Agenda AST Site Visit April 20-21, 2017

Thursday April 20, 2017

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 (S. Balachandar, Martin Schulz)
9:05-9:30   Agenda, Review Recommendations, Management, Internships, Educational Impact (Jackson)
9:30-10:30  Overview, Scope and Coupling, Y3 Accomplishments (Balachandar) (RQ 1,2,6)
10:30-10:45  Coffee break
10:45-11:30 Integration of experiments and simulations (Rollin/Diggs) (RQ 2,6)
11:30-11:50  CMT-nek (Jason Hackl) (RQ 4,5,6)
11:50-1:00   Lunch (RT will meet in small conference room)
1:00-1:50    V&V and UQ (Haftka, Park, Kim) (RQ 2,6)
1:50-2:40    Dynamic Load Balancing (Ranka, Banerjee) (RQ 3)
2:45-3:00    Coffee break
3:00-3:50    CS/BE results at scale (Lam, Stitt) (RQ 4,5,6)
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 21, 2017

7:45    Van pickup at University Hilton
8:00-9:00  Continental Breakfast (RT will meet in small conference room)
9:00-10:30  Overview of Scientific Goals and Accomplishments – I
            Nalini Kumar (Florida; Exascale; 15 mins)
            David Zwick (Florida; Simulations and CMT-nek; 15 mins)
            Fred Ouellet (Florida; Simulations and UQ; 15 mins)
            Yash Mehta (Florida; Physics Microscale and Modelling; 15 mins)
            Yiming Zhang (Florida; UQ; 15 mins)
            Carlo Pascoe (Florida; Exascale & FPGA; 15 mins)
10:30-10:45  Coffee Break
10:45-11:15  Overview of Scientific Goals and Accomplishments – II
            Kyle Hughes (Florida; UQ and experiments; 15 mins)
            Heather Zunino (ASU; expansion of multiphase flows; 15 mins)
11:15-12:15  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
## Attendee List

### Faculty

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### Review Team

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# AST Meeting Agenda

## Thursday
- Review Recommendations, Management, Internships, Educational Impact (Jackson)
- Overview, Scope and Integration, Y3 Accomplishments (Balachandar; RQ 1,2,6)
- Integration of Experiments & Simulations (Rollin/Diggs; RQ 2,4)
- CMT-nek (Hackl; RQ 4,5,6)
- V&V and UQ (Haftka, Park, Kim; RQ 2,6)
- Dynamic Load Balancing (Ranka; RQ 3,4,5)
- CS/BE results at scale (Lam, Stitt; RQ 4,5,6)
- Student Lightning Round
- Poster Session (25)
- Dinner

## Friday
- Overview of Scientific Goals
- Center Response to AST Questions (Balachandar)
- RT Deliberations/Summary
Review Team Recommendations – 2016

- **RQ 1 – Recommendations on Scope**
  - Consider simpler experiment for code validation
  - Compaction not yet accounted for
  - Consider contingency plans to meet year 5 goals

- **RQ 2 – Recommendations on Experiments/Simulation Coupling**
  - Develop and document detailed V&V plan
  - Include more detail on how data from ASU experiment will be extracted
  - V&V experts should work closer with Eglin

- **RQ 3 – Recommendations on Dynamic Load Balancing**
  - Continue efforts on GPUs and host CPUs
  - Discuss dynamic aspects of load balancing
  - Center should take advantage of lab expertise on load balancing

- **RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts**
  - Adopt rigorous software development and documentation practices
  - Feedback loop between physics and CS/BE efforts
  - More staff with in-depth knowledge on CMT-nek with strong ties to CS

- **RQ 5 – Recommendations on Scalability Results**
  - Scalability tests for CMT-nek
  - Use existing allocations on Titan & Mira
  - Use testbeds for upcoming machines

- **RQ 6 – Additional Recommendations**
  - Develop strategy to use lower fidelity runs for hero runs
  - Increase efforts on rigorous code verification for CMT-nek
  - Clarify how microscale results are used at mesoscale subgrid models
  - Scalability of FPGA approach
  - More talks by students
Review Team Recommendations – 2016

- **RQ 1 – Recommendations on Scope**
  - Consider simpler experiment for code validation
  - Compaction not yet accounted for
  - Consider contingency plans to meet year 5 goals

- **Answer to RQ 1**
  - Primarily addressed in Overview Talk (Balachandar)
  - Narrowed focus to only 4 experiments that feed into Demonstration Problem
    - ASU expansion
    - Sandia shock tube
    - Eglin mesoscale
    - Eglin microscale
  - Reduce importance of compaction
  - Revised experimental plans include lower volume fraction

- **RQ 2 – Recommendations on Experiments/Simulation Coupling**
  - Develop and document detailed V&V plan
  - Include more detail on how data from ASU experiment will be extracted
  - V&V experts should work closer with Eglin

- **Answer to RQ 2**
  - Primarily addressed in Overview (Balachandar), Integration (Rollin, Diggs), and UQ (Haftka, Park, Kim) talk
  - Fine-tuned detailed V&V workflow within each experiment/simulation and across scales
  - Recent work at ASU includes image de-warping, Fourier analysis, void tracking, PIV (Heather Zunino Talk)
  - Angela and Kyle are leading the UF-Eglin interaction
Review Team Recommendations – 2016

RQ 3 – Recommendations on Dynamic Load Balancing
- Continue efforts on GPUs and host CPUs
- Discuss dynamic aspects of load balancing
- Center should take advantage of lab expertise on load balancing

Answer to RQ 3
- Primarily addressed in CS talk (Ranka)
- New CPU/GPU work
- New work on load balancing

RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
- Adopt rigorous software development and documentation practices
- Feedback loop between physics and CS/BE efforts
- More staff with in-depth knowledge on CMT-nek with strong ties to CS

Answer to RQ 4
- Primarily addressed in BE (Lam, Stitt) and CMT-nek (Hackl) talks
- Closing the loop: Behavioral Emulation & design-space exploration on CMT-nek
  - Perform large-scale validation (100k+ MPI ranks) on DOE systems (Cab, Vulcan, Titan) and performed predictive simulations to million+ MPI ranks
  - Lectures on CMT-nek formulation and code during Winter Break 2016-2017 for CCMT staff and leadership
- New staff
### RQ 5 – Recommendations on Scalability Results

- Scalability tests for CMT-nek
- Use existing allocations on Titan & Mira
- Use testbeds for upcoming machines

#### Answer to RQ 5

- Primarily addressed in BE (Lam, Stitt) and Multiphase (David Zwick) talks
- Scaling studies routinely use 8k to 131k cores on Vulcan
- New emulation up to 1M cores; significant effort on benchmarking
- CS uses Titan (GPU dev)
- Large ASU experiment (meso and micro) ongoing on Mira
- Using Knights Landing (CS/BE)

### RQ 6 – Additional Recommendations

- Develop strategy to use lower fidelity runs for hero runs
- Increase efforts on rigorous code verification for CMT-nek
- Clarify how microscale results are used at mesoscale subgrid models
- Scalability of FPGA approach

#### Answer to RQ 6

- Primarily addressed by Overview (Bala), Integration (Rollin, Diggs), CMT-nek (Hackl), UQ (Haftka, Park, Kim), BE (Lam, Stitt) talks
- Multi-fidelity surrogate based strategy has been developed and is being demonstrated with 1D (lower fidelity) and 2D (higher fidelity) mesoscale shock tube simulations
- CMT-nek comparisons to Rocflu for shock/particle interaction
- Balachandar will present current approach on coupling microscale to macroscale
- Scalability of FPGA approach (multi-FPGA scalability projection will be presented)
Review Team Recommendations – 2016

- RQ 6 – Additional Recommendations
  - Lightning round before Student Poster session
  - More talks by students
- Comments on Education and Collaborations
  - UF courses/student internships/CCMT sponsored multiphase workshop

- Answer to RQ 6
  - Included in Agenda
  - Friday morning devoted to student talks (8 total)
  - Internships and Educational Impact to be addressed (Jackson)
  - Details of CCMT sponsored multiphase workshop on CCMT website

Leadership

**Physics and Code Development**
- S. (Bala) Balachandar
- Siddharth Thakur (ST)
- Thomas Jackson
- Paul Fischer
- Ju Zhang
- Bertrand Rollin

**UQ and V&V**
- Raphael Haftka
- Nam-Ho Kim

**Experiments**
- Ronald Adrian
- Charles Jenkins
- Donald Littrell

**CS/Exascale**
- Sanjay Ranka
- Herman Lam
- Gregory Stitt
- Scott Parker

UF members in red
### Internship Program - Completed

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<th>Dates</th>
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<td>Dr. Kathy Prestridge</td>
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<tr>
<td>Kevin Cheng</td>
<td>LLNL</td>
<td>May-Aug, 2014</td>
<td>Dr. Maya Gokhale</td>
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<td>Nalini Kumar</td>
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<td>March-Aug, 2015</td>
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<td>May-Aug, 2015</td>
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### Internship Program - Planned

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<tr>
<td>Yash Mehta</td>
<td>LLNL</td>
<td>Summer, 2017</td>
<td>Dr. Kambiz Salari</td>
</tr>
</tbody>
</table>
Internship Program – Not Yet Planned

- Brad Durant, PhD (MAE, Physics and UQ)
- Joshua Gorno, PhD (MAE, Physics and UQ)
- Kyle Hughes, PhD (MAE, Experiments and UQ)
- Brandon Osborne, PhD (MAE, Physics)
- Fred Ouellet, PhD (MAE, Physics and UQ)
- Prashanth Sridharan, PhD (Physics)
- Mason Rawson, MS (ECE, Exascale)
- Trokon Johnson, PhD (ECE, Exascale)

Graduated Students

- 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

- Subbu Annamalai, PhD (2015), Dr. S. Balachandar, MAE
  - Postdoc in center thru March 2017
  - Senior Systems Engineer, Optym, Gainesville FL

- Georges Akiki, PhD (2016), Dr. S. Balachandar, MAE
  - Postdoc in center thru March 2017
  - Postdoctoral Associate, LANL
Additional Information

- Additional Graduate Program Announcements
  - David Zwick – NSF Fellowship Graduate Program (started Aug 2016)
  - Georges Akiki - MAE Best Dissertation Award (TSFD; May 2017)
  - Chandler Moore – incoming PhD student; NSF Fellowship Graduate Program

- Other metrics (Y1 – Y3)
  - Publications: 82
  - Presentations: 69

- Deep Dive Workshops
  - Exascale & CS Issues, Feb 3-4, 2015, University of Florida
  - Multiphase Physics, Oct 13-14, 2016, Tampa FL

- Center Webpage
  - http://www.eng.ufl.edu/ccmt/

Educational Programs

- Institute for Computational Science (ICE)
  - One of key initiatives in the College of Engineering
  - Educational mission
    - Graduate certificate in Scientific Computing
    - Required for all CCMT students
    - Offers ICE fellowships to incoming graduate students
  - Research mission
    - Coordinating computational multidisciplinary research
    - Foster interdisciplinary research through graduate fellowship
    - Complements our investment in HPC infrastructure
    - Yearly 6 fellowships for incoming students
Educational Programs under ICE

- Profs. Kim & Haftka
  - Yearly course in Verification, Validation and Uncertainty Quantification
  - A new course started in 2014 in anticipation of CCMT
  - Lessons learned from the research in CCMT are immediately reflected in the course

- Prof. Sanjay Ranka
  - Teaches yearly a specialized course for HPC for computational scientists (as part of the Computational Engineering Certificate)

Additional Educational Programs

- Prof. S. Balachandar
  - Fall, 2016 – new graduate course on multiphase flows (30 graduate students)

- Profs. Greg Stitt/Herman Lam
  - Discusses exascale challenges and the NGEE work in the reconfigurable computing course (EEL5721/4720) and digital design (EEL4712)
  - Uses the CCMT center as a motivational example in Introduction to Electrical and Computer Engineering (EEL3000)
## Additional Educational Programs

- **Profs. Alan George/Ian Troxel**
  - EEL6763 (Parallel Computer Architecture), Spring 2016 and 2017 terms
  - Student enrollment – 2016 (70); 2017 (30)
  - DOE, CCMT, and NGEE project have significantly influenced this course (and vice-versa) since the PSAAP-II grant began
    - New lecture discussions (on Exascale, simulation, etc.) taken from CCMT research into the classroom
    - Option for a CMT-oriented course project (we've had several teams do so)
    - Use of equipment (e.g., Novo-G, Xeon Phi) closely related to CCMT for course projects on various topics
    - An offer to alumni of this course to continue (as volunteer or for credit) for summer studies related to NGEE

## 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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</thead>
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<tr>
<td>Exascale</td>
<td>X</td>
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<tr>
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<tr>
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<td></td>
<td></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
</tbody>
</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 this summer in PS&T Building to add 6 new office spaces for students
- All meetings held in PS&T Building
3rd Annual CCMT Picnic

Do you have any questions?
CCMT
Integration & Accomplishments

S. Balachandar

Review Team Recommendations – 2016

- RQ 1 – Recommendations on Scope
  - The project has defined a very broad scope. Assess if the Year 5 goals are still realistic. Compaction (is hard) not yet accounted for

