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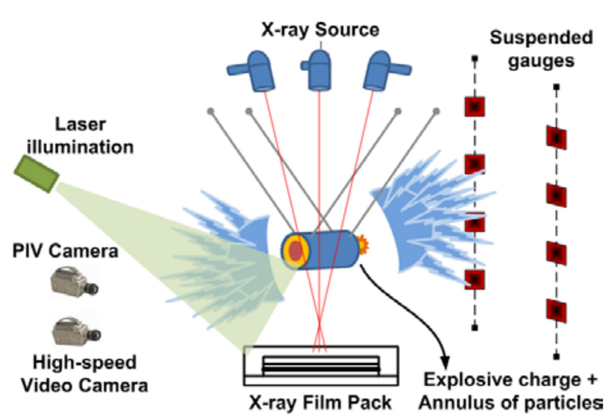
CENTER FOR COMPRESSIBLE MULTIPHASE TURBULENCE

TST Review

December 1-2, 2016



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Center for Compressible Multi-Phase Turbulence

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Agenda for TST Site Visit December 1 and 2, 2016

<u>Thursday December 1, 2016</u>

7:45	Van pick up at University Hilton
8:00-8:45	Full Breakfast (Review team caucus)
8:45-9:45	T1 - CCMT Overview/Highlights/AST Response (S. Balachandar)
9:45-10:30	T2 - Microscale (Tom Jackson/Yash Mehta)
10:30-10:45	Coffee break
10:45-11:45	T3 - Macroscale (Bertrand Rollin/Subbu Annamalai)
11:45-1:00	Lunch
1:00-2:00	T4 - UB (Chanyoung Park)
2:00-2:50	T5 - CS (S. Ranka)
2:50-3:00	Coffee break
3:00-3:50	T6 - Exascale (H. Lam/G. Stitt/ N. Kumar)
3:50-4:10	T7 - Internship presentations by David Zwick, Goran Marjanovic, Georges Akiki
4:10-4:30	T8 – PIEP Modeling (Georges Akiki)
4:30-5:15	Social with Students/Posters
5:15	Transportation to University Hilton by CCMT Faculty
6:00-7:30	Dinner at the University Hilton, hosted by CCMT Faculty

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Friday December 2, 2016

8:00	Van pickup at University Hilton
8:15-9:00	Continental Breakfast
9:00-9:30	T9 - ASU Experiments (Blair Johnson)
9:30-10:00	T10 - Eglin Experiments (Angela Diggs/Kyle Hughes)
10:00-10:45	T11 - CMT-nek (Jason Hackl/David Zwick)
10:45-11:30	Discussions between TST and CCMT PIs
11:30	Box Lunch; Transportation to hotel and/or airport as needed

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TST Review December 1-2, 2016 Attendee List

Faculty

S. Balachandar "Bala"	University of Florida	bala1s@ufl.edu
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Blair Johnson	Arizona State University	bajohn48@asu.edu
Chanyoung Park	University of Florida	cy.park@ufl.edu

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Melanie DeProspero	University of Florida	mel7703@ufl.edu

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Overview and Integration

S. Balachandar

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AST Meeting Agenda

Thursday
- Overview and Integration
- Microscale
- Macroscale
- *Lunch*
- Uncertainty Budget
- CS
- Exascale
- Internship presentations
- PIEP Modeling
- *Dinner at University Hilton with CCMT Faculty and Staff*

Friday
- ASU Experiments
- Eglin Experiments
- CMT-nek
- Discussions between TST and CCMT PIs
- *Lunch and transportation to airport*

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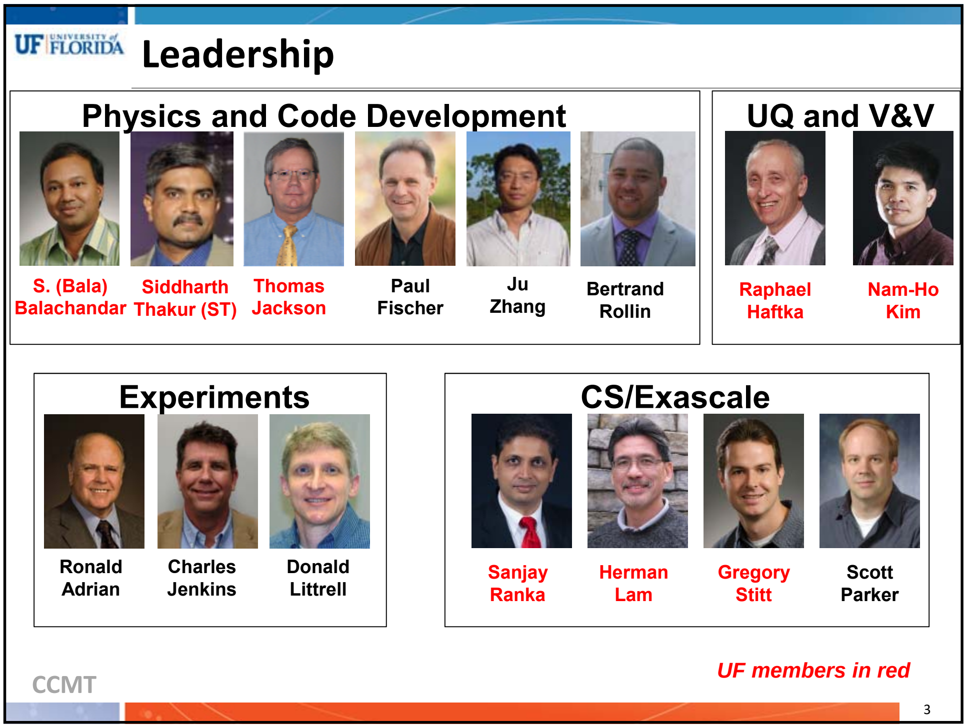
2


UF UNIVERSITY of FLORIDA
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
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Research Staff & Senior PhD Students
Georges Akiki
Subramanian Annamalai
Tania Banerjee
Jason Hackl
Chanyoung Park
Angela Diggs (Eglin AFB)
Blair Johnson (ASU)
Carlo Pascoe
Nalini Kumar
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4

Current Students (Undergraduate & Graduate)

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5

Outline

- Demonstration problem
- Sequence of events and physics models
- Simulation roadmap
- Uncertainty quantification and reduction
- Y2.5 accomplishments
- Goals for next year
- Response to AST comments

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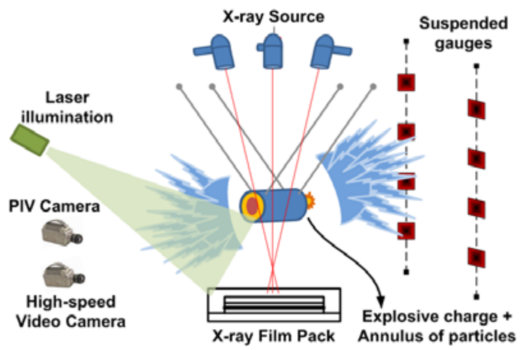
6

Demonstration Problem

- Explosive-driven cylindrical annulus of particles



- Integrated effort toward predictive simulations
- Experimental measurements for validation

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Demonstration Problem

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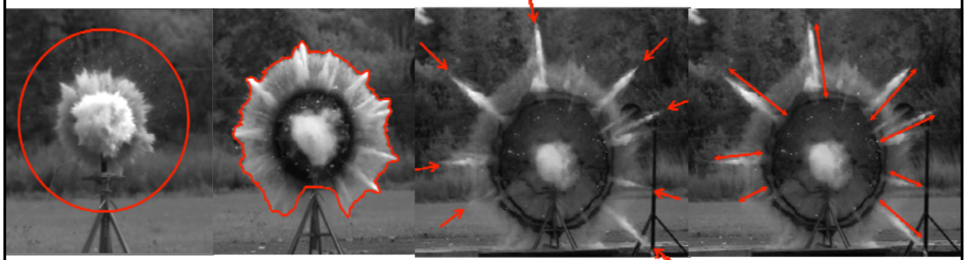
Prediction Metrics

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



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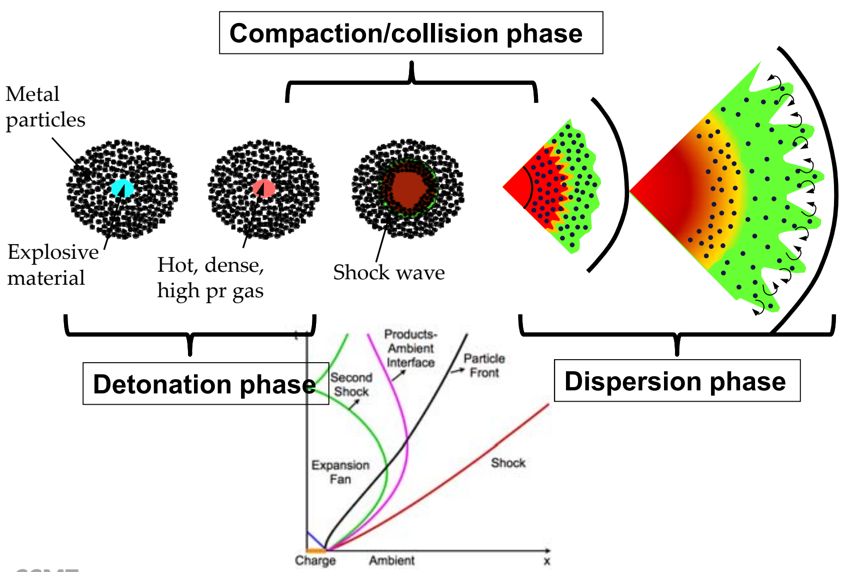
| 9

Sequence of Events



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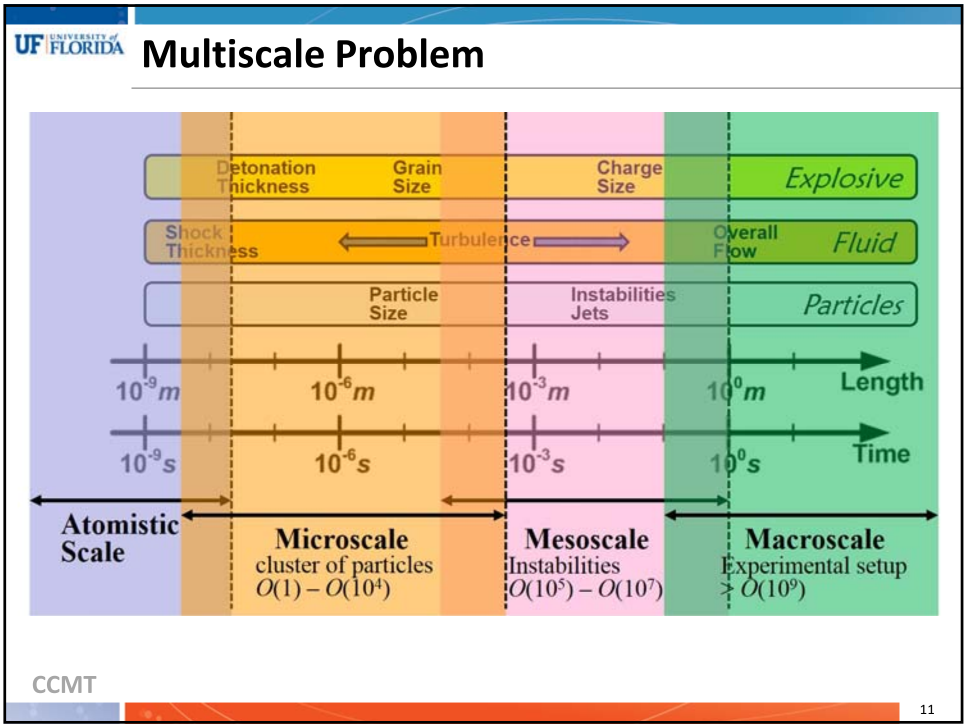
10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Multiscale Problem
Detonation Thickness
Grain Size
Charge Size
Explosive
Shock Thickness
Turbulence
Overall Flow
Fluid
Particle Size
Instabilities Jets
Particles
10^-9 m
10^-6 m
10^-3 m
10^0 m
Length
10^-9 s
10^-6 s
10^-3 s
10^0 s
Time
Atomistic Scale
Microscale
cluster of particles
O(1) – O(10^4)
Mesoscale
Instabilities
O(10^5) – O(10^7)
Macroscale
Experimental setup
> O(10^9)
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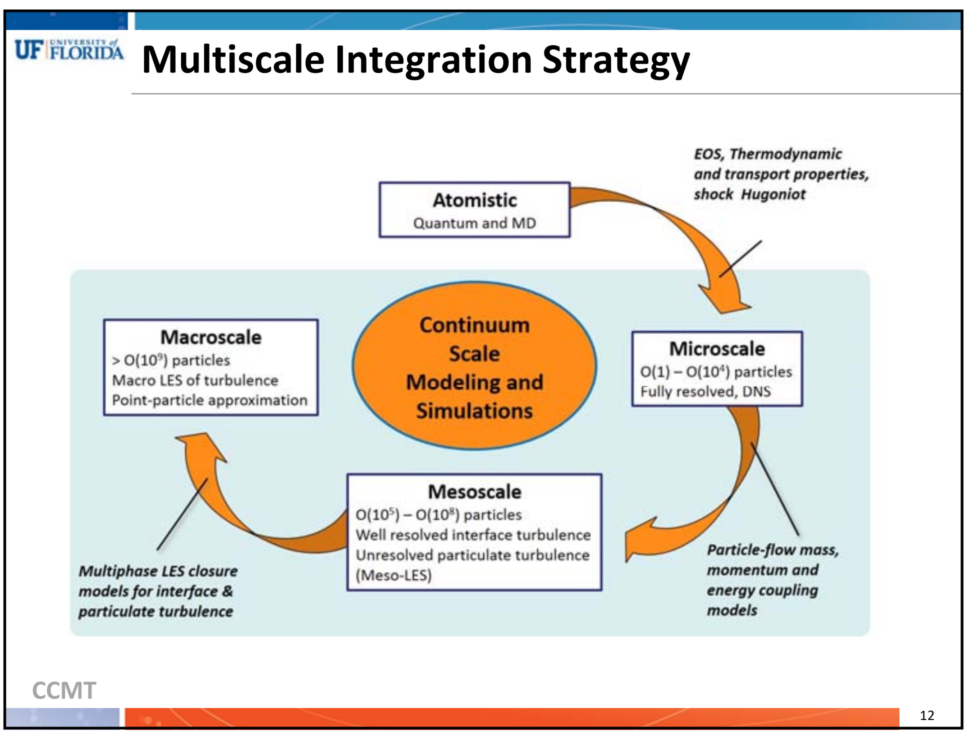
11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Multiscale Integration Strategy
EOS, Thermodynamic and transport properties, shock Hugoniot
Atomistic
Quantum and MD
Macroscale
> O(10^9) particles
Macro LES of turbulence
Point-particle approximation
Continuum Scale Modeling and Simulations
Microscale
O(1) – O(10^4) particles
Fully resolved, DNS
Mesoscale
O(10^5) – O(10^8) particles
Well resolved interface turbulence
Unresolved particulate turbulence
(Meso-LES)
Multiphase LES closure models for interface & particulate turbulence
Particle-flow mass, momentum and energy coupling models
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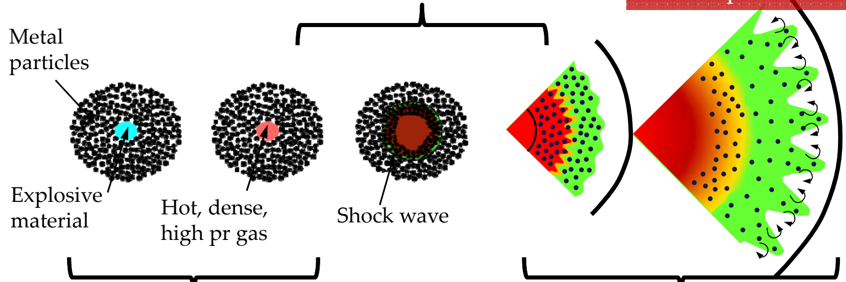
12

Physical Models – Sources of Error

T8:Deformation model

Compaction/collision phase

T4:Collision model
T5:Compaction model



Detonation phase

T1:Detonation model

Dispersion phase

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

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13

Sources of Errors & Uncertainties

- T1: Detonation modeling
- T2: Multiphase turbulence modeling
- T3: Thermodynamics & transport properties
- T4: Particle-particle collision modeling
- T5: Compaction modeling (dense-to-dilute transition)
- T6: Point-particle force modeling
- T7: Point-particle thermal modeling
- T8: Particle deformation and other complex physics

Advance state-of-the-art in multiphase turbulence and point-particle models

- T9: Discretization and numerical approximation errors
- T10: Experimental and measurement errors & uncertainties

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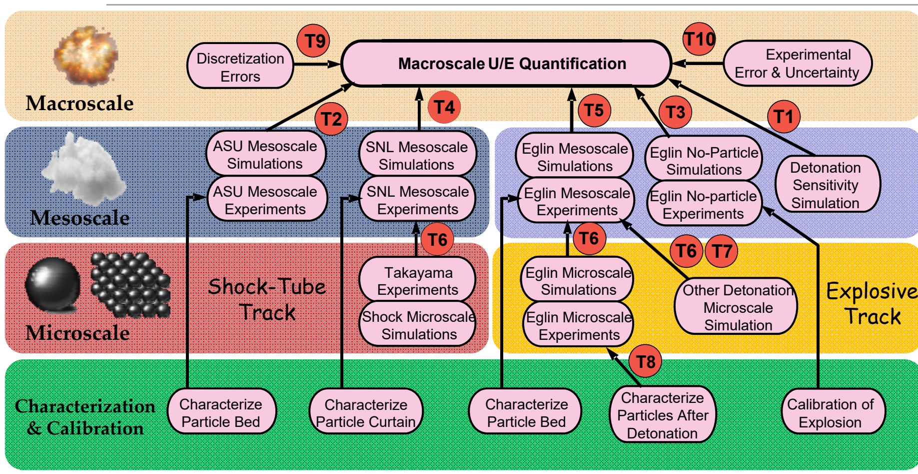
14

Uncertainty Budget – Overall Plan



- Integrates all the center activities
- Uncertainty reduction through iterative improvement

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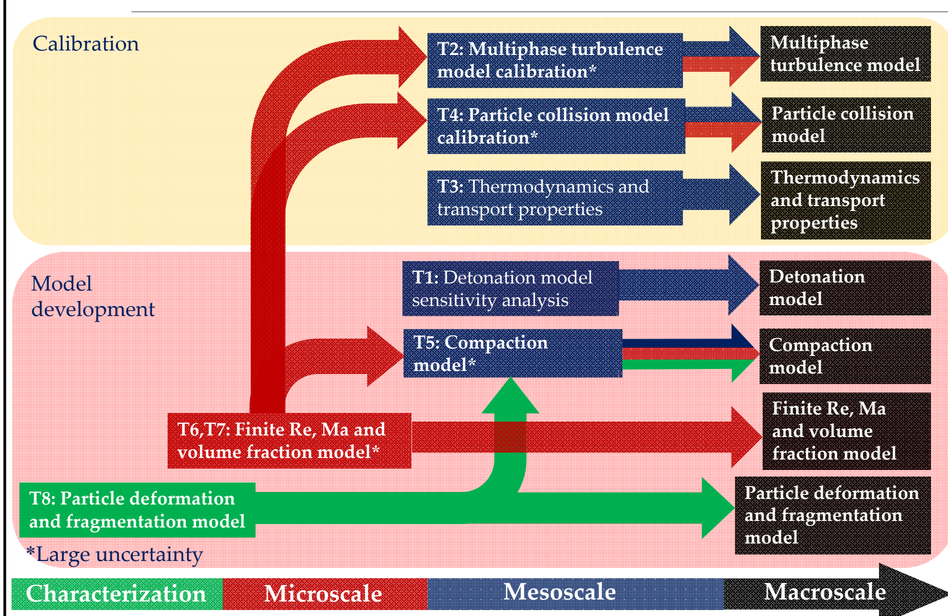
15

Multiscale Uncertainty Propagation



16

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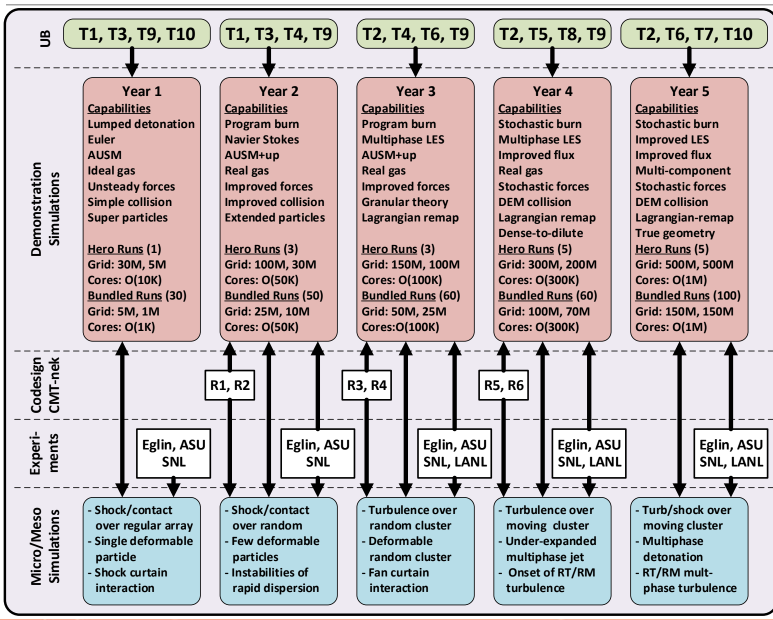
Simulation Roadmap



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17

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Demonstration Simulations

T1, T3, T9, T10	T1, T3, T4, T9	T2, T4, T6, T9	T2, T5, T8, T9	T2, T6, T7, T10
Year 1	Year 2	Year 3	Year 4	Year 5
Capabilities	Capabilities	Capabilities	Capabilities	Capabilities
Lumped detonation	Program burn	~~Program burn~~	Stochastic burn	Stochastic burn
Euler	Navier Stokes	Multiphase LES	Multiphase LES	Improved LES
AUSM	AUSM+up	~~AUSM+up~~	Improved flux	Improved flux
Ideal gas	Real gas	Real gas	Real gas	Multi-component
Unsteady forces	~~Improved forces~~	~~Improved forces~~	Stochastic forces	Stochastic forces
Simple collision	Improved collision	Granular theory	DEM collision	DEM collision
Super particles	~~Extended particles~~	Lagrangian remap	Lagrangian remap	Lagrangian-remap
			Dense-to-dilute	True geometry
Hero Runs (1)	Hero Runs (3)	Hero Runs (3)	Hero Runs (5)	Hero Runs (5)
Grid: 30M, 5M	Grid: 100M, 30M	Grid: 150M, 100M	Grid: 300M, 200M	Grid: 500M, 500M
Cores: O(10K)	Cores: O(50K)	Cores: O(100K)	Cores: O(300K)	Cores: O(1M)
Bundled Runs (30)	Bundled Runs (50)	Bundled Runs (60)	Bundled Runs (60)	Bundled Runs (100)
Grid: 5M, 1M	Grid: 25M, 10M	Grid: 50M, 25M	Grid: 100M, 70M	Grid: 150M, 150M
Cores: O(1K)	Cores: O(50K)	Cores:O(100K)	Cores: O(300K)	Cores: O(1M)

- Uncertainty Budget drives yearly simulation
- T1 – T10 will be computed Year-2 to Year-5

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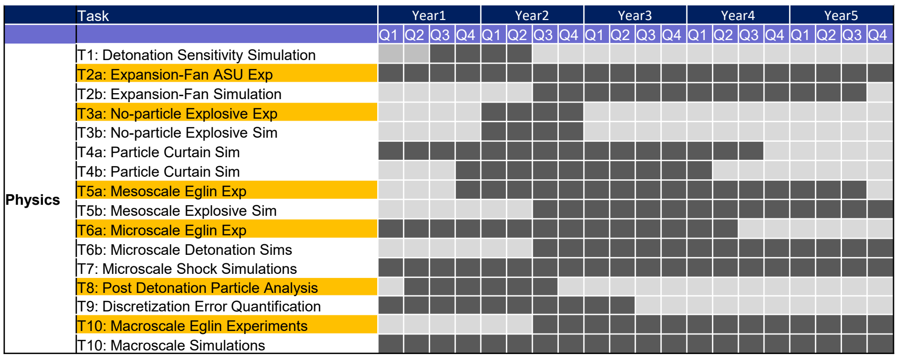
18

