16-bit Fixed | 3x3 | 15.5x | 19.8x | 19.4x | 19.0x | 18.4x |
| 5x5 | 12.9x | 18.6x | 19.3x | 19.1x | 17.7x |
| 7x7 | 10.5x | 18.2x | 19.7x | 20.5x | 17.2x |
| 9x9 | 8.1x | 15.3x | 16.9x | 18.6x | 14.7x |
| Avg | 11.8x | 18.0x | 18.9x | 19.5x |

| 32-bit Float | 3x3 | 14.6x | 19.4x | 19.0x | 18.6x | 17.9x |
| 5x5 | 12.2x | 17.0x | 18.6x | 18.7x | 17.8x |
| 7x7 | 9.9x | 15.2x | 16.9x | 17.3x | 14.8x |
| 9x9 | 5.8x | 9.0x | 8.9x | 9.4x | 8.3x |
| Avg | 10.6x | 15.4x | 15.8x | 16.0x |
Do you have any questions?

Appendix
Dynamic Routing

- Replaced static routing method with dynamic routing
  - Improve BE-SST scaling: large static routing table not required for increasing number of cores (Fig. 1)
  - Build-time benefits: Config build time not a bottleneck for large simulation (Fig. 2)

Parallel Performance of BE-SST

- Simulations of Vulcan System with 5-D Torus Topology*
  - 4K, 32K, 128K core
  - Improved parallel performance with increase in problem size
  - For e.g., 128k core simulation
    - Without parallelization (1 rank): ~1 day;
    - With 256-rank parallelization: 17 min.

* Run using BE-SST installed on Titan
Comparison Interconnects between 5-D Torus and non-blocking fat tree architecture in BE-SST

- In simulating equal # of nodes in BE-SST, 5-D torus configuration uses ~1.7 times the # of interconnects in fat-tree.
- In simulating equal # of cores in BE-SST, 5-D torus configuration uses ~4.7 times the # of interconnects in fat-tree.

Comparison GCM* between 5-D torus and non-blocking fat tree archs in BE-SST (Build-time)

- In simulating equal # of nodes in BE-SST, GCM* for fat-tree configuration is approx. the same as the GCM* of 5-D torus.
- In simulating equal # of cores in BE-SST, fat-tree configuration consumes only ~40% of GCM* consumed by 5-D torus configuration.
**BE-SST performance on fat-tree architecture**

Comparison GC time between 5-D Torus and non-blocking fat tree architecture in BE-SST

- In simulating equal # of nodes in BE-SST, GCT for 5-D torus configuration is **approx. same** as the GCM of fat-tree topology.
- In simulating equal # of cores in BE-SST, 5-D torus configuration consumes ~3.7 times the GCM of interconnects in fat-tree topology.

---

**Multi-fidelity Prediction of CMT-nek**

*Experimental setup*

- Design of experiment (DOE)
  - Element size (ES) = 5, 9, 13, 17, 21
  - Elements per processor (EPP) = 8, 32, 64, 128, 256
  - Number of processors (NP) = 16, 256, 2048, 16384, 131072

- 125 total data points
  - **BE simulation**: all 125 runs
  - **CMT-nek**: 22 runs
  - **CMT-bone**: 67 runs

- Multi-fidelity surrogate model
  - Fitting CMT-nek using **corrected fitting of BE simulation**
  - For large problems, low-fidelity BE simulation is **computationally cheaper** than high-fidelity CMT-nek or CMT-bone
Multi-fidelity Prediction of CMT-nek

Initial RMSE comparison:
- BE-simulation vs CMT-nek at all experimental points
- Overall root mean squared error (RMSE) 74%

Accuracy of corrected BE sim.
- At 10 left-out CMT-nek test points
- Overall RMSE < 10% with 7 or more CMT-nek data
- Reducing computation budget
  - Supplementing high-fid. (CMT-nek) with low-fid. (BE simulation) runs

Extrapolation Towards Large-scale Runs

- Extrapolation necessary for exascale prediction
  - But challenging due to limited runs
- Develop MFS using:
  - 7 (out of 22) runs of CMT-nek (high-fidelity), at 256 and 2k processors
  - All 125 BE simulations (low-fidelity)
- Extrapolate using MFS towards 16k (11 runs) & 128k (4 runs) processors

Extrapolation: Validation

- Extrapolate using MFS towards 16k (11 runs) and 128k (4 runs) processors
  - Linear fit to CMT-nek: poor result
  - High-order fitting leads to overfitting due to limited samples (7 CMT-nek runs with 3 variables)
  - MFS: relative errors less than 11%

Extrapolation: Prediction of CMT-nek

- MFS prediction towards one million processors with UQ
  - 64 elements per processors (9 CMT-nek runs)
  - MFS predictions
- Monotonic trend with small curvature in logarithmic coordinate
CMT-nek: CS Update

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352 514 4213

Members

Keke Zhai
Mohamed Gadou
Adeesha Malavi
Tania Banerjee
David Zwick
Jason Hackl
Sai Chenna
Sanjay Ranka
Exascale Simulation: CS Challenges

Dynamic Load Balancing

Future Architectures and Hybrid Processors

Parallelization on a million+ processors

Energy and Performance Tradeoffs

Feasible space

Time

Energy

Accomplishments (past year)

- Dynamic load balancing of CMT-nek for moving particles
- Results for CMT-bone with DVFS on heterogeneous platform
- Support for CMT-bone on KNL (architectures with multi level memories)
- Support for CMT-nek on GPU (in progress)
Talk Overview

- CMT-bone/CMT-nek
- Dynamic Load Balancing
  - Colocation of particles with spectral elements
  - Mapping/Remapping
- Hybrid Multicore Processor
  - Traditional Core (Autotuning)
  - GPU (Manual Tuning)
  - Hybrid Core Mapping
  - KNL (Multi-level Memories)
  - Power/Energy Modeling
  - Dynamic Voltage Scaling
- Conclusions

CMT-bone and CMT-nek workflow

Each cube represents a spectral element – formulation of the finite element method that uses high degree piecewise polynomials as basis functions.

Performance per Flop Improvement

Dynamic Load Balancing: Expansion Fan

CMT-nek Simulation

ASU Experiment
Demonstration Problem

CMT-nek Simulation

Eglin Blast Pad Experiment

Overview of Dynamic Load Balancing

Step 1: Domain decomposition
Happens during initialization only

Step 2: Elements to processor mapping
Happens during initialization and on every remapping

Step 3: Decide when to trigger a remap
- Rebalance after every k time steps (user set up)
- Rebalance automatically after certain time steps (adaptive load balancing)

Step 4: Transfer elements and particles and reset other data structures
Spectral Bisection

P1 – 8 particles
P2 – 11 particles
P3 – 8 particles
P4 – 5 particles

Elements to Processor Mapping

P1 – 8 particles
P2 – 11 particles
P3 – 8 particles
P4 – 5 particles
P4 – 8 particles

(a) Default elements to processor mapping, agnostic of particles
Elements to Processor Mapping

(b) Elements to processor mapping, after taking into account both elements and particles

Overview of Element to Processor Mapping Algorithm

- Centralized
  - Easy to accomplish
  - There is a bottleneck where only processor P0 is working
  - Have more information to achieve better decision

- Distributed
  - There is no bottleneck at all
  - Each processor communicates with each other to get partial information
  - Use limited information to make decisions
  - MPI_allgatherv is taking most of the time on Quartz

- Hybrid
  - Combination of centralized and distributed
  - Utilize broadcast in replace of MPI_allgatherv to reduce communication time
**The Centralized Algorithm**

Each processor sends element load array to P0

- P0
  - 3 6 4 5
  - 8 8 10 8
- P1
  - 8 8 10 8
- P2
  - 7 3 7 3

**The Distributed Algorithm**

Each processor computes local prefix sum and the exclusive prefix sum of the element load on each processor

- P0
  - Prefix sum: 3 9 13 18
  - 18 34 20
- P1
  - Exclusive prefix sum: 8 16 26 34
- P2
  - Exclusive prefix sum: 7 10 17 20
The Hybrid Algorithm

The hybrid algorithm is similar to the distributed algorithm except for the step that get the global element->processor mapping. Each processor sends the mapping to P0.