  - Answer to RQ 1
    - Narrowed focus to only 4 integrated experimental/simulation campaigns
    - Clearly identified one or two target physical models for each campaigns
    - Will reduce the importance of compaction

- RQ 2 – Recommendations on Experiments/Simulation Coupling
  - Develop and document a detailed V&V plan. Show the overall V&V workflow

  - Answer to RQ 2
    - Will discuss UB workflow within each exp/sim problem and across the different scales

- RQ 6 – Additional Recommendations
  - How microscale results are used at mesoscale

  - Answer to RQ 6
    - Quasi-steady drag model, PIEP model, Force fluctuation, etc.
Outline

- Background
- Scope of the center (RQ1)
- V&V and UQ workflow (RQ2)
- Microscale informed models for meso/macroscale (RQ6)
- Y3 accomplishments

Demonstration Problem
**Prediction Metrics**

<table>
<thead>
<tr>
<th>PM-1: Blast Wave Location</th>
<th>PM-2: Particle Front Location</th>
<th>PM-3: Number of Instability Waves</th>
<th>PM-4: Amplitude of Instability Waves</th>
</tr>
</thead>
</table>

**Sequence of Events**

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

- **Compaction/collision phase**

- **Dispersion phase**
**Physical Models – Sources of Error**

- **T8:** Deformation model  
- **Compaction/collision phase**
  - Metal particles
  - Explosive material: Hot, dense, high pr gas
  - Shock wave

- **T1:** Detonation model  
- **Detonation phase**

- **T4:** Collision model  
- **T5:** Compaction model  
- **T6:** Point particle force model  
- **T7:** Point particle heat transfer model

**Multiscale Integration Strategy**

- **Macroscopic**
  - $O(10^7)$ particles
  - $O(10^8)$ of turbulence
  - Point-particle approximation

- **Mesoscopic**
  - $O(10^9)$ to $O(10^7)$ particles
  - Well resolved interface turbulence
  - Unresolved particulate turbulence

- **Microscopic**
  - $O(10^7)$ particles
  - Fully resolved, DNS

- **Atomistic**
  - Quantum and MD

- **Continuum Scale Modeling and Simulations**
  - Multi-scale LES closure models for interface & particulate turbulence

- **EOS, Thermodynamic and transport properties, shock Hugoniot**
Multiphysics Scope (From Site Visit)

- Our focus will be on
  - Turbulence at the rapidly expanding material front
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities
  - Gas-particle coupling
  - Self-assemble of explosive-driven particles

- 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
Amendment to Scope

- Our focus will be on
  - Turbulence at the rapidly expanding material front
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities
  - Gas-particle coupling
  - Self-assemble of explosive-driven particles

- We have added an intermediate configuration that minimizes
  - Compaction effect and associated modeling (T5)

- Revised plan includes
  - Mesoscale and demonstration experiments with lower $\phi$
  - Use hollow spheres (thin glass beads)

Uncertainty Budget – Overall Plan

- 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 Budget Workflow

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

Empty Success (Small error, but Large Uncertainty)

Useful Failure
Uncertainty Budget Workflow

- Experiments → Experimental input → Simulations
- Input uncertainty → Target model error → Computed Metrics
- Measured Metrics → Target model error
- Target model error → Uncertainty/error reduction
- Propagated uncertainty → Stochastic variability
- Discretization error → Neglected feature/physics
- Uncertainty/error reduction → Large?
- Large? → Target model improvement

UB Workflow - Experiment Worksheet

- Experimental input
  - ...
- Input uncertainty
  - ...
- Prediction metrics
  - ...
- Uncertainty & error quantification (UQ)
  - ...
- Uncertainty & error reduction (UR)
  - ...

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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 error

UB Workflow Simulation Worksheet

- Neglected physics and features
  - ...
- Discretization error quantification (UQ)
  - ...
- Uncertainty quantification (UQ)
  - ...
- Uncertainty reduction efforts (UR)
  - ...
- Model form and parameter improvement (MI)
  - ...
UB Workflow Simulation Worksheet

- Neglected physics and features
  - Particle curtain gap, initial particle velocity, non-sphericity, ...
- Discretization error quantification
  - Finite $\Delta x$, finite $\Delta t$, finite number of computational particles
- Uncertainty quantification (UQ)
  - Run 18,000 1D simulations varying random initial particle location, varying shock, particle and curtain properties
- Uncertainty reduction efforts (UR)
  - Perform 2D & 3D simulations with the spanwise gap
- Model form and parameter improvement (MI)
  - Sensitivity analysis of force coupling models (T6)
  - Sensitivity analysis of particle-particle interaction model (T4)

UQ Propagation Across Scale

- Demonstration
- Eglin Mesoscale
- ASU Expansion Fan
- Sandia Shock-tube
- Eglin Micro

Target Model
Propagated Model
Other Simulation Efforts

- 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

Timeline

Sandia ST  ASU EF  Eglin Micro  Eglin Meso  Demonstration  Micro Sim  Multiphase Jet  Sedimentation  Instability

Year 1  Year 2  Year 3  Year 4  Year 5

✎: Coupling to Higher Scale
Essence of Euler-Lagrange Simulation

\[ \frac{\partial \mathbf{u}_g}{\partial t} = \mathbf{g}_{\text{inv}} + \mathbf{g}_{\text{vis}} + \mathbf{g}_{\text{turb}} + f_{gp} + f_{\text{ext}} \]

Fluxes (T3)  
Turbulence closure (T2)  
Detonation source (T1)

\[ \mathbf{U}_g = \left\{ \frac{\alpha_g \rho_g}{\alpha_g \rho_g \mathbf{u}_g} \right\} \]

Force coupling (T6)  
Particle-particle (T4)

\[ \frac{d\mathbf{u}_{p,i}}{dt} = f_{pp} + f_{gp,i} \]

Compaction Model (T5)

Commonly used models are based on:
- Uniform flow
- Quasi-steady flow
- Isolated particles
- Low Mach number, modest Reynolds number

But the actual conditions are:
- Strong non-uniformity
- Highly unsteady
- Very large Mach and Reynolds numbers
- Particle-Particle interaction
  - Fluid-mediated
  - Direct collision
**Faxén Theorem (1924)**

- Stokes flow (Re = 0 limit)
  
  $$\text{Stokes Drag} = 3\pi \mu d u$$

  - Undisturbed flow at the particle

  Uniform
  
  Undisturbed
  
  Ambient flow

  Perturbation

  Stokes flow

  Faxén Theorem:  
  
  $$\text{Drag} = 3\pi \mu d u^3$$

---

**Why We Need Faxén Theorem**

- Shock-particle interaction

  - Post-Shock
    
    $$p_2, \rho_2, u_2, T_2$$

  - Pre-Shock
    
    $$p_1, \rho_1, u_1 = 0, T_1$$

  $$\text{drag} = 3\pi \mu d u$$

- Flow-mediated particle-particle interaction

  A generalized Faxén Theorem has been developed
**Generalized Faxén Theorem**

- Expressed in terms of undisturbed flow seen by the particle
  - Can be any spatially varying flow (shock thickness << $d'$)
  - Can be rapidly varying flow
- Framework applies for force, heat transfer, pressure, volume, etc.

\[
m_p \frac{d\vec{v}}{dt} = F_{sp} = \sqrt{\rho} \frac{D\vec{u}}{Dt} + \frac{3\pi \mu \vec{u}}{D} + \int_{-\infty}^{t} \left( K_s + K_{sv} \right) \left( \frac{D\rho\vec{u}}{Dt} \right) d\xi + \int_{-\infty}^{t} K_{sv} \left( \frac{D\rho\vec{u}}{Dt} \right) d\xi
\]

**Finite-Size Models for Single Particle**

- Fan-Particle Interaction ($M_s = 1.22$) (inviscid simulation)
Micro-Macro Integration Strategy

1. We have a rigorous theoretical single particle force model

2. From microscale simulations have the best empirical single particle force model at finite Re, Ma

3. Beyond force model – model for particle temperature, pressure

4. Beyond single particle
   - Mean volume fraction effect
   - Systematic inclusion of particle-particle interaction

5. Back effect on gas (modeling of pseudo turbulence)
   - Reynolds stress closure, etc.
Random Pack – Drag Force

- Mean volume fraction effect
- Fluid-mediated particle-particle interaction
- Pseudo turbulence

Mach 3.0 & 10% Volume Fraction

Random Pack – Transverse Force

- Mean volume fraction effect
- Fluid-mediated particle-particle interaction
- Pseudo turbulence

Mach 3.0 & 10% Volume Fraction
Particle-Particle Interaction (PIEP) Model

Particle-Particle Interaction Assumption

- Two-step process
  - Evaluate undisturbed velocity
  - Faxén theorem

Undisturbed Velocity:

\[ u_{un}(x_i) = u_{macro} + \tilde{u}_{N-i} \]

\[ u_{un}(x_i) \approx u_{macro} + \sum_{j=1}^{N} \tilde{u}_{j-i} \]
**Pairwise Interaction Model**

\[ F = 3\pi \mu d \bar{u}_{un}^S + m_f (1 + C_m) \frac{D\bar{u}_{un}}{Dt}^S + m_f C_{IL} \bar{u}_{un}^S \times \bar{\omega}_{un}^S \]

*Undisturbed Velocity:*

\[ u_{un}(x_i) = u_{macro} + \bar{u}_{N \rightarrow i} \]

\[ u_{un}(x_i) \approx u_{macro} + \sum_{j=1}^{N} \bar{u}_{j \rightarrow i} \]

---

**Mesoscale Simulations With PIEP Model**

- Matlab and Fortran black boxes with PIEP model

**Neighbor Info**

\( \phi_i; N, x_j, v_j, \Omega_j, d_j \)

**Particle Info**

\( x_i, v_i, \Omega_i, d_i \)

**Flow Info**

\( u, \omega, \frac{Du}{Dt} @ x_i \)

**C_{F,avg}(Re, Ma, \phi)**

- Drag, Lift, Torque

**PIEP model**
PIEP Model vs DNS (drag)

$R^2 = 0.00$

PIEP Model vs DNS (Lift)

$R^2 = 0.60$
Drafting, Kissing & Tumbling Validation

DEM w/ Standard Drag Model

DEM w/ PIEP Model

DNS

Velocity contours

80 Sphere Sedimentation Validation

DNS

DEM

Velocity Distribution

Height vs radial position
Convergence of Euler-Lagrange Approach

- Shock thickness depends on grid (~10 $\Delta x$)

Point-particle

Finite-size particle

With decreasing $\Delta x$ convergence becomes an issue:
- the shock becomes sharper and
- $\bar{u}^T$ differs from $\bar{u}$ at the particle
- $\bar{u}^T$ depends on gas velocity at

Test case condition:
- Stationary single point particle
- 1-Way Coupling
- Particle diameter: 115 $\mu$m
- Grid size range: 800 to 3.125 $\mu$m

With decreasing $\Delta x$ only finite size force converges.
Standard EL approach fails!!!
Y3 Accomplishments

1. Macroscale – Hero Run
2. Mesoscale – CMT-nek simulation of expansion fan
3. Microscale – Shock + Contact
4. Validation experiments & Forensic UQ
5. CMT-nek
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 3
- Use existing code to perform petascale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)
- Develop capabilities for the next hero run: real gas EOS, reactive burn, collision modeling

Presentation
- Bertrand Rollin
2: Mesoscale Simulations

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

Year 3
- Scalable 2-way coupled particle capability in CMT-nek
- CMT-nek simulations of ASU experiment
- Incorporating PIEP model into Nek5000 and CMT-nek
- Mesoscale simulations of expansion fan over a bed of particles

Presentation
- David Zwick, Bertrand Rollin

ASU rarefaction experiment

<table>
<thead>
<tr>
<th>particle properties</th>
<th>( N_{\text{hex}} )</th>
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<tr>
<td>Gas DOF</td>
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<tr>
<td>MPI ranks</td>
<td>8192</td>
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3: 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 3
- Shock propagation over a structured array
- Shock propagation over a random array
- PIEP model validation & improvement
- Shock + Contact (detonation condition)

Presentation
- Yash Mehta
4: Validation 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 3
- Blast pad experiments at Eglin AFB
- Mesoscale gas-gun experiments at Eglin
- Forensic UQ
- Experimental studies of gas-particle mixtures under sudden expansion at ASU

Presentation
- Angela Diggs, Heather Zunio (ASU) & Kyle Hugh
5: 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 3
- Develop and release microscale version of CMT-nek for microscale simulations
- Develop and release mesoscale version of CMT-nek for mesoscale simulations
- Shock capturing with EVM
- CMT-bone development
- CMT-nek in nek5000 repository

Presentation
- Jason Hackl and David Zwick

6: UQ Workflow

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

Year 3
- 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
- Rafi Haftka, Chanyoung Park, Nam-Ho Kim, Herman Lam, Fred Ouellet, Yiming Zhang
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 3
- Enhanced BE methods with network models, interpolation schemes, and benchmarking for CMT-bone AppBEs
- 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, Nalini Kumar, Carlo Pascoe, Yiming Zhang

8: Dynamic Load Balancing

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

Year 3
- 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
- Tania Banerjee & Sanjay Ranka
Do you have any questions?
Integration of Experiments and Simulations

Angela Diggs and Bertrand Rollin
Bring predictive capabilities to particle-laden flow simulations under extreme conditions.