Timeline: T1-T10 Uncertainty Reduction



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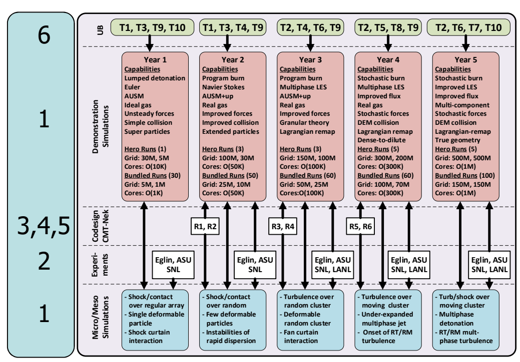
19

Year 2.5 Key Accomplishments

1. Simulations
2. Validation Experiments
3. CMT-nek development
4. Energy & thermal aware computing
5. Exascale emulation
6. UB



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20

1: Demonstration Problem (Macroscale)

Goal

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

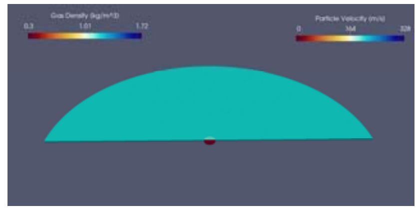
Year 2.5

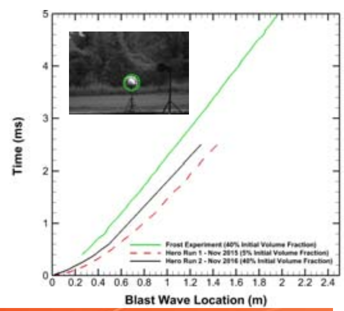
- Use existing code to perform petascale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)
- Develop capabilities for the next hero run: real gas EOS, reactive burn, collision modeling, higher volume fraction

Presentation

- Bertrand Rollin, Subbu Annamalai

3-D demonstration Simulations





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21

1: Mesoscale Simulations

Goal

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

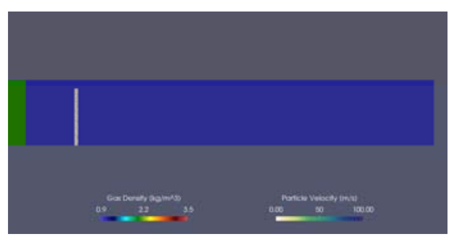
Year 2.5

- Many mesoscale simulations of shock propagation over a bed of particles
- Mesoscale simulations of expansion fan over a bed of particles

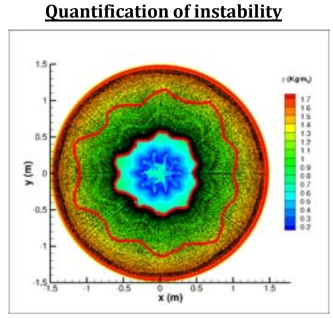
Presentation

- Bertrand Rollin & Subbu Annamalai

Shock tube



Quantification of instability



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22

1: Microscale Simulations

Goals

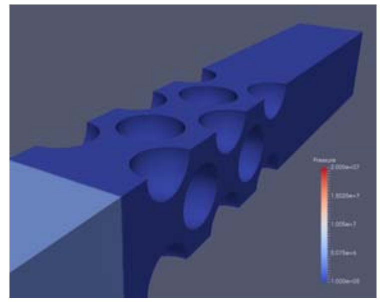
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation to the demonstration problem

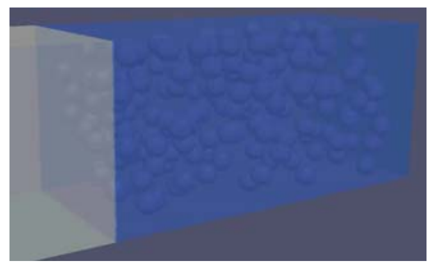
Year 2.5

- Highly resolved simulations of shock propagation over a structured array
- Highly resolved simulations of shock propagation over a random distribution
- Binary superposition model

Presentation

- Tom Jackson & Yash Mehta





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23

1: Microscale Simulations

Goals

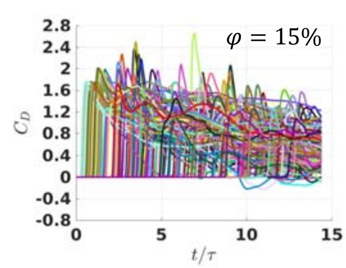
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation to the demonstration problem

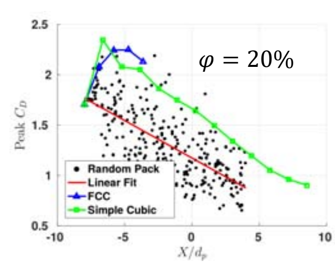
Year 2.5

- Highly resolved simulations of shock propagation over a structured array
- Highly resolved simulations of shock propagation over a random distribution

Presentation

- Yash Mehta





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24

1: New Point-Particle Framework

Goals

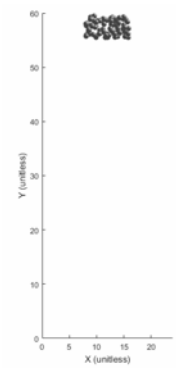
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation to the demonstration problem

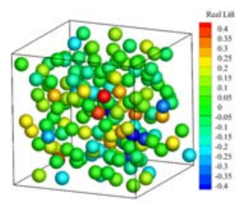
Year 2.5

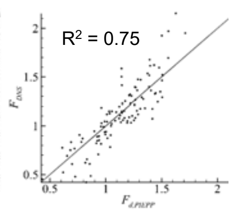
- Development of Pairwise Interaction Point-Particle (PIEP) model
- Rigorous testing of PIEP model and extension to shock-particle interaction
- Characterization of pseudo-turbulence and Reynolds stress and other closures

Presentation

- Georges Akiki and Yash Mehta







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25

2: Validation Experiments

Goals

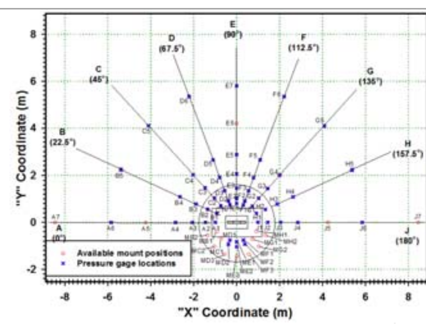
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

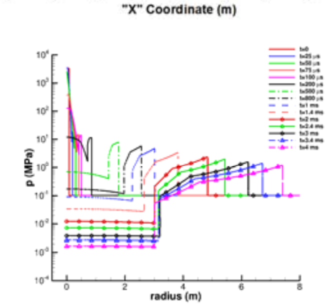
Year 2.5

- Blast pad experiments at Eglin AFB
- Mesoscale gas-gun experiments at Eglin
- Continued micro- and mesoscale explosive dispersal experiments at Eglin
- Experimental studies of gas-particle mixtures under sudden expansion at ASU

Presentation

- Blair Johnson (ASU) & Kyle Hugh





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26

3: CMT-nek Development

Goals

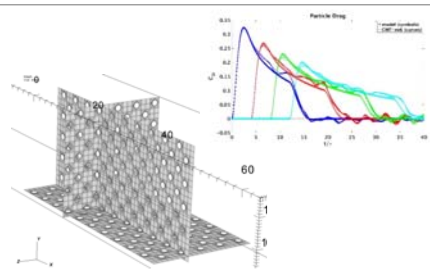
- Co-design an exascale code (CMT-nek) for compressible multiphase turbulence
- Perform micro, meso and demonstration-scale simulations
- Develop & incorporate energy and thermal efficient exascale algorithms

Year 2.5

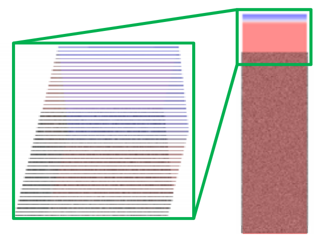
- Develop and release microscale version of CMT-nek for microscale simulations
- Develop and release mesoscale version of CMT-nek for mesoscale simulations
- CMT-bone development
- CMT-nek in nek5000 repository

Presentation

- Jason Hackl and David Zwick



Micro simulation - 4000 MPI ranks



131,000 elements, LX1=12,
20 billion particles, 131K MPI ranks

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27

3: CMT-bone

Goals

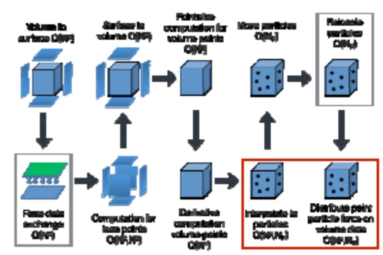
- Co-design an exascale code (CMT-nek) for compressible multiphase turbulence
- Perform micro, meso and demonstration-scale simulations
- Develop & incorporate energy and thermal efficient exascale algorithms

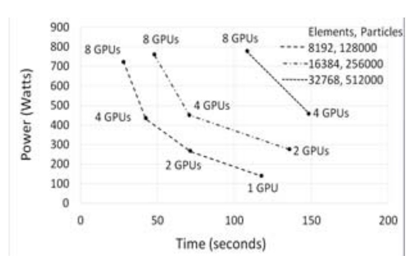
Year 2.5

- Develop and release first version of CMT-nek for microscale simulations
- Develop and release first version of CMT-nek for mesoscale simulations
- CMT-bone development
- CMT-nek in nek5000 repository

Presentation

- Jason Hackl and David Zwick





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28

4: Energy & Thermal Aware Computing

Goal

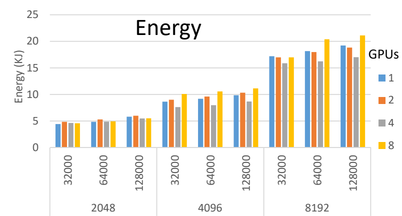
- Derive computationally intensive portions of the CMT-nek code and understand its performance, thermal and energy issues

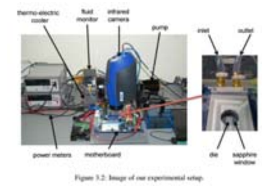
Year 2.5

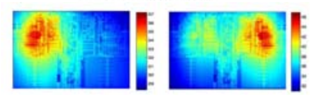
- Carried out extensive investigation of performance and energy issues for CMT-bone
- Hybrid CPU-GPU implementation of CMT-bone and optimization
- Thermal aware optimization
- Load balancing with particles

Presentation

- Tania Banerjee & Sanjay Ranka







Thermal aware optimization

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29

5: Exascale Emulation

Goal

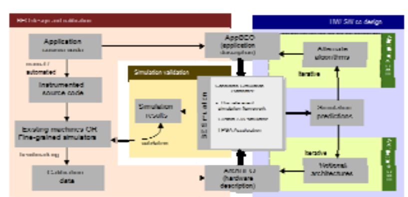
- Develop behavioral emulation (BE) methods and tools to support co-design for algorithmic design-space exploration and optimization of key CMT-bone kernels & applications on future Exascale architectures

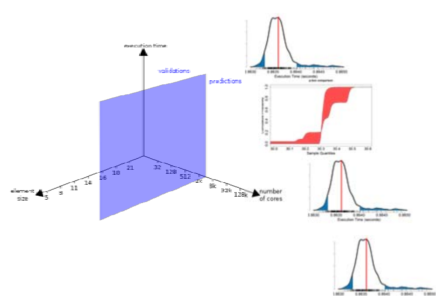
Year 2.5

- Enhanced BE methods with network models, interpolation schemes, and energy/thermal bechmarking for CMT-bone AppBEOs
- Performed large-scale experiments on DOE platforms
- Completed SST-based BE simulator
- Improved throughput and scalability for FPGAs

Presentation

- Herman Lam, Greg Stitt





CMT-bone-BE on Vulcan

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30

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6: Uncertainty Budget

Goals

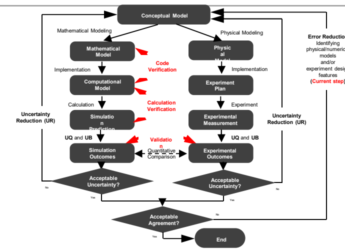
- Develop UB as the backbone of the Center
- Unified application of UB for both physics and exascale emulation

Year 2.5

- 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

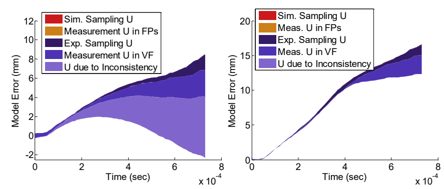
Presentation

- Rafi Haftka, Chanyoung Park, Nam-Ho Kim



UQ Framework

UB for Sandia shock tube problem



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Major Goals For Next Year

- Bigger hero run of demonstration problem with more physics
- Mesoscale simulations of SNL, ASU and Eglin experiments
- Microscale simulations of shock + contact over particles
- Development and implementation of pairwise interaction point-particle model
- UB of other meso and macroscale problems
- CMT-nek micro and mesoscale simulations with shock
- Energy and thermal aware hybrid implementation of CMT-nek
- NGEE on multiple FPGAs and performance comparison against simulation

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32

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AST Review Report
Spring 2016
(Response)

CCMT PSAAP II Center
University of Florida
August 31, 2016

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General Comments and Kudos

The review itself was very well prepared and organized (e.g., all documents and slides were sent to the review team early) and accompanied by excellent logistics. Overall, the center has been very responsive to lab, TST and AST recommendations and has shown nice progress compared to last year.

Overall, the review team had a positive impression of CCMT and the overall project. In particular, the following items stuck out:

- The review team was pleased to see the UQ work is being adopted across the entire project. A very good example showing the impact of these efforts was the identification of cancelling errors in the AUSM1+up method.
- The work showed good progress on the microscale physics modeling.
- The review team commends the center on progress made on the Behavioral
- Emulation (BE) work in Y2. In particular, the integration of UQ into the BE thrust to track the impact of multiple parameters at once is innovative and should be expanded on.

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34

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General Comments and Kudos

- The evolving story on the surrogate-based modeling approach using FPGAs is credible and provides reasonable results.
- The current work to support node heterogeneity, in particular GPGPUs, is very promising and has already shown good results.
- The review team is pleased with your success in incorporating CMT-nek into the nek5000 repository, which will generate a viable code maintenance strategy.
- Based on the recommendations from 2016, the center performed validation of CMT-bone against CMT-nek using LLNL's Veritas. The results were interesting and already led to a refinement of the proxy app CMT-bone.

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35

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Key Areas of Concern

The review team had five areas of concerns along with recommendations to mitigate them. The remainder of this report is structured around them:

- The center has a broad scope, especially for a smaller PSAAP-II center. In particular, targeting the Frost Experiment as the validation target is a lot to take on.
- While both experimental and simulation efforts are strong, the coupling between the two aspects offers room for improvements.
- On the simulation code side, dynamic load imbalance can prevent the center from being successful, unless it is properly addressed.
- Even though significant advances have been made since the last review, the efforts to integrate the CS/BE efforts with the production code work around CMT-nek should be further improved
- The review team would have liked to see more results at scale, in particular for CS/BE related efforts, to understand the scaling implications of the proposed and presented approaches.

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36

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Areas of Concern - Scope

The review team had five areas of concerns along with recommendations to mitigate them. The remainder of this report is structured around them:

- The center has a broad scope, especially for a smaller PSAAP-II center. In particular, targeting the Frost Experiment as the validation target is a lot to take on.

- A simpler and a more controlled version Frost's experiment is in preparation at Eglin Air Force Base. While still cylindrical in configuration (to conform with past blast-pad experiments and historical data from Eglin) some of the challenges of Frost's experiment will be addressed, e.g. unknown casing, limited diagnostics, boundary conditions, etc.

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Experimental/Simulation Coupling

The review team had five areas of concerns along with recommendations to mitigate them. The remainder of this report is structured around them:

- While both experimental and simulation efforts are strong, the coupling between the two aspects offers room for improvements.

- Experiments have indeed been out of phase with the simulations in the past
- First round Micro/meso experiments at Eglin had outpaced the Center's M&S capability
- To re-couple these efforts, the center has assigned Kyle and Angela to act as a liaison between Eglin and the simulation team. Their responsibilities are to
  - Maintain steady communication between the experimental, simulation and UQ teams (Kyle is part of UQ team)
  - Guarantee that simulations guide improvement of experiments and vice-versa

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38

Experimental/Simulation Coupling

While both experimental and simulation efforts are strong, the coupling between the two aspects offers room for improvements.

- Develop and document a detailed V&V plan that explicitly documents how/which experiments are supporting which simulation efforts and vice versa, as new physics are added to the code.
- Have a flow diagram that shows the overall V&V workflow, as well as a timeline showing the dependencies between experiments, simulations and code development efforts.

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Experimental/Simulation Coupling

- Simulation/experiment plans are being documented by the physics team
- The flow diagrams of the mesoscale V&V workflows have been prepared
- The flowchart includes processes for uncertainty budget (UB) and uncertainty reduction (UR) to show their impact on V&V
- The flow diagrams of the other scales will be prepared based on the mesoscale flow diagram
- Dependencies of simulations/experiments of different scales are clarified by the physics team

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Experimental/Simulation 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.

Work even closer with the team at Eglin AFB

- More detailed simulation requirements should be characterized for the validation. This could help fine-tune the experimental setup before the actual experiments are conducted and with that ease and improve the validation later on.

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Experimental/Simulation Coupling

- UQ of the ASU experiment is being carried out by Justin Mathew
- The physic team is working on the ASU shock tube model and the ASU experiment plan is being discussed and refined
- In discussion with the UB team three evenly distributed notches will be made on the particle casing in the Eglin blast pad experiment to identify possible cause of particle fingers
- The mesoscale gas gun experiments and sabot are being prepared and examined at UF
- The Eglin mesoscale simulation is being prepared for validation of the physics for modeling particle cloud behavior
- The UQ of Eglin microscale experiments is being carried out at UF
- The Eglin microscale simulations are being performed to replicate the experiment

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Dynamic Load Balancing

On the simulation code side, dynamic load imbalance can prevent the center from being successful, unless it is properly addressed.

- The load balancing problem has a number of facets that we will analyze:
  - Multiobjective Load balancing for performance, energy and thermal issues.
  - Simultaneous Load balancing for *spectral elements and particles*:
    - The distribution of spectral elements is static and well organized. While this balance is aimed at optimum performance, a dynamic component to load balancing is introduced when we consider thermal & energy effects
    - The particles move about throughout simulation, and this will require dynamic load balancing capabilities for both performance and thermal management.
  - Challenge: the base code is in Fortran 77, that does not allow for effective dynamic memory allocation

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43

Integration of CS/BE & CMT-nek Efforts

- Even though significant advances have been made since the last review, the efforts to integrate the CS/BE efforts with the production code work around CMT-nek should be further improved
- How advances by CS/BE teams will be transferred into the main code base since center has lost expert personnel in CMT-nek

- New hires in the area of software engineer are being made which will help us with the transfer of CS/BE efforts back into CMT-nek

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Scalability Results

- ➢ Experiments on scalability of CMT-nek – Leveraging NEK 5000, which has been shown to scale to large numbers of cores, as the base for the new code is a sound approach and comes with the promise of achieving a similar scalability for the new code. However, this assumption needs to be verified and the review team is therefore suggesting running more and earlier scalability tests to show that this is really the case.
- ➢ The current results on up to 8K cores are showing good initial results, but it is a large jump from there to hundreds of thousands of cores and the scalability of any code at such target scales can be impacted by even small code additions.

- The CMT-nek and CS teams are demonstrating scalability of CMT-nek on Vulcan/Mira and the hybrid version of CMT-bone on Titan. This work will continue as more particle features and two-way coupling aspects are introduced.

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Additional Recommendations: CMT-nek

Integration and feedback from CS and BE team

- ➢ CMT-nek feeds into CS performance analysis and GPU porting
- ➢ CMT-nek feeds into BE through proxy application CMT-bone
- ➢ What feeds back into CMT-nek?

- Proxy apps will follow CMT-nek to github
- Training CS and BE personnel in CMT-nek will enable them to specifically identify and plan places for their discoveries to enhance CMT-nek
- Dedicated software expert will help will the implementation of improvements back into CMT-nek

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46

Additional Recommendations: CMT-nek

Application requirements to direct CS and BE

- Simulation groups must bound the parameter space for BE work
- Hero runs should be goals

- CS and BE will be integrated into migration of microscale and mesoscale groups from RocFlu to CMT-nek
- CS and BE will be briefed on large simulations as they occur
- Everyone will get together on Arora

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47

Additional Recommendations: UQ

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

- We are employing multi-fidelity surrogate technology to emulate the Hero Runs with an aid of other cheaper but approximate simulations
- Various existing multi-fidelity surrogates have been studied and tested to be apply for the parameter study and UQ of the Hero Runs

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48

Additional Recommendations: UQ

The center should clarify in more detail how they will work across the envisioned scales.

- How they will first take advantage of microscale results to address mesoscale subgrid scale, and then eventually macro-scale modeling.
- A dedicated presentation would be helpful

- The stochastic properties of a random distribution of particles will be measured and quantified from the microscale simulation, which will then be deployed in the mesoscale simulation. Once validated the model will eventually be used in the macroscale
- We will have a dedicated presentation at next AST

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49

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Do you have any questions?

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2016 PSAAP II Center Review Outbrief

Martin Schulz, Review Team Chair

Kudos

- We are pleased to see UQ work is being adopted across the entire project, e.g. AUSM+up identifying cancelling errors.
- There is good progress on the microscale physics modeling, e.g. PIEP.
- We are pleased to see dedicated CCMT personnel working with Eglin AFB and ASU experimental teams.
- We believe your comparisons of models with experiments represent a step forward from Y1.
- The RT commends you on progress made on BE work in Y2.
  - Integration of UQ into BE work is innovative.
  - You have created a surrogate-based modeling approach using the FPGA as a surrogate model and are evolving a credible story with reasonable results.

Kudos (cont)

- Leveraging nek5000 is a sound strategy.
- RT is pleased with your success in incorporating CMT-nek into the nek5000 repository.
- Validation of CMT-bone against CMT-nek using Veritas is productive.
- Integration of BE into SST appears to be a viable strategy moving forward.
- Your GPGPU and on-node load-balancing work is coming together.
  - We look forward to seeing dynamic aspects next year.

Kudos (cont)

- The review was well-prepared and well-organized.
  - Students understand where they fit in and are empowered.
  - RT appreciates receiving presentation slides early.
  - Logistics are excellent.
- You are generally responsive to lab, TST and AST recommendations.
- There is an impressive number of students associated with CCMT and they appear to work well together.
- Overall the RT sees nice progress compared to Y1.

Concerns

1. You have defined a very broad scope, e.g. the Frost Experiment is a lot to take on.
2. We believe you need stronger coupling between experimental and simulation efforts.
3. Dynamic load-balancing can prevent you from being successful if you are not able to deal with it.
4. More coupling is needed between CS/BE efforts and CMT-nek integration.
5. We would like to see more scalability results.

Concern #1: Scope

You have defined a very broad scope, e.g. the Frost Experiment is a lot to take on.

- Step back and assess your ongoing work to determine what parts are essential to meet your Y5 goals.
  - Are your goals realistic now that you have completed Y2 out of 5?
  - What do you need to do to lower risk of incompletion?
  - Identify what you would not do if you have to cut something.
  - For example:
    - Compaction is not yet accounted for and relies on particle material used.
    - Compaction is different for spherical versus cylindrical geometry.
    - Jump from microscale to mesoscale is big.

Concern #2: Experimental/Simulation Coupling Recommendations

- Be explicit about how experiments are supporting simulations (and vice versa) as new physics is inserted into the code. Document the V&V plan.
  - Flow diagram showing your V&V workflows.
  - Timeline showing dependencies between experiments and simulations.
- Clarify how you plan to extract velocity fluctuation measurements in the ASU experiments.