![Diagram of processor mappings]

Rebalancing Time: Total Overhead Time (Vulcan)

Overhead expressed as number of time steps:
- 1.00 for the centralized
- 0.77 for the distributed,
- 0.84 for the hybrid algorithm
Expansion testcase: CMT-nek on Vulcan

- Time per time step:
  - 20.00 s for the original code
  - 2.52 s for the load balanced code
- There was no need to load balance during the simulation since the time per time step didn't increase over the threshold set to trigger load balancing.

Expansion testcase: Adaptive Load Balancing

- User-triggered load balancing algorithm: load balance every 500 time steps.
- Adaptive load balancing algorithm: first load balance after 4000 time step.
- Time per time step from step 4,000 to 6,000 for adaptive and user-triggered load-balancing algorithms was 3.78 s and 4.17 s, respectively.
- Giving us an overall improvement of 9.4%.
Performance comparison between CMT-nek and Nek5000

- Performance of CMT-nek without particles is about the same as Nek5000 without particles.
- Performance of CMT-nek with particles is about half of the performance of Nek5000 with particles.

Performance of CMT-nek with particles using multiple-thread

- Performance using 2 threads is about 2 time performance using 1 thread.
**Expansion testcase: Power consumption on Mira (Using MonEQ)**

- Core power and DRAM power reduced by about 5% and 2% respectively, leading to an overall reduction of 3.5% of total power when load balancing is used.
- Energy consumption of the load balanced code is better because of reduced time as well as reduced power consumption.

**Rebalancing Time: Total Overhead (Quartz)**

- Overhead expressed as number of time steps:
  - 1.94 for the centralized
  - 3.35 for the distributed
  - 1.82 for the hybrid algorithm
- This shows that the overhead for load balancing is very small.
Expansion testcase: CMT-nek on Quartz

- Time per time step:
  - 9.92 s for the original code
  - 0.995 s for the load balanced code
- Adaptive load balancing were used and it first happened at 4077 time step.

Expansion testcase: Power consumption on Quartz (using Libmsr)

- Power consumption is comparable.
Nek5000 User Meeting

- To be held at Tampa, on April 17 and 18.
- Load balancing will be of interest since Nek5000 is being enhanced with particles.
- Potentially, there will be a wider user base for load balancing.

Hybrid Multicore Architectures

Multi-objective Load decomposition

<table>
<thead>
<tr>
<th>CPU Attribute</th>
<th>Description</th>
<th>GPU Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency</td>
<td>2.4GHz</td>
<td>Model</td>
<td>K40m</td>
</tr>
<tr>
<td>Sockets</td>
<td>2</td>
<td>Frequency</td>
<td>745MHz</td>
</tr>
<tr>
<td>Cores/Socket</td>
<td>12</td>
<td>SMs</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cores/SM</td>
<td>192</td>
</tr>
</tbody>
</table>

Multi-objective Optimization on Hybrid Systems using DVFS, Mohamed Gadou, Sankeerth Mogili, Tania Banerjee, Sanjay Ranka, submitted to ICCP 2018
**CPU: Power-Performance Tradeoffs**

- **Observations:**
  - Using 24 cores causes very high power consumption
  - Using 8 and 4 cores is power as well as performance efficient

---

**CPU: Energy-Performance Tradeoffs**

- **Observations:**
  - Using 24 cores with lower frequencies results in an energy and performance efficient configuration
Observations:
- Using 8 GPUs causes very high power consumption
- Using 4 and 2 GPUs is power as well as performance efficient

Observations:
- Using 4 GPUs with lower frequencies results in an energy and performance efficient configuration
Theoretical formulation

Minimize

\[ E(n, m, f, g, S) \]

Subject to

\[ T(n, m, f, g, S) \leq T_1 - O(n, m, f, g, S) \]

\[ n \leq N \]

\[ m \leq M \]

\[ f \in F \]

\[ g \in G \]

\[ S \leq 16128 \]

\[ \text{Minimize} \quad E_{CPU}(n, f, X) + E_{GPU}(m, g, S-X) \]

Subject to

\[ T_{CPU}(n, f, X) \leq T_1 - C_{CPU}(m+n, S) \]

\[ n \leq N \]

\[ m \leq M \]

\[ f \in F \]

\[ g \in G \]

\[ X \leq S \]

\[ \frac{T_{CPU}(n, f, X)}{f} \times P_{CPU}(n, f) \]

\[ \frac{T_{GPU}(m, g, S-X)}{g} \times P_{GPU}(m, g) \]

CPU Experiments

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>x, problem size in terms of number of elements (57)</td>
<td>1024, 1152, 1280, 1408, 1536, 1664, 1792, 1920, 2048, 2176, 2304, 2432, 2560, 2688, 2816, 2944, 3072, 3200, 3328, 3456, 3584, 3712, 3840, 3968, 4096, 4224, 4352, 4480, 4608, 4736, 4864, 4992, 5120, 5248, 5376, 5504, 5632, 5760, 5888, 6016, 6144, 6272, 6400, 6528, 6656, 6784, 6912, 7040, 7168, 7296, 7424, 7552, 7680, 7808, 7936, 8064, 8192</td>
</tr>
<tr>
<td>f, frequency in MHz (5)</td>
<td>1200, 1500, 1800, 2100, 2400</td>
</tr>
<tr>
<td>n, number of cores (5)</td>
<td>1, 2, 4, 8, 12</td>
</tr>
</tbody>
</table>
CPU Experiments

- Time per time step for processing a problem size of 8192 spectral elements and 256,000 particles
- Experiments show time decreases by increasing CPU counts and frequency

- CPU communication time for processing 8192 spectral elements and 256,000 particles
- Communication time first decreases and then increases as processors are increased because volume of data communicated per core decreases in the beginning but the total communication volume begins to increase later
**Assumptions**

- Performance using lower clock frequencies may be derived from that using the highest clock frequency
  \[ T_{CPU}(n, f, x) = k \times \frac{f_{\text{max}}}{f} \times T_{CPU}(n, f_{\text{max}}, x) \]
- Power consumption does not depend on problem size
  \[ P_{CPU}(n, f, x) = P_{CPU}(n, f) \]
- \( n \) = CPU count, \( f \) = CPU frequency, \( x \) = problem size

Example: Power lookup table:

<table>
<thead>
<tr>
<th>( f )</th>
<th>( n )</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>93.24</td>
<td>97.33</td>
<td>101.32</td>
<td>114.46</td>
<td>127.50</td>
<td></td>
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<tr>
<td>1500</td>
<td>96.67</td>
<td>100.78</td>
<td>108.32</td>
<td>122.95</td>
<td>136.79</td>
<td></td>
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<tr>
<td>1800</td>
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<td>102.88</td>
<td>111.53</td>
<td>131.86</td>
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<td>106.31</td>
<td>117.11</td>
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</tr>
<tr>
<td>2400</td>
<td>102.65</td>
<td>108.12</td>
<td>123.94</td>
<td>145.54</td>
<td>167.08</td>
<td></td>
</tr>
</tbody>
</table>

**Performance Prediction Error**

- Prediction error is within 3% for 99% of the tests
  \[ T_{CPU}(n, f, x) = k \times \frac{f_{\text{max}}}{f} \times T_{CPU}(n, f_{\text{max}}, x) \]
Power Prediction Error

- Prediction error is within 5% for 99% of the tests
- \[ P_{CPU}(n,f,x) = PCPU(n,f) \]

<table>
<thead>
<tr>
<th>Error percent range</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-1</td>
<td>723</td>
</tr>
<tr>
<td>1-2</td>
<td>430</td>
</tr>
<tr>
<td>2-3</td>
<td>304</td>
</tr>
<tr>
<td>3-4</td>
<td>186</td>
</tr>
<tr>
<td>4-5</td>
<td>48</td>
</tr>
<tr>
<td>5-6</td>
<td>9</td>
</tr>
<tr>
<td>6-7</td>
<td>6</td>
</tr>
<tr>
<td>7-8</td>
<td>2</td>
</tr>
<tr>
<td>8-25</td>
<td>2</td>
</tr>
</tbody>
</table>

GPU Experiments

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y ), problem size in terms of number of elements (57)</td>
<td>Same problem sizes as described for CPUs.</td>
</tr>
<tr>
<td>( g ), frequency in MHz (3)</td>
<td>875, 810, 745</td>
</tr>
<tr>
<td>( m ), number of GPUs (4)</td>
<td>1, 2, 4, 8</td>
</tr>
</tbody>
</table>
**GPU Experiments**

- Time per time step for processing a problem size of 8192 spectral elements and 256,000 particles.
- Experiments show time decreases by increasing CPU counts and frequency.