Review Team Recommendations – 2016

- RQ 2 – Recommendations on Experiments/Simulation Coupling
  - Include more detail on how data from ASU experiment will be extracted
  - V&V experts should work closer with Eglin

  Answer to RQ 2
  - Recent work includes image de-warping, Fourier analysis, void tracking, PIV
  - Angela and Kyle are leading the UF-Eglin interaction

- RQ 6 – Additional Recommendations
  - Develop strategy to use lower fidelity runs for hero runs

  Answer to RQ 6
  - 2D and sub-domain runs have been used for hero run tests and development since year 1. We are now openly integrating them into a multi-fidelity strategy for model validation and for prediction metric studies
Outline

- **Demonstration Problem**
  - Hero Run
  - Eglin’s Macroscale Experiment (Blastpad)

- **Model Validation Problems**
  - Eglin’s Micro and Mesoscale Experiments
  - SNL’s Multiphase Shock Tube

---

Physical Models – Sources of Error

- **T8**: Deformation model
  - Compaction/collision phase
  - Metal particles
  - Explosive material
  - Hot, dense, high pr gas
  - Shock wave

- **T4**: Collision model
- **T5**: Compaction model

- **Detonation phase**
  - **T1**: Detonation model

- **Dispersion phase**
Demonstration Problem: Hero Run 2

- **Features:**
  - 30 Million computational cells
  - 5 Million computational particles
  - \( r_{\text{max}} = 4.00 \text{m} \)
  - \( t_{\text{max}} = 2.50 \text{ms} \)
  - 4096 cores

---

### Hero Run: Evolution

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<th>Properties</th>
<th>Hero Run 1</th>
<th>Hero Run 2</th>
<th>Hero Run 3A</th>
<th>Hero Run 3B</th>
<th>Hero Run 3C</th>
<th>Hero Run 4</th>
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<td>40 % - Frozen</td>
<td>10 % - Frozen</td>
<td>10 % - Frozen</td>
<td>10 % - Frozen</td>
<td>40 %</td>
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<td>1 mode in azimuthal direction</td>
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<td>60 M</td>
<td>60 M</td>
<td>60 M</td>
<td>120 M</td>
</tr>
<tr>
<td>No. of cores</td>
<td>512</td>
<td>4096</td>
<td>5760</td>
<td>5760</td>
<td>5760</td>
<td>16384</td>
</tr>
</tbody>
</table>
The Jones-Wilkins-Lee (JWL) equations of state are used to predict the pressures of high energy substances and are:

\[
P_{JWL}(\rho, \varepsilon) = A(1 - \frac{\varepsilon}{\rho V})e^{-\frac{\rho V}{R_1}} + B(1 - \frac{\varepsilon}{\rho V})e^{-\frac{\rho V}{R_2}} + \omega \rho e^{-\frac{\rho V}{R_3}}
\]

\[
T_{JWL}(\rho, \varepsilon) = \left(\frac{1}{\rho c_0^2}\right)(P - A e^{-\frac{\rho V}{R_1}} - B e^{-\frac{\rho V}{R_2}})
\]

where \( V = \frac{\rho}{\rho_0} \) and \( \rho_0, A, B, C, R_1, R_2 \) and \( \omega \) are parameters for the substance.
**Hero Run 3**

- Features:
  - 60 Million computational cells
  - 15 Million computational particles
  - \( t_{\text{max}} = 2.50 \text{ms} \)
  - \( r_{\text{max}} = 4.00 \text{m} \)
  - 5760 cores

---

**Demonstration Problem: Predictions**

**Blast Wave Location (PM-1)**

- Time vs. Blast Wave Location (m)
- Time vs. Blast Wave Location (m)
**Demonstration Problem: Predictions**

**Particle Front Location (PM-2)**

- **Initial configuration.** Explosive charge surrounded by a ring of particles (5%PVF). The rest of the domain is filled with air.

- **Initial perturbation** in the particle volume fraction (PVF). It is single mode with wavenumber equal 10, amplitude 0.14 and no phase shift.
**Prediction Metric: Maximum PVF Ratio**

Maximum PVF ratio is defined as the ratio between the particle volume fraction (PVF) of the sector with the highest PVF and the PVF of the sector with the smallest.

![Schematic of a sector. We used 1024 sectors](image)

\[
\text{Max. PVF Ratio} = \frac{PVF_M}{PVF_L}
\]

Maximum Particles Ratio as a function of time for unperturbed and perturbed cases. The error bars are a 90% confidence intervals.

---

**Modal Filtering**

- The noise in the data has a normal distribution with mean zero and standard deviation smaller than 6e-5.

- The signal is one order of magnitude bigger than the noise standard deviation for the perturbed case.

- Moving average method will be used as a noise filter in the future optimization process.
Outline

- Demonstration Problem
  - Hero Run
  - Eglin’s Macroscale Experiment (Blastpad)

- Model Validation Problems
  - Eglin’s Micro and Mesoscale Experiments
  - SNL’s Multiphase Shock Tube

AFRL Blastpad Experimental Setup

- Instrumentation:
  - 54 pressures probes
  - Momentum traps (instrumented possible)
  - Four high speed video cameras
  - Linear optical transducers

- Six shots
  - 2 bare charges
  - 1 charge w/tungsten (notched)
  - 1 charge w/steel (notched)
  - 2 charges w/steel (un-notched)
Blastpad Charge Sizing

- A critical design parameter is the ratio of the mass of the particles to the mass of the charge (M/C ratio)
- Based on a sampling of the literature that reported jets in their results, M/C ratio of 10 was chosen:

<table>
<thead>
<tr>
<th>Paper Title</th>
<th>First Author</th>
<th>Charge Mass [g]</th>
<th>Particle Mass [g]</th>
<th>M/C Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle jet formation during explosive dispersal of solid particles</td>
<td>Frost</td>
<td>1.6</td>
<td>226.2</td>
<td>141.375</td>
</tr>
<tr>
<td>Particle momentum effects from the detonation of heterogeneous explosives</td>
<td>Frost</td>
<td>435</td>
<td>4350</td>
<td>10</td>
</tr>
<tr>
<td>Explosive dispersal of solid particles</td>
<td>Zhang</td>
<td>2400</td>
<td>26000</td>
<td>10.83333</td>
</tr>
</tbody>
</table>

- The charge mass was chosen to match legacy blastpad data (released to UF)

Dimensions in inches

- Minimize Case Influence

- Case fracture may be a possible mechanism for jetting instability [Zhang et al. 2001, Xu et al. 2013]
- Reduce the influence of the case:
  - Thin phenolic tubing (3/16") for the case
  - Failure energy ~0.06% of explosive energy
  - No case between the explosive and particles
  - Case notched on outer surface to control case failure
Preliminary Particle Characterization

- **Steel Particles**
  - Multiple vendors surveyed. Criteria were high particle roundness (sphericity) and narrow particle spread
  - Vendor: Osprey Sandvik
  - Size range (confirmed with particle sizer): 75-125 µm
  - SEM shows mostly spherical particles

- **Tungsten Particles**
  - Government provided
  - Size range (confirmed with particle sizer): 100-130 µm
  - SEM shows mostly spherical particles

Collaboration: Input Measurement Uncertainty

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Explosive length [mm]</td>
<td>AFRL measurement</td>
</tr>
<tr>
<td>Explosive diameter [mm]</td>
<td>AFRL measurement at 5 locations</td>
</tr>
<tr>
<td>Explosive density [kg/m³]</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Explosive quality</td>
<td>AFRL X-ray</td>
</tr>
<tr>
<td>Particle diameter [mm]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle density [kg/m³]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle volume fraction</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Ambient pressure [kPa]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Ambient temperature [°C]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Probe locations [m]</td>
<td>CCMT measurement</td>
</tr>
</tbody>
</table>

Pre-test collaboration ensures input parameter measurements are performed to quality requested by UF CCMT UQ team.
Future Experiments

- Previous feedback from AST/TST shows concern with modeling the compaction regime
- Future experiments at lower volume fraction will allow a focus on multi-disperse effects, vice compaction
  - 5, 10, 15, 20% volume fraction explosive experiments
  - Similar range to Multiphase Shock Tube at Sandia
  - Achievable by mixing “micro bubbles” (hollow glass spheres) with metal powder
- Future experiments likely at mesoscale due to AFRL budget constraints

Blastpad Simulation Setup

Preliminary Simulation Details:
- 5.16 million cells in two dimensions
- To be run on 1024 cores using LLNL’s Quartz machine
- Bottom five boundaries are slipwalls
- Remaining three are outflows
- 65 probes set in locations of experimental sensors
## Blastpad Simulation Parameters

<table>
<thead>
<tr>
<th>Properties</th>
<th>Comp B</th>
<th>Steel</th>
<th>Tungsten</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter (μm)</td>
<td>-</td>
<td>100 μm</td>
<td>115 μm</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>1712</td>
<td>7660</td>
<td>15540</td>
</tr>
<tr>
<td>Specific heat (J/kg K)</td>
<td>1223.6</td>
<td>510</td>
<td>134</td>
</tr>
<tr>
<td>Outer diameter (in)</td>
<td>3.25</td>
<td>6.88</td>
<td>5.12</td>
</tr>
<tr>
<td>Depth (thickness) (in)</td>
<td>0.75</td>
<td>0.75 (2 cm)</td>
<td>0.75 (2 cm)</td>
</tr>
<tr>
<td>Energy = (dens x int energy/unit vol)</td>
<td>8.5 GPa (products); 0.662 GPa (unreacted)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Computational Particles</td>
<td>-</td>
<td>10 M</td>
<td>10 M</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometry outer diameter</td>
<td>16 m</td>
</tr>
<tr>
<td>Simulation time</td>
<td>6 ms</td>
</tr>
<tr>
<td>Charge/mass ratio</td>
<td>10</td>
</tr>
</tbody>
</table>
Outline

- **Demonstration Problem**
  - Hero Run
  - Eglin’s Macroscale Experiment (Blastpad)

- **Model Validation Problems**
  - Eglin’s Micro and Mesoscale Experiments
  - SNL’s Multiphase Shock Tube

---

Key Physics

- Collision model
- Collision phase
- Shock-particle Interaction phase
- Dispersion phase
- Point particle force model
Mesoscale Experiments: November 2015

Summary of 7 mesoscale explosive shots of interest.

<table>
<thead>
<tr>
<th>Test #</th>
<th>Driver</th>
<th>Particles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nov15-1</td>
<td>RP-80 + 1 N5</td>
<td>0.5 g Tungsten powder</td>
</tr>
<tr>
<td>Nov15-2</td>
<td>RP-80 + 1 N5</td>
<td>0.5 g Tungsten powder</td>
</tr>
<tr>
<td>Nov15-3</td>
<td>RP-2 + 1 N5</td>
<td>0.5 g Tungsten powder</td>
</tr>
<tr>
<td>Nov15-4</td>
<td>RP-80 + 1 N5</td>
<td>0.5 g Tungsten powder</td>
</tr>
<tr>
<td>Nov15-5</td>
<td>RP-80 + 1 N5</td>
<td>0.5 g Tungsten powder</td>
</tr>
<tr>
<td>Nov15-6</td>
<td>RP-80 + 1 N5</td>
<td>0.5 g Tungsten powder</td>
</tr>
<tr>
<td>Nov15-7</td>
<td>RP-80 + 2 N5</td>
<td>0.5 g Tungsten powder</td>
</tr>
</tbody>
</table>

Summary of Microscale Experiments
Preliminary Simulation Results

Simulation Details:
- Axisymmetric
- Ideal gas equation of state
- Point-particle model
- Explosive modeled as high-density, quiescent gas
- Time-shifted to align with experimental times
- 1-way coupled
- Mean input quantities used

Comparison of experimental results with simulation
(simulation credit: Joshua Gamo)

Microscale Simulations Progression

- Plan for gradually including more sophisticated machinery into the simulation
  - JWL instead of ideal gas to improve handling of explosive products
  - Reactive burn instead of constant property gas to improve initial conditions
  - Introduction of more realistic geometry
- Current geometry has a solid backwall for the explosive
  - In reality there is a sizable hole in the back of the explosive where the detonator attaches

Cross Section View
Not to scale
All dimensions in mm
Uncertainty Propagation

- The simulation is too expensive to sample many times
  - Instead, batches of runs with varying uncertain inputs are conducted
  - Kriging is chosen as a surrogate technique for its low interpolation error
  - Construction of Kriging surrogate will allow Monte Carlo sampling of the simulation
- Uncertain input ranges for the surrogate are taken from UQ
- Simulation prediction metrics with uncertainty can be used to perform meaningful validation

Example of how batches of runs are used to construct a kriging surrogate. The surrogate is sampled many times to construct confidence intervals for the simulation.