Concern #2: Experimental/Simulation Coupling Recommendations (cont)

- Work closely with Eglin AFB to characterize simulation requirements for validation.
- Enhance ASU experiments:
  - Consider ways to image structural details within the particle bed.
  - Consider ways to characterize the impact of wall contribution to void structure.

Concern #3: Dynamic Load-balancing Recommendations

- Start working on dynamic global load-balancing now, not only in CMT-bone but also in CMT-nek:
  - Using current state of code/physics.
  - Because code without load-balancing is likely to not scale well (if at all).
- Build upon your initial success with CMT-bone on-node load-balancing.
- Work with lab experts and other PSAAP II Centers.

Concern #4: CS/Code Coupling

- The RT does not understand how/when changes in – and lessons learned from - CMT-bone and CMT-bone-BE will flow back into CMT-nek.
- Tighter integration of current physics code tested at scale with all features might help drive CS work.
- Recommendations:
  - Assign staff for the transition of CMT-bone to CMT-nek.
  - To lower risks and barriers for bringing new contributors to CMT-nek up to speed, consider adoption of more rigorous software development and documentation practices.
  - Identify app requirements for the CS group.

Concern #5: Scalability

- We realize nek5000 is a sound strategy but we would like to see experimental data for CMT-nek to support this hypothesis.
  - You have shown simulations to 8K cores – it is a large jump to hundreds of thousands of cores.
- Recommendations:
  - Perform ongoing scaling studies on CMT-nek with current physics on the complete integrated software stack.
    - Utilize your ALCC allocation on Mira and Titan.
    - Utilize lab testbeds as early as possible, e.g. upcoming Sierra testbeds.
    - And on your performance simulators.

Additional Recommendations

- For next year's review clarify how you will take advantage of microscale results to address mesoscale subgrid scale modeling (eventually also for macroscale).
- Develop a strategy to use lower-fidelity runs to augment the Hero Runs in order to explore parameter space more broadly.
- Next year (or at the next TST meeting) present analysis of the scalability of the FPGAs:
  - How large a problem can be solved with what level of hardware?
  - What is the relationship?

Additional Recommendations (cont)

- Perform rigorous code verification to distinguish model errors from numerical errors as CMT-nek grows.
  - Apply trend approach to look at order of magnitude of the error (as opposed to absolute error).
  - Look at mixed orders of accuracy from DG to time integration of particles.
- We would like to hear more talks from students in future reviews.
- Have each student with a poster present a short (60-90 second) overview via a “lightning round”.
- For the 2017 Review, present one talk addressing status for each of the five areas of concern.

CCMT 11/29/2016 2015 PSAAP II Center Annual Review 63

Education and Collaborations

- We appreciate the numerous courses (including new ones) related to CCMT effort being offered by UF.
- We look forward to the CCMT-sponsored Multiphase Flow Workshop in October.
- There is noticeable increase in CCMT outreach to DOE labs.
- Student internships appear to be going well.

CCMT November 29, 2016 2015 PSAAP II Center Annual Review 64

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Microscale Simulations and Modeling

T.L. Jackson & Y. Mehta

UF UNIVERSITY of FLORIDA

NNSA

UF UNIVERSITY of FLORIDA

Microscale Team


Siddharth Thakur (ST)


Thomas Jackson


Ju Zhang


Georges Akiki


Brandon Osborne


Yash Mehta


Prashanth Sridharan

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2

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Goals

- Perform DNS simulations of shock propagating over a random pack of particles in air
- Advance modeling to next generation point-particle force and temperature models for meso/macroscale simulations that take into account neighboring particles

Frost et al. 2012

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3

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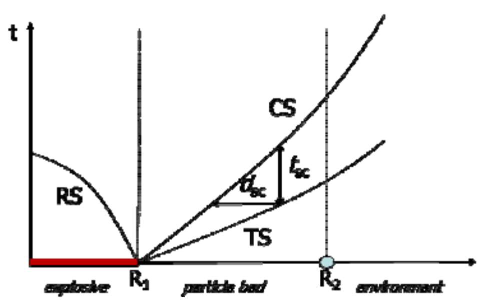
Features to Capture – Early Time Behavior



- TS – transmitted shock
- RS – reflected shock
- CS – contact surface
- d_{sc} – distance between CS and TS
- t_{sc} – time between CS and TS arrival

- Reactive burn
- Microscale simulations
  - Shock-particle interaction (M, ϕ)
  - Shock-contact interaction (M, ϕ, t_{sc})

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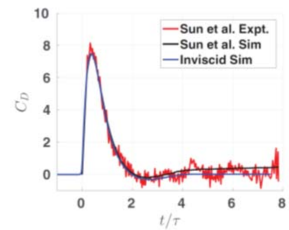
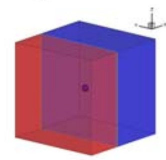
Time Scale Analysis

- Shock-particle $\tau = d_p/u_s$
- Acoustic $\tau_a = d_p/c$
- Inviscid $\tau_i = d_p/u_{ps}$
- Viscous diffusional $\tau_v = \delta_v^2/\nu_m$
- Particle motion $\tau_p = \rho_p\, d_p^2/18\mu_m$





- Ratios: $\frac{\tau_p}{\tau} \sim \frac{\rho_p}{\rho_m} Re \sim 10^4$ $\quad \frac{\tau_v}{\tau} = \frac{u_s}{u_{ps}} \sim 2$

- Inviscid simulations will accurately capture peak and short time evolution of force

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5

Governing Equations

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u}) = 0,$$

$$\frac{\partial (\rho \vec{u})}{\partial t} + \vec{\nabla} p + \vec{\nabla} \cdot (\rho \vec{u} \vec{u}) = 0,$$

$$\frac{\partial E}{\partial t} + \vec{\nabla} \cdot [(E + p)\vec{u}] = 0,$$

$$E = \rho\left(e + \tfrac{1}{2}\vec{u} \cdot \vec{u}\right),$$

$$p = p(\rho, e)$$

- 3-D Euler equations
- Ideal gas equation of state
- Implemented in finite volume, in-house code – Rocflu
- Body conforming grids are used

- Assumptions
  - Particles are stationary
  - Neglect viscous effects
  - No particle deformation

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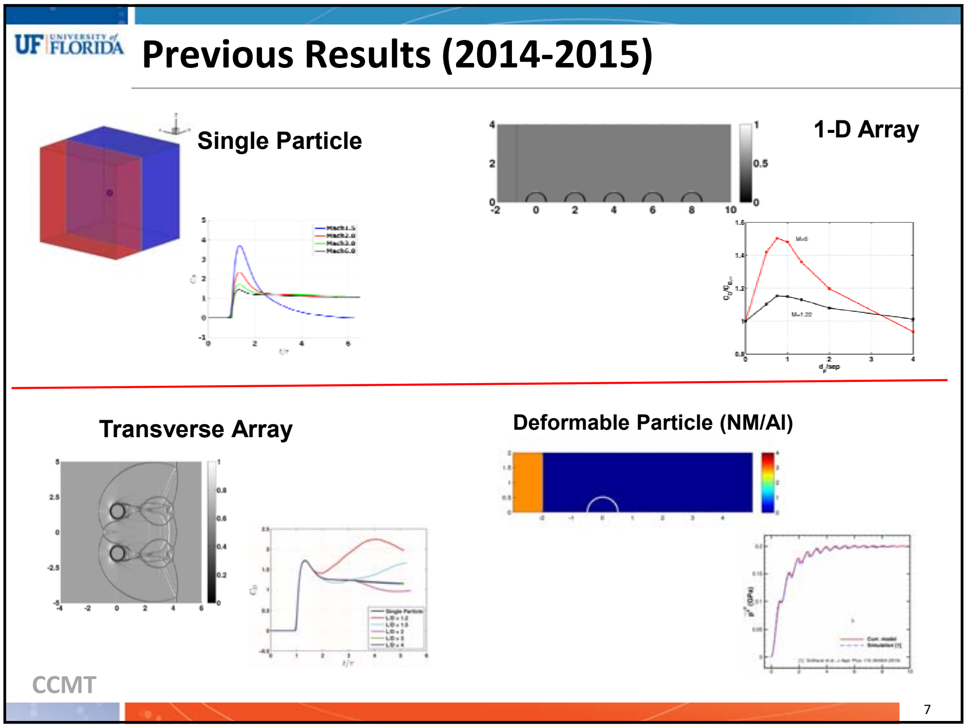
6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Previous Results (2014-2015)
Single Particle
1-D Array
Transverse Array
Deformable Particle (NM/Al)
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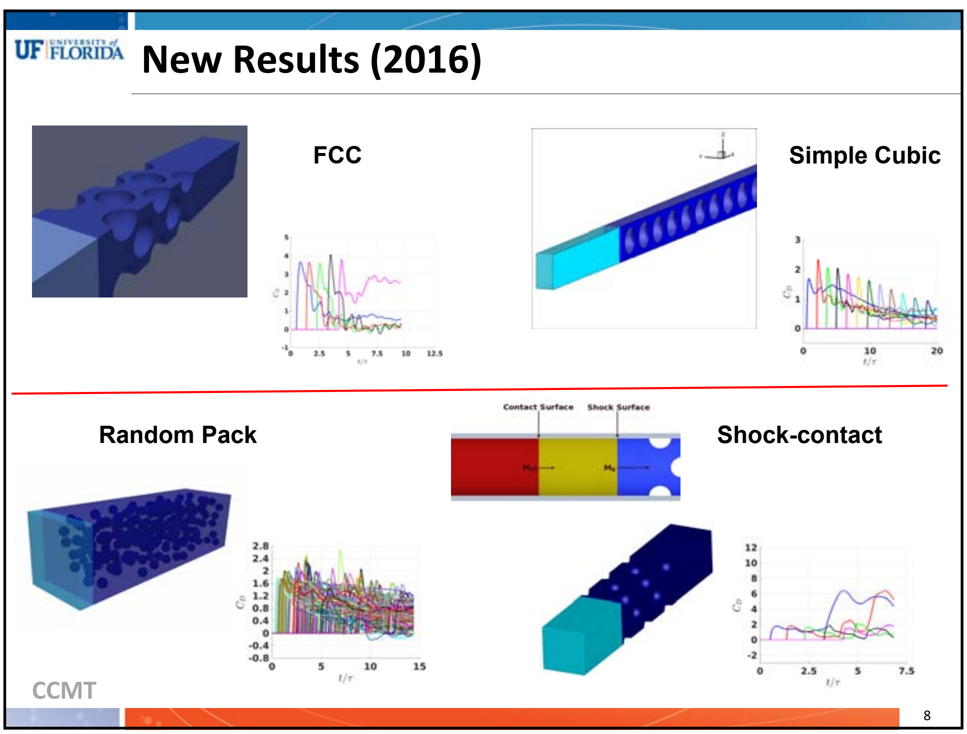
7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New Results (2016)
FCC
Simple Cubic
Random Pack
Contact Surface
Shock Surface
Shock-contact
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8

Outstanding Challenges

- Simulations with a large cluster of moving particles
  - Dynamic gridding (immersed boundary method?)
  - How to handle particle-particle interaction?
- Simulations of detonation-induced particle deformation
  - Numerical issue of particle mass preservation
  - Material modeling and EOS
- Upscaling of the microscale results
  - Point-particle force model (effect bow shock & wave drag)
  - Heat transfer model, deformation model, etc
  - PIEP model extension to compressible flows and testing
  - Validation

Outstanding Challenges

- Additional features
  - Reactive burn
  - Shock-contact problem
  - Viscous effects
  - Non-ideal EOS for detonation products

Outline of Microscale Simulations & Modeling

- Shock interaction – volume fraction and Mach number effects
  - Simple cubic array
  - Face-centered cubic (FCC) array
  - Random distribution of particles
- Point-Particle Model Development

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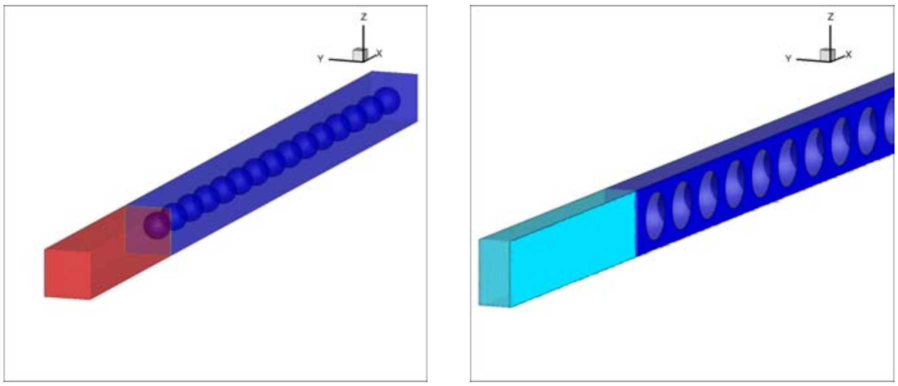
Shock Interaction with Simple Cubic Array



Density contour along X-Z cut-plane

- Shock Mach numbers, $M_s = 3.0$ and volume fractions, $\varphi = 10\%, 20\%$
- Transverse periodicity – particle curtain

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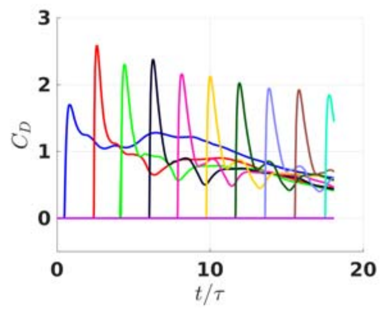
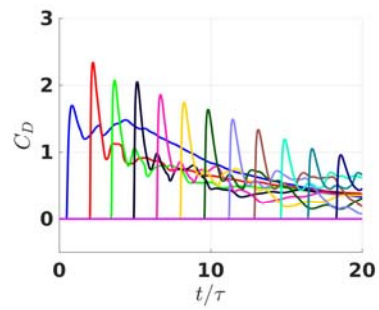
Shock Interaction with Simple Cubic Array



$M_s = 3.0; \varphi = 10\%$



$M_s = 3.0; \varphi = 20\%$

- Clear effect of volume fraction compared to 1-D array
- Local shocklets lead to energy dissipation and weakening of the transmitted shock

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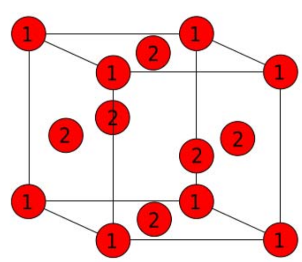
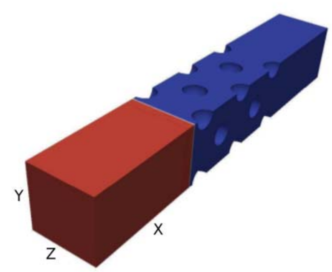
13

Shock Interaction with FCC Array





	$\varphi = 10\%$	$\varphi = 20\%$	$\varphi = 30\%$	$\varphi = 40\%$
$M_s = 1.5$	RUN1	RUN5	RUN9	RUN13
$M_s = 2.0$	RUN2	RUN6	RUN10	RUN14
$M_s = 3.0$	RUN3	RUN7	RUN11	RUN15
$M_s = 6.0$	RUN4	RUN8	RUN12	RUN16

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14

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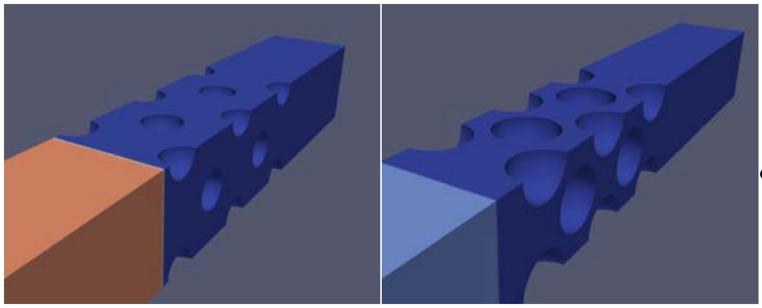
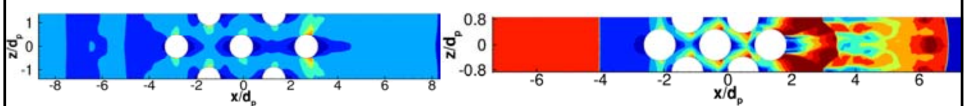
Shock Interaction with FCC Array

$M_s = 1.5$
$\varphi = 10\%$



$M_s = 6$
$\varphi = 40\%$



- Even for structured array, ensuing flow is quite complicated
- There is a strong effect of the particles on the flow

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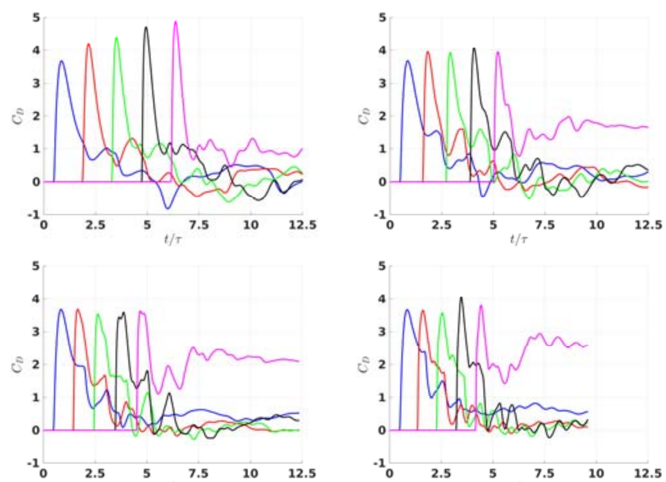
FCC - Effect of Volume-fraction; $M_s = 1.5$

$\varphi = 10\%$ $\varphi = 20\%$

$\varphi = 30\%$ $\varphi = 40\%$



- At higher volume fractions the last plane of particles will move faster, resulting in curtain spreading

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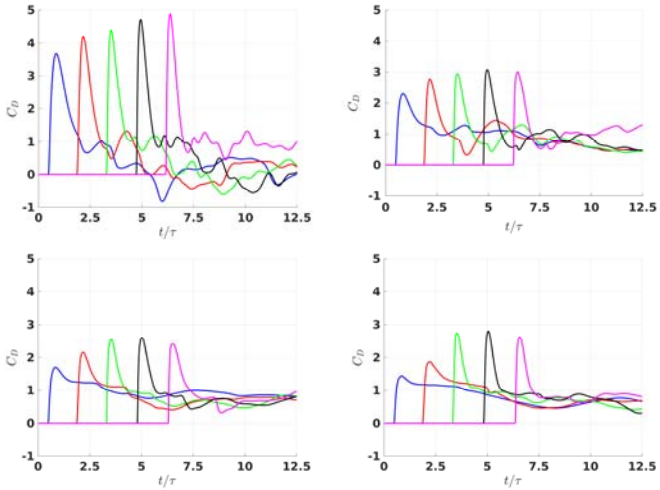
FCC - Effect of Mach number; $\varphi = 10\%$

$M_s = 1.5$ $M_s = 2.0$

$M_s = 3.0$ $M_s = 6.0$



- There is a high variability for peak forces

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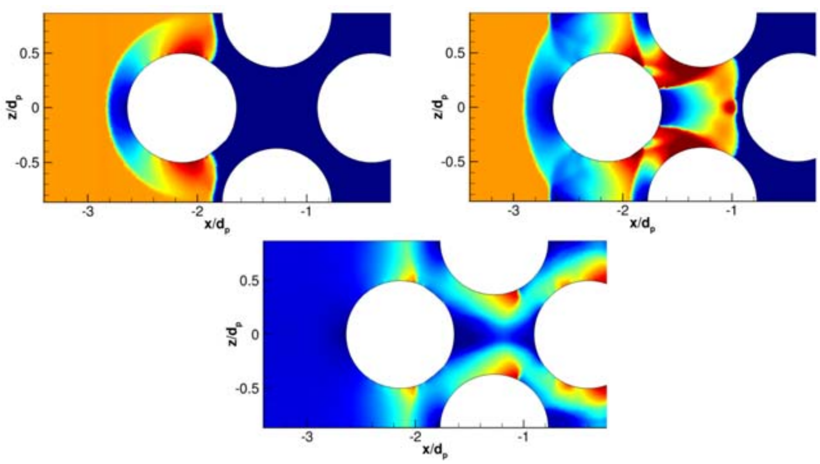
Shock Interaction with FCC Array



- Shock focusing leads to increase in drag force
- Shocklets result in energy dissipation and decrease in drag force

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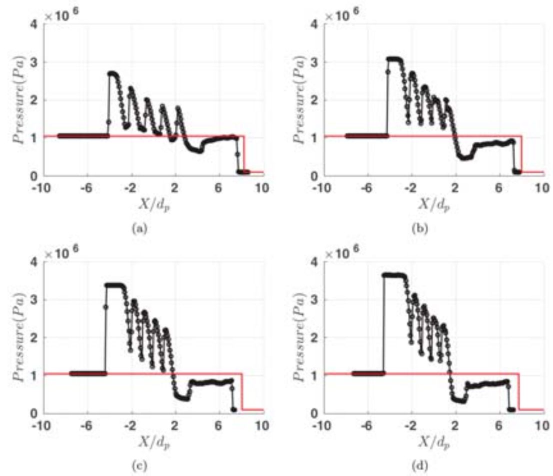
Shock Interaction with FCC Array

$\varphi = 10\%$ $\varphi = 20\%$

$\varphi = 30\%$ $\varphi = 40\%$



- Energy dissipation leads to pressure attenuation downstream of particle bed

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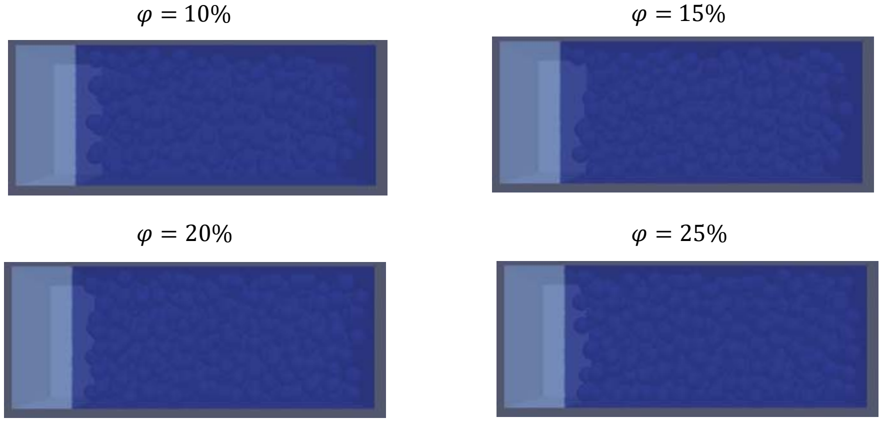
Shock Interaction with Random Pack of Particles

$\varphi = 10\%$ $\varphi = 15\%$

$\varphi = 20\%$ $\varphi = 25\%$



- Mach 3.0 shock traveling through the particle beds

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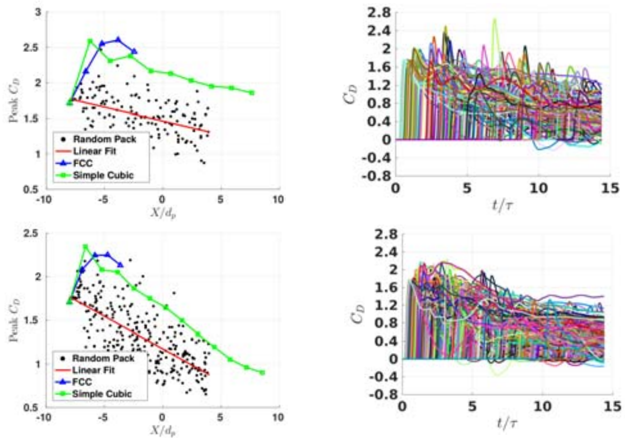
Shock Interaction with Random Pack of Particles