---

- Total communication time when GPUs are used to solve the problem.
Assumptions

- Performance using lower clock frequencies may be derived from that using the highest clock frequency
  \[ T_{GPU}(m, g, y) = k \times \frac{g_{max}}{g} \times T_{GPU}(m, g_{max}, y) \]
- Power consumption does not depend on problem size
  \[ P_{GPU}(m, g, y) = P_{GPU}(m, g) \]
- \( m = \text{GPU count}, g = \text{GPU frequency}, y = \text{problem size} \)
- Example: Power lookup table:

<table>
<thead>
<tr>
<th>( g )</th>
<th>( m )</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>745</td>
<td>89.79</td>
<td>169.91</td>
<td>314.53</td>
<td>550.91</td>
<td></td>
</tr>
<tr>
<td>810</td>
<td>93.51</td>
<td>176.05</td>
<td>324.59</td>
<td>567.11</td>
<td></td>
</tr>
<tr>
<td>875</td>
<td>98.80</td>
<td>185.46</td>
<td>341.26</td>
<td>589.41</td>
<td></td>
</tr>
</tbody>
</table>

Performance Prediction Error

- Prediction error is within 5% for 99% of the tests

<table>
<thead>
<tr>
<th>Frequency</th>
<th>0-1</th>
<th>1-2</th>
<th>2-3</th>
<th>3-4</th>
<th>More</th>
</tr>
</thead>
<tbody>
<tr>
<td>Error percent range</td>
<td>273</td>
<td>137</td>
<td>35</td>
<td>9</td>
<td>2</td>
</tr>
</tbody>
</table>
Power Prediction Error

- Prediction error is within 10% for 99% of the tests

Summary of CPU and GPU experiments

- Assumption that performance at lower clock frequencies may be derived from the performance of the application at the highest clock frequency holds both for CPUs and GPUs
- Assumption that power consumption does not depend on problem size holds for both CPUs and GPUs
- The above assumptions help to reduce the number of required experiments further
## Hybrid Experiments

### Parameters and Values

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Load ((x, y))</td>
<td>(x = \text{CPU load}) (y = \text{GPU load}) ((1024, 7168), (1152, 7040), (1280, 6912), (1408, 6784), (1536, 6656), (1664, 6528), (1792, 6400), (1920, 6272), (2048, 6144), (2176, 6016), (2304, 5888), (2432, 5760), (2560, 5632), (2688, 5504), (2816, 5376), (2944, 5248), (3072, 5120), (3200, 4992), (3328, 4864), (3456, 4736), (3584, 4608), (3712, 4480))</td>
</tr>
<tr>
<td>(f)</td>
<td>1200, 1500, 1800, 2100, 2400</td>
</tr>
<tr>
<td>(g)</td>
<td>745, 810, 875</td>
</tr>
<tr>
<td>(n)</td>
<td>2, 4, 8, 12</td>
</tr>
<tr>
<td>(m)</td>
<td>1, 2, 4, 8</td>
</tr>
</tbody>
</table>

### Hybrid Experiments Table

<table>
<thead>
<tr>
<th>CPU</th>
<th>GPU</th>
<th>Predicted Energy (J)</th>
<th>Actual Energy (J)</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>elements</td>
<td>count</td>
<td>GHz</td>
<td>elements</td>
<td>count</td>
</tr>
<tr>
<td>2540</td>
<td>8</td>
<td>2.4</td>
<td>5652</td>
<td>2</td>
</tr>
<tr>
<td>2621</td>
<td>8</td>
<td>2.4</td>
<td>5571</td>
<td>2</td>
</tr>
<tr>
<td>2621</td>
<td>8</td>
<td>2.4</td>
<td>5571</td>
<td>2</td>
</tr>
<tr>
<td>2540</td>
<td>8</td>
<td>2.4</td>
<td>5652</td>
<td>2</td>
</tr>
<tr>
<td>2293</td>
<td>8</td>
<td>2.4</td>
<td>5899</td>
<td>2</td>
</tr>
<tr>
<td>1474</td>
<td>4</td>
<td>2.4</td>
<td>6718</td>
<td>2</td>
</tr>
</tbody>
</table>

- Error in prediction for some of the best predicted configurations for minimum energy consumption
Hybrid Experiments

- Energy versus performance pareto optimal curve. Red line shows the predicted curve, while blue line is obtained from actual data.

Pareto Curves for Energy Versus Runtime

- Data for each Pareto-optimal point contain the following information in order: CPU load (%), CPU count, GPU count, CPU frequency (GHz), GPU frequency (MHz), energy (J), time (s).
Pareto Curves for different input sizes

- Power versus performance pareto optimal curve. Red line shows the predicted curve, while blue line is obtained from actual data.

- Center for Compressible Multiphase Turbulence
CMT-nek CPU-GPU interaction model

- GPU performs computational work
- Host CPU core is used for inter process communication
- Idle CPU cores will be used for computation

![Diagram of CPU-GPU interaction]

**Tesla K20x:**
- 14 Processors
- 192 Cores
- 48k shared memory
- 64k registers
- 1310 GFLOP/s Peak
- 732MHz clock frequency
- 6GB DDR5

**Host:**
- AMD Opteron
- 16 cores
- 2.2GHz clock frequency

CMT-nek on GPU

- Based on the implementation of CMT-bone on GPU for fluid, with support for new enhancements (viscous flow)
- New code for particles
- High level Architecture
  - Assign one element to a SM to minimize array data reading from the global memory
  - Dispatch threads equal to number of grid points (lx * ly *lz) when calculations are required for each grid point
  - Dispatch threads equal to (number of faces * lx * lz) when calculations are required for each face
Challenges in porting CMT-nek

- **Hardware perspective: Memory constraints**
  - 48KB cache per SM
    - For 512 grid points per element, one array requires 4k memory. Can hold only 12 such arrays. Total array requirement is about 50.
    - Solution: Reduce grid points or split kernels so a kernel requires only few arrays.
  - 64K registers per SM
    - For 512 grid points per element, one thread can have 125 registers. Additional registers will be stored in the global memory.
    - Solution: Split kernels, change the order of calculations to reuse registers.