Outline

- Demonstration Problem
  - Hero Run
  - Eglin’s Blastpad Case

- Model Validation Problems
  - Eglin’s Micro and Mesoscale Experiments
  - SNL’s Multiphase Shock Tube
New Particle Curtain Experiments


Key Physics

Collision model

Collision phase

Shock impact

Shock-particle Interaction phase

Dispersion phase

Point particle force model
3D Particle Curtain Simulation

- Features:
  - 18 Million computational cells
  - 6 Million computational particles

Large-Scale Bundle Runs Planning

- Comparison between mesoscale 1D/2D/3D simulations and the new SNL experiments with non-tophat initial particle volume fraction profile
  - Modeling initial volume fraction profile using Beta distribution
  - Expected outputs: particles position data at time t
  - Runs for:
    - 5 different Mach numbers: 1.24, 1.40, 1.45, 1.66, 1.92
    - Initial particle volume fraction
    - Random initial particle locations
    - 2 Beta distribution parameters
    - Curtain thickness
  - Required 18000 simulations (full factorial design):
    - 5 (Mach numbers) x 16 (initial particle volume fractions) x 5 (random initial particle locations) x 5 (curtain thickness) x 9 (two beta distribution parameters)
  - Required subset of 1D, 2D and 3D simulations and Multi-Fidelity model prediction will be applied.
### Initial Particle Volume Fraction Study

<table>
<thead>
<tr>
<th>Simulations ($M = 1.66$)</th>
<th>Particle Volume Fraction (%)</th>
<th>Curtain thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Run 1</td>
<td>10</td>
<td>3.1</td>
</tr>
<tr>
<td>Run 2</td>
<td>15</td>
<td>2</td>
</tr>
<tr>
<td>Run 3</td>
<td>Distribution</td>
<td>3.4</td>
</tr>
</tbody>
</table>


### Particle Curtain Initial Volume Fraction Effects

- The initially “gaussian” particle volume fraction profile appears to allow for better prediction than the 10% and 15% uniform volume fraction cases
Do you have any questions?
CMT-nek: A compressible multiphase DGSEM extension to nek5000

Jason F. Hackl

Review Team Recommendations – 2016

- RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
  - Adopt rigorous software development and documentation practices
    - [http://travis-ci.org/UFCCMT/Nek5000](http://travis-ci.org/UFCCMT/Nek5000) automated regression testing,
      Doxygen committed with code, [http://github.com/Nek5000/NekDoc](http://github.com/Nek5000/NekDoc)
  - Feedback loop between physics and CS/BE efforts
  - CMT-nek team collaborating with CS & exascale for particle load-balancing; Ongoing application to large simulations of ASU experiment.
  - More staff with in-depth knowledge on CMT-nek with strong ties to CS
  - Lectures on CMT-nek formulation and code during Winter Break 2016-2017 for CCMT staff and leadership.

- RQ 5 – Recommendations on Scalability Results
  - Scalability tests for CMT-nek
    - Only needed for particles; Eulerian code is a trivial subset of nek5000, which already scales well. Production runs and method verification routinely use 8K to 131K cores on vulcan.
  - Use existing allocations on Titan & Mira
    - CS on titan (GPU dev)
    - Large ASU experiment (meso and micro) ongoing on Mira.
CMT-nek team

Prof. Paul Fischer, UIUC, Argonne
Li Lu, UIUC
Jason Hackl, UF
Brad Durant, UF
David Zwick, UF
Goran Marjanovic, UF

Accomplishments

- Discontinuous Galerkin SEM of high-order terms
  - Entropy viscosity for stabilizing shocked flow
- Particle tracking, 2-way coupling
- Rarefaction over particle bed (ASU experiment)
  - Mesoscale: 2-way coupled point particles
  - Microscale: Inviscid forces on arrays of spheres
- Interaction between shocks and cylinder, sphere
Outline

1. Brief review of CMT-nek framework
   a. Discontinuous Galerkin method for gas flow solver
   b. Lagrangian particles and scaling

2. Accomplishments
   - High-order terms and artificial viscosity
   - Particle tracking, 2-way coupling
     • Production rarefaction through particle bed @ meso- and microscale
   - Shock-particle interactions
     • Release for microscale simulation of shocked flows

3. Current and near-future work
   - Shocked mesoscale flows

---

Discontinuous Galerkin Spectral Elements

Steps to DGSEM for a conservation law \( \frac{\partial U_i}{\partial t} + \nabla \cdot H_i(U, \nabla U) = R_i \)

1. Inner product with test function \( v \)
2. Integrate by parts on hexahedral \( \Omega_e \)
3. Numerical flux \( H^* \) in surface integral
   - Weak boundary conditions
   - Couples elements together
4. Isoparametrically map \( \Omega_e \) to \([-1, 1]^d\)
5. Approximate integrals with quadrature
6. Approximate \( U \) & \( v \) with Lagrange polynomials
   - \( N \) Gauss-Legendre-Lobatto (GLL) nodes
   - Nested tensor product \( \sim O(N^d) < N^3 \times N^3 \)

Matrix ops within \( \Omega_e \):

\[
\int_{\Omega_e} f(x) \, dV = \int_{-1}^{1} f(r) J \, d^3r \approx \sum_{j=1}^{N} \omega_j f(r_j)
\]

\[
\int_{-1}^{1} \frac{\partial U_i}{\partial t} J \, d^3r = \int_{-1}^{1} \frac{\partial v}{\partial x_j} \frac{\partial v}{\partial r_k} H_j \, J \, d^3r - \sum_{j=1}^{6} \int_{-1}^{1} H^* N_j A J \, d^2r + \int_{-1}^{1} v J R J \, d^3r
\]

### Discontinuous Galerkin Spectral Elements

Nested tensor products of per-element $N \times N$ matrix operators for...

- Differentiation
  $$\frac{\partial}{\partial x_i} = \frac{\partial}{\partial r_i} \frac{\partial}{\partial r_k} \approx [r_{k,n}] [D_k f]$$

- Volume integrals
  $$\int f \, dv = \int_{N^3} f \, dV$$
  (Integration of $N^3$ quadrature points \(\rightarrow\) diagonal mass matrix $B$)

- Surface integrals
  $$\int_{\partial r_i} f$$
  (Face restriction $E$, diagonal $B_A$ on $N^2$ face points)

**Equations**

$$v^T B \left[ \frac{\partial U}{\partial t} \right] = v^T D_i^k B \left[ r_{k,n} \right] \left[ H_i \right] - v^T E^T B_A \left[ H^*(E[U, \nabla U]) \right] + v^T BR$$

Discretize LHS with explicit TVD RK3

---

### CMT-nek: Convective terms in DGSEM

The 3rd variable's flux = convective + diffusive

$$H_{i \gamma} = H_{i \gamma} \left( U \right) + H_{i \gamma} \left( U, \nabla U \right)$$

#### Volume fractions of gas

$$\phi_g = 1 - \phi_p$$

$$\phi_p = \lim_{V \rightarrow 0} \frac{V_2}{V}$$

... and particles

Conserved variables...

- Mass
  $$H_z = (U_2, U_3, U_4)^T$$

- Momentum
  $$H_z = \phi_g \left[ \begin{array}{c} \rho u \\ \rho v \\ \rho w \\ \rho E \\ \rho \end{array} \right]$$

- Energy
  $$H_z = \phi_g \left[ \begin{array}{c} \rho E + p \\ \rho \end{array} \right]$$

Here, quadrature needs $M > N$ nodes

- Interpolate onto $M = 3(N-1)/2$ Gauss-Legendre points to "dealias" integrals.

---


CMT-nek: Entropy viscosity method (EVM)

Diffusive flux from \emph{entropy viscosity} (NOT Navier-Stokes)

\[
\begin{align*}
\mathbf{H}^d_{ij} &= -\phi_g \nu \mathbf{\nabla} \rho \\
\mathbf{H}^d_{i+1,j} &= -\phi_g \left( \mu_s \rho \sigma_{ij} + \nu_s \mathbf{u}_j \right) \frac{\partial \rho}{\partial x_i} \\
\mathbf{H}^{d_{\text{EN}}} &= \left\{ - \mathbf{E}_{\mathbf{A}} \left[ \left( \mathbf{H}^d_{i} \cdot \mathbf{n} \right) - \left\{ \left( \mathbf{H}^d_{i} \cdot \mathbf{n} \right) \right\} \right] \\
&+ \mathbf{D}_{\mathbf{A}} \left( \mathbf{u} \right) \mathbf{E}_{\mathbf{A}} \left[ \mathbf{U} - \left\{ \{ \mathbf{U} \} \right\} \right] \right\} \\
&= \frac{1}{2} \left( \mathbf{u}^- + \mathbf{u}^+ \right) \\
\end{align*}
\]

Mass
\[
\mathbf{H}^m_{ij} = -\phi_g \nu \mathbf{\nabla} \rho
\]

Momentum
\[
\mathbf{H}^m_{i+1,j} = -\phi_g \left( \mu_s \rho \sigma_{ij} + \nu_s \mathbf{u}_j \right) \frac{\partial \rho}{\partial x_i} + \frac{1}{2} \left( \mathbf{u}^- + \mathbf{u}^+ \right)
\]

Energy
\[
\mathbf{H}^{e_{\text{EN}}} = - \phi_g \left[ \mu_s \rho u_j \sigma_{ij} + \nu_s \left( \frac{\partial (\rho e)}{\partial x_i} + \frac{1}{2} \left| \mathbf{u} \right|^2 \frac{\partial \rho}{\partial x_i} \right) \right]
\]

Entropy and its residual
\[
s = \log \left( \frac{e^{rac{1}{\rho}}}{\rho} \right), \quad \mathbf{R}_s = \frac{\partial s}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{s})
\]

\[
\mu_s = cb_h(x)^2 \frac{|R_s|}{\|s - \{s\}\|_\infty} \max_{x} \left( \frac{1}{\Omega_x} \right) \text{Tent between maximum @ vertices}
\]


cmt-nek: Lagrangian particles

Governing equations of \(i\)th particle
\[
\begin{align*}
\frac{d\mathbf{X}_p}{dt} &= \mathbf{V}_p \\
\frac{d\mathbf{V}_p}{dt} &= -\mathbf{F}_{hyd}(\mathbf{X}_p, \mathbf{V}_p)
\end{align*}
\]

Particle force from models\(^1\) and gas properties at \(\mathbf{X}_p\)
\- Barycentric interpolation from \(N^3\) GLL grid points
\- Same Runge Kutta time marching as DGSEM

**Back-coupling to gas** (e.g. momentum equations)
\- Gaussian kernel \(G\)
\[
\phi_g = \sum_{i=1}^{N_p} V_p^{(i)} G(\mathbf{x} - \mathbf{X}_p^{(i)})
\]
\[
\mathbf{R}(\mathbf{x}) = p \nabla \phi_g - \sum_{i=1}^{N_p} F_{hyd}^{(i)} G(\mathbf{x} - \mathbf{X}_p^{(i)})
\]

\(^1\)Ling, Balachandar & Parmar (2016) Phys. Fluids 28, 033304

ASU rarefaction experiment

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N_{\text{gas}})</td>
<td>8192</td>
</tr>
<tr>
<td>Gas DOF</td>
<td>1E6</td>
</tr>
<tr>
<td>SPL</td>
<td>78</td>
</tr>
<tr>
<td>MPI ranks</td>
<td>8192</td>
</tr>
</tbody>
</table>

David Zwick, April 21
CMT-nek: scaling

nek5000's guts (F77) & sinews (C, MPI1) gird CMT-nek

Largest values of key parameters so far

<table>
<thead>
<tr>
<th>MPI Ranks</th>
<th>N_elements</th>
<th>Grid points</th>
<th>Particles</th>
<th>Wall time</th>
</tr>
</thead>
<tbody>
<tr>
<td>131,072</td>
<td>4,194,304</td>
<td>250 M</td>
<td>20 B</td>
<td>12 hours</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>20.6 B</td>
</tr>
</tbody>
</table>

Particles, Strong Scaling

Accomplishments: inviscid sphere array

CMT-nek predictions & model dev on Mira

Elements | Spheres | Rows |
---------|---------|------|
23424    | 95      | 21   |

Volume fraction 3%

Convergence study in ρ

Accomplishments: Mach 3 shock-sphere

- $2^{20}$ - element mesh from GridPro, far-field $h=0.1075a$
  - $N = 5$, 125M DOF in surrounding $10a \times 10a \times 10a$ box
- 8192 cores on Vulcan

Shock physics$^1$
- Incident wave diffraction
- Mach stem formation, radial spread of triple point

EVM Artificial viscosity
- Localized at shocks
- Scales as$^2$ $h/p$

$^2$Persson & Peraire AIAA 2006-112
**Shock over cylinder: CMT-nek vs RocFlu**

CMT-nek
- $N=9$ ($p=8$)
- 576 DOF on cylinder
- 50K DOF in surrounding 2x2 box

RocFlu
- 300 DOF on cylinder
- 140K DOF in surrounding 2x2 box

Validation of cylinder drag coefficient


**Conclusion**

**Current capabilities**
- Mesoscale flows without shocks
- Microscale flows with shocks

**Pending Milestones**
- Publication
- CUBIT installation and training for mesh generation
- Shock capability for mesoscale simulations
- Fully compressible Navier-Stokes

**Future Work**
- CS feedback; GPU port
- Numerics
  - Implicit time marching
  - Refined smoothing of the viscosity
Uncertainty Budget
Validation and Uncertainty Reduction