$\varphi = 10\%$ $\varphi = 15\%$

$\varphi = 20\%$ $\varphi = 25\%$



- There is a high variability for the peak drag and a clear downward trend

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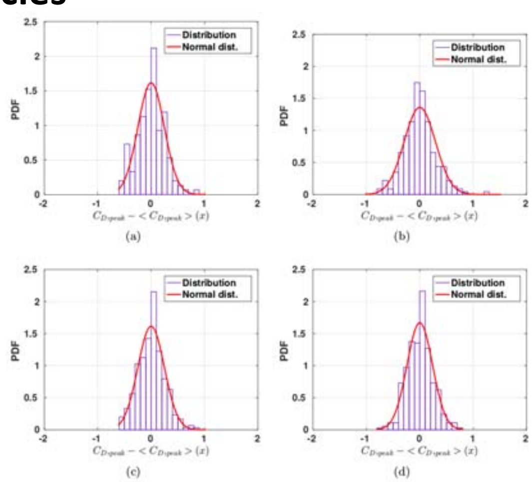
Shock Interaction with Random Pack of Particles

$\varphi = 10\%$ $\varphi = 15\%$

$\varphi = 20\%$ $\varphi = 25\%$



- Force fluctuation follows normal distribution around the mean(x) drag

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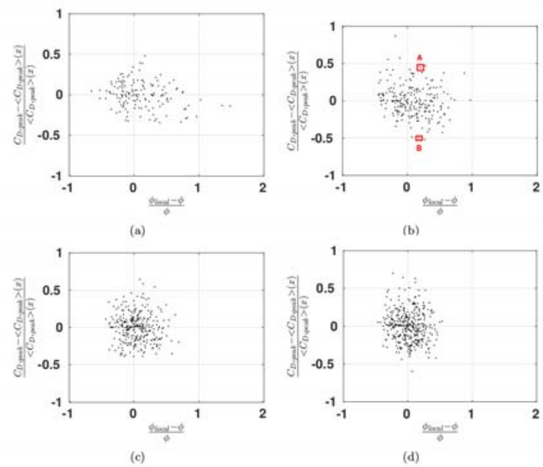
Shock Interaction with Random Pack of Particles

$\varphi = 10\%$ $\varphi = 15\%$



$\varphi = 20\%$ $\varphi = 25\%$

- Force fluctuation does not correlate with local volume fraction

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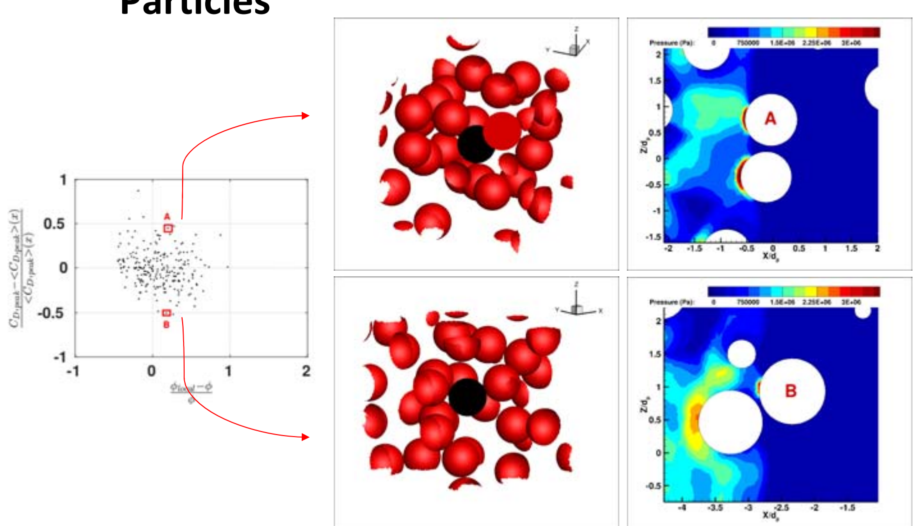
Shock Interaction with Random Pack of Particles



- Force fluctuation is dependent on local neighborhood of particles

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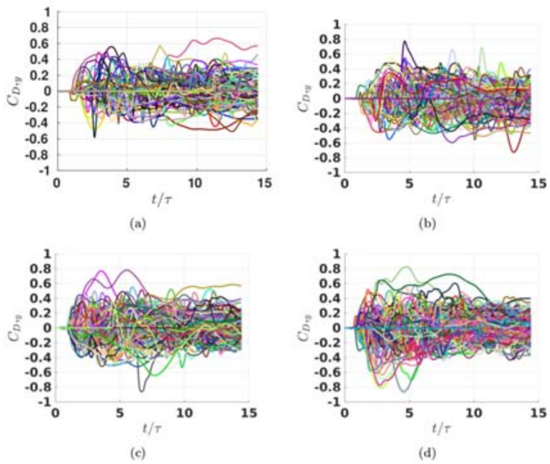
Shock Interaction with Random Pack of Particles

$\varphi = 10\%$ $\varphi = 15\%$

$\varphi = 20\%$ $\varphi = 25\%$



- Fluid mediated particle-particle interaction leads to transverse forces
- Mean transverse force over the entire bed is zero

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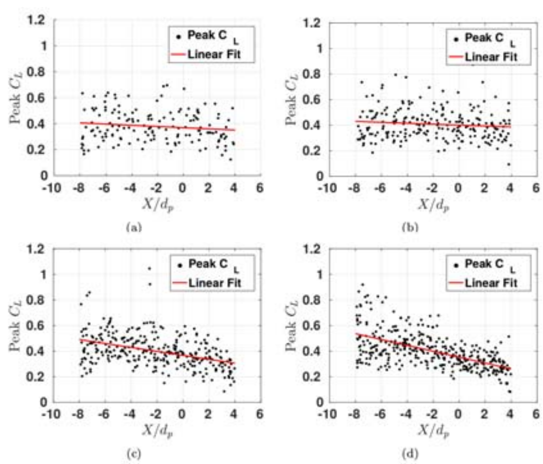
Shock Interaction with Random Pack of Particles

$\varphi = 10\%$ $\varphi = 15\%$

$\varphi = 20\%$ $\varphi = 25\%$



- Total transverse force shows same trend as the streamwise drag force

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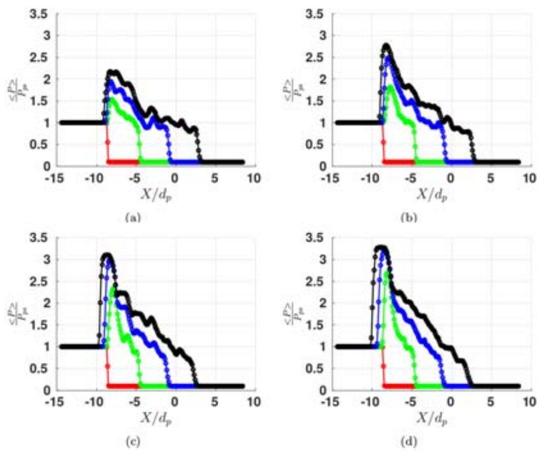
Shock Interaction with Random Pack of Particles

$\varphi = 10\%$ $\varphi = 15\%$

$\varphi = 20\%$ $\varphi = 25\%$



- Pressure drop across transmitted shock increases as volume fraction increases

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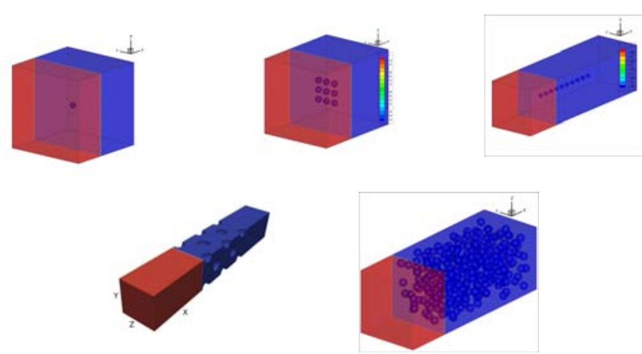
27

Fully Resolved Simulations - Summary

- Complex physical mechanisms at play during shock particle interaction
- Strong effect of shock Mach number and volume fraction on drag force
- Supersonic flow leads to shocklets and bow shocks
- Energy dissipation causes pressure attenuation behind the particle bed
- Signification variation in force due to fluid mediated particle-particle interaction



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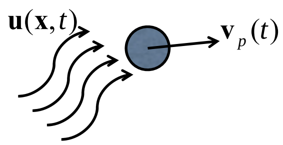
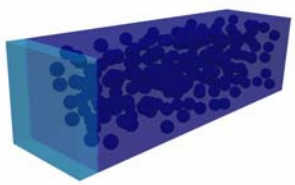
Point-Particle Model Development



Commonly used models are based on:

- Uniform flow
- Quasi-steady flow
- Isolated particles
- Low Mach number, modest Reynolds number



But reality:

- Highly unsteady and spatially non-uniform flow
- Large Mach and Reynolds numbers
- Closely clustered particles
- Particles can deforms
- Real gas & turbulence effects

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Physics-Based Modeling

- Isolated particle
  - Rigorous point-particle formulation with empirical extension to finite Re and Mach condition
- Particle-particle interaction (current status)
  - Simple volume fraction correction to point-particle model for predicting average behavior
- Particle-particle interaction (New Development)
  - A novel Pairwise-Interaction Extended Point-particle (PIEP) model for predicting average & fluctuation behavior

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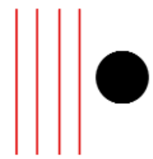
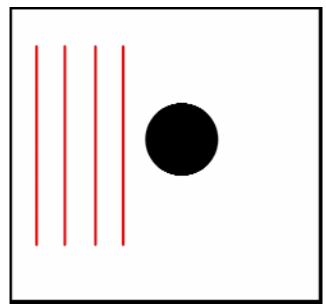
Shock Particle Interaction Modeling

$$F(t) = ?$$



$$F(t) = F_{UD}(t) + F_D(t)$$



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Shock Particle Interaction Modeling

$$F_{UD}(t) = F_{SG}(t)$$

$$F_D(t) = F_{QS}(t) + F_{IU}(t) + F_{VU}(t)$$

- F_{SG} = Stress Gradient
- F_{QS} = Standard Drag
- F_{IU} = Inviscid Unsteady
- F_{VU} = Viscous Unsteady

Current Model (Generalized Faxen Theorem)

$$F_{UD}(t) = \forall \left(\overline{\rho \frac{Du}{Dt}}^{\forall} \right)$$

$$F_D(t) = 6\pi\mu a \left(\overline{u}^S \right) + \forall \int_{\varepsilon=-\infty}^{t} \left(K_{iu} \left[\overline{\frac{d\rho u}{dt}}^{\forall} \right] \frac{C_0}{a} \right) d\varepsilon$$

$$K_{iu} = \exp\left[-(t-\varepsilon)\frac{C_0}{a} \right] \cos\left[-(t-\varepsilon)\frac{C_0}{a} \right]$$

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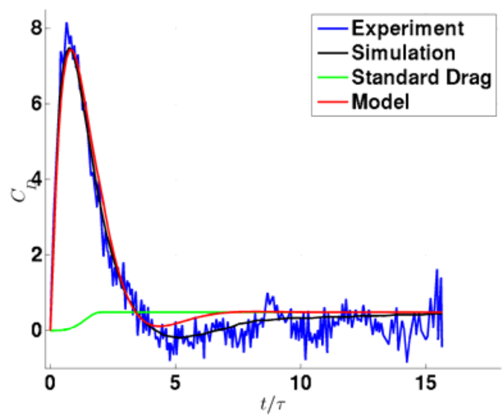
32

Shock Particle Interaction Modeling



- Force on a spherical particle for shock Mach number $M_s = 1.22$

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33

Shock Particle Interaction modeling-Summary

- We have state-of-the-art single particle model
- There is a need to extend this model for super-critical Mach numbers and include volume fraction effects
- Pair-wise interaction is a novel way to account for effect of volume fraction

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34

Shock Particle Interaction modeling

- As shock travels over (1), it diffracts the flow field
- (R) sees the flow diffracted by (1) + shock
- (R) diffracts the both these flow fields
- $F_R = F_{shock} + F_{1-R}$

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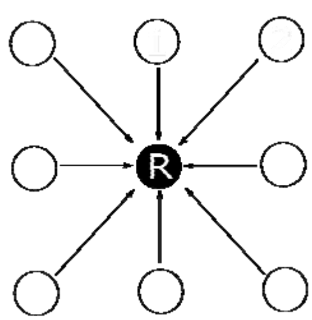
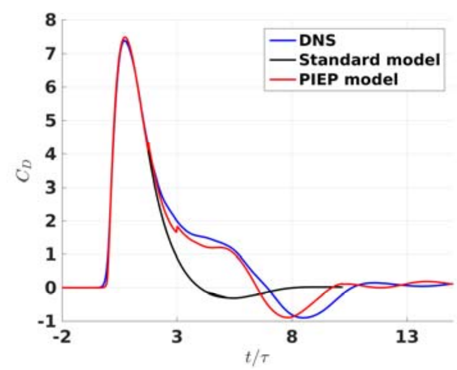
35

PIEP – Streamwise Force

- Shock interaction with transverse array of particles





- Force found by superposition
- $\text{Force}_{part-R} = \text{Force}_{shock} + 4 * \text{Force\_diff}_{part-1} + 4 * \text{Force\_diff}_{part-2}$

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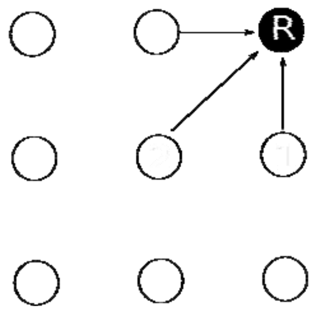
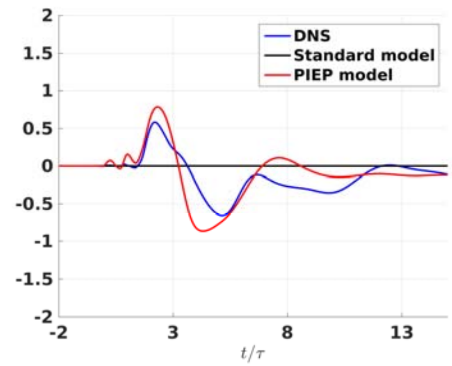
36

PIEP - Transverse Force





- $\text{Force}_{\text{part-R}} = 2 * \text{Force\_diff}_{\text{part-1}} + 1 * \text{Force\_diff}_{\text{part-2}}$

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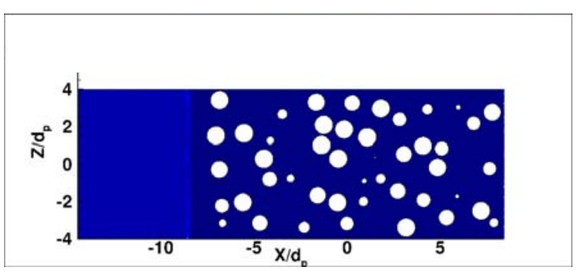
37

Future Work – Viscous simulations

- Viscous simulations
- Moving particles
- PIEP models



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38

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Journal Publications (2015-2016)

- Sridharan, P., Jackson, T.L., Zhang, J. and Balachandar, S. (2015). Shock interaction with 1-D array of particles in air. ***Journal of Applied Physics***, Vol. 117, 075902.
- Sridharan, P., Jackson, T.L., Zhang, J., Balachandar, S., and Thakur, S. (2016). Shock interaction with deformable particles using a constrained interface reinitialization scheme. ***Journal of Applied Physics***, Vol. 119, 064904, 18 pages.
- Mehta, Y., Jackson, T. L., Zhang, J., & Balachandar, S. (2016). Numerical investigation of shock interaction with one-dimensional transverse array of particles in air. ***Journal of Applied Physics***, *119*(10), 104901.
- Akiki, G., Jackson, T.L., & Balachandar, S. (2016). Force variation within arrays of mono-disperse spherical particles. ***Physical Review Fluids***, 1, 044202.
- Mehta, Y., Neal, C., Jackson, T.L., Balachandar, S., Thakur, S. (2016). Shock interaction with three-dimensional face centered cubic array of particles in air. ***Physical Review Fluids***, 1, 054202.
- Annamalai, S., Balachandar, S. Sridharan, P. and Jackson, T.L. (2016). A pressure evolution equation for the particulate phase in inhomogeneous compressible disperse multiphase flows. ***Physical Review Fluids***, (submitted).
- Akiki, G., Jackson, T.L., & Balachandar, S. (2016). PIEP model for a random array of monodisperse spheres. *Journal of Fluid Mechanics*, under review.
- Neal, C., Mehta, Y., Salari, K., Jackson, T.L., Balachandar, S., Thakur, S. (2016). Shock propagation in air over a random bed of spherical particles. (in preparation).

39

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Do you have any questions?

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Full System Simulations

Subbu Annamalai
Bertrand Rollin

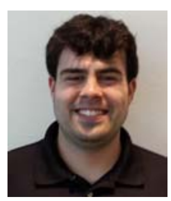
UF UNIVERSITY of FLORIDA

NNSA

Macro/Mesoscale Team


Bertrand Rollin


Subbu Annamalai


Fred Ouellet


Rahul Koneru


Giselle Fernandez


Joshua Garno

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Explosive-Driven Particle-Laden Flows

Sarychev peak (source: wikipedia)

- Fundamental physics involved
  - Explosive-driven flow
  - Shock/particle interaction
  - Turbulence/particle interaction

- Bring predictive capabilities to particle-laden flow simulations under extreme conditions

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Goals

- **The Demonstration Problem**
  - Perform the largest, most accurate multiphase flow possible (Hero Run)
- **Experimental - Macro/Meso Team collaboration**
  - Simulation of Eglin blast-pad experiment
  - Simulation of Eglin microscale and mesoscale experiments
- **UB – Macro/Meso Team collaboration**
  - Quantify prediction metrics PM-3 and PM-4
  - Model the JWL equation of state using surrogate modeling
  - Shock-particle interaction

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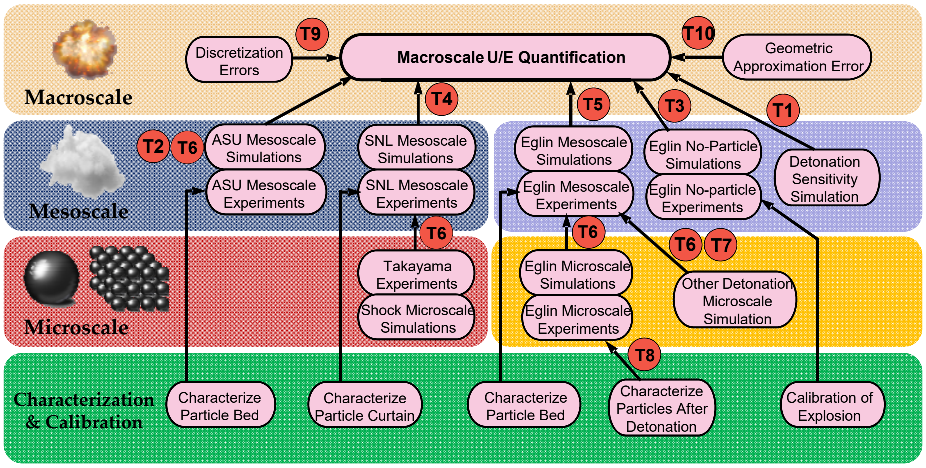
Demonstration Problem



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Outline

- **Macroscale**
  - Simulating the demonstration problem
  - Quantifying prediction metrics PM-3 and PM-4
  - Simulation of Eglin blast-bad experiment
- **Mesoscale Simulations**
  - Shock - Particle Curtain Interaction
  - Explosive dispersal of tungsten particles (Eglin experiment)
- **Modeling**
  - Surrogate Modeling of the real gas equation of state
  - Force & pressure modeling using generalized Faxén’s theorem

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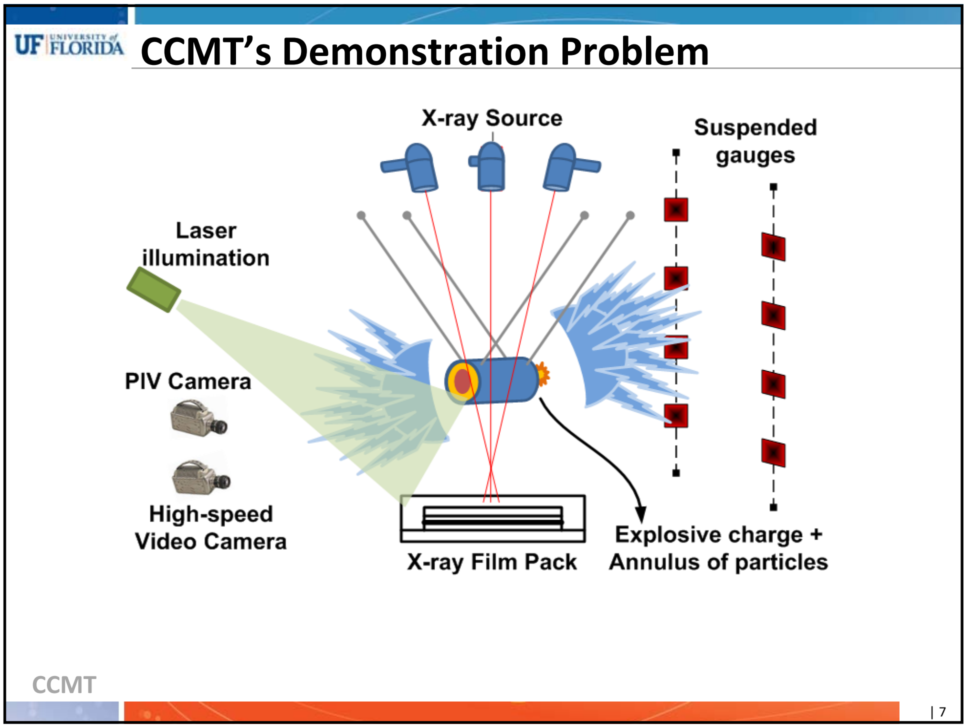
CCMT's Demonstration Problem
X-ray Source
Suspended gauges
Laser illumination
PIV Camera
High-speed Video Camera
X-ray Film Pack
Explosive charge + Annulus of particles
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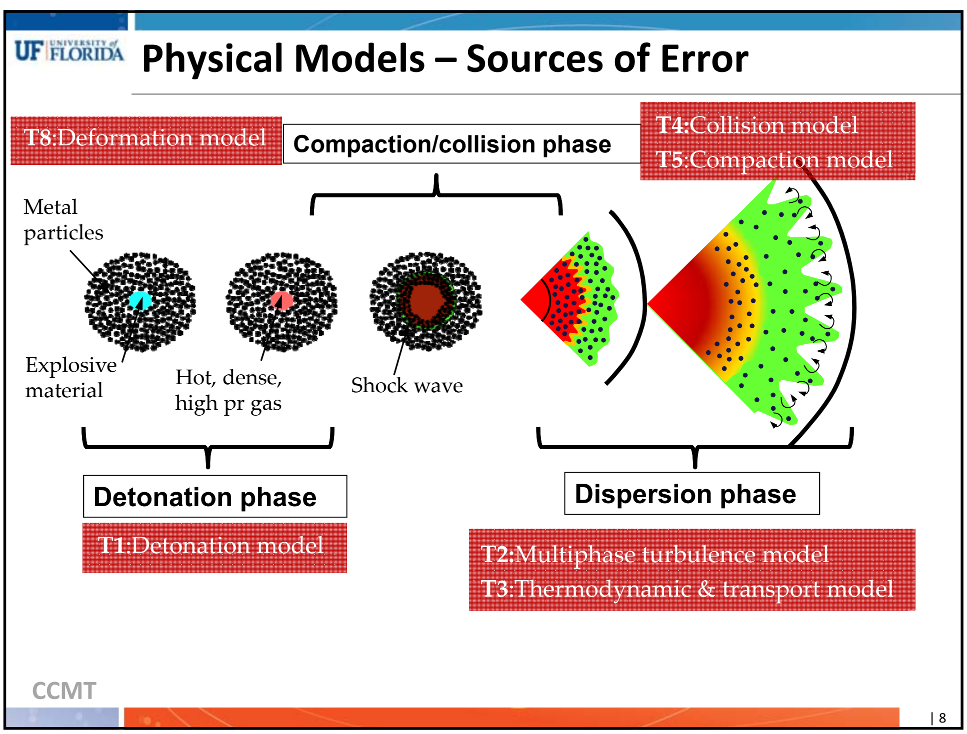
| 7