- **Coding perspective**
  - A number of nek5000 libraries such as routines for spectral methods must be ported to GPU for full GPU support
  - MPI calls require GPU kernels to be stopped and data to be transferred to CPU

Preliminary results

- CMT-nek total time for 100 time steps(s)
- 125 elements
- For different lx1 (Initial size of the grid) and lxd (finer mesh) values

<table>
<thead>
<tr>
<th>(lx1, lxd)</th>
<th>1 CPU</th>
<th>4 CPUs</th>
<th>16 CPUs</th>
<th>1GPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>(6,10)</td>
<td>37.47</td>
<td>14.47</td>
<td>7.15</td>
<td>9.77</td>
</tr>
<tr>
<td>(8,12)</td>
<td>86.78</td>
<td>32.68</td>
<td>15.00</td>
<td>14.66</td>
</tr>
<tr>
<td>(10,16)</td>
<td>205.94</td>
<td>74.27</td>
<td>30.72</td>
<td>27.57</td>
</tr>
</tbody>
</table>
Multi-Level Memories

**KNL Overview**
- Chip: 36 Tiles interconnected by 2D Mesh
- Tile: 2 Cores + 2 VPU/core = 1 MB L2

**Memory:**
- MCDRAM: 36 GB on-package; High BW
- DDR4: 6 channels @ 2400 up to 384 GB
- I/O: 16 lanes PCIe* Gen3, 4 lanes of OMI for chipset

**Node:**
- 1-Socket only

**Fabric:**
- Intel® Omni-Path Architecture on-package (not shown)

**Vector Peak Perf:**
- 3+TF. DP and 6+TF SP Flops

**Scalar Perf:**
- 2x over Knights Corner

**Streams Test (7k/4):**
- MCDRAM = 500+; DDR< 30+

"> 5x Higher BW than DDR"

---

CMT-bone on Intel KNL

- Running time is total time taken to complete 1 time step.
- Running time as Number of processes being varied.

**Single node**
- CMT-bone
- 7x7x7 grid size
- 1.8GHz frequency
- 32 MPI ranks
- 2 OpenMP threads

---

Page 122 of 167
Increasing number of OpenMP threads enhances overall performance.
Using 64 MPI processes + 2 OpenMP threads yields in lowest running time.

Changing MCDRAM mode or clustering mode changes in performance.
Using MCDRAM in cache mode yields in speed up of 1.8x
CMT-bone on Different Platforms

- Only 1 cpu + 1 gpu was used for GPU based platforms
- Intel Broadwell was a 16 core processor
- KNL is faster than Intel Broadwell and gpu accelerated Systems

Summary of Accomplishments

- Dynamic load balancing of CMT-nek for moving particles
- Results for CMT-bone with DVFS on heterogeneous platform
- Support for CMT-bone on KNL (architectures with multi level memories)
- Support for CMT-nek on GPU (in progress)
Publications

8. Keke Zhai, Tania Banerjee, David Zwick, Jason Hackl and Sanjay Ranka, Dynamic Load Balancing for Compressible Multiphase Turbulence, accepted International Conference on Supercomputing, 2018

Conclusions: Overall Improvement
Do you have any questions?

CPU Experiments

- Constant of proportionality, for total execution time

<table>
<thead>
<tr>
<th>f</th>
<th>n</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>0.975</td>
<td>0.965</td>
<td>0.965</td>
<td>0.935</td>
<td>0.905</td>
<td></td>
</tr>
<tr>
<td>1500</td>
<td>0.985</td>
<td>0.985</td>
<td>0.975</td>
<td>0.955</td>
<td>0.915</td>
<td></td>
</tr>
<tr>
<td>1800</td>
<td>0.995</td>
<td>0.995</td>
<td>0.990</td>
<td>0.985</td>
<td>0.975</td>
<td></td>
</tr>
<tr>
<td>2100</td>
<td>0.990</td>
<td>0.990</td>
<td>0.990</td>
<td>0.990</td>
<td>0.970</td>
<td></td>
</tr>
</tbody>
</table>

- Constant of proportionality, for communication time

<table>
<thead>
<tr>
<th>f</th>
<th>n</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>0.82</td>
<td>0.88</td>
<td>0.82</td>
<td>0.72</td>
<td>0.62</td>
<td></td>
</tr>
<tr>
<td>1500</td>
<td>0.86</td>
<td>0.86</td>
<td>0.86</td>
<td>0.77</td>
<td>0.70</td>
<td></td>
</tr>
<tr>
<td>1800</td>
<td>0.90</td>
<td>0.90</td>
<td>0.90</td>
<td>0.83</td>
<td>0.80</td>
<td></td>
</tr>
<tr>
<td>2100</td>
<td>0.95</td>
<td>0.95</td>
<td>0.95</td>
<td>0.92</td>
<td>0.90</td>
<td></td>
</tr>
</tbody>
</table>
Hardware-Software Autotuning

Algorithm: dudr-4loop
\[
\begin{align*}
\text{do } & k = 1, N_z \\
\text{do } & j = 1, N_y \\
\text{do } & i = 1, N_x \\
\text{do } & l = 1, N_x \\
\text{dudr}(i, j, k) & = dudr(i, j, k) + a(i, l) * u(l, j, k, ie) \\
\end{align*}
\]
\text{enddo} \text{ enddo} \text{ enddo} \text{ enddo}

Algorithm: dudr-4loop-fused
\[
\begin{align*}
\text{do } & k = 1, N_z \cdot N_y \\
\text{do } & i = 1, N_x \\
\text{do } & l = 1, N_x \\
\text{dudr}(i, k) & = dudr(i, k) + a(i, l) * u(l, k, ie) \\
\end{align*}
\]
\text{enddo} \text{ enddo} \text{ enddo}

Algorithm: dudr-4loop-permuted-and unrolled
\[
\begin{align*}
\text{do } & k = 1, N_z \\
\text{do } & i = 1, N_x \\
\text{do } & j = 1, N_y \\
\text{do } & l = 1, N_x, 2 \\
\text{dudr}(i, j, k) & = dudr(i, j, k) + a(i, l) * u(l, j, k, ie) \\
\text{dudr}(i, j, k+1) & = dudr(i, j, k+1) + a(i, l+1) * u(l+1, j, k+1, ie) \\
\end{align*}
\]
\text{enddo} \text{ enddo} \text{ enddo} \text{ enddo}

Number of 4-loop implementations for dudr
\[N_x=N_y=N_z=10\]
\[= 4! \cdot 4^4 \]
\[= 24 \cdot 256 = 6144 \text{ variants}\]

Total number of variants = 98,240 (N=10)

Total number of variants = 217,728 (N=20)

Exhaustive search may not be feasible

Genetic Algorithm

- Compile and run each individual
- Set fitness value for each individual based on performance and energy
- Generate Initial Population
  - i=1
- Population Selection
- Add new individuals using crossover and mutation
  - i=i+1
- Report the best individual

Yes
No

i < n ?

Report the best individual
### Comparison of GA with Exhaustive Approach

#### Comparison of performance by platform

<table>
<thead>
<tr>
<th>Platforms</th>
<th>CMT-nek time (seconds)</th>
<th>Exhaustive Autotuning</th>
<th>GA based Autotuning</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Time</td>
<td>Search Space</td>
<td>% Less</td>
</tr>
<tr>
<td>IBM BG/Q</td>
<td>5.57</td>
<td>2.54</td>
<td>9771</td>
</tr>
<tr>
<td>AMD Opteron</td>
<td>1.81</td>
<td>1.02</td>
<td>9771</td>
</tr>
<tr>
<td>AMD Fusion</td>
<td>1.36</td>
<td>0.95</td>
<td>3265</td>
</tr>
</tbody>
</table>

#### Comparison of energy consumption by platform

<table>
<thead>
<tr>
<th>Platforms</th>
<th>CMT-nek energy (Joules)</th>
<th>Exhaustive Autotuning</th>
<th>GA based Autotuning</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Energy</td>
<td>Search Space</td>
<td>% Less</td>
</tr>
<tr>
<td>IBM BG/Q</td>
<td>292.1</td>
<td>131.7</td>
<td>9771</td>
</tr>
<tr>
<td>AMD Fusion</td>
<td>17.6</td>
<td>11.98</td>
<td>3265</td>
</tr>
</tbody>
</table>

#### Results (AMD Fusion @ Sandia)

- **Runtime Comparison**
- **Energy Comparison**

---

### Performance (varying hardware parameters)

- **Best Time (seconds)**
  - **Line Size - Associativity**
  - **Capacity Tuning**
  - **Line Size Tuning**