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

Uncertainty Budget Team

- PIs: Raphael Haftka and Nam-Ho Kim
- Research Scientist: Chanyoung Park
- Students
  - Giselle Fernandez (Instability signal to noise ratio)
  - Kyle Hughes (UQ of Eglin exp.)
  - Justin T. Mathew (UQ of ASU/SNL experiments) (New student)
  - Sam Nili (Mesoscale 1D/2D force model potential errors)
  - Yiming Zhang (UQ and multi-fidelity correction of BE emulation)
- Undergraduate students
  - Shirly Spath (UQ of Eglin exp.)
**Collaborations**

- Giselle Fernandez
- Rahul Koneru
- Brad Durant
- Frederick Ouellet
- Siddharth Thakur
- Yash Mehta
- S. Balachandar
- Thomas Jackson
- Bertrand Rollin
- Jason Hackl
- Ronald Adrian
- Blair Johnson
- Heather Zunino
- Herman Lam
- Nalini Kumar
- Aravind Neelakantan
- Sanjay Ranka
- Tania Banerjee
- Angela Diggs
- Mike Jenkins
- Don Littrell

**AST Questions and Answers**

- **RQ2 – Recommendations on Exp/Sim Coupling**
  - Work closer with the team at Eglin
    - How we followed and identified unrecognized uncertainties and realized we are doing forensic UQ.
    - While both experimental and simulation efforts are strong, the coupling between the aspects leave room for improvements.
    - Sandia shock tube experiments progress
    - Eglin mesoscale and macroscale progress

- **RQ6 –Additional Recommendations**
  - Develop strategy for use of lower fidelity runs to augment the hero runs
    - Multi-fidelity surrogate for exploring parameter space of the Hero runs with an aid of cheap lower fidelity simulation runs
    - Multi-fidelity surrogate also for predicting computational times with exascale team.
Forensic UQ

- In the course of digging deeper into experiments and models we realized that we perform **forensic uncertainty quantification**
  - We discover anomalies
  - We discover or help discover **unrecognized** errors and uncertainties
  - We have the advantage of being outsiders to both modeling and experiments

- **Forensic UQ tools**
  - Document all the experimental details (crime scene)
  - Clarify details with experimentalists (witnesses)
  - Quantify uncertain inputs and prediction metrics (forensics lab)
  - Identify unrecognized uncertainties via simulation (culprits)

- Forensic UQ of the microscale experiment (Kyle Hughes) next

---

Microscale Experiments: February 2015

- Surprising evidence that the flow is strongly coupled with particles:
  - Mean shock arrival times increase as the number of particles is increased

- A possible explanation is high volume fraction in the initial plane of the particles:

Overhead schematic of the test set-up.

Source: Black, Littrell, and Delcambre, internal written report, 3/7/2015
Preliminary Microscale Validation

- Simulation Details:
  - Single particle
  - Axisymmetric
  - Point-particle model
  - Explosive modeled as high-density, quiescent gas
  - Time-shifted to align with experimental times (Kyle Hughes, detective)
  - 1-way coupled
  - Simulation credit: Joshua Garno

Comparison of experimental results with simulation

Lessons Learned from Eglin Microscale Exp

- Kyle Hughes surprised everybody by finding that the small number of particles show significant coupling with the flow

- Uncertainty quantification for validation of even this “simplified” problem required extensive back and forth between UQ, simulation, and experimental teams (~5+ months)
  - Underscores importance of clear communication
  - Written documentation of information source increases rigor

- Start simulation of the problem
  - Simulations are challenging and require a significant ramp-up time
  - Inputs/assumptions can help drive the forensic UQ
The neglected gap appeared to be the largest uncertainty source. The uncertainty in the initial volume fraction (input uncertainty) was the second largest uncertainty source.
Mesoscale Validation Forensic UQ

- The largest uncertainty was surmised to be absence of the particle curtain gaps in the 1D mesoscale simulation.
- The newest shock tube experiment without gap revealed that the effect of the gaps was minimal (Forensic UQ).

- The second largest uncertainty in the initial volume fraction was characterized in detail and reduced using X-ray (Forensic UQ).
- We found that maximum volume fraction was used as ‘top-hat’ profile in simulations.
- Detailed analysis by Justin Mathew working together with Justin Wagner narrowed uncertainty in volume fraction.

Before and After

- Carried out UQ roughly.
- 19%-23% for Experiment #1 (previously).
- 20.1%-21.7% for Experiment #1.
- Found much larger uncertainties in curtain thickness.
Error Identification and ER

- Experiments
- Input uncertainty
- Simulations
- Target model

- Measured Metrics
- Error reduction (ER)
  - Reduced the error significantly by implementing AUSM+up

- Error discovery by groups of runs
  - Noisy response due to AUSM+

- Uncertainty/error reduction

The Coupling of Simulation and Experimental Efforts for Improvements of CMT physics models

- Propagated uncertainty
- Stochastic variability
- Discretization error
- Neglected feature/physics
V&V Plan With UR and ER for Improvements

- The CCMT V&V plan is to improve key CMT physics models based on V&Vs of simulations in different scales dominated by the key CMT physics.
- The coupling of simulation and experimental efforts of each scale highlights the target model error by removing influences of other error sources (ER) and uncertainties (UR).
- Emphasizes identifying unrecognized uncertainties through forensic UQ and better experiment data extraction process.
- The mesoscale shock tube V&V will be presented to demonstrate how the plan was applied.

Shock Tube Experiment

- To observe shock-particle interactions in dense gas-solid flows.
- Point particle force model is the key physics (Bertrand Rollin).
- Upstream and downstream particle front positions are prediction metrics.

Experiments of Justin Wagner (SNL)

- Initial curtain thickness of 2 mm at t=0.
- Curtain thickness after impact.
Key Uncertainties and Prediction Metrics

- Key uncertainties (highest 6 out of 24)

<table>
<thead>
<tr>
<th>#</th>
<th>Uncertainty Source</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Measurement bias in particle front positions</td>
<td>Systematic bias uncertainty because of the gap between the particle curtain and wall</td>
</tr>
<tr>
<td>2</td>
<td>Particle volume fraction</td>
<td>Measurement uncertainty (21%±2%) Local variation in particle curtain</td>
</tr>
<tr>
<td>3</td>
<td>Initial particle positions</td>
<td>Variability in initial particle positions</td>
</tr>
<tr>
<td>4</td>
<td>Particle diameters</td>
<td>Variability in particle diameters</td>
</tr>
<tr>
<td>5</td>
<td>Curtain thickness</td>
<td>Local curtain thickness variation</td>
</tr>
<tr>
<td>6</td>
<td>Pressure at driver section</td>
<td>Very small measurement noise</td>
</tr>
</tbody>
</table>

- Prediction metrics
  - Particle front positions **averaged** over initial particle positions
  - 4 repeated experiments
  - 10 repeated simulations with random initial particle positions

Target Modeling Setting

- Experiments → Experimental input → Simulations
- Measured Metrics → Target model error → Computed Metrics
- Uncertainty/error reduction
- Large?

- Uncertainty/Error
  - Sampling uncertainty
  - Measurement uncertainty
  - Measurement processing error
  - Propagated uncertainty
    - Stochastic variability
    - Discretization error
    - Neglected feature/physics

- Particle force model

- Input uncertainty
Highlights of 1D Shock Tube Sim. (Before UR)

- Comparison between the 1D simulation (Sam Nili and Giselle Fernandez) and the experiment (Justin Wagner)

- UQ revealed large uncertainty in the model error estimate [-1,7] mm
- 2D simulation (Bertrand Rollin and Rahul Koneru) with the gaps appeared to show neglected gaps in the 1D simulation as largest source of uncertainty
- Next step is uncertainty reduction and error reduction
Uncertainty Reduction (UR)

- **Experiments** → **Experimental input** → **Simulations** → **Input uncertainty** → **Target model improvement**

**UR1:** Recognized uncertainty due to particle curtain gap in the experiments
- Comparison between the 2D with gap and the shock tube experiments *with* gap
- Comparison between the 1D and the new shock tube experiments *without* gap

**UR2:** Reduced the uncertainty in the initial volume fraction

**UR1 – Option1: 2D Simulation With Gap**

- Predicted DFP of 2D simulation *(Rahul Koneru)* corresponding the measured DFP
- Uncertainty due to inconsistency of the 1D simulation due to missing gap effect was reduced by modeling gap through 2D simulation
- The uncertainty reduction revealed that model improvement is needed
**UR1 – Option 2: Removing Gap from the Exp.**

- Predicted DFP of 1D simulation corresponding the measured DFP
- Uncertainty due to inconsistency of the 1D simulation due to missing gap effect was reduced by conducting new experiments without gap
- The experiment results without gap (Justin Wagner) are almost identical to those with gap

**UR2: Reducing Uncertainty in Init. VF**

- Preliminary UQ on initial VF was conservative including data noise in the uncertainty of the initial VF calculation
- Estimated uncertainty in initial VF estimated at 19%-23%
- Revised UQ (Justin Mathew and Chanyoung Park) filters out data noise and considers uncertainty in the measurement processing due to the noise
- 20.1%-21.7% is newly estimated uncertainty
On-Going Error Reduction

Experiments → Experimental input → Simulations

- Input uncertainty
- Target model error
- Computed Metrics
- Target model improvement
- Large?

Measured Metrics → Target model error

- Sampling uncertainty
- Propagated uncertainty
- Neglected feature/physics

- Reducing numerical error in the hybrid Eulerian-Lagrangian mesoscale shock tube simulation by using finite size particles

Computed Metrics → Measured Metrics

- Uncertainty/error reduction
- Large?

Convergence of Euler-Lagrange Approach

- Shock thickness depends on grid (~10 Δx)

- With decreasing Δx only finite size force converges. Standard EL approach fails!!!
Target Model Improvement Prioritization

- Experiments → Experimental input → Simulations
- Input uncertainty → Target model improvement
- Measured Metrics
  - Particle force model improvement
  - GSA to identify influential force models
- Uncertainty/Error reduction

Uncertainty/Error reduction
- Stochastic variability
- Discretization error
- Neglected feature/physics

Uncertainty/Error reduction
- Target model error

Target Model Error Reduction Potentials

- Global sensitivity analysis (GSA) quantifies target model error reduction potentials of individual particle force models (Sam Nili)
- GSA shows chances of large change of front position when one force model is improved
Further ER Plans

Experiments → Experimental input → Simulations

- Input uncertainty
- Target model error
- Large?
- Target model improvement
- Neglected feature/physics

Measured Metrics → Target model error

- Uncertainty/error reduction

Computed Metrics

- Error in the approximated initial volume fraction model
- Modeling Gaussian VF profile instead of tophat type VF profile using X-ray images

Eglin AFB Experiment Planning

Past exp. : Forensic UQ

Future exp. : Uncertainty reduction
Summary of Eglin Experiments

- Macroscale explosive tests (focusing on uncertainty reduction)
  - Propagating all sub-scale uncertainties & validation (no calibration)
  - Casing with notches (UR for controlling jet formation)
  - Bare charge tests (UR for reactive burn simulation)
  - CT scan (UQ for volume fraction), SEM (UQ for particle size), Pycnometer (UQ for particle density)

- Microscale explosive experiments (focusing on forensic UQ)
  - Strong coupling between flow and particle (unrecognized uncertainty)
  - Inconsistent timing in opening valve and x-rays (unrecognized)
  - Particle velocity processing error due to x-ray positions (unrecognized)
  - Particle diameter and density (UQ)
  - Unrecoverable shock locations, but contact lines (changing prediction metric)

Ex: Casing Design for UR

- Casing fracture can be a possible cause of jet formation [Zhang et al. 2001, Xu et al. 2013]
  - In order to minimize/control the casing effect, 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 will be introduced to the casing to attempt to control the failure
Multi-Fidelity Surrogate Model for Augmenting the Hero Runs in Order to Explore Parameter Space

RQ 6 – Additional Recommendations

- Develop a strategy to use lower-fidelity runs to augment the Hero Runs in order to explore parameter space more broadly
Multi-Fidelity Surrogate

- Multi-fidelity surrogate (MFS) can simulate high-fidelity runs (e.g. the Hero Runs) with the aid of lower-fidelity runs
- It was found that MFS is most useful for increasing computational efficiency
- An analytical example showed that MFS is as accurate as the surrogate with high-fidelity data only with 1% of computational cost
- MFS can take into account the model error in the low-fidelity model via scaling and discrepancy

1D/2D/3D Mesoscale Simulation Runs

- Comparison between mesoscale 1D/2D/3D simulations and the new SNL experiments with a non-tophat initial VF profile
  - Chanyoung and Justin (UB team) / Brad (Physics team)
  - Modeling initial VF profile model using Beta distribution
  - Expected outputs: particle front positions at time \( t \)
  - Runs for
    - 5 different Mach numbers: 1.24, 1.40, 1.45, 1.66, 1.92
    - Initial volume fractions
    - Random initial particle locations
    - 2 beta distribution parameters
    - Curtain thickness
  - Required 18000 Simulation runs (full factorial design):
    - 5 (Mach numbers) \( \times 16 \) (initial volume fractions) \( \times 5 \) (random initial particle locations) \( \times 5 \) (curtain thickness) \( \times 9 \) (two beta distribution parameters)
  - Required subset of 1D simulation runs for 2D and 3D and multi-fidelity model prediction will be applied
Data Extraction from the Experiments

RQ 2 – Recommendations on Coupling

- The plan should include how data will be extracted from the experiments

  - For example, how are the PIs planning to extract velocity fluctuation measurements in the ASU experiments, etc.