Physical Models – Sources of Error
T8:Deformation model
Compaction/collision phase
T4:Collision model
T5:Compaction model
Metal particles
Explosive material
Hot, dense, high pr gas
Shock wave
Detonation phase
T1:Detonation model
Dispersion phase
T2:Multiphase turbulence model
T3:Thermodynamic & transport model
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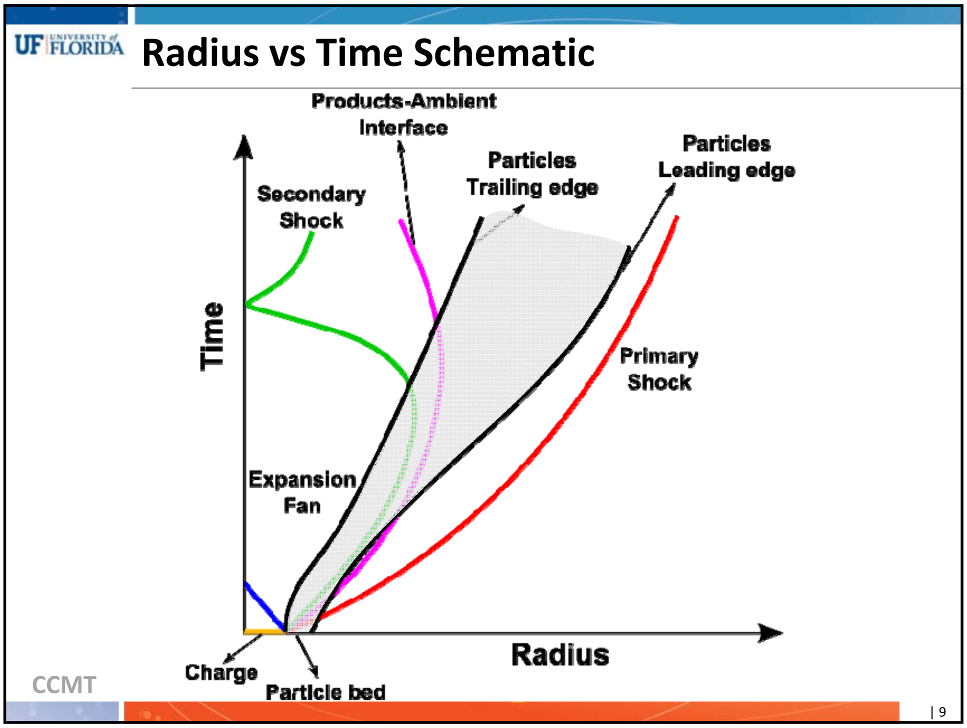
| 8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Radius vs Time Schematic
Products-Ambient Interface
Particles Trailing edge
Particles Leading edge
Secondary Shock
Time
Primary Shock
Expansion Fan
Radius
Charge
Particle bed
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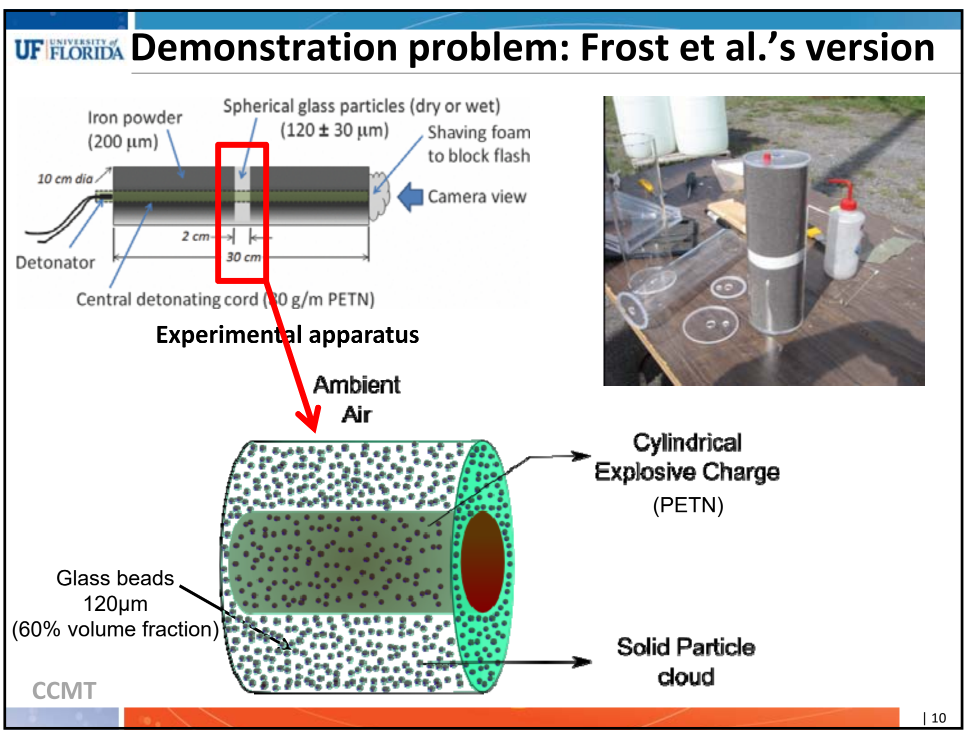
| 9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Demonstration problem: Frost et al.'s version
Iron powder (200 μm)
Spherical glass particles (dry or wet) (120 ± 30 μm)
Shaving foam to block flash
10 cm dia
Camera view
2 cm
30 cm
Detonator
Central detonating cord (10 g/m PETN)
Experimental apparatus
Ambient Air
Cylindrical Explosive Charge (PETN)
Glass beads 120μm (60% volume fraction)
Solid Particle cloud
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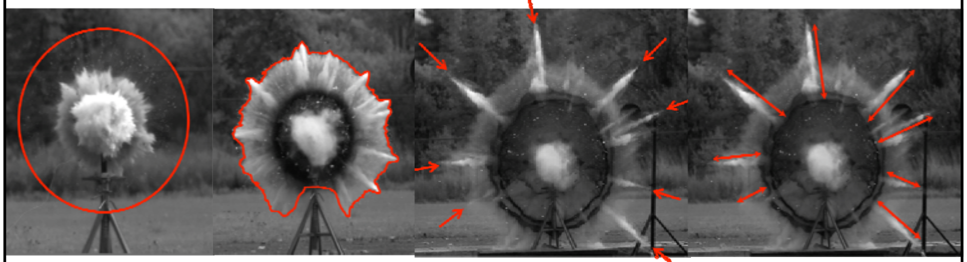
Explosive Dispersal of Particles – Experiment

PM-1: Blast Wave Location

PM-2: Particle Front Location

PM-3: Number of Instability Waves

PM-4: Amplitude of Instability Waves



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Hero Runs: Comparison

Properties	Hero Run 1	Hero Run 2	Hero Run 3
Reactive burn	No	No	Yes
Equation of state	Ideal	JWL	JWL
Density of products (kg/m^3)	1770	1770	1666
Pressure of products (GPa)	4	13	12
Kinetic energy of products (kJ/m^3)	0	0	60.5
Initial Particle volume fraction	5 %	40 %	60 %
No. of computational particles	5 M	5 M	15 M
No. of cores	512	4096	4096

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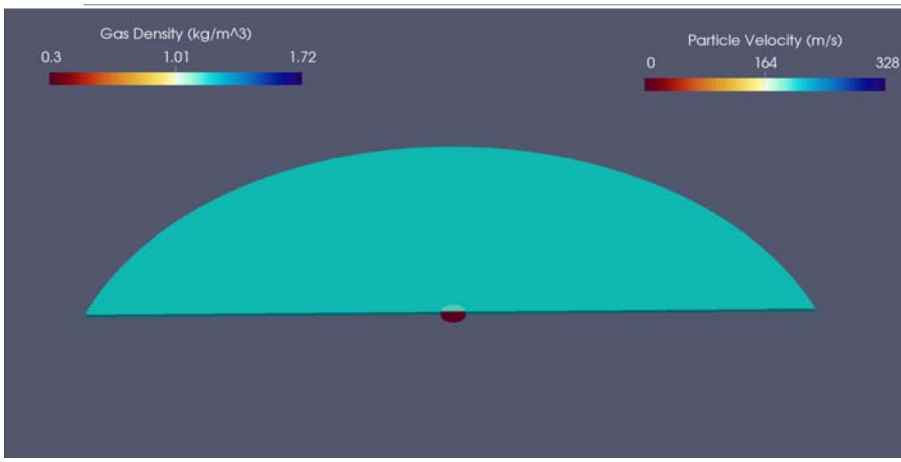
Demonstration Problem: Simulation



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

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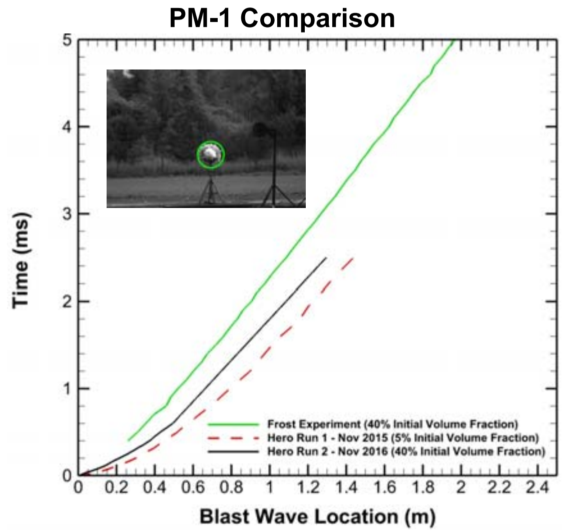
| 13

Demonstration Problem: Predictions



- Data from Frost experiment video starts at 0.400 milliseconds
- Possible sources of discrepancy: Collision/Compaction model, …

- The blast wave is slower in the experiment than in our current simulations
- The Larger initial volume fraction is improving PM-1's prediction

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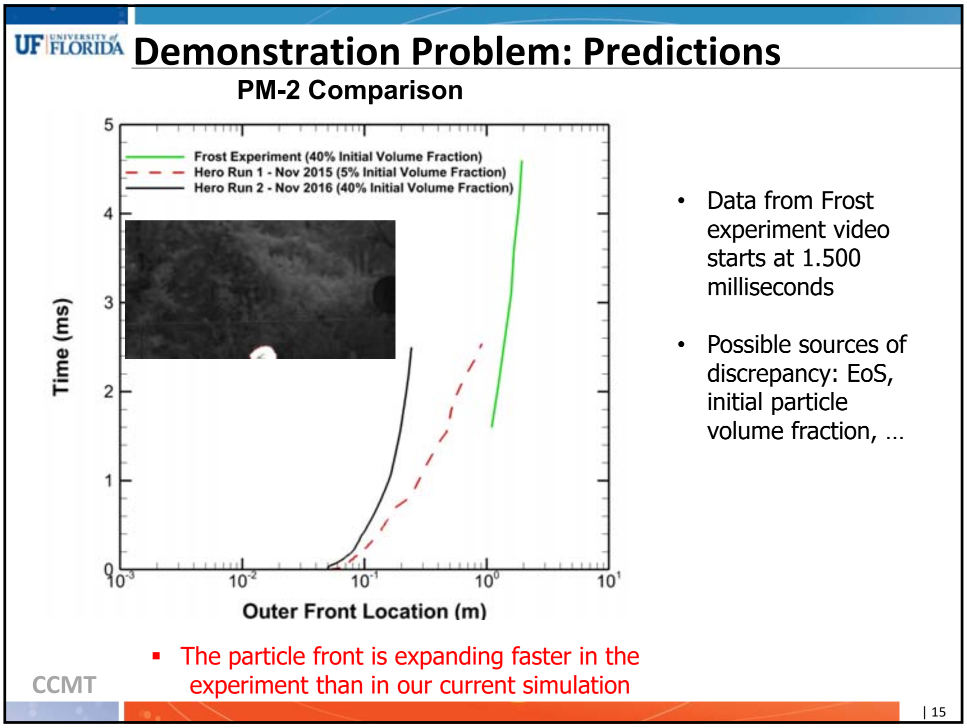
| 14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Demonstration Problem: Predictions
PM-2 Comparison
Frost Experiment (40% Initial Volume Fraction)
Hero Run 1 - Nov 2015 (5% Initial Volume Fraction)
Hero Run 2 - Nov 2016 (40% Initial Volume Fraction)
Time (ms)
Outer Front Location (m)
Data from Frost experiment video starts at 1.500 milliseconds
Possible sources of discrepancy: EoS, initial particle volume fraction, …
The particle front is expanding faster in the experiment than in our current simulation
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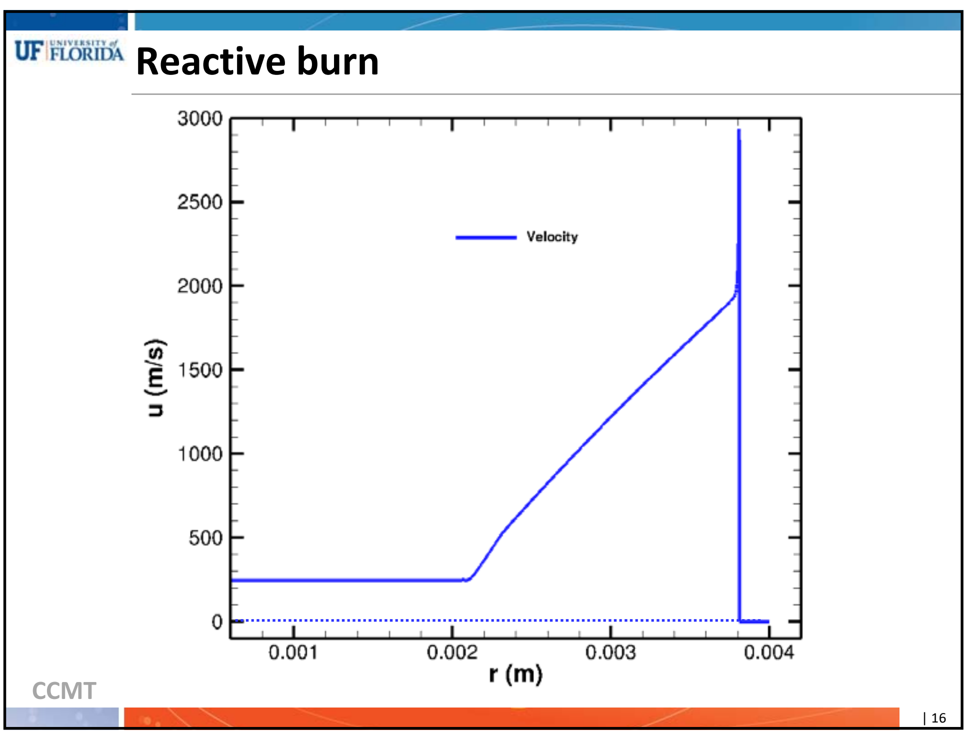
| 15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Reactive burn
Velocity
u (m/s)
r (m)
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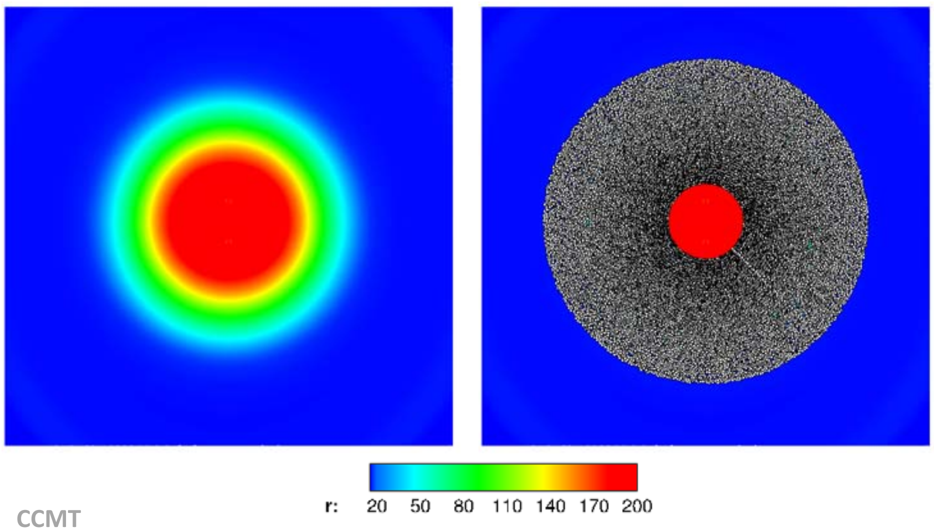
Working towards Hero Run 3

t = 25 μs

Density contour

2d with particles



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Outline

- **Macroscale**
  - Simulating the demonstration problem
  - Quantifying prediction metrics PM-3 and PM-4
  - Simulation of Eglin blast-bad experiment
- **Mesoscale Simulations**
  - Shock - Particle Curtain Interaction
  - Explosive dispersal of tungsten particles (Eglin experiment)
- **Modeling**
  - Surrogate Modeling of the real gas equation of state
  - Force & pressure modeling using generalized Faxén’s theorem

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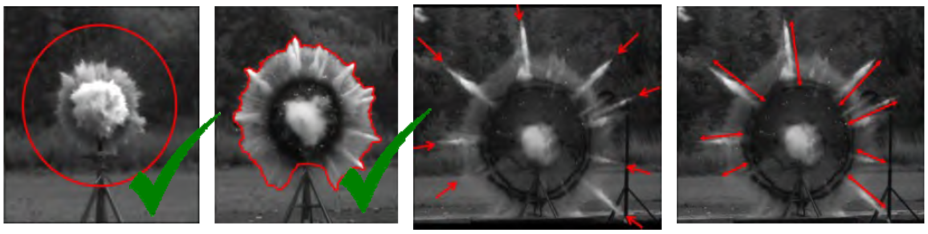
Prediction Metrics

CCMT prediction metrics are:



PM-1	PM-2	PM-3	PM-4
Blast wave location	Particle front location	Number of instability waves	Length of instability waves

Can we predict these metrics in simulations?

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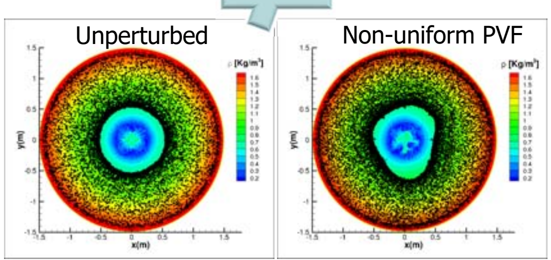
Experiment vs. Simulations

Experiments → Instabilities waves



Simulations → Are there instabilities? How can we measure?

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PVF Initial Perturbation

- Goal: optimization of perturbation parameters to get large instability waves

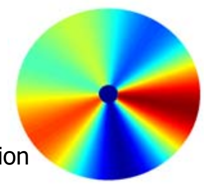
$$\phi^p(\theta) = \phi_0^p\left[1 + A_1 cos(k_1\theta) + A_2 cos(k_2\theta + \Phi_{12}) + A_3 cos(k_3\theta + \Phi_{13})\right]$$

PVF   Base PVF

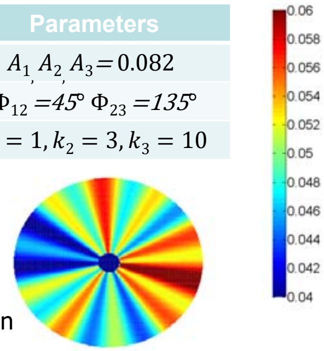
Parameters
$A_1, A_2 = 0.1 \quad A_3 = 0$
$\Phi_{12} = 45°$
$k_1 = 2, k_2 = 3$

Parameters
$A_1, A_2, A_3 = 0.082$
$\Phi_{12} = 45°\ \Phi_{23} = 135°$
$k_1 = 1, k_2 = 3, k_3 = 10$

Bi-modal Perturbation



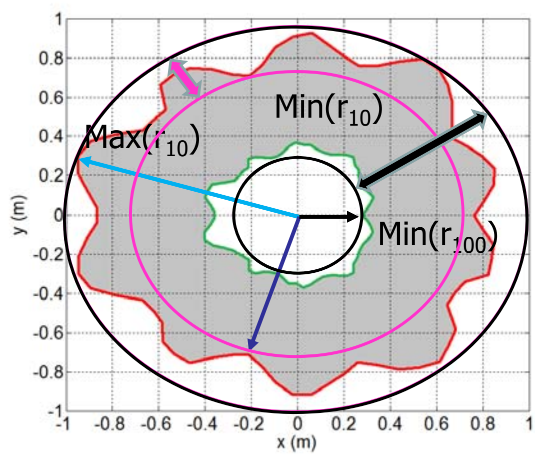
Tri-modal Perturbation

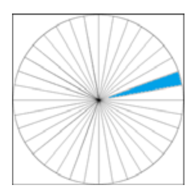


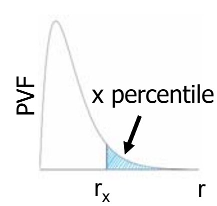
Schematic of Metrics

Definition of instability length and curtain thickness

r_{10}
r_{100}



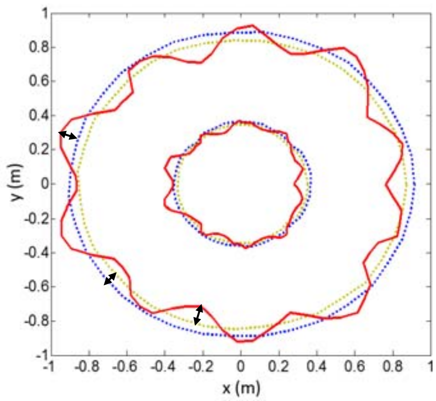


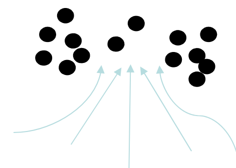


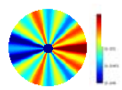
Instability Length (IL)= *Max(r_{10})-Min(r_{10})*

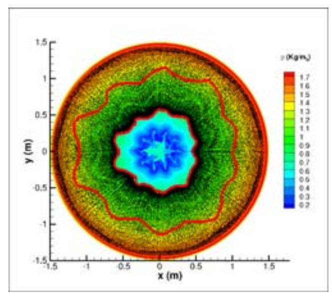
Curtain Thickness (CT)= *Max(r_{10})-Min(r_{100})*

Sample Simulation Result









k_1=2, k_2=3, k_3=10
Unperturbed PVF(t=0)=4%
Unperturbed PVF(t=0)=6%

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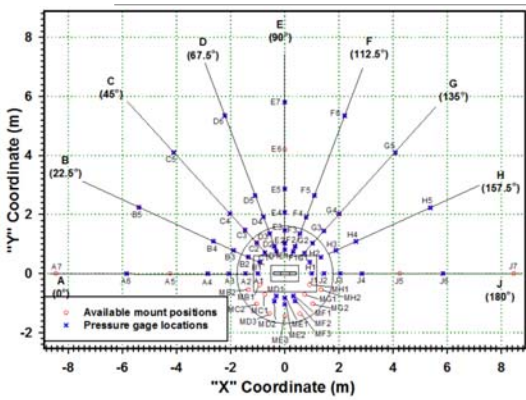
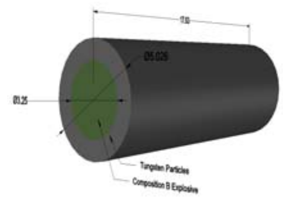
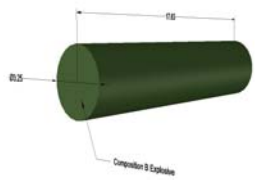
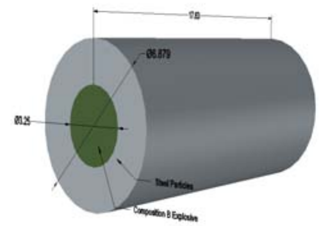
Blast Pad Experimental Setup



Location of pressure transducers (54 total)







Schematic of proposed cylindrical charges

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| 25

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Blast Pad Simulation Parameters