Genetic Algorithm based Autotuning Approach for Performance and Energy Optimization, Tania Banerjee and Sanjay Ranka (SUSCOM, to appear)

GEM5 environment
- Instruction set architecture: X86
- CPU model: Out-of-order CPU
- Memory model: Classic, DDR3
- Clock frequency: 1GHz
Uncertainty Budget
Validation and Uncertainty Reduction

Chanyoung Park, Raphael (Rafi) T. Haftka and Nam-Ho Kim
Department of Mechanical & Aerospace Engineering

Uncertainty Budget Team

- **PIs:** Raphael Haftka and Nam-Ho Kim
- **Research Scientist:** Chanyoung Park
- **Students**
  - Kyle Hughes (UQ of Eglin exp.)
  - Samaun Nili (Mesoscale 1D/2D force model potential errors)
  - Yiming Zhang (UQ and multi-fidelity correction of BE emulation)
  - Giselle Fernandez (Instability signal to noise ratio)
  - Tanner Johns (UQ of ASU experiments)
  - Eric Maltz (UQ of Eglin exp.)

- **Tanner Johns (New undergrad students)**
Summary of Past Work

- Year 1: Integrate with physics team
- Year 2: Integrate with exascale team
  - UQ for SNL simulation and experiments
  - Initial UQ for CS and exascale activities
- Year 3: Engage with the demonstration problem
  - Forensic UQ for Eglin and SNL experiments
  - Validation by blind prediction for CS and exascale
- Year 4: Engage with the demonstration problem
  - UQ for demonstration problem
  - Finalizing UQ and validation for shock-tube simulation and experiment

Outline

- Unique aspects of UQ at CCMT
- UQ of demonstration problem
- VVUQ workflow of demonstration problem
- Summary of Sandia Shocktube Campaign
- Forensic UQ of micro- & meso-scale experiments
Unique Aspects of UQ at CCMT

- Separated treatment of error from uncertainty
  - Uncertainty reduction to reveal model error
  - Error reduction through model update
- Global sensitivity analysis to identify model error potentials
- Forensic UQ
- Measurement processing uncertainty
- Method of multiple lines for extrapolation
- Multi-fidelity surrogate modeling

Reducing Uncertainty to Expose Errors

- Reducing uncertainty in model error estimate (UR)
  - Large uncertainty prevents observation of model error
  - Will require substantial uncertainty reduction
  - Hidden model error due to canceling errors
  - Identify models where refinement matters and possibly experimental bias
- Reducing model error (ER)
  - Identifying/ranking error sources
In the course of digging deeper into experiments and simulations we realized that we perform forensic uncertainty quantification.

- Simulation driven UQ: quantifying uncertainty in measurement of inputs for simulation
- Discover anomalies in simulations from UQ of the simulation
- Identify/help to discover unrecognized uncertainties and errors based on UQ

Forensic UQ tools:

- Document all the details (crime scene)
- Clarify details with experimentalists and physicists (witnesses)
- Quantify uncertainties (forensics lab)
- Identify unrecognized uncertainties and errors via simulation (culprits)

Outline:

- Unique aspects of UQ at CCMT
- UQ of demonstration problem
  - VVUQ workflow of demonstration problem
  - Summary of Sandia Shocktube Campaign
  - Forensic UQ of micro- & meso-scale experiments
Demonstration Problem (Eglin Macro)

- Composition B
- Particle to charge mass ratio: 13

Design of Macroscale Eglin Experiments

- Design of macroscale experiment
  - Took over measurement processing for UQ:
    - CT scan (UQ of volume fraction)
    - SEM (UQ of particle size)
    - Pycnometer (UQ of particle density)
  - Casing with notches (UR of measurement)
  - Bare charge experiments (UQ of explosive)
  - Multiple cameras to observe the experiment with different angles (UR of measurement)
### UQ of Experimental Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Quantity</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Explosive Length</td>
<td>44.75 ± 0.08 cm</td>
<td>Tape Measure</td>
</tr>
<tr>
<td>Explosive Diameter</td>
<td>8.194 ± 0.008 cm</td>
<td>Caliper</td>
</tr>
<tr>
<td>Explosive Mass</td>
<td>4100 ± 24 g</td>
<td>Mass Balance</td>
</tr>
<tr>
<td>Particle Diameter</td>
<td>TBD</td>
<td>SEM</td>
</tr>
<tr>
<td>Particle Density</td>
<td>7.66 ± 0.03 g/cm³</td>
<td>Pycnometer</td>
</tr>
<tr>
<td>Particle Volume Fraction</td>
<td>TBD</td>
<td>CT Scanner</td>
</tr>
<tr>
<td>Ambient Pressure</td>
<td>101.8 ± 0.8 kPa</td>
<td>Eglin Weather Station</td>
</tr>
<tr>
<td>Ambient Temperature</td>
<td>32 ± 7 °C</td>
<td>Eglin Weather Station</td>
</tr>
<tr>
<td>Probe Locations</td>
<td>±1%</td>
<td>Tape Measure</td>
</tr>
</tbody>
</table>

- **Forensic UQ**
  - UB team collected the uncertainty information
  - The information was used for planning the experiment

### UQ Driven Experiment Planning

- Steel particles chosen for validation experiments (75-125 µm)
- To closely match monodisperse and spherical assumptions of the simulation
- Allocated 3 experiments with steel / 2 bare charge / 1 with tungsten
- Particle bed characterization
  - SEM of particles and particle density via pycnometer
  - Steel mock CT scan

- SEM of single steel particle at 1000x zoom
- SEM of several steel particles at 100x zoom
- Steel mock CT scan
- SEM of single tungsten particle, 500x zoom
UQ-Driven Casing Design

- Casing fracture can be a possible cause of jet formation
- In order to minimize/control the casing effect (uncertainty reduction), two measures were taken:
  - Thin phenolic tubing (3/16") was chosen for the outer casing with a failure energy estimated to be 0.06% of the energy of the explosive
  - Notches were introduced to the casing to attempt to control the failure

Negligible Effect of Notched Casing

- Case notches did not appear to have an effect compared to the un-notched data
- Variability is small between 3 data sets (2 tests with notched case and 1 case with un-notched case)
- Jets were formed for all cases
UQ-Driven Measurement Plan

- Phantom v1212 sampled at 12000 fps (Camera 1/4) and Phantom v711 sampled at 7500 fps
- Instrumentation suite consisting of 54 in-ground pressure transducers (sampled at 1 MHz), 6 optical linear encoders, 8 unconfined momentum traps and 4 high-speed cameras
- Tests performed on AFRL Blastpad (Kyle Hughes talk)

Camera 1 vs Camera 3

- Cameras 1 and 4 contain significant perspective errors if used to measure shock position on the centerline
- Camera 3 shows three shock structures due to end-cap effects
- To find the shock time of arrival (TOA) along the 90-degree, camera 3 is used
- Shocks analyzed normal to the ground to examine the shock data for ground effects
Error in the particle force model (T6) was estimated from the Sandia campaign. Propagating the error and uncertainty in the particle force model through CMT-nek Hero 1 provides the error and uncertainty in the macroscale prediction. Errors from other campaigns will be propagated when they are completed.