  - The PIs should consider ways to explain structural details within the particle bed and document ways to characterize the impact of wall contribution to void structure.

  - RQ 2 – Recommendations on Experiments/Simulation Coupling
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)

Data Extraction from Eglin Experiments

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

- 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
Data Extraction from Eglin Experiments

- Eglin macroscale blastpad experiment
  - SEM of particles and particle density via pycnometer
  - Steel mock CT scan
  - Comp B x-rays

Data Extraction from ASU Shock Tube

- SEM shows particle diameters tending to the lower end of nominal ranges
  
  \[
  \begin{array}{c|c}
  \text{mean} & \text{sd} \\
  \hline
  108.6 & 8.09 \\
  157.2 & 28.1 \\
  \end{array}
  \]

- CT scan-based volume fraction measurement
- Working on UQ in particle bed locations
Lessons Learned in Year 3

- Unrecognized epistemic uncertainties can be identified from the coupling of simulation and experiment (Forensic UQ)
  - Negligible influence of gap of the shock tube experiment
  - Strong coupling between gas and a small number of particles
  - Parametric study anomalies in the particle force model
- Multi-fidelity surrogate models can augment computationally expensive runs
  - Physics: Used as a strategy to use lower-fidelity runs to augment parametric study of hero runs
  - Exascale: Multi-fidelity surrogates have been used to predict CMT-nek execution time by combining data from different fidelities
- Different force model errors contribute simultaneously to the single prediction metric
  - Enough information to quantify uncertainty, but not enough to reduce it
  - **Global sensitivity analysis** can help to identify target models where refinement will influence most prediction metrics

Summary

- **Year 1:** Explore
  - Map uncertainty sources
  - initial UQ and UR for multiphase shock tube (MST) simulation
- **Year 2:** Integrate with other teams
  - Full range of UQ and UR for MST simulation
  - UQ of Eglin, SNL, and ASU experiments
  - Initial UQ for CS and Exascale activities
- **Year 3:** Bite into demonstration problem
  - UQ for demonstration problem and fingers phenomenon,
  - Guiding experiments
  - Validation by blind prediction for CS and exascale
Do you have any questions?

Influence of Gap on Front Position (PM)

- Front positions were obtained from schlieren images that capture the side view of the entire particle curtain.
- 2D half particle curtain model with 99000 particles (Top view).
- Approximately 0-10% measurement bias in measured downstream front positions.
What are Our Criteria for Success?

- 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

Calibrated A for Measuring VF (Linear)

- Initial UQ cumulated the uncertainty in the calibration (model-form uncertainty) in the linear fit and the noise
- The uncertainty in the initial VF was very conservative
- Correlated noise model is applied to filter the noise effect out and to exclusively consider the uncertainty in calibration

Considering uncertainty in coefficients
The influence of the gap on experiments and simulations are not consistent.

Experiments are insensitive to the presence of the gaps while 2D sims are not.

Explanation on the unexpected observation is that boundary layer growth over time < 800 μsec mitigated possible movement of particles along sides ahead of the bulk.

![Graphs showing 2D simulations and experiments with and without gaps](image)
CMT-nek: CS Update

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Members

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Mohamed Gadou
Sankeerth Reddy Mogili
Tania Banerjee

Sanjay Ranka
Exascale Simulation: CS Challenges

Dynamic Load Balancing

Energy and Performance Tradeoffs

Future Architectures and Hybrid Processors

Parallelization on a million+ processors

Review Team Questions – 2016

- RQ 3 – Recommendations on Dynamic Load Balancing
  - Continue efforts on GPUs and host CPUs
    - Completed code that divides data structures and computation on CPU+GPUs. Tested on Titan.
    - Discuss dynamic aspects of load balancing
      - Developed initial implementation for serializing, deserializing, communication and dynamic load balancing. Tested on Titan, Vulcan and Mira.
  - Center should take advantage of lab expertise on load balancing
    - Conducted a detail literature survey including correspondence with lab personnel.
Talk Overview

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

CMT-bone

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

Multi-Level Memories

Dynamic Voltage Scaling

Power/Energy Performance Trade-offs

CMT-nek CMT-bone

Dynamic Load Balancing

Auto Tuning

Hybrid Core Mapping

Dynamic Load Balancing

Multi-Level Memories

Dynamic Voltage Scaling

Hybrid Core Mapping

Multi-level Memories

Dynamic Load Balancing

Auto Tuning

Hybrid Core Mapping

Multi-objective Load decomposition

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<th>CPU Attribute</th>
<th>Description</th>
</tr>
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<tr>
<td>Manufacturer</td>
<td>Intel</td>
</tr>
<tr>
<td>Model</td>
<td>Xeon E5-2695 v2</td>
</tr>
<tr>
<td>Frequency (GHz)</td>
<td>2.4</td>
</tr>
<tr>
<td>Number of Cores (sockets)</td>
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<tr>
<td>Memory (GB)</td>
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</table>

<table>
<thead>
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<th>GPU Attribute</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer</td>
<td>NVIDIA</td>
</tr>
<tr>
<td>Model</td>
<td>Tesla K80(Kepler)</td>
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<tr>
<td>Number of GPUs</td>
<td>8</td>
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<tr>
<td>Number of Cores/SM</td>
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<td>Global Memory (GB)</td>
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<td>Shared Memory (SM) (KB)</td>
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<td>L1 Cache (KB)</td>
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<tr>
<td>Number of Registers (SM)</td>
<td>1430</td>
</tr>
<tr>
<td>Peak performance (GFlops)</td>
<td>1430</td>
</tr>
</tbody>
</table>

Hybrid Multicore Architectures
**Problem formulation**

Minimize  

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

Subject to  

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

\[ n \leq N \]

\[ m \leq M \]

\[ f \in F \]

\[ g \in G \]

\[ S \]

\[ T \]

\[ T_1 \]

\[ O \]

\[ E : \text{Energy consumed} \]

\[ n : \text{Number of CPUs} \]

\[ m : \text{Number of GPUs} \]

\[ f : \text{CPU Frequency} \]

\[ g : \text{GPU Frequency} \]

\[ N : \text{Total available CPUs} \]

\[ M : \text{Total available GPUs} \]

\[ F : \text{Set of available CPU frequencies} \]

\[ G : \text{Set of available GPU frequencies} \]

\[ S : \text{Problem size} \]

\[ T : \text{Computation Time} \]

\[ T_1 : \text{Constrained time} \]

\[ O : \text{Communication overhead} \]

\[ ECPU(n, f, X) + EGPU(m, g, S-X) \]

\[ TCPU(n, f, X) \leq T_1 - C_o(m+n, S) \]

\[ TGPU(m, g, S-X) \leq T_1 - C_o(m, S-X) \]

\[ n \leq N \]

\[ m \leq M \]

\[ f \in F \]

\[ g \in G \]

CPU: Computation and Computation Time

- Single node CMT-bone
- 8192 elements
- 128000 particles
- 7x7x7 grid size
- Strong scaling
**CPU: Power Consumption**

- Observations:
  - Power consumption does not vary with workload
  - Power consumption increases as:
    - More cores are used
    - Clock frequency is increased

**CPU: Energy Consumption**

- Energy consumption first decreases and then increases with frequency
**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
GPU: Computation and Communication Time

- Strong scaling
- Single node
- CMT-bone
- 8192 elements
- 128000 particles
- 7x7x7 grid size

GPU: Power Consumption

- Observations:
  - Power consumption increases as
    - More GPUs are used
    - Clock frequency is increased
  - Power consumption does not vary with workload
**GPU: Energy Consumption**

- Total energy consumption
  - remains nearly constant for 1, 2 and 4 GPUs
  - increases as 8 GPUs are used
    - Due to significantly more power consumption for the 8 GPUs

**GPU: Power Performance Tradeoff**

- Using 8 GPUs is the most performance efficient setup
- while using 1 GPU is the most power efficient setup
GPU: Energy-Performance Tradeoff

- Using 4 GPUs at 666 MHz frequency is the most energy efficient.
- The other configurations with 4 GPUs give reasonable performance while at the same time being energy efficient.

Hybrid: Load Balancing between CPU and GPU

- The lowest value depends on CPU and GPU frequencies as well as the number of processing elements of each type.
Hybrid: Power-Performance Tradeoff

- The triplets represent (#Cores, #GPUs, % load on cores)

Hybrid: Energy-performance Tradeoffs

- The triplets represent (#Cores, #GPUs, % load on cores)
Multi-Level Memories

Running time is total time taken to complete 100 time steps.

Optimizations on KNL include autotuning, vectorization AVX-512 instructions, using OpenMP + MPI, using MCDRAM as cache.
KNL is faster than an Intel IvyBridge by about 4 times
KNL is faster than Tesla K40m GPU by about 3 times
KNL is the most energy efficient platform

Load Balancing: Expansion Fan
Load Balancing: Cylindrical Scattering

Dynamic Load Balancing

- Step 1: Initial Partitioning of Elements and Particles
- Step 2: Decide when to trigger a remap
  - Rebalance after every $k$ time steps
  - Rebalance when processing time per step gets higher beyond a threshold
  - Generate an element to processor mapping
- Step 3: Transfer elements and particles
  - Serialize
  - Deserialize
  - Reset other data structures
Load Balancing: Literature Survey

- Pearce O, Gamblin T, de Supinski BR, Amato N, MPMD Framework for Offloading Load Balance Computation, Olga Pearce, Todd Gamblin, Bronis de Supinski, Nancy Amato, IPDPS, Chicago, IL, USA, May 2016.
- Pearce O, Gamblin T, de Supinski BR, Schulz M, Amato N, Quantifying the Effectiveness of Load Balance Algorithms, International Conference on Supercomputing (ICS), June 2012.

Load Balancing: Literature Survey (continued)

Initial Partitioning

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

Elements to Processor Mapping

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

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

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

- P1 – 8 particles
- P2 – 8 particles
- P3 – 8 particles
- P4 – 8 particles
After n time steps

P1 – 4 particles P2 – 3 particles P3 – 12 particles P4 – 12 particles

Remapping

P1 – 7 particles P2 – 8 particles

- Determine new mapping of elements to processors
- Transfer elements and particles using serialization
- Deserialize newly received elements and particles
- Reinitialize other supporting data structures
During rebalancing, some arrays are reinitialized while others are transferred. Currently we reuse nek5000 initialization routines, as a result there are some significant additional and redundant operations happening.
CMT-nek on Vulcan

- Ran out of time on Vulcan after 8hrs whereas load balanced version finished in 3.5 hours
- More than 5 times improvement in average performance

CMT-nek on Mira (setup from previous slide)

- Power consumption by both the Chip Core and DRAM domains improved by using load balancing
- Thus energy consumption of the load balanced code is better because of reduced time as well as reduced power consumption
CMT-bone on Titan

More than 1.3 times improvement in average performance

Hardware-Software Autotuning

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

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

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

Number of 4-loop implementations for dudr
\[N_z = N_y = N_x = 10\]
\[= 4! \cdot 4^3 = 6144\] variants
Total number of variants = 198,240 \(N=10\)
Total number of variants = 217,728 \(N=20\)
Exhaustive search may not be feasible

More than 1.3 times improvement in average performance
Genetic Algorithm

- Compile and run each individual
- Set fitness value for each individual based on performance and energy
- Generate initial population
- $i = 1$

Comparison of GA with Exhaustive Approach

<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 19771</td>
<td>9771</td>
</tr>
<tr>
<td>AMD Opteron</td>
<td>1.81</td>
<td>1.02 19771</td>
<td>45.6</td>
</tr>
<tr>
<td>AMD Fusion</td>
<td>1.36</td>
<td>0.95 3265</td>
<td>30</td>
</tr>
</tbody>
</table>

<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 9771</td>
<td>54.9</td>
</tr>
<tr>
<td>AMD Fusion</td>
<td>17.6</td>
<td>11.98 3265</td>
<td>32</td>
</tr>
</tbody>
</table>
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

Power for most configurations is nearly the same. Thus, energy requirements are similar.

Publications
Conclusions: Overall Improvement

- Algorithmic
- Hardware

Performance per Flop Improvement

Overall Improvement \( \propto X^Y \)

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

Sai Chenna (M.S./Ph.D.)
Trokon Johnson (Ph.D.)
Nalini Kumar (Ph.D.)
Aravind Neelakantan (M.S./Ph.D.)