Properties	Tungsten	Comp B
Diameter	100 µm	-
Density	19250 kg/m³	1712 kg/m³
Specific heat	134 J/kg K	1223.6 J/kg K
Outer diameter	5.12 in	3.25 in
Depth (thickness)	0.75 in (2 cm)	0.75 in
Energy = (dens x int energy/unit vol)	-	8.5 GPa (products); 0.662 GPa (unreacted)
Computational Particles	10 M	-
Super-particle loading	18.176	-

Geometry outer diameter	16 m
Simulation time	6 ms
Charge/mass ratio	10

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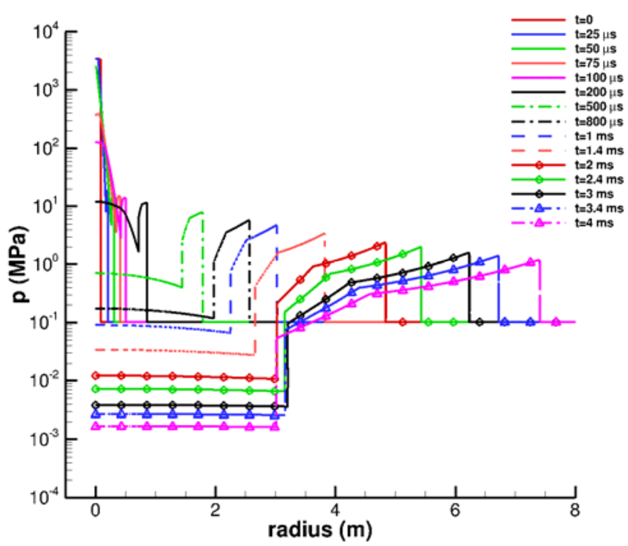
| 26

Blast Pad Simulation (Bare charge 1d results)



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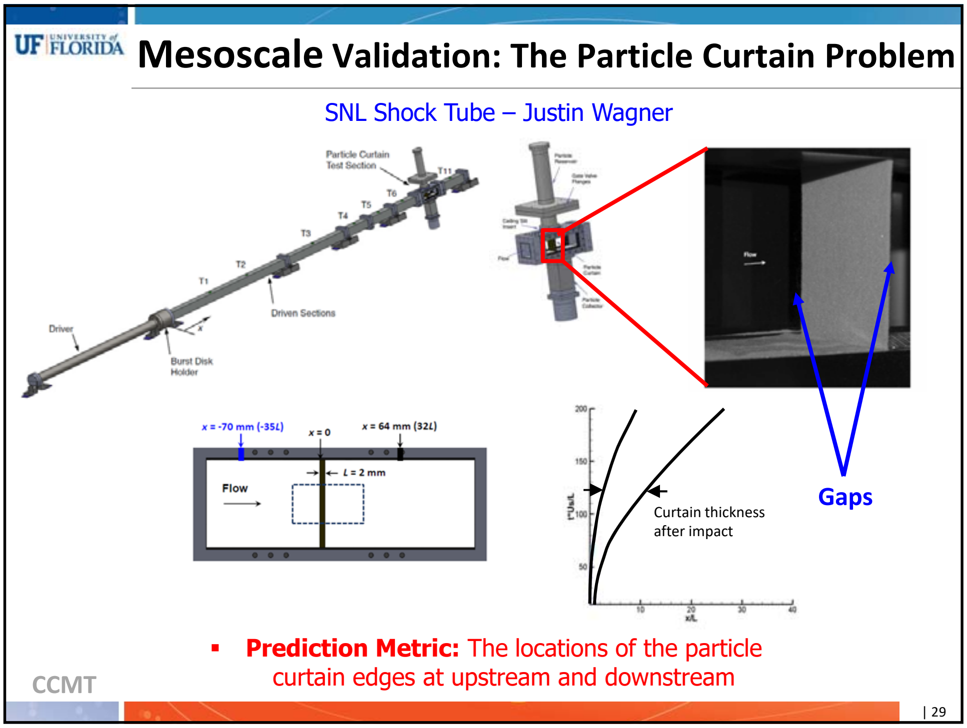
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Mesoscale Validation: The Particle Curtain Problem
SNL Shock Tube – Justin Wagner
Particle Curtain Test Section
Driven Sections
Driver
Burst Disk Holder
x = -70 mm (-35L)
x = 0
x = 64 mm (32L)
L = 2 mm
Flow
Curtain thickness after impact
Gaps
Prediction Metric: The locations of the particle curtain edges at upstream and downstream
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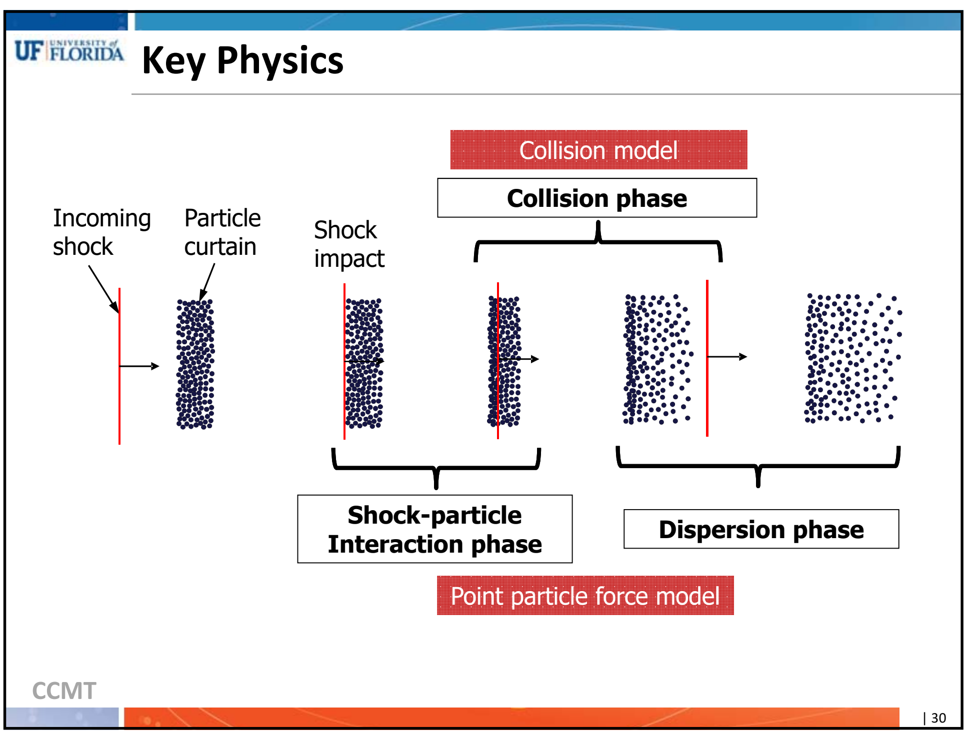
| 29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Key Physics
Collision model
Collision phase
Incoming shock
Particle curtain
Shock impact
Shock-particle Interaction phase
Dispersion phase
Point particle force model
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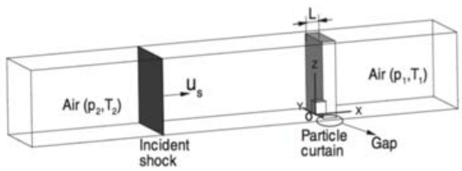
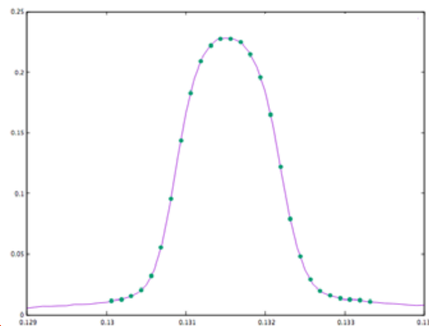
| 30

Experimental Variability & Uncertainty

Simulations (M = 1.66)	Particle Volume Fraction (%)	Curtain thickness (mm)
Run 1	10	3.1
Run 2	15	2
Run 3	Distribution	3.4
Run 4	19	2



Adapted From: Y. Ling et al. Phys. Fluids **24**, 113301 (2012)



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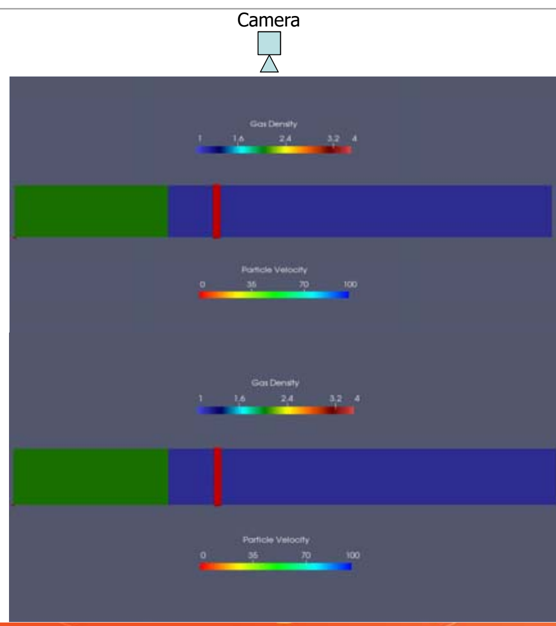
Simulation Results – No Gap



Run 2

Run 3

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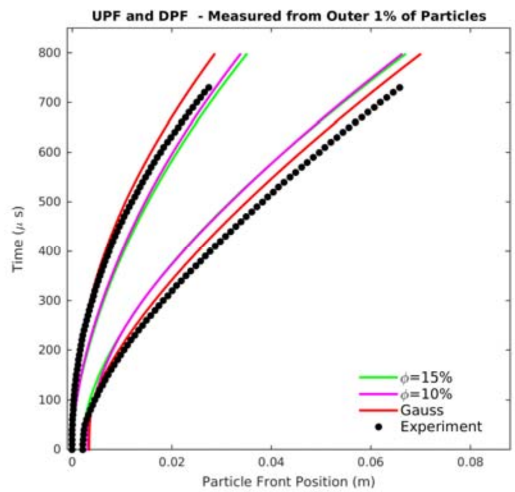
Particle Curtain Front Locations



- The initially "gaussian" particle volume fraction profile appears to allow for better prediction than the 10% and 15% uniform volume fraction cases

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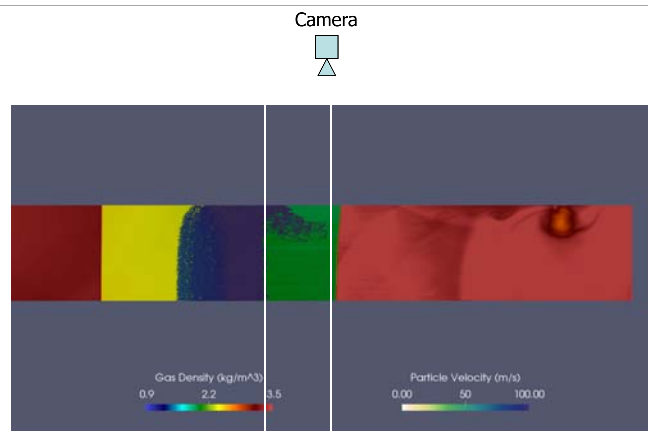
Effect of Gap



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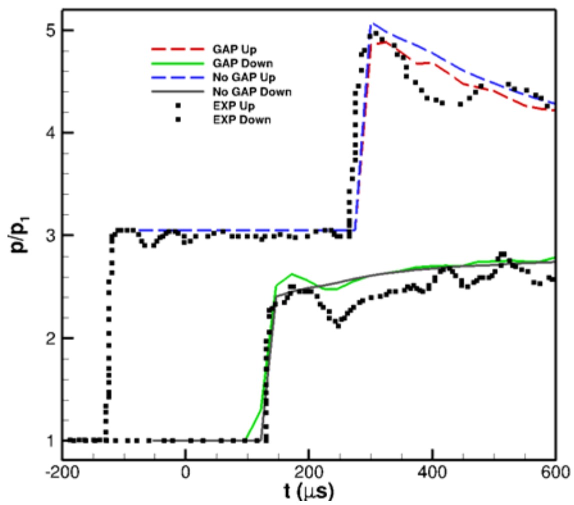
Pressure Measurement



- Signature of the presence of the sidewall gaps in the pressure measurement downstream of the curtain

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| 35

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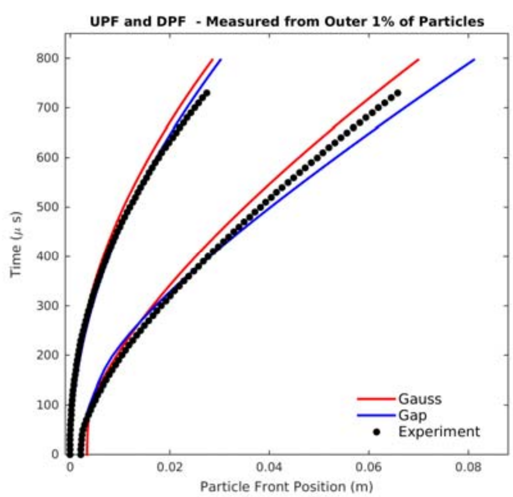
Particle Curtain Front Locations



- Particles initially near the gap travel ahead of particles in the core of the curtain

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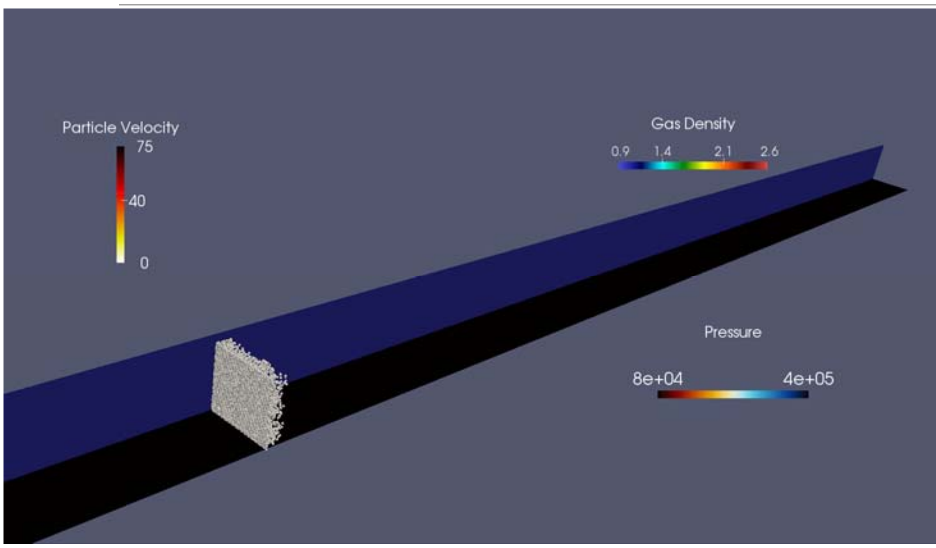
| 36

Particle Curtain Simulation



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

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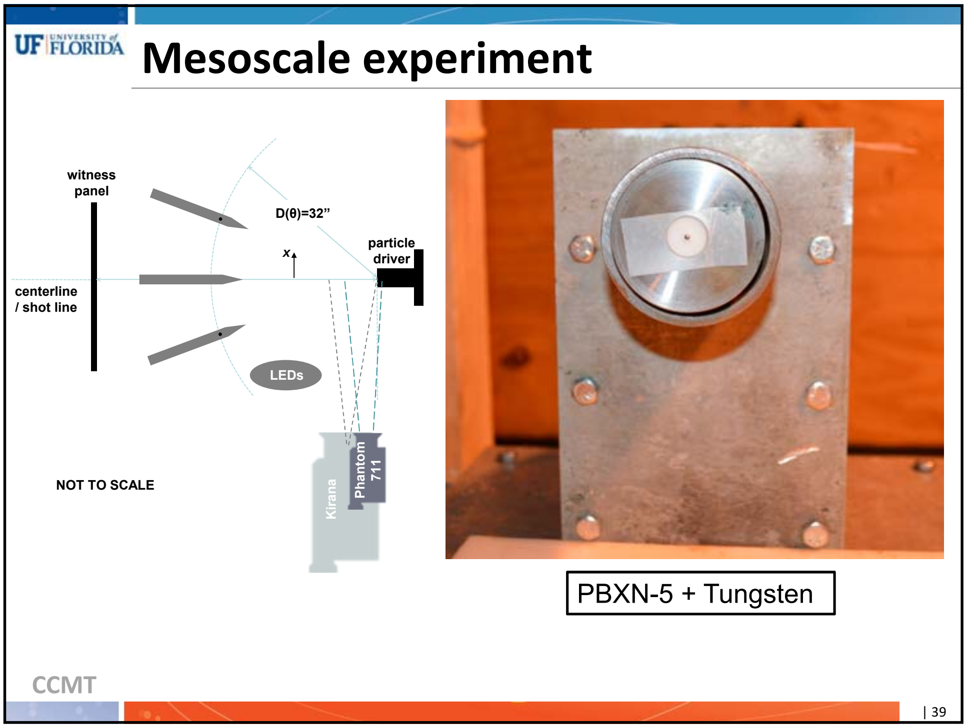
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Mesoscale experiment
witness panel
D(θ)=32"
particle driver
x
centerline / shot line
LEDs
Phantom 711
Kirana
NOT TO SCALE
PBXN-5 + Tungsten
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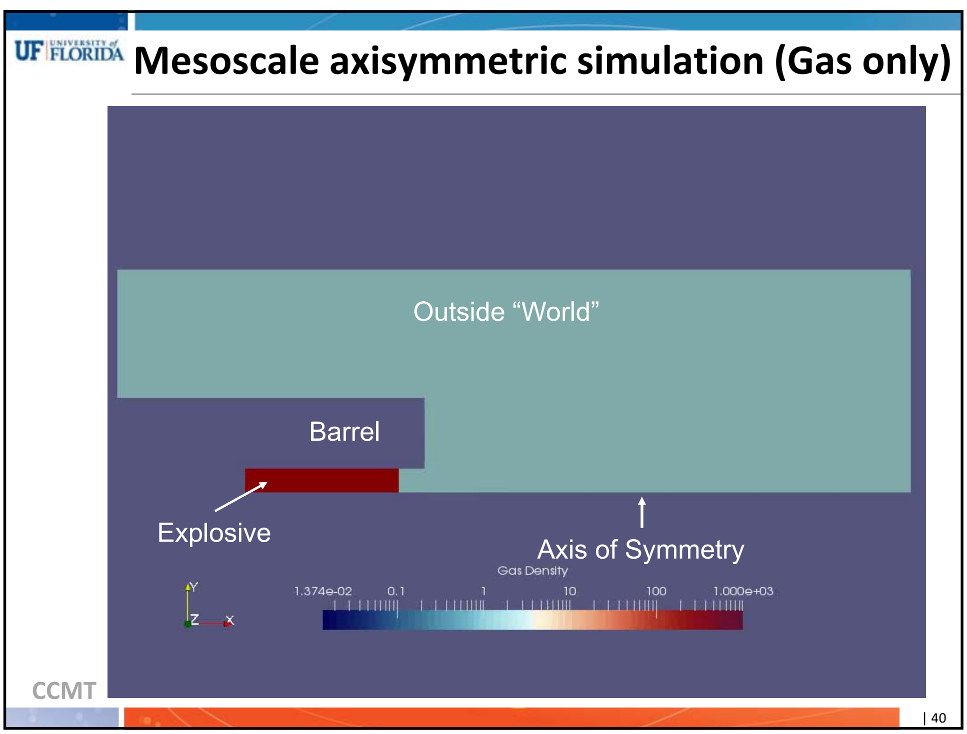
| 39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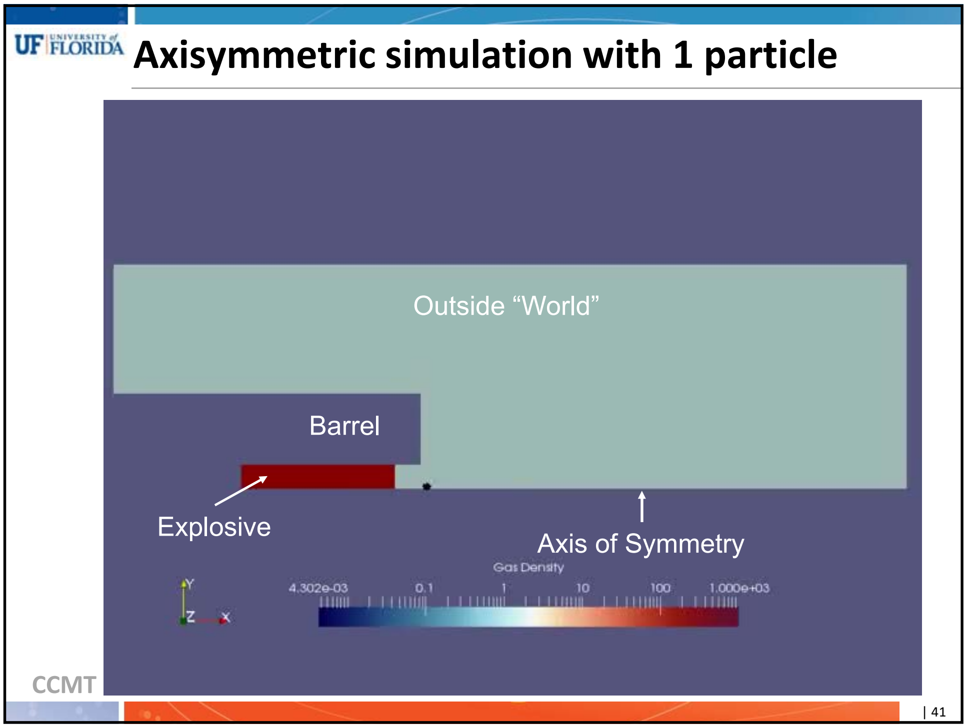
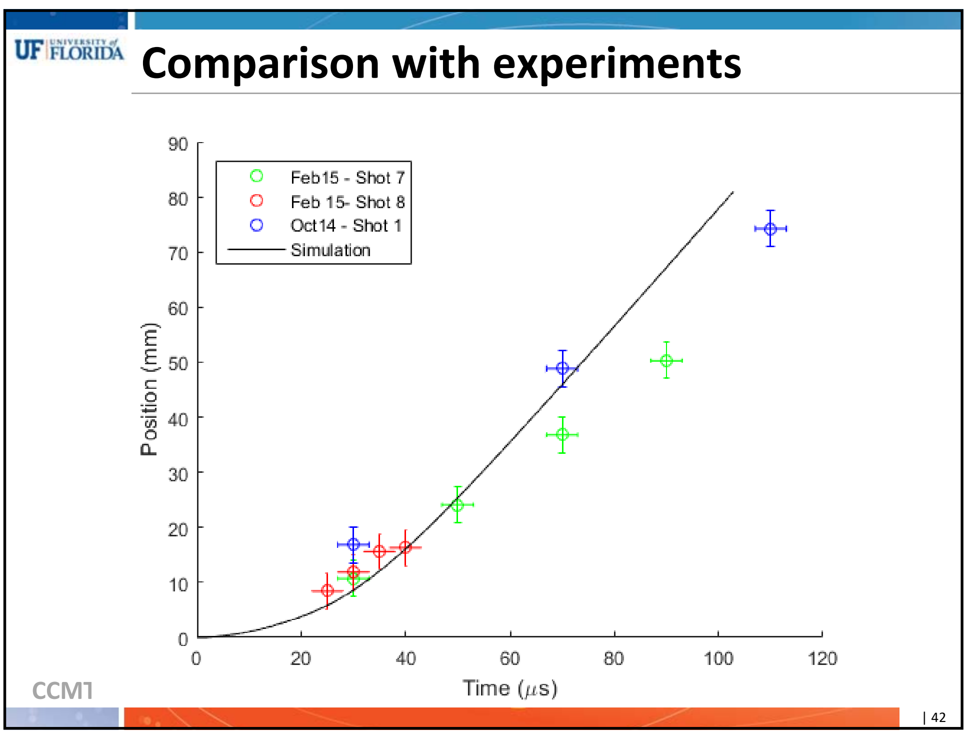
Mesoscale axisymmetric simulation (Gas only)
Outside "World"
Barrel
Explosive
Axis of Symmetry
Gas Density
1.374e-02
0.1
1
10
100
1.000e+03
Y
Z
X
CCMT
| 40


UF FLORIDA
Axisymmetric simulation with 1 particle
Outside "World"
Barrel
Explosive
Axis of Symmetry
Gas Density
4.302e-03
0.1
1
10
100
1.000e+03
CCMT
| 41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Comparison with experiments
Feb15 - Shot 7
Feb 15- Shot 8
Oct14 - Shot 1
Simulation
Position (mm)
Time (µs)
0
10
20
30
40
50
60
70
80
90
0
20
40
60
80
100
120
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| 42

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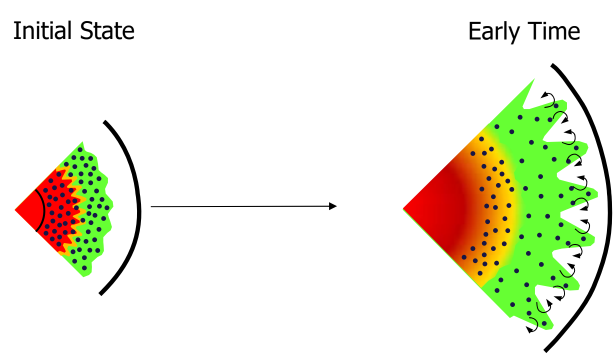
| 43

Handling Cells with Mixed EoS



- A short time after detonation, there are both pure explosive products and pure air
- At later time, pure species still exist but a mixture region will form where two equations of state must be satisfied
- The goal is to find a way to simplify and speed up the gas computations in this zone

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Looking at the Big Picture

The Jones-Wilkins-Lee (JWL) equations of state are used to predict the pressures of high energy substances and are:

$$P_{JWL}(\rho, e) = A\left(1 - \frac{\omega}{R_1 V}\right)e^{-R_1 V} + B\left(1 - \frac{\omega}{R_2 V}\right)e^{-R_2 V} + \omega \rho e$$

$$T_{JWL}(P, \rho) = \left(\frac{1}{\rho \omega C_v}\right)\left(P - Ae^{-R_1 V} - Be^{-R_2 V}\right)$$

where $V = \frac{\rho_o}{\rho}$ and $\rho_o, A, B, C, R_1, R_2$ and ω are parameters for the substance.