Outline

- Unique aspects of UQ at CCMT
- UQ of demonstration problem
- VVUQ workflow of demonstration problem
- Summary of Sandia Shocktube Campaign
- Forensic UQ of micro- & meso-scale experiments
V&V and UQ Workflow

- Experiments
- Experimental input
- Simulations
- Input uncertainty
- Forensic
- Measured QoI
- Target model error estimate
- Computed QoI
- Large?
- Model Improvement
- Uncertainty/Error Reduction
- Uncertainty/Error Reduction
- Large?
- Propagated uncertainty
- Stochastic variability
- Discretization error
- Neglected feature/physics
- Uncertainty/Error
- Uncertainty/Error
- Reduction
- Reduction
- Large?
- Target model error estimate
- Error
- Error
- Large?
- Simulations
- Input uncertainty
- Experiments

Discretization Error Estimation

- **Goal**: Estimate the discretization error of multiphase problems
- **Difficulty**: Grid size can be smaller than the particle size
- **Solution**: Use the finite size of the particles (Samaun Nii)

- Point particle shows an abrupt change in force
- Finite size particle shows a gradual increase in force
Convergence of Quasi-Static Force

- Can’t afford to have the converged grid size, but can estimate discretization error
- Local force profiles are different, but overall forces are similar

Point particle

Finite size particle

Propagation of Error and Uncertainty

- Couplings of simulation and experiment for error estimation of the key CMT physics (T2, T4, T5, T6) of the demonstration simulation
- Applying Forensic UQ and UR/ER to the couplings for successful validation
Propagation of Knowledge from Forensic UQ

Design of Eglin Macroscale Experiment

UQ found substantial uncertainty in pressure ratio

ASU Vertical Shocktube Exp.

SNL Shocktube Experiments

Eglin Gas-gun Experiments

Eglin Microscale Experiments

Experienced experiments need more UQ involvements in measurement processes

Planning experiment with UQ team

Measuring uncertainties by UQ team

Designed notches to minimize uncertainty due to casing

Used cameras in different angles

Casing design was modified to be thicker

Found substantial uncertainty due to casing

Outline

- Unique aspects of UQ at CCMT
- UQ of demonstration problem
- VVUQ workflow of demonstration problem
- Summary of Sandia Shocktube Campaign
- Forensic UQ of micro- & meso-scale experiments
Summary of Sandia Campaign

- Sandia campaign has reached useful failure after vigorous uncertainty reduction campaign
- Uncertainty in experimental data extraction process was significant
  - The uncertainty in data extraction process overwhelmed the experimental variability
  - Reduced uncertainty in data extraction because it was more critical than increasing repeatability
- Experiment configuration limited validation
  - Experiment plan need to consider simulation limitations
  - Actively involved in Eglin experiment plan
- VVUQ framework was developed and is being used for the demonstration problem

Shock Tube Experiment

- To observe shock-particle interactions in dense gas-solid flows
- Point particle force model is the key physics (Bertrand Rollin)
- Quantity of interest (QoI): Upstream and downstream particle front positions
Initial Uncertainties and QoI

- Key uncertainties (highest 6 out of 24)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measurement bias in particle front positions</td>
<td>Uncertainty in systematic bias due to gap between particle curtain and wall</td>
</tr>
<tr>
<td>Particle volume fraction</td>
<td>Measurement uncertainty</td>
</tr>
<tr>
<td>Initial particle positions</td>
<td>Variability in initial particle positions</td>
</tr>
<tr>
<td>Particle diameters</td>
<td>Variability in particle diameters</td>
</tr>
<tr>
<td>Curtain thickness</td>
<td>Local curtain thickness variation</td>
</tr>
<tr>
<td>Pressure at driver section</td>
<td>Very small measurement noise</td>
</tr>
</tbody>
</table>

- Quantity of interest
  - Particle front positions **averaged** over initial particle positions
  - 4 repeated experiments
  - 10 repeated simulations with random initial particle positions

Reducing Large Noisy Error due to AUSM+

- Groups of runs identified large noise error in the behavior of average downstream front position for varying diameter
- The physics team advanced the upgrade schedule of AUSM+ to AUSM+up
- Model improvement substantially reduced the error

![Graph showing comparison of AUSM+ and AUSM+up](image-url)
AUSM+ vs. AUSM+up (1D)

- Large noisy error due to AUSM+ was identified (Forensic UQ)
- Uncertainty reduction (UR) by implementing AUSM+up
- Discrepancy between simulation and experiment was significantly increased (discovered hidden error)

Quantifying U. due to Gap Using 2D Sim.

- 2D half particle curtain model was used to study the effect of gap
- Approximately 0-10% measurement bias in measured downstream front positions was expected

Biased estimation in 2D simulation:

- Biased FPs due to gap
- Unbiased FPs
The uncertainty due to gap should be considered in UQ (Forensic UQ).
2D simulation was used to estimate the uncertainty due to gap.
The second largest uncertainty was the uncertainty in the initial volume fraction (measurement uncertainty).

Reducing U. due to Gap and U. in Initial VF

- Identified large error in AUSM+
- Reduced the error by AUSM+up
- Reduced uncertainty due to gap
- Identified / reduced measurement U in initial VF

New experiments without gaps were conducted.

Maximum initial volume fraction 19-23% was reduced to 20-22%.
The new experiment without gap removed the largest uncertainty due to gap was conducted.

The second largest measurement uncertainty in the initial volume fraction was reduced by rigorous UQ.

Reducing Error in Initial VF Input

- Identified large error in AUSM+
- Reduced the error by AUSM+up
- Reduced uncertainty due to gap
- Identified / reduced measurement U in initial VF
- Identified error in initial VF
- Reduced error in initial VF
Identified unrecognized error in the initial volume fraction input and was reduced (Forensic UQ and ER)
The particle force model was applied in CMT-nek for ASU campaign
Pseudo turbulence in 3D
81/625/6875 simulation runs for UQ of 3D/2D/1D

Target Model Error Reduction Potentials
- Global sensitivity analysis (GSA) quantifies target model error reduction potentials of individual particle force models (Samaun Nili)
- GSA shows chances of large change of front position when one force model is improved
- Error in UFP is likely to be dominated by error in Quasi-Steady force model
- DFP was significantly influenced by errors in Quasi-Steady, Added Mass and Pressure Gradient force models
Outline

- Unique aspects of UQ at CCMT
- UQ of demonstration problem
- VVUQ workflow of demonstration problem
- Summary of Sandia Shocktube Campaign
- Forensic UQ of micro- & meso-scale experiments

Design of Macroscale Eglin Experiments

- Lessons learned from Frost experiment
  - Need to have cameras with different angles
  - Casing may influence particle jets
- Lessons learned from the mesoscale experiment
  - Casing fractions hampered observing the particle cloud movement
  - Limited means for observing the movement
- Lessons learned from the microscale experiment
  - Casing fractions caused issues regarding shock forming and particle movement observation
  - Particle velocity processing error due to x-ray positions
Experimental Setup: February 2015

Experimentalists: Littrell, Delcambre, and Black

Side view photograph showing the concave pressure probe array.

Summary of test shots performed in October 2014 and February 2015. Particles were 2-mm tungsten spheres.

<table>
<thead>
<tr>
<th>Test #</th>
<th>Arrangement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oct14-1</td>
<td>Single</td>
</tr>
<tr>
<td>Oct14-2</td>
<td>Ring of 7</td>
</tr>
<tr>
<td>Oct14-3</td>
<td>Grid of 16</td>
</tr>
<tr>
<td>Feb15-1</td>
<td>Single</td>
</tr>
<tr>
<td>Feb15-2</td>
<td>Single</td>
</tr>
<tr>
<td>Feb15-3</td>
<td>Diamond of 4</td>
</tr>
</tbody>
</table>

Overhead schematic of the test set-up.