Carlo Pascoe (Ph.D.)
Ajay Ramaswamy (M.S.)
Mason Rawson (B.S./M.S.)
Review Team Questions & Recommendations - 2016

- RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
  - Feedback loop between physics and CS/BE efforts
  - "Closing the loop": predictive BE simulation of CMT-nek design space

- RQ 5 – Recommendations on Scalability Results
  - Scalability is a major objective in Year 3; will emphasize scalability studies in benchmarking results, predictive BE simulation, and FPGA acceleration

- RQ 6 – Additional Recommendations
  - Scalability of FPGA approach
  - A multi-FPGA scalability projection will be presented

Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts & Y3 achievements

- BE-SST simulator & tools for CMT-bone-BE simulations
- Multi-fidelity surrogate model for performance prediction
- BE simulation of CMT-nek design space
- Adding energy models to BE
- Accelerating BE simulations with FPGAs

- Summary, conclusions, & future work
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---

Co-Design Using **Behavioral Emulation**

**HW/SW co-design**

- Algorithmic & architectural design-space exploration (DSE)

**Coarse-grained BE simulation**

- Balance of simulation speed & accuracy for rapid design-space evaluation
Goal & Accomplishments

Goal: Develop Coarse-grained Behavioral Emulation methods & tools

- To support co-design for algorithmic & architecture DSE
- For purpose of optimization of key kernels in CMT-nek

On existing & future architectures, up to Exascale

Year 1 & 2 Accomplishments:

- Developed & explored BE methods at device level (Year 1)
- Scaled experiments beyond device level and performed predictive simulations of larger & notional systems (8k MPI ranks) (Year 2)
- Developed and performed experiments on SMP software & FPGA-based simulators (Year 1)
- Begin development of SST-based BE simulator (BE-SST); Explored FPGA-acceleration methods for rapid design space reduction & UQ (Year 2)

Year 3 Accomplishments:

- BE method enhancement: network models, interpolation schemes, energy & thermal modeling
- Perform large-scale validation (100k+ MPI ranks) on DOE systems (Cab, Vulcan, Titan) and performed predictive simulations to million+ MPI ranks
- Closing the loop: Behavioral Emulation & design-space exploration on CMT-nek
- Completed development of v1.0 of SST-based BE simulator
- Validation of dataflow, pipelined approaches; multi-FPGA scalability prediction

Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts & Y3 achievements

- BE-SST simulator & tools for CMT-bone-BE simulations
- Multi-fidelity
- BE simulation
- Adding energy
- Accelerating
- Summary, etc.
**BE-SST Simulator**

- Developed by extending Structural Simulation Toolkit (SST) from SNL
  - Framework for parallel simulations
  - Supported by developers and vendors
  - Flexibility in designing custom components

<table>
<thead>
<tr>
<th>SST Capabilities</th>
<th>BE Influences</th>
<th>BE-SST</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Parallel simulations</td>
<td>• Software Definitions</td>
<td>• Parallel discrete event simulation environment</td>
</tr>
<tr>
<td>• Discrete event simulation</td>
<td>• Probabilistic Simulation</td>
<td>• Distributed component queues</td>
</tr>
<tr>
<td>• Clock and event queues</td>
<td>• Abstract Network Definitions</td>
<td>• Software Definitions</td>
</tr>
<tr>
<td>• Network Models</td>
<td>• Abstract Hardware Definitions</td>
<td>• Probabilistic Simulation</td>
</tr>
<tr>
<td>• Component Models</td>
<td></td>
<td>• Abstract Network Models</td>
</tr>
</tbody>
</table>

**BE-SST model enhancements**

- Communication model enhancements:
  - Dynamic generation of network routes provide better performance scaling and parallel performance
  - Overhead modeling at both sender/receiver endpoints

- Interpolation API allows easy switching between different interpolation methods for better accuracy
  - Polynomial Interpolation
  - Lagrange Interpolation

- Improved scalability and robustness of software product
  - Reduced storage by deleting handled events from queues
  - Switched from static routes to runtime routing
Parallel Performance of BE-SST

- BE simulations of 3d-mesh system running CMT-bone-BE
  - Simulations of machines with up to a million cores
  - With dynamic routing

- System config build time is not a bottleneck for large simulations

BE-SST running on 64 cores of HiPerGator@UF

![Graph showing event simulation time, system config build time, and total simulation time vs. simulated system size (in cores).]

* See poster from Ajay Ramaswamy

Outline

- Review & Overview:
  - Behavioral Emulation (BE)

  **Research thrusts & Y3 achievements**

  - BE-SST simulator & tools for CMT-bone-BE simulations
  - Multi-fidelity
  - BE simulation
  - Adding energy
  - Accelerating

- Summary

  RQ 5 – Recommendations on Scalability Results
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

- **Cab @ LLNL**
  - TLCC2 cluster
  - 8-core Intel Xeon; 16 cores/node; 1k nodes; 20k cores
  - 32GB/node

Application Case Study: CMT-bone-BE

- CMT-nek & CMT-bone (proxy-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 vector 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
    - Benchmarking technique: in situ
  - 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 CMT-bone-BE on Titan

- Average % error between CMT-bone-BE simulation and execution time is 4%
- Maximum error is 17%

\[
\% \text{ error} = \frac{\sum_{i=1}^{N} |\text{measurement}_i - \text{simulated}_i|}{\sum_{i=1}^{N} \text{measurement}_i} \times 100
\]
BE Simulations of CMT-bone-BE on **Vulcan**

- **BE simulation**
- **Measured**

**CMT-bone-BE Execution**

- **BE Simulation**

- Average % error between CMT-bone-BE simulation and execution time is 4%
- Maximum error is 9%

---

**In situ vs. Micro-kernel Benchmarking**

- Micro-kernel benchmarking for calibration to support **notional exploration**
  - E.g., no source available
- **Initial study** – simulation of two, 2048-core systems
  - **Vulcan**: Average error is **comparable** with in situ methods
  - **Titan**: Average error is 20% compared to 4% (in situ)
- A suitable **combination** of the two methods is best for DSE

---

*See posters from Nalini Kumar, Aravind Neelakantan, and Trokon Johnson*
Outline

- Review & Overview:
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Research thrusts & Y3 achievements

- BE-SST simulator & tools for CMT-bone-BE simulations
- Multi-fidelity surrogate model for performance prediction
- BE simulation
- Adding energy
- Accelerating BE simulations

Summary, conclusions, & future work

Assessing Behavioral Emulation

- Motivation
  - Improve BE models via validation and uncertainty estimation
  - Verify trends among CMT-nek, CMT-bone, and CMT-bone-BE
  - Reduce computational budget by fitting to CMT-nek using Multi-Fidelity Surrogate (MFS) BE simulation
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

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

Trends of CMT-nek, -bone, and -bone-BE

- Similar trends across three applications:
  - Left: Linear in (element size)$^3$
  - Right: Linear in elements/processor

- CMT-bone-BE has different slope – captures only spectral element solver kernel of nek/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

---

Multi-fidelity Prediction of **CMT-bone**

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

**Accuracy of corrected BE sim.**
- At 20 left-out CMT-bone test points
- Overall RMSE < 5% with 15 or more CMT-bone data

* See posters from Aravind Neelakantan and Yiming Zhang
Outline

- Review & Overview:
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- Research thrusts & Y3 achievements

  - RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
  - Feedback loop between physics and CS/BE efforts

  - BE simulation of CMT-nek design space
  - Adding energy models to BE
  - Accelerating BE simulations with FPGAs

Motivation & Approach

- Motivation: Very large design space
  - CMT-nek provides various algorithmic and parametric options
  - Rapid algorithmic DSE helps in performance evaluation of these options on future exascale systems

- Iterative DSE steps:
  - Identify optimization candidates (i.e. most expensive subroutines) via profiling
  - Create and validate models of algorithms for these subroutines
  - Use BE to predict performance
CMT-nek Profiling: Gas vs Particle Solver

- Execution time primarily depends on input parameters:
  - Particles/gridpoint (α), element size, elements/process

- Observations:
  - Particle solver becomes more expensive than gas solver with
    - Increasing element size and particles/gridpoint
  - David (CMT-nek) is developing particle phase of CMT-nek

- Conclusions:
  - Alternate algorithms for particle solver phase provide 14x speedup!
  - Reaches a theoretical maximum of 24x for larger element sizes
CMT-nek Alternate Algorithms

- Explore accuracy vs execution time trade-off of algorithm design choices for portions of CMT-nek particle solver
- **Time Integration** - solve differential equations to calculate particle properties
  - Current: Runge-Kutta 3 (rk3) – 3 stage time integration
  - Alternate: Backward Differentiation Formula (bdf) – single stage time integration
- **Particle Interpolation** - interpolates fluid properties acting on particles:
  - Current: Barycentric Interpolation
  - Alternate: Reduced Barycentric Interpolation

Validation of Particle Solver Models

CMT-nek particle solver (rk3 time integration & Barycentric interpolation) - Validation results on Vulcan

- Fixed particles/gridpoint = 0.1
  - Element sizes: 5,7,9,13,17,21
  - Elements/process: 4,8,16,32,64
- Fixed element resolution = 5
  - Elements/process: 4,8,16,32,64
  - Particles/gridpoint: 0,1,0.33,1,3.33,10

- Observed an average error of 2.57% in simulations
- Reduced Barycentric Interpolation – average error 2%
- Bdf time integration – average error 2.44%
Simulator Predictions: Time Integration

Simulation predictions on Vulcan

- Both algorithms vary
  - Non linearly w.r.t element size and elements/process
  - Linearly w.r.t particles/gridpoint
- bdf time integration provides 3x speedup over rk3
  - # of particles/gridpoint can be 3x large using bdf time integration

Simulator Predictions: Interpolation

Simulation predictions on Vulcan

- Both algorithms vary
  - Non linearly w.r.t element size and elements/process
  - Linearly w.r.t particles/gridpoint
- Reduced barycentric interpolation provides 5x speedup over current approach
  - Reaches max. speedup of 8 for larger element sizes
  - # of elements/process can be quadrupled using reduced barycentric interpolation

* See posters from Sai Chenna and David Zwick
Outline

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  - BE-SST simulator & tools for CMT-bone-BE simulations
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- Summary, conclusions, & future work

Energy Benchmarking & Modeling

Goal: Create an extendable, configurable, portable, and scalable benchmarking methodology for generating energy models to be integrated into ArchBEOs for scaling studies

Energy Measurement Tools: Score-P, libmsr, RAPL
Energy Benchmarking Infrastructure

Tangible Result

Tool for Data Visualization

Output Data

Auto Instrumentation

API Wrapper

API

HW counter

CCMT

Processor Granularity Energy/Power Consumption Data

Visualization using Vampir

Calibration Data Generation

Score-P

Open Source Plugins

X86Energy Plugin

libmsr

Intel : RAPL

Vampir

- Allows easy visualizing of trace data generated by Score-P

Score-P

- Is open source
- Generates profiling and tracing data
- Is portable across HPC systems
- Is scalable to large, HPC code

Open Source Plugins

- Are configurable to vary overhead and API settings
- Allow extensions to a variety of hardware counters
Thermal Aware Computing Lab (TACL)

- **Purpose**
  - Develop detailed understanding of processor level thermal effects on performance and energy consumption
  - Develop thermal- and energy-aware optimizations for multicores
    - Initial analysis on Intel Knights Landing
  - Working with experimentalist (Kyle Hughes) for IR thermography experience

- **Equipment**
  - Flir A35c IR Camera
  - Knights Landing (KNL)

*See posters from Mason Rawson and Tanya Banerjee*

Outline

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

- **Research thrusts**
  - BE-SST simulator & tools for CMT-BE simulations
  - Multi-fidelity surrogate model for performance prediction
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- **RQ 6 – Additional Recommendations**
  - Scalability of FPGA approach
**BE 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

**Landscape of FPGA-acceleration Studies**

Original Project Target
- 1 large, Exascale sim distributed over many FPGAs

NGEEv1* Progress
- 1 small, microscale sim limited to a single FPGA

NGEEv1 Enhancements
- Ongoing improvements to allow for sims at larger scale

NGEEv1 Parameter Sweeps
- Multi-FPGA DSE* limited to a single simulation per device

(NEW) Pipelined Simulations for Rapid DSE and MC Simulations
- Fully-expanded dataflow pipeline (maximum throughput)
- Collapsed dataflow pipeline (greatly improved scalability)
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. Extracting DFG from BE simulation configuration

   Configuration Mapping

```
AppBEO
<table>
<thead>
<tr>
<th>recv</th>
</tr>
</thead>
</table>
ArchBEO
```

2. Mapping DFG to FPGA Pipeline

```
<table>
<thead>
<tr>
<th>send</th>
<th>mem</th>
<th>recv</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
```

**Event Attributes**
- Type: sim
- Subgraph name
- Port: src
- Parameters: (op, M, id)

**Pipeline Simulation**
- pp1, pp2, pp3, pp4
- send, mem, recv

1. Extracting DFG from BE simulation configuration

```
<table>
<thead>
<tr>
<th>dfg</th>
</tr>
</thead>
<tbody>
<tr>
<td>send</td>
</tr>
<tr>
<td>recv</td>
</tr>
</tbody>
</table>
```

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. Extracting DFG, then identify subgraphs & dependencies

```
<table>
<thead>
<tr>
<th>dfg</th>
</tr>
</thead>
<tbody>
<tr>
<td>send</td>
</tr>
<tr>
<td>recv</td>
</tr>
</tbody>
</table>
```

2. Mapping DFG to FPGA Pipeline

```
<table>
<thead>
<tr>
<th>send</th>
<th>mem</th>
<th>delay</th>
<th>recv</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
```