- What is the iterative scheme in our code really doing?

Inputs:
ρ_m, e_m, Y_{exp}

↓

Outputs:
1) Common pressure/temperature for both EoS
2) Internal energy attributed to the air and the products
3) Density attributed to the air and the products

- If we compute the common pressures and temperatures outside of the code, a curve fit can be applied

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| 45

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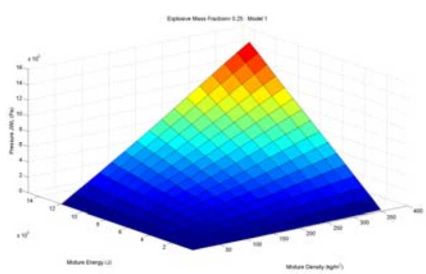
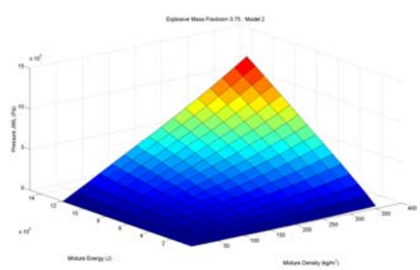
Surrogate Model - Development





- Kriging method used to generate two models for mixed cell pressure and temperature in terms of ρ_m, e_m and Y_{exp} using 200 sampling points
- Domain Space: $(\rho_m, e_m, Y_{exp}) \rightarrow [(0.1{,}350), (1.25e5, 1.5e7), (0{,}1)]$
  - Model 1: Used both relative and absolute errors in choosing sampling points
  - Model 2: Used only absolute errors in choosing sampling points
- Average relative errors :
  - Pressure (1): 1.00%
  - Temperature (1): 0.04%

Pressure (2): 0.94%
Temperature (2): 0.04%

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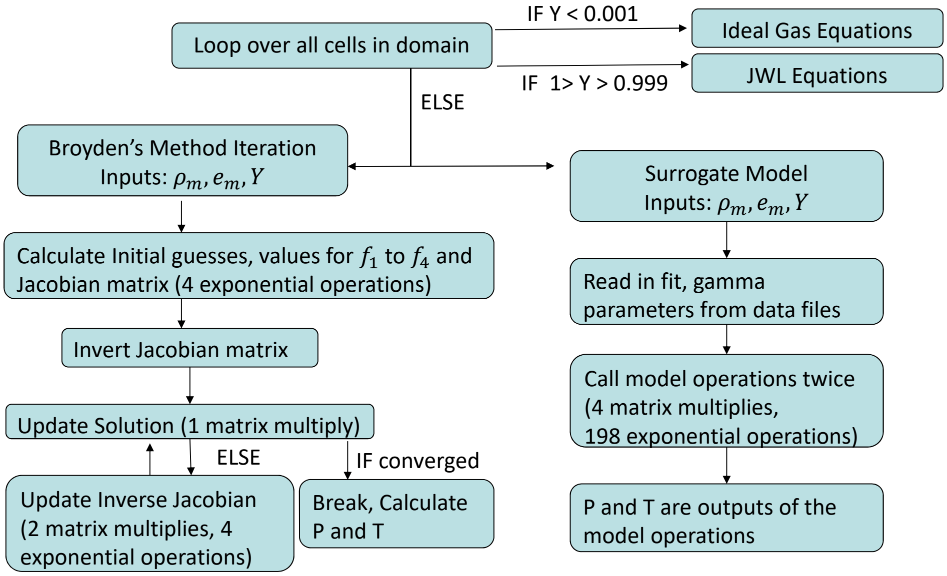
| 46

Flowchart – Iterative vs. Surrogate



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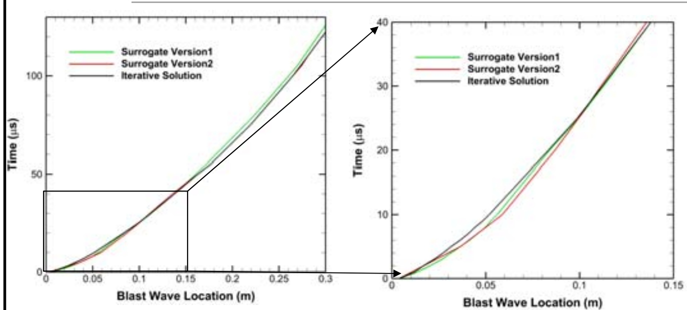
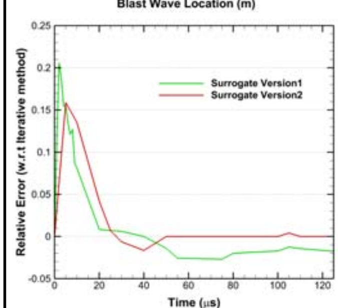
Model Results – Blast Wave



Simulation Description:

- 2D, Cylindrical grid
- Outer radius = 0.3 m
- 150,000 cells
- Gas-Only
- Simulation out to 125 μs



- Results show relatively large errors in tracking the blast wave at early times for both models
- Model 2 appears to be better suited to track the wave
- Improvements need to be made to reduce the initial error spike
  - More sampling points
  - Full density range with same density of sampling points

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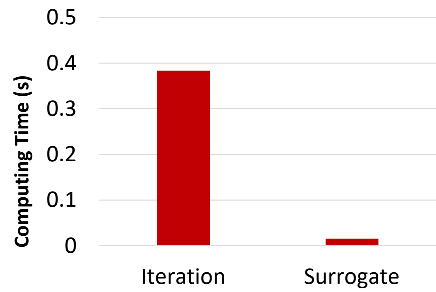
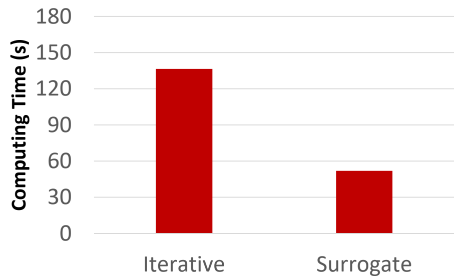
Surrogate Model Results – Computation Time



- Wall clock time to calculate pressure and temperature for 1000 points:
  - Iteration: 0.383 s
  - Surrogate: 0.015 s
  - Ratio: 25.533



- Wall clock time to compute 1000 time steps in Rocflu:
  - Iteration: 136.444 s
  - Surrogate: 51.835 s
  - Ratio: 2.632
- Results averaged over three runs
- The improvement ratio is grid dependent

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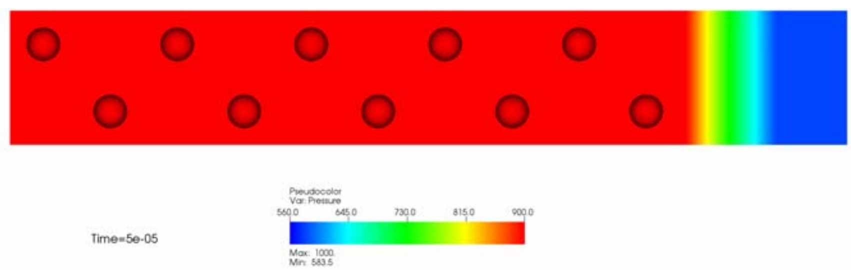
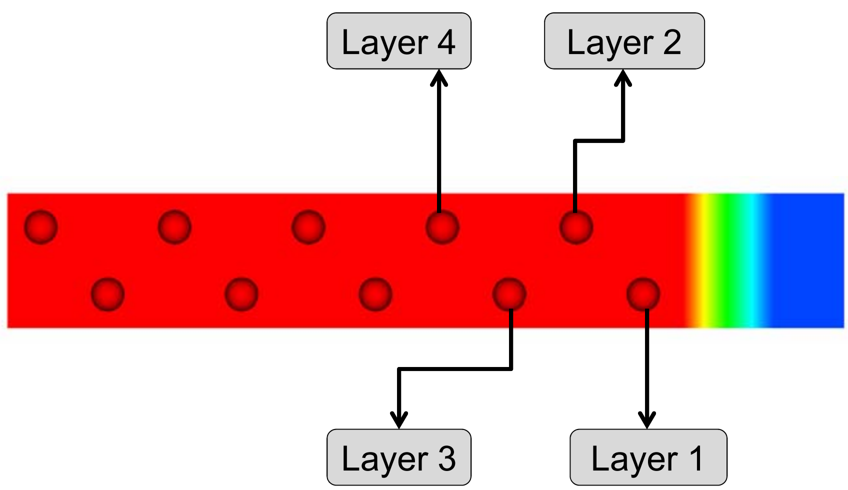
Improved Forces – Generalized Faxén's Theorem

$$\mathbf{F}_{inv}(t) = \frac{4}{3}\pi R^3 \rho \overline{\frac{D\mathbf{u}}{Dt}}^V + 4\pi R^3 \int_{\tilde{\xi}=-\infty}^{\tilde{t}} K_{iu}(\tilde{t}-\tilde{\xi}) \left[\frac{D}{Dt}\overline{(\rho \mathbf{u}_r)}^S\right]_{\tilde{t}=\tilde{\xi}} d\tilde{\xi} .$$

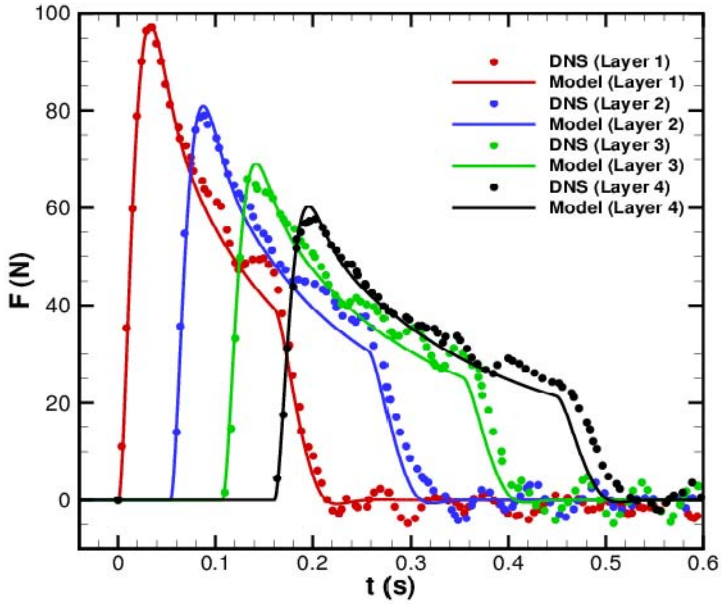


Simulation of an expansion fan over an array of spheres using CMT-nek

Expansion fan – Multi-particle system



Expansion fan – Multi-particle system



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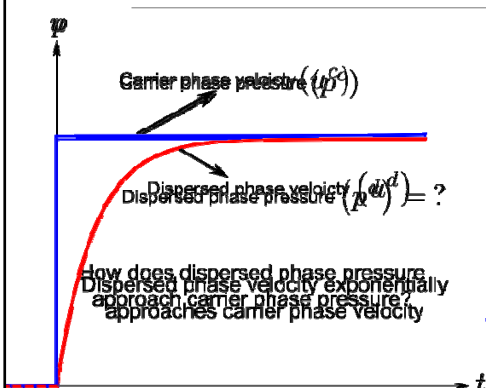
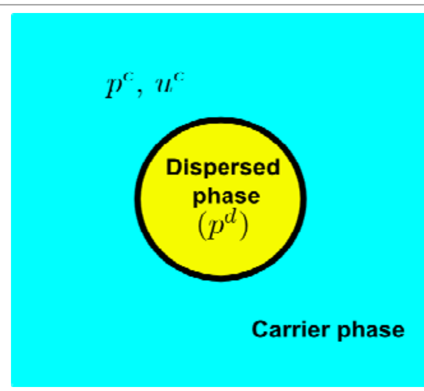
Pressure evolution inside the particle





$$\frac{d\mathbf{u}^d}{dt} = \frac{\mathbf{u}^c - \mathbf{u}^d}{\tau_{pV}}$$

$$\tau_{pV} = \frac{(2\tilde{\rho}+1)R_0^2}{9\nu^c\Phi_V}$$

Momentum balance → Stokes drag

$$\frac{dp^d}{dt} = ?$$

$$\tau_{pP} = ?$$

Pressure equilibration equation

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Pressure Equilibration Equation

The volume-averaged particle phase pressure expressed purely in terms of "undisturbed" time-variation of the carrier phase properties is given as below:

$$\overline{p^d}^V(t)-\overline{p_0^d}^V = \frac{R_0}{a_0^c}\int_{\tilde{\xi}=-\infty}^{\tilde{t}} K_p(\tilde{t}-\tilde{\xi})\,\frac{\mathrm{d}}{\mathrm{d}t}\overline{p^c}^S\Big|_{\tilde{t}=\tilde{\xi}}\mathrm{d}\tilde{\xi} + R_0\int_{\tilde{\xi}=-\infty}^{\tilde{t}} K_w(\tilde{t}-\tilde{\xi})\,\frac{\mathrm{d}}{\mathrm{d}t}\overline{(\rho u_r)^c}^S\Big|_{\tilde{t}=\tilde{\xi}}\mathrm{d}\tilde{\xi}$$

- $\overline{p^d}^V(t)-\overline{p_0^d}^V$: Change in particle pressure (volume averaged)
- $K_p(\tilde{t}-\tilde{\xi})$: Response to unit-step change in ambient pressure
- $\frac{\mathrm{d}}{\mathrm{d}t}\overline{p^c}^S$: Time-varying ambient pressure (surface averaged)
- $K_w(\tilde{t}-\tilde{\xi})$: Response to unit-step change in ambient radial momentum
- $\frac{\mathrm{d}}{\mathrm{d}t}\overline{(\rho u_r)^c}^S$: Time-varying ambient radial momentum (surface averaged)

R_0 : Mean particle radius, a_0^c : Ambient speed of sound

$K_p, K_w = f(\tilde{\rho}, \tilde{a})$ where $\tilde{\rho}$: density ratio, $\tilde{a}$: Speed of sound ratio

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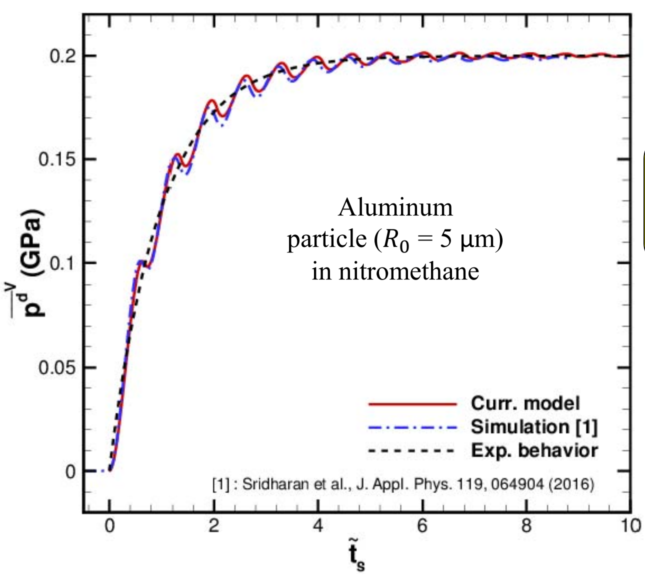
Pressure Evolution: Shock Ma = 1.11



Exp. behavior (black-dash line) analogous to particle equation of motion:

$$\frac{\mathrm{d}\overline{p^d}^V}{\mathrm{d}t} = \frac{p^c_{\mathrm{final}} - \overline{p^d}^V}{\tau_{pP}}$$

$\tau_{pP} = R_0/u_s$ is the particle time-scale

Similar agreements also observed for higher Mach numbers and particles with larger radii.

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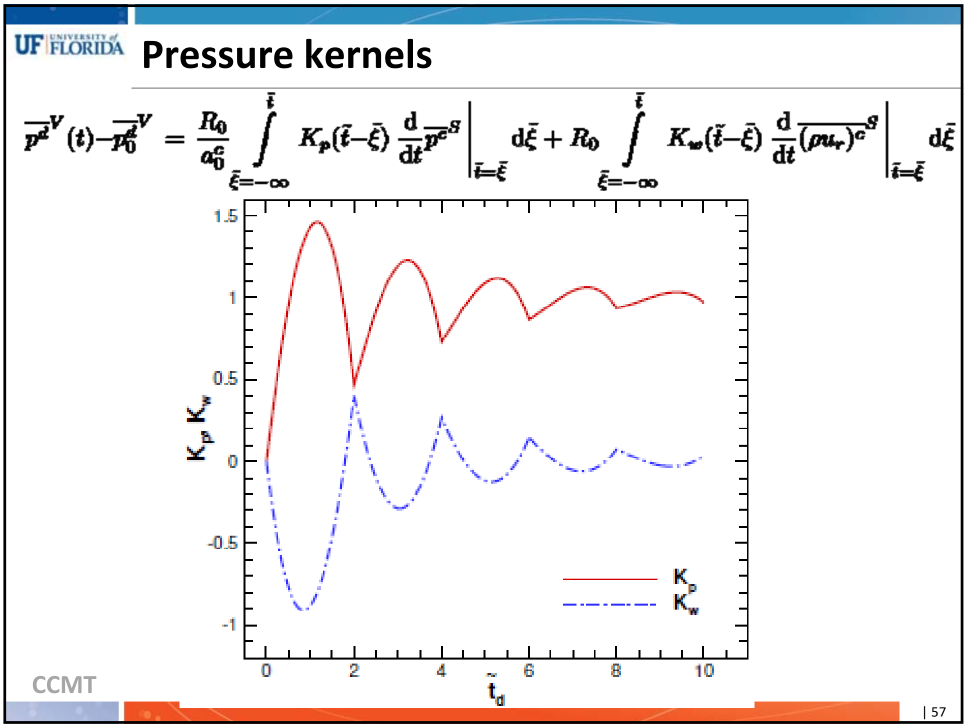
Pressure kernels
$\overline{p^d}^V(t) - \overline{p_0^d}^V = \frac{R_0}{a_0^c} \int_{\tilde{\xi}=-\infty}^{\tilde{t}} K_p(\tilde{t}-\tilde{\xi}) \frac{d}{dt}\overline{p^c}^S \Big|_{\tilde{t}=\tilde{\xi}} d\tilde{\xi} + R_0 \int_{\tilde{\xi}=-\infty}^{\tilde{t}} K_w(\tilde{t}-\tilde{\xi}) \frac{d}{dt}\overline{(\rho u_r)^c}^S \Big|_{\tilde{t}=\tilde{\xi}} d\tilde{\xi}$
K_p, K_w
$\tilde{t}_d$
K_p
K_w
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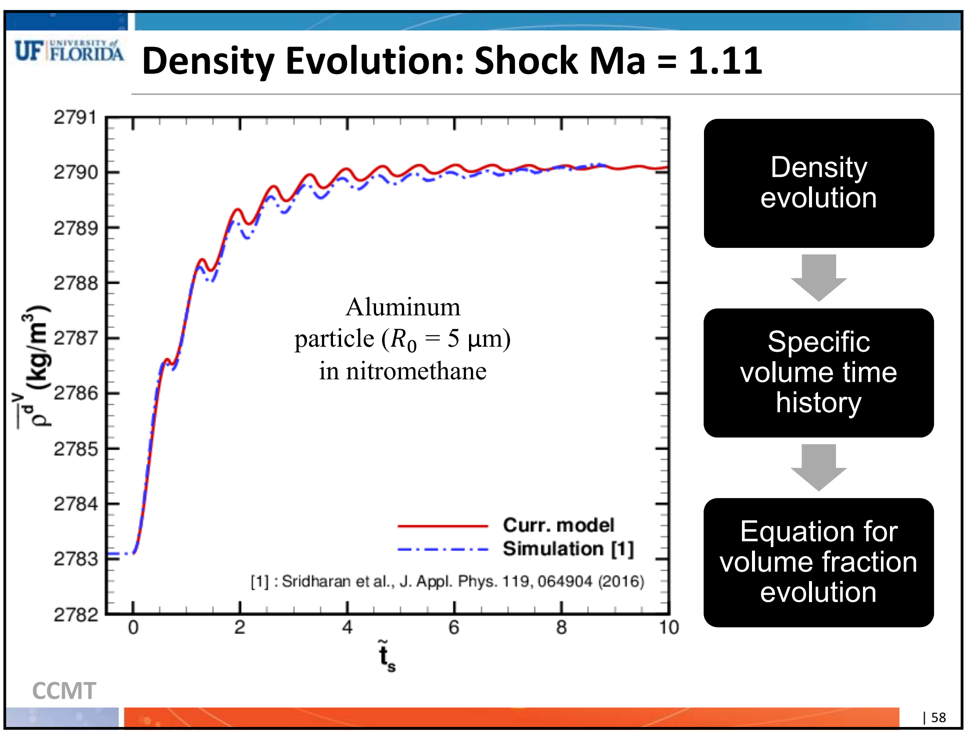
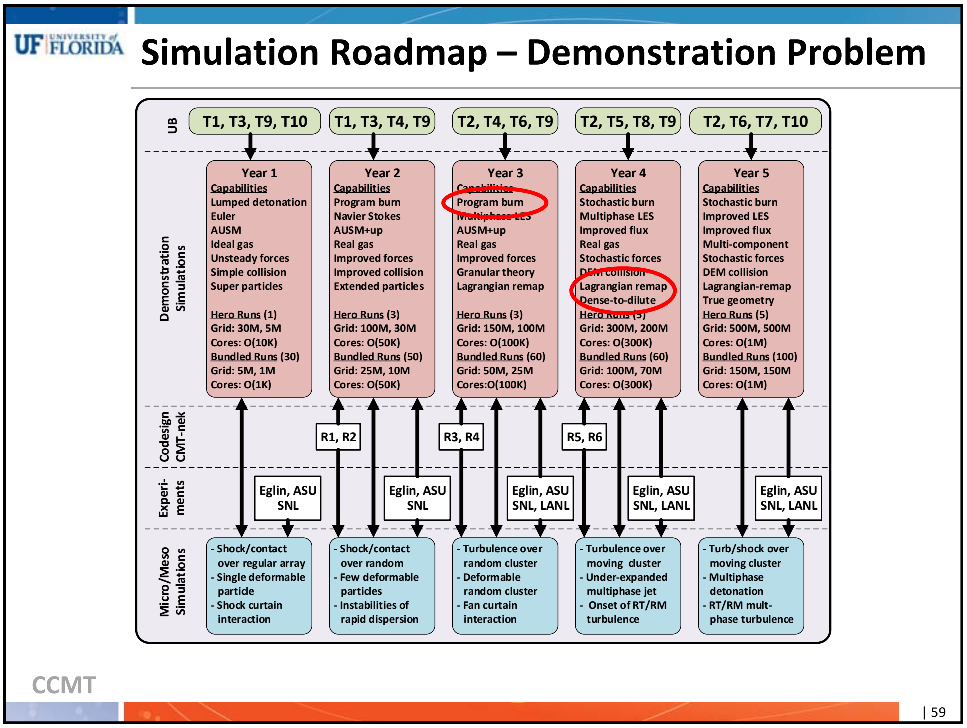
| 57