Sources: Myles Delcambre, Internal CCMT Fall 2014 presentation
Black, Littrell, and Delcambre, Eglin internal written report, 3/7/2015

Major Uncertainty Sources: Casing Fracture

- Casing fragmentation is challenging to include in the simulation
- Designed new microscale explosives with a reduced amount of explosive and increased casing size (modeling after the mesoscale/p-rad)
  - Pro: Casing would only deform slightly and can probably be included with some additional approximations
  - Con: Detonator remains a significant amount of the total explosive (multi-species modeling required)

Pictures of the microscale casing pre- and post-shot

Pictures of the p-rad casing pre- and post-shot
Microscale Gas Only Simulation

- Micro-scale gas-only simulation and experiment shows a good agreement
- This confirms that the error with a particle is solely due to the particle force model

Error Estimation of Micro Sim. With One Particle

- The validated particle force model from the Sandia campaign is used
- The uncertainties in the inputs (particle diameter, density and explosive density) were propagated
- The uncertainty in the time of the experimental data will to be converted in terms of particle location for error estimation
**UQ in ASU Experiment**

- **Goals:**
  - Plan new validation experiments that consider simulation limitations and uncertainty quantification goals.
  - **Identify** and **quantify** sources of experimental uncertainty to have a greatest influence on simulation inputs.
  - UQ is involved in the experiment (Justin Mathew, Kyle Hughes, Tanner Jones).

- Shock tube overview:
  - Four 32cm length segments.
  - Particle diameter: 45-90 microns.
  - Pressure ratio: 10-20.
  - Initial bed height: 32 cm.

---

**Uncertain Experimental Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Quantity</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Driven section pressure</td>
<td>? kPa</td>
<td>Calculation based on shock speed</td>
</tr>
<tr>
<td>Driver section pressure</td>
<td>100.68±0 kPa</td>
<td>Static pressure sensor</td>
</tr>
<tr>
<td>Volume of particle bed</td>
<td>383.5-385.6 cm³</td>
<td>CT scanner</td>
</tr>
<tr>
<td>Initial volume fraction</td>
<td>59-65%</td>
<td></td>
</tr>
<tr>
<td>Initial mean volume fraction</td>
<td>60-61%</td>
<td>( \varphi_{mean} = \frac{m}{hA} \cdot \frac{1}{p_{glass}} ) (Justin)</td>
</tr>
<tr>
<td>Particle diameter (before)</td>
<td>67±8 μm</td>
<td>SEM</td>
</tr>
<tr>
<td>Particle diameter (after)</td>
<td>68±22 μm</td>
<td>SEM</td>
</tr>
<tr>
<td>Particle density</td>
<td>2.44±0.006 g/cm³</td>
<td>Pycnometer</td>
</tr>
<tr>
<td>Tube geometry</td>
<td>Negligible</td>
<td></td>
</tr>
</tbody>
</table>

- **UB team** actively involved in measurements and uncertainty estimation (forensic UQ)
- The measured and calculated driven section pressure were different (forensic UQ).
Particle Characterization – Shape/Size

- Glass particles: 45-90 microns in diameter, 2.44±0.006 g/cm³ (Kyle Hughes and Justin Mathew at UF)
- Scanning electron microscope (SEM) Images show largely homogenous groups of particles with no apparent source of significant variation

Particle Bed Characterization – Initial VF

- To verify estimates of ~61% average volume fraction measured during ASU experiments, a mock particle bed was created for a CT scan
  - The mock tube was only 7 mm in diameter (versus ~40 mm shock tube diameter)
  - Observed a mysterious volume fraction increase in the radial direction
Comparison between Sim. and Exp. Results

- Mach number 1.494 (Oct/12 Exp #4)
- The height data from the experiments is based on high speed camera image that yields uncertainty in the measured height.

![Graph comparing Sim. and Exp. Results]

Timeline

- Target model
  - T2: Multiphase turbulence model
  - T4: Collision model
  - T5: Compaction model
  - T6: Particle force model

- Eglin Macroscale Simulations
- Eglin Macroscale Experiments
- ASU Mesoscale Simulations
- SNL Mesoscale Simulations
- SNL Shocktube Experiments
- Eglin Gas-gun Experiments
- Eglin Microscale Simulations
- Eglin Microscale Experiments

- Y5Q2 (on going)
- Y4Q4 (completed)
- Y5Q3 (on going)
Lessons Learned in Year 4

- Important to separate error from uncertainty for simulation development stage
  - Uncertainty reduction reveals simulation errors
  - Forensic UQ has been fully exercised for different scales
  - Experience from micro- and meso-scale experiments were applied to macro-scale demonstration experiment
  - It is important that UQ team needs to be involved in experiment planning
  - SNL shock tube simulation/experiment demonstrated that meaningful validation can be possible after reducing uncertainty
  - Based on 3D simulation, an important source of error is from 1D approximation

Summary of Simulation Run Plan

- Groups of simulation runs (Mesoscale)
  - 1D/2D/3D simulations with a tophat initial VF profile for the new SNL experiments
  - 1D/2D/3D simulations with a bell-shaped initial VF profile for the new SNL experiments
  - Estimating discretization error of 1D/2D/3D simulations with finite volume particles
  - 1D/2D/3D simulations with finite volume particles and compare it to the new SNL experiment
- Groups of simulation runs (Mesoscale)
  - 2D/3D simulation (CMT-nek) and the ASU experiment (Justin and Chanyoung)
  - Axisymmetric mesoscale with a single particles, JWL and reactive burn
  - Axisymmetric gas gun with particles
Summary of Simulation Run Plan

- Groups of simulation runs (Macroscale)
  - 1D macroscale with particles, JWL and reactive burn
  - 3D (or 2D) macroscale with particles, JWL and reactive burn with a case model

Do you have any questions?
Data Extraction from Shock Tube Experiment

- X-ray to measure particle volume fraction profile
  - A processing model from X-ray image intensity to volume fraction
  - Need calibration for attenuation coefficient
  - Uncertainty in the volume fraction is from
    1) Uncertainty in the experiment
    2) Uncertainty in the calibration process (model form uncertainty)

ASU Experiments Forensic UQ

<table>
<thead>
<tr>
<th>Experiment</th>
<th>$\frac{P_4}{P_1}$</th>
<th>Mach</th>
<th>Calc $\frac{P_4}{P_1}$</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0920_4</td>
<td>9.5</td>
<td>1.152</td>
<td>1.947</td>
<td>79.50</td>
</tr>
<tr>
<td>1012_5</td>
<td>13.3</td>
<td>1.393</td>
<td>4.851</td>
<td>63.52</td>
</tr>
<tr>
<td>1012_6</td>
<td>9.2</td>
<td>1.212</td>
<td>2.475</td>
<td>73.09</td>
</tr>
</tbody>
</table>
Data Extraction from Eglin Experiments

- Eglin microscale experiment (Forensic UQ)
  - Input UQ: particle diameter and density
  - Output UQ: particle positions and contact line

  ![Simacon image of the Eglin microscale experiment](image1)
  ![Multiple exposure x-ray of single particle](image2)

- Eglin mesoscale gas gun experiment
  - Computerized tomography (CT) scans of particle packet, SEM of particles, particle density via pycnometer
  - Simacon and X-ray images to track particle cloud movements

  ![CT scans of particle packet for the Eglin mesoscale gas gun experiment](image3)
  ![Eglin mesoscale gas gun experiment](image4)
CCMT
Student Lightning Round

DSE* of CMT-nek using BE**

Sai Prabhakar Rao Chenna
Advisor: Dr. Herman Lam, Dr. Greg Stitt
Department: ECE, UF

- Goals
  - Use BE methods & tools to perform extensive DSE on CMT-nek design space
  - Perform trace-driven simulations to optimize CMT-nek performance on HPC systems

- Simulation roadmap
  - Early DSE to enhance CMT-nek performance on future exascale systems

* DSE - Design Space Exploration
**BE – Behavioral Emulation
Uncertainty Quantification of Shock Tubes

Brad Durant
Advisor: S. Balachandar, T.L. Jackson
Department: MAE, UF

- **Goals**
  - Reproduce measurement processing from Sandia shock tube to identify sources of uncertainty
  - Propagate identified sources of uncertainty from experiments into simulations

- **Simulation roadmap**
  - T6: Force coupling
  - T4: Particle-particle interaction

Particles Departure from Axisymmetry

Maria Giselle Fernandez
Advisor: Dr. Raphael T. Haftka and Dr. S. Balachandar
Department: MAE, UF

- **Goals**
  - Determine what initial perturbation in particles leads to the maximum departure from axisymmetry

- **Simulation roadmap**
  - Collaboration with UB and Macroscale teams studying particles departure from axisymmetry
**CMT-bone on KNL and DVFS based Systems**

Mohamed Gadou  
Advisor: Prof. Sanjay Ranka  
Department: CISE, UF

- **Goals**
  - Multiobjective Optimization of CMT-bone on DVFS based hybrid Systems
  - Performance optimization of CMT-bone on Intel KNL

- **Simulation roadmap**
  - Our research roadmap is closely tied with CMT-nek development.