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
Simulations of CMT-bone-BE on Vulcan

<table>
<thead>
<tr>
<th>Simulation Method</th>
<th>Num. of MPI Ranks</th>
<th>Num. of Timesteps</th>
<th>Num. of Events</th>
<th>% Logic Utilization</th>
<th>FPGA Ck Frequency</th>
<th>Latency to First Output</th>
<th>Mega Sims/second</th>
</tr>
</thead>
<tbody>
<tr>
<td>BE-SST</td>
<td>128</td>
<td>1</td>
<td>5,952</td>
<td>NA</td>
<td>NA</td>
<td>66</td>
<td>280 – 320</td>
</tr>
<tr>
<td>FEP</td>
<td>128</td>
<td>1</td>
<td>5,952</td>
<td>66%</td>
<td>280 - 320 MHz</td>
<td>118</td>
<td>280 – 320</td>
</tr>
<tr>
<td>CP</td>
<td>128</td>
<td>1</td>
<td>5,952</td>
<td>2%</td>
<td>315 - 355 MHz</td>
<td>458</td>
<td>1.68 – 1.99</td>
</tr>
</tbody>
</table>

- BE software and BE FPGA simulations produce similar results
- Fully-expanded approach provides greatest performance at cost of more resources
- Collapsed approach allows for greatly reduced resource utilization and increased scalability at cost of slightly reduced performance

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

*Fully-expanded performance of CMT-Bone-BE with varied MPI ranks and simulation timesteps on a single Stratix V SG5MDK1F40C2 (d) 300 MHz*
Fully-Expanded & Collapsed Pipeline Tradeoffs

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

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>% LU</th>
<th>Num. of Events</th>
<th>Lat to First Out (cycles)</th>
<th>Mega Sims /second*</th>
<th>Giga Events /second*</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>1</td>
<td>2</td>
<td>1,344</td>
<td>278</td>
<td>10.5</td>
<td>14.1</td>
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<tr>
<td>32</td>
<td>4</td>
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<td>980</td>
<td>10.5</td>
<td>56.3</td>
</tr>
<tr>
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<td>113</td>
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<tr>
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<td>10.5</td>
<td>225</td>
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<td>2,880</td>
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<td>60.3</td>
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<td>5.23</td>
<td>241</td>
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<tr>
<td>64</td>
<td>32</td>
<td>46</td>
<td>92,160</td>
<td>10,252</td>
<td>5.23</td>
<td>482</td>
</tr>
<tr>
<td>128</td>
<td>1</td>
<td>2</td>
<td>5,952</td>
<td>458</td>
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<td>15.6</td>
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<td>5,228</td>
<td>2.62</td>
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<tr>
<td>128</td>
<td>32</td>
<td>47</td>
<td>190,464</td>
<td>10,316</td>
<td>2.62</td>
<td>498</td>
</tr>
</tbody>
</table>

Collapsed Pipeline Single-FPGA Performance/Scalability

*Collapsed performance of CMT-Bone-BE with varied MPI ranks and simulation timesteps on a single Stratix V S5GSMD8K1F40C2 @ 335MHz
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

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### Collapsed Pipeline Single-FPGA Performance/Scalability

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>% LU</th>
<th>Num. of Events</th>
<th>Lat to First Out (cycles)*</th>
<th>Mega Sims /second*</th>
<th>Giga Events /second*</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>32</td>
<td>44</td>
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<td>10.5</td>
<td>450</td>
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<td>46</td>
<td>92,160</td>
<td>10,252</td>
<td>5.23</td>
<td>482</td>
</tr>
<tr>
<td>128</td>
<td>32</td>
<td>47</td>
<td>190,464</td>
<td>10,316</td>
<td>6.22</td>
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<td>1,148,056</td>
<td>3.19e-4</td>
<td>36</td>
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</tbody>
</table>

*Collapsed performance of CMT-Bone-BE with varied MPI ranks and simulation timesteps on a single Stratix V S5GSMD8K1F40C2 @ 335MHz

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### 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</th>
<th>FPGAs</th>
<th>Num. of Events</th>
<th>Lat to First Out (cycles)*</th>
<th>Mega Sims /second*</th>
<th>Giga Events /second*</th>
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</thead>
<tbody>
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<td>1K</td>
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<td>3.19e-4</td>
<td>2,299</td>
</tr>
</tbody>
</table>

*Predicted collapsed performance of CMT-Bone-BE with varied MPI ranks and simulation timesteps on multiple Stratix V S5GSMD8K1F40C2 @ 335MHz

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Novo-GF#
- 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

* See poster from Carlo Pascoe
Summary & Conclusions

- **BE methods & tools**
  - BE-SST v1.0: parallel BE simulator based on SST
  - Reduction of computational budget using **MFS models**
  - Began energy & thermal modeling

- **Large-scale experiments**
  - Validation (**100k+ MPI ranks**) on Titans, Vulcan, and Cab
  - Predictive simulations to **million+ MPI ranks**

- **CMT-nek DSE using BE simulation**
  - Profiling of key CMT-nek particle solver routines
  - Accuracy/performance tradeoffs using **BE simulation**

- **FPGA acceleration of BE simulation**
  - Validation of dataflow, pipelined approaches (**FEP, CP**)
  - Performance/scalability **tradeoff analysis** for FEP & CP

---

Do you have any questions?
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**
  - Profile CMT-nek to identify candidates for DSE
  - Perform algorithmic DSE of CMT-nek using BE methods & tools

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

* DSE - Design Space Exploration
**BE – Behavioral Emulation
UQ of Sandia Shock Tube Experiments

Brad Durant
Advisor: Prof. S. Balachandar
Department: MAE, UF

- Goal
  - Carry out bundle runs in 1-D, 2-D and 3-D using Dakota for UQ for Sandia shock tube
  - Perform sensitivity analysis of various underlying models for force coupling and particle-particle interactions
- Simulation roadmap
  - T6: Force coupling
  - T4: Particle-particle interaction

Particles Jet Formation Study

M. Giselle Fernandez
Advisor: Prof. Raphael T. Haftka and S. Balachandar
Department: MAE, UF

- Goals
  - Measurement of PM3 and PM4 in simulations
  - Optimization of initial PVF conditions that grow into jets
- Simulation roadmap
  - Validation of PM4 and PM4
Optimization of CMT-nek on CPUs/GPUs

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

- Goals
  - Optimization of CMT-bone on hybrid architecture with multiple CPUs/GPUs
  - Performance/Energy modeling of CMT-bone on HMPs
  - Implementation of CMT-bone on Intel KNL

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

---

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 0.5 g packet of particles
  - Validate Rocflu models governing particle motion

- Simulation roadmap
  - Real Gas
  - EL-AUSM+UP
  - Improved Forces
  - Program Burn
Support for Benchmarking & AppBEO Creation

**Trokon Johnson**

Advisors: Dr. Herman Lam, Dr. Greg Stitt
Department: ECE, UF

- **Goals**
  - Benchmarking automation
  - Benchmarking for CMT-nek DSE*
  - Formalize AppBEO creation process

- **Simulation roadmap**
  - Support for BE* in early DSE of CMT-nek code development
  - Automate & formalize process for BE

*DSE – Design Space Exploration
*BE – Behavioral Emulation

---

Forensic Uncertainty Quantification

**Kyle Hughes**

Advisor: Prof. Nam-Ho Kim
Department: MAE, UF

- **Goals**
  - Quantify uncertainty of past experiments to provide meaningful validation
  - Assist with planning of future experiments to minimize uncertainty

- **Simulation roadmap**
  - Act as a liaison between simulationalists and experimentalists
Compressible Multiphase Turbulence Modeling

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

- Goals
  - Develop multiphase compressible LES model
  - Improved force modeling
  - Validation and integration into Rocflu and CMT-nek

- Simulation roadmap
  - Implement single phase LES and extend it to multiphase flows
  - Validate existing force-models and develop new models in collaboration with microscale team
  - Perform mesoscale simulations

Simulation Roadmap

Improving Accuracy and Scalability of Behavioral Emulation (BE) Methodology

Nalini Kumar
Advisors: Dr. Herman Lam, Dr. Greg Stitt
Department: ECE, UF

- Goals
  - Apply BE methodology, demonstrated for device and system simulations, to simulation of large-scale systems
  - Design & validate simulation models of existing machine architectures
  - Improve communication modeling in BE

- Simulation roadmap
  - Design and evaluate BE simulation framework which will enable early design-space exploration to aid and assist CMT-nek code developers

Simulation Roadmap
CMT-nek Microscale Simulation

Goran Marjanovic
Advisor: Prof. S. Balachandar
Department: MAE, UF
- Goals
  - Demonstrate CMT-nek capabilities
  - Verification
  - Validation
- Simulation roadmap
  - Microscale simulation
  - Expansion over curtains of particles

Simulation Roadmap

Uncertainty Quantification of Shock Tubes

Justin Mathew
Advisor: Prof. Kim and Prof. Haftka
Department: MAE, UF
- Goals
  - Reproduce measurement processing from Sandia and ASU shock tubes to identify sources of uncertainty
  - Propagate identified sources of uncertainty from experiments into simulations
- Simulation roadmap
  - T2: Multiphase turbulence modeling and uncertainty
  - T4: Validation, UQ and UR of the shock tube simulation

Simulation Roadmap
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 (Inviscid and Viscous)
  ➢ Integration of force models in Meso-Macro scale simulations

Multi-objective optimization on Hybrid Systems using DVFS

Sankeerth Reddy Mogili
Advisor: Prof. Sanjay Ranka
Department: CISE, UF

● Goals
  ➢ Power Minimization
  ➢ Energy Optimization
  ➢ Time per time-step minimization

● Simulation roadmap
  ➢ Our research roadmap is closely tied with CMT-nek development
### Behavioral Emulation (BE) Models

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

- **Goals**
  - Validation and uncertainty estimation of BE
  - Reduce computation budget of CMT-nek (with UB team)
  - Verify trend among CMT-nek, CMT-bone, and CMT-bone-BE

- **Simulation roadmap**
  - BE helps in simulating CMT-nek on exascale systems (notional architectures)

---

### Eulerian-Lagrangian Interphase Coupling UQ and UR

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

- **Goals**
  - Identify and quantify potential errors for numerical force models of Eulerian-Lagrangian multi-phase dispersed
  - Reduce the errors by model improvement

- **Simulation roadmap**
  - T4: Verification and validation of the shock tube simulation
  - Uncertainty reduction via model improvement
Shock and Contact Interaction with Particles

Brandon Osborne
Advisor: Prof. S. Balachandar
Department: MAE, UF

- **Goals**
  - DNS of shock and contact interaction with structured and random arrangements of particles
  - Development of models for predicting particle motion

- **Simulation roadmap**
  - Microscale simulations for shock-contact-particle interaction

---

Surrogate Modeling of the Equation of State

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

- **Goals**
  - Develop a surrogate model for use in evaluating the equation of state in mixed air/product cells
  - Perform and analyze simulations of the Eglin blastpad experiments

- **Simulation roadmap**
  - Real gas equation of state capabilities in code
  - Analysis of instabilities of rapid dispersion
FPGA Pipelined Simulations for CMT-nek

Carlo Pascoe
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

Simulation Roadmap

BE-SST* Simulator

Ajay Ramaswamy
Advisor: Dr. Lam, Dr. Stitt
Department: ECE, UF

- Goals
  - Use SST framework to develop BE methods and run parallel, scalable simulations
  - Run simulations of large HPC systems
  - Improve communication models and interpolation API

Simulation roadmap
- BE-SST simulator enables scalable design space exploration on exascale systems

Simulation Roadmap

*SST: Structural Simulation Toolkit from Sandia National Laboratory
Energy and Thermal Modeling

Mason Rawson
Advisor: Dr. Lam, Dr. Stitt
Department: ECE, UF

- Goals
  - Design and implement a framework for assessing performance and energy consumption tradeoffs across entire HPC systems
  - Understand processor level thermal effects on performance and energy consumption

- Simulation roadmap
  - Explore design space of future HPC systems to incorporate power and energy

---

RocSDT: Shock-Particle Interaction

Prashanth Sridharan
Advisor: Dr. Thomas L. Jackson
Department: MAE, UF

- Goals
  - Investigate aluminum spherical particles under various shock loading conditions
  - Implement modelling technology to create robust level-set algorithms that handle mixture of deforming and rigid particles

- Simulation roadmap
  - Preliminary research conducted to produce transient force/drag histories
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-bone and CMT-nek by utilizing dynamic load balancing
  - Simulation roadmap
    - This simulation includes moving particles and gas to simulate the actual particle movement within a fixed box

Correction of Performance Emulation

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

- Goals
  - Quantify similarity and difference between run times of CMT codes
  - Develop correction schemes for BE emulation to predict performance of CMT codes
  - Simulation roadmap
    - Using advanced data analytics to assist performance emulation at different stages in the simulation roadmap
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

Two-way Coupling in CMT-nek

David Zwick
Advisor: Dr. S. Balachandar  
Department: MAE, UF

- Goals
  - Understanding of physics in ASU experiment through simulation
  - Development of state-of-the-art Eulerian-Lagrangian capabilities in CMT-nek

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