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**Eglin Explosive Barrel Ejection Simulations**

Joshua Garno  
Advisor: Dr. S. Balachandar  
Department: MAE, UF

- **Goals**
  - Simulate trajectory of 1, 9 and many particle configurations
  - Simulate dispersal of 0.5g packet of particles
  - Validate Rocflu models governing particle motion

- **Simulation roadmap**
  - Real Gas
  - EL-AUSM+UP
  - Improved Forces
  - Reactive Burn
Macroscale Explosive Dispersal of Particles

Kyle Hughes
Advisor: Prof. Kim, Balachandar, and Haftka
Department: MAE, UF

- Goals
  - Perform forensic uncertainty quantification of past experiments to inform future experiments
  - Design validation experiments to meet simulation assumptions and capabilities
  - Perform uncertainty quantification of validation experiments

- Simulation roadmap
  - Tie experiments performed at LANL and Eglin AFB to simulations using uncertainty quantification

Simulation Roadmap

Uncertainty Quantification of ASU Shock Tube

Tanner Jones
Advisor: Dr. Kim, Dr. Haftka, Dr. Park
Department: MAE, UF

- Goals
  - Identify sources of uncertainty in experimental procedures
  - Propagate identified sources of uncertainty from experiments into simulations
  - Validate CMT-nek simulation capabilities

- Simulation roadmap
  - Multiphase turbulence modeling and uncertainty
  - Conduct forensic UQ

Simulation Roadmap
Compressible Multiphase Turbulence Modeling

Rahul Babu Koneru
Advisor: Dr. S. Balachandar
Department: MAE, UF

- Goals
  - Improve drag models at high Mach numbers and dense regimes
  - Extend LES models to compressible multiphase flows
  - Validation and integration into CMT-nek
- Simulation roadmap
  - Validate existing force models and develop new models
  - Implement single phase LES and extend it to multiphase flows

CMT-nek Microscale Simulations

Goran Marjanovic
Advisor: Prof. Balachandar
Department: MAE, UF

- Goals
  - Demonstrate CMT-nek capabilities
  - Validation
  - Verification
- Simulation roadmap
  - Microscale simulations
    - Expansion wave propagating over particle beds
Microscale – Shock Particle Interaction

Yash Mehta
Advisor: Prof. S. Balachandar
Department: MAE, UF

- Goals
  - Fully resolved DNS of shock interaction with particles
  - Developing models for predicting particle motion and force history

- Simulation roadmap
  - Simulating shock interaction with random bed of particles
  - Integration of force models in Meso-Macro scale simulations

Data-driven Point-Particle Force Modeling

W. Chandler Moore
Advisor: Prof. Balachandar
Department: MAE, UF

- Goals
  - Test the PIEP model at high volume fractions
  - Improve the PIEP model using DNS data

- Simulation roadmap
  - This work uses data from microscale simulations to improve force models which bridge the gap between microscale simulations and the demonstration simulations
Multi-fidelity Surrogate Modeling for Co-design

Aravind Neelakantan
Advisor: Dr. Lam, Dr. Stitt
Department: ECE, UF

- Goals
  - Reduce computational budget of HPC codes (parent app)
  - Low-cost model validation over larger design space
  - Extrapolation of parent app towards large scale run

- Simulation roadmap
  - MFS and BE helps in simulating CMT-nekon exascale systems (notional architectures)

Discretization Error in Euler-Lagrange Simulation

Samaun Nili
Advisor: Prof. Kim, Haftka & Balachandar
Department: MAE, UF

- Goals
  - To estimate the discretization error in a 1D Euler-Lagrange simulation of an interaction between the shock wave and particle-laden
  - To achieve mesh convergence for 1D shock particle-laden interaction problem via model implementation improvement

- Simulation roadmap
  - T4: Verification and validation of the shock tube simulation
  - Uncertainty reduction via model implementation improvement
Surrogate Modeling of the Equation of State

Frederick Ouellet  
Advisor: Dr. S. Balachandar  
Department: MAE, UF

- **Goals**
  - Develop surrogate models for use in evaluating equations of state (EoS) in mixed air/product cells
  - Perform and analyze macroscale simulations of the Frost and Eglin blastpad experiments

- **Simulation roadmap**
  - Real gas equation of state capabilities in code
  - Analysis of instabilities of rapid dispersion

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FPGA Pipelined Simulations for CMT-nek

Carlo Pascoe, Ryan Blanchard  
Advisors: Dr. Herman Lam, Dr. Greg Stitt

- **Design-space exploration (DSE) critical in optimization of CMT-nek for potential Exascale architectures**
  - CMT-nek has huge design space (DS)
  - BE is a potential solution, but is it enough?
  - Complement and accelerate BE approach via FPGA acceleration
  - Propose pipelined data flow simulations as useful technique for rapid exploration under certain circumstances

- **Goal:** Pipeline simulations to explore a different design option every cycle
  - After some initial latency, quickly explore large number of different configurations – fast DSE

- **Ideal for an FPGA**
  - Pipeline is bounded by resources rather than I/O
  - Multiple FPGAs can be used to explore a vast input space – almost embarrassingly parallel
  - **Up to eight orders-of-magnitude faster DSE**
**BE-SST Simulator**

Rajashekar Rajagopalan  
Trokon Johnson  
Advisor: Dr Herman Lam,  
Dr Greg Stitt  
Department: ECE, UF  

- **Goals**  
  - Use SST framework to develop BE methods and run parallel, scalable simulations  
  - Simulations and validations of large HPC systems  
  - Improve communication models and Interpolation API  

- **Simulation roadmap**  
  - BE-SST simulator enables scalable Design Space Exploration on exascale systems

**Dynamic Load Balancing for CMT-nek**

Keke Zhai  
Advisor: Prof. Sanjay Ranka  
Department: CISE, UF  

- **Goals**  
  - To reduce simulation time and decrease power consumption on CMT-nek by utilizing dynamic load balancing algorithms  

- **Simulation roadmap**  
  - This simulation includes moving particles and gas to simulate the actual particle movement within a fixed box
Adaptive Sampling For Design Space Exploration Using Behavioral Emulation

Yiming Zhang
Advisor: Prof. Raphael T. Haftka & Prof. Nam H. Kim
Department: MAE, UF

- Goals
  - Produce sampling plans and predictions using probabilistic models for the validation and usage of Behavioral Emulation of HPC architectures
- Simulation roadmap
  - Assist validation and usage of Behavioral Emulation for algorithmic & architectural design-space exploration at different stages

Gas-Particle Mixtures Under Sudden Expansion

Heather Zunino
Advisor: Prof. Ronald Adrian
Department: SEMTE, ASU

- Goals
  - Perform repeatable experiments on a vertical shocktube at ASU
  - Examine expansion fan, flow structures, and instabilities
  - Provide data for validation of computational codes
- Simulation roadmap
  - The shocktube experiment at ASU will provide data for validating the codes being developed at UF
David Zwick
Advisor: Prof. Balachandar
Department: MAE, UF

- Goals
  - Development of state-of-the-art Eulerian-Lagrangian capabilities in CMT-nek
  - Understanding the physics of particles interacting with expansion waves

- Simulation roadmap
  - Detailed modeling of particle simulations of ASU experiment in CMT-nek

**The End**