Density Evolution: Shock Ma = 1.11
$\overline{\rho^d}^V$ (kg/m^3)
$\tilde{t}_s$
Aluminum
particle (R_0 = 5 μm)
in nitromethane
Curr. model
Simulation [1]
[1] : Sridharan et al., J. Appl. Phys. 119, 064904 (2016)
Density evolution
Specific volume time history
Equation for volume fraction evolution
CCMT
| 58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Simulation Roadmap – Demonstration Problem
UB
T1, T3, T9, T10
T1, T3, T4, T9
T2, T4, T6, T9
T2, T5, T8, T9
T2, T6, T7, T10
Demonstration Simulations
Year 1
Capabilities
Lumped detonation
Euler
AUSM
Ideal gas
Unsteady forces
Simple collision
Super particles
Hero Runs (1)
Grid: 30M, 5M
Cores: O(10K)
Bundled Runs (30)
Grid: 5M, 1M
Cores: O(1K)
Year 2
Capabilities
Program burn
Navier Stokes
AUSM+up
Real gas
Improved forces
Improved collision
Extended particles
Hero Runs (3)
Grid: 100M, 30M
Cores: O(50K)
Bundled Runs (50)
Grid: 25M, 10M
Cores: O(50K)
Year 3
Capabilities
Program burn
Multiphase LES
AUSM+up
Real gas
Improved forces
Granular theory
Lagrangian remap
Hero Runs (3)
Grid: 150M, 100M
Cores: O(100K)
Bundled Runs (60)
Grid: 50M, 25M
Cores:O(100K)
Year 4
Capabilities
Stochastic burn
Multiphase LES
Improved flux
Real gas
Stochastic forces
DEM collision
Lagrangian remap
Dense-to-dilute
Hero Runs (5)
Grid: 300M, 200M
Cores: O(300K)
Bundled Runs (60)
Grid: 100M, 70M
Cores: O(300K)
Year 5
Capabilities
Stochastic burn
Improved LES
Improved flux
Multi-component
Stochastic forces
DEM collision
Lagrangian-remap
True geometry
Hero Runs (5)
Grid: 500M, 500M
Cores: O(1M)
Bundled Runs (100)
Grid: 150M, 150M
Cores: O(1M)
Codesign CMT-nek
R1, R2
R3, R4
R5, R6
Experi-ments
Eglin, ASU SNL
Eglin, ASU SNL
Eglin, ASU SNL, LANL
Eglin, ASU SNL, LANL
Eglin, ASU SNL, LANL
Micro/Meso Simulations
- Shock/contact over regular array
- Single deformable particle
- Shock curtain interaction
- Shock/contact over random
- Few deformable particles
- Instabilities of rapid dispersion
- Turbulence over random cluster
- Deformable random cluster
- Fan curtain interaction
- Turbulence over moving cluster
- Under-expanded multiphase jet
- Onset of RT/RM turbulence
- Turb/shock over moving cluster
- Multiphase detonation
- RT/RM mult-phase turbulence
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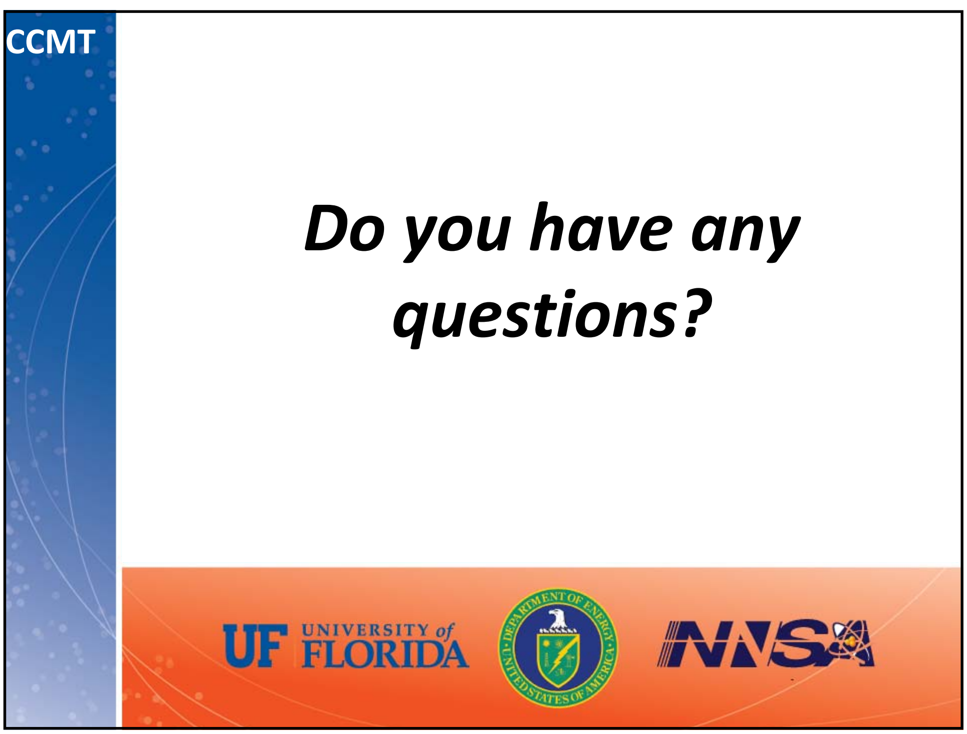
| 59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Do you have any questions?
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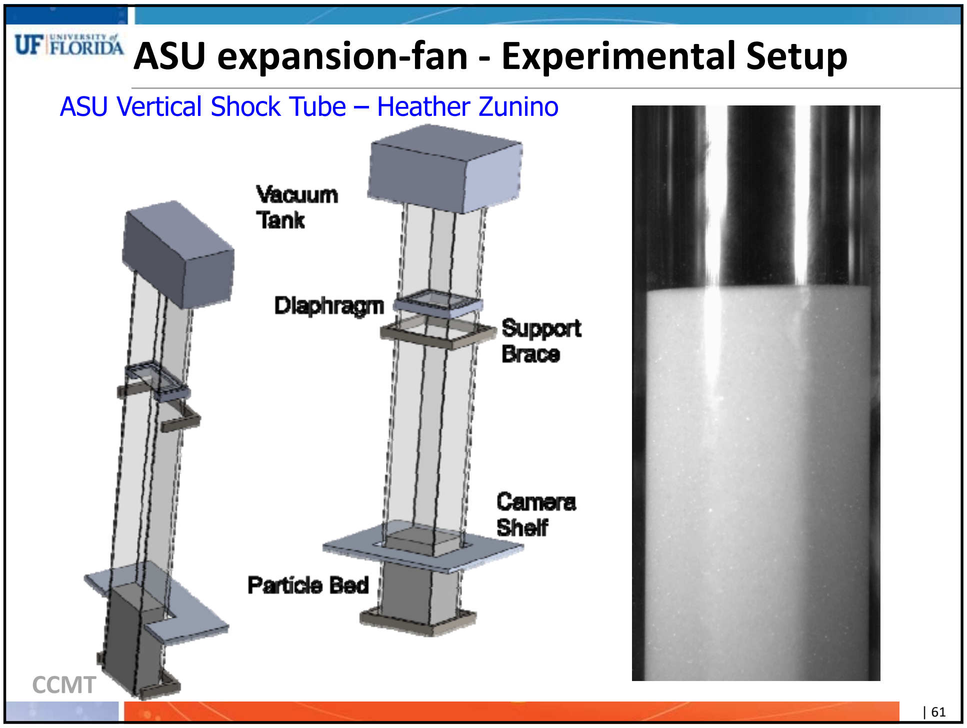
DEPARTMENT OF ENERGY UNITED STATES OF AMERICA
NNSA


ASU expansion-fan - Experimental Setup
ASU Vertical Shock Tube – Heather Zunino
Vacuum Tank
Diaphragm
Support Brace
Camera Shelf
Particle Bed
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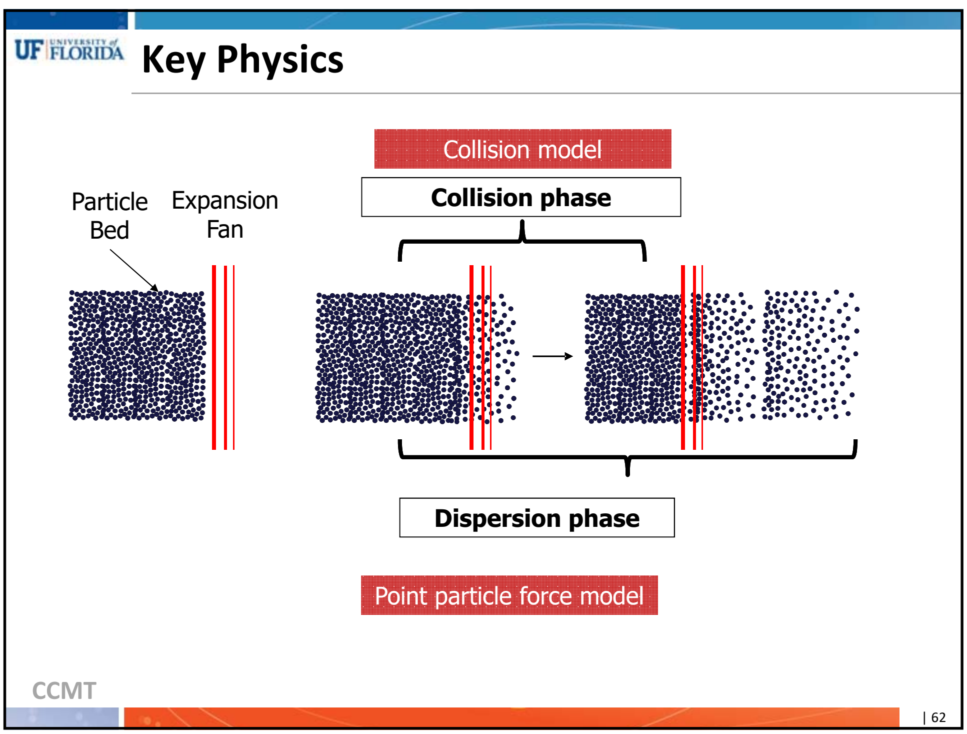
| 61


Key Physics
Collision model
Collision phase
Particle Bed
Expansion Fan
Dispersion phase
Point particle force model
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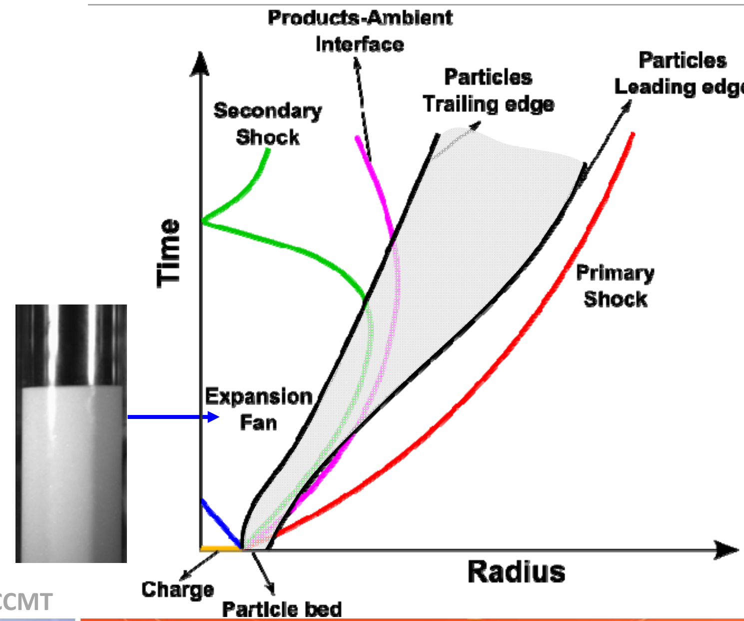
Features to Capture



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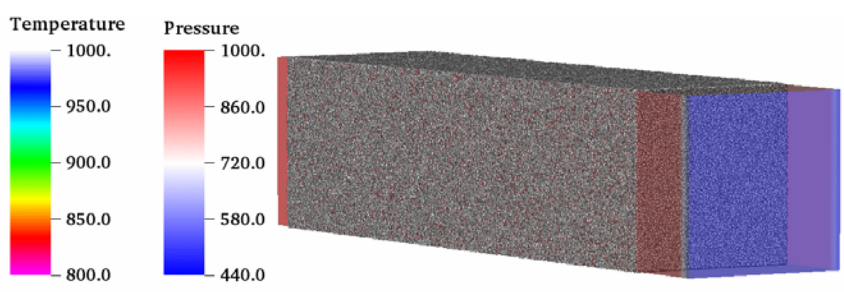
Particles – Expansion Fan Interaction

- 1-way coupled capability run with new physics:
  - Quasi-steady, inviscid unsteady, and undisturbed forces
  - Finite Reynolds and Mach number corrections
- 131k processors for 11 hours on Vulcan
- ~250 million grid points
  - 131,072 spectral elements
  - 12x12x12 grid points per element
- ~20 billion particles



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Uncertainty Budget

Validation and Uncertainty Reduction

Chanyoung Park

Department of Mechanical & Aerospace Engineering, University of Florida

---

Uncertainty Budget Team

Raphael T. Haftka, PhD

Nam-Ho Kim, PhD

Chanyoung Park, PhD

Kyle Hughes

Sam Nili

Yiming Zhang

Giselle Fernandez

- PI: Raphael T. Haftka and Nam-Ho Kim
- Research Scientist: Chanyoung Park
- Students
  - Giselle Fernandez (Signal to noise ratio)
  - Kyle Hughes (UQ of Eglin exp.)
  - Justin T. Mathew (UQ of ASU/SNL experiments)
  - Sam Nili (Mesoscale 1D/2D simulations)
  - Yiming Zhang (Validation and UQ of BE emulation)
- Undergraduate students
  - Shirly Spath (UQ of Eglin exp.)

Justin T. Mathew

(New student)

Shirly Spath (Undergrad)

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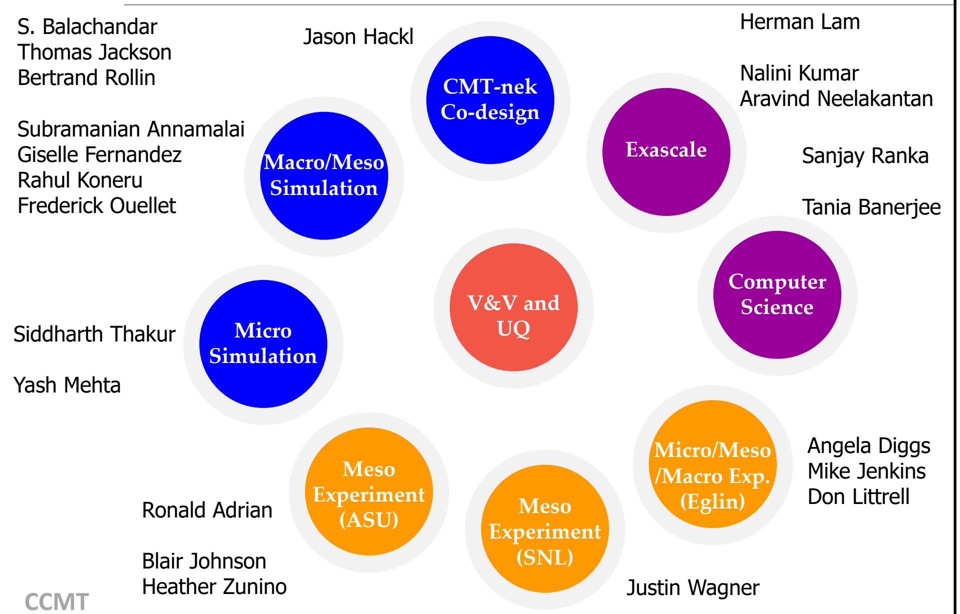
2

Collaborations



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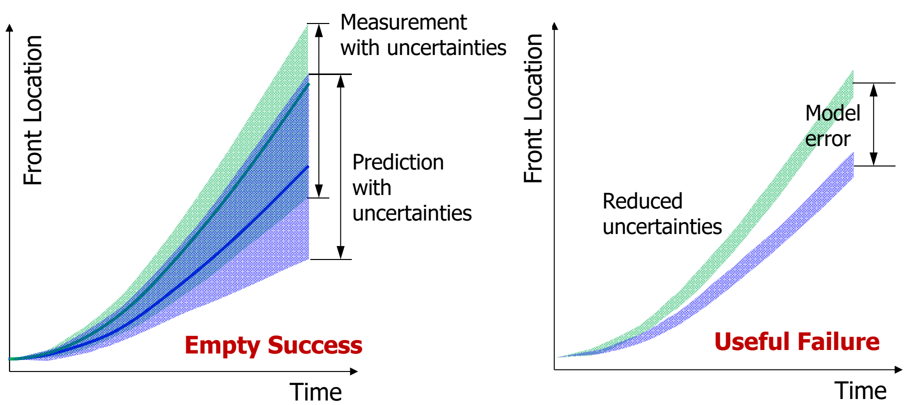
3

Objective and Approach

- In order to **validate** the prediction capability of the demonstration problem
  - Establish appropriate UQ and **uncertainty reduction (UR)** frameworks



- Empty validation success and useful validation failure

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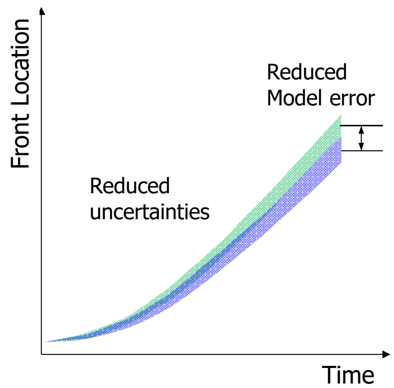
4

Objective and Approach

- In order to validate the prediction capability of the demonstration problem
  - Establish appropriate UQ and **uncertainty reduction (UR)** frameworks



- Multiple physical and numerical models contribute model error
- Calculate error reduction potentials of models for **identifying** important physical and numerical models to support **error reduction (ER)**

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Accomplishments and Collaborations

- **Model error estimation**: Estimated model error of 1D/2D mesoscale simulation with uncertainty
- **Uncertainty budget**: Quantified the contributions of uncertainty sources to the uncertainty in the mesoscale model error estimate
- **Reducing uncertainty in model error**: Modeled gap effect with 2D mesoscale simulation to reduce uncertainty due to inconsistency in 1D
- **Identifying error** in 1D simulation with AUSM+
- Revisit UQ of past experiments and influence plan for future experiments
- Additional collaborations
  - Comparison between CMT-bone, CMT-bone-BE and BE emulation
  - Modeling JWL-EOS surrogate for efficient computing

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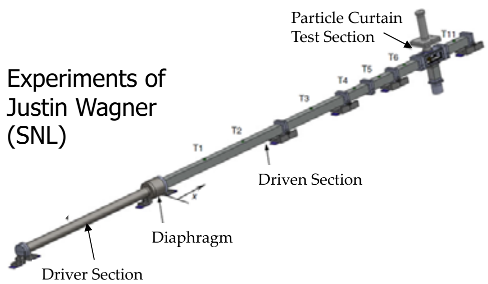
Mesoscale Validation, UQ and UB

- **Goals**
  - Validating the particle force models and numerical models regarding solving multiphase shock problem
  - Estimating the errors and uncertainties in the physics models through 1D/2D/3D simulations
  - Quantifying the contributions of uncertainty sources on the uncertainty in the estimated errors for **uncertainty reduction**
  - Prioritizing/identifying physical/numerical models to be improved for **error reduction**

Experiments of Justin Wagner (SNL)



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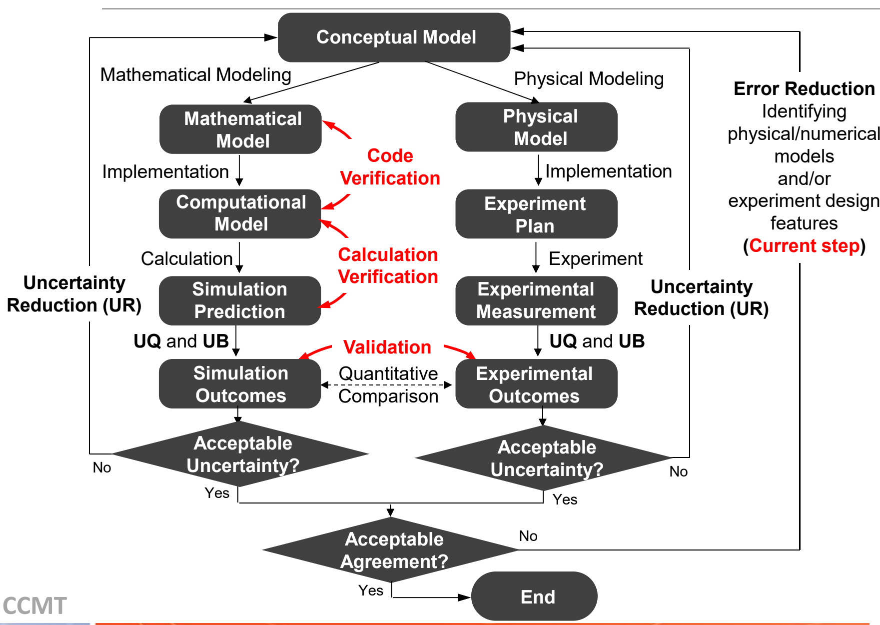
7

V&V, UQ, UR and ER Progress Flowchart



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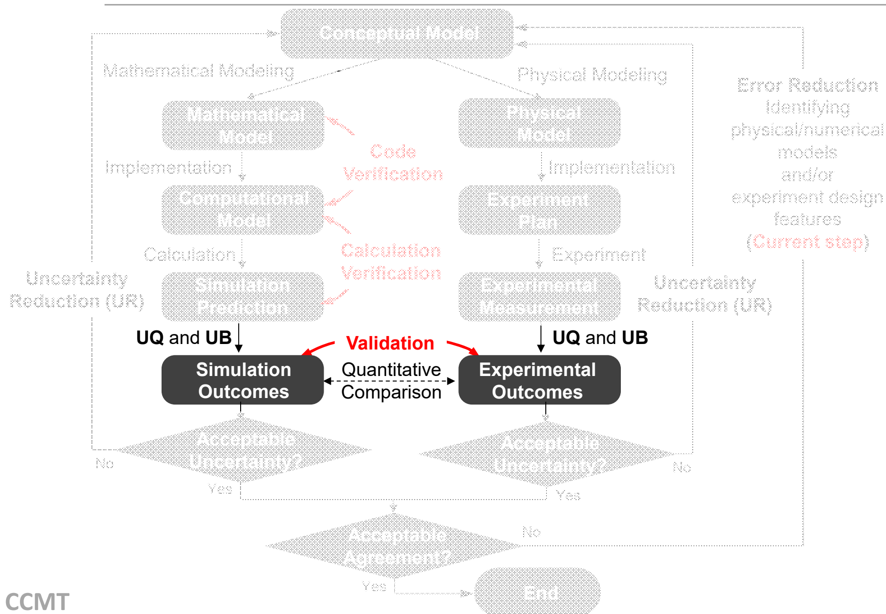
8

UQ and UB (First Iteration)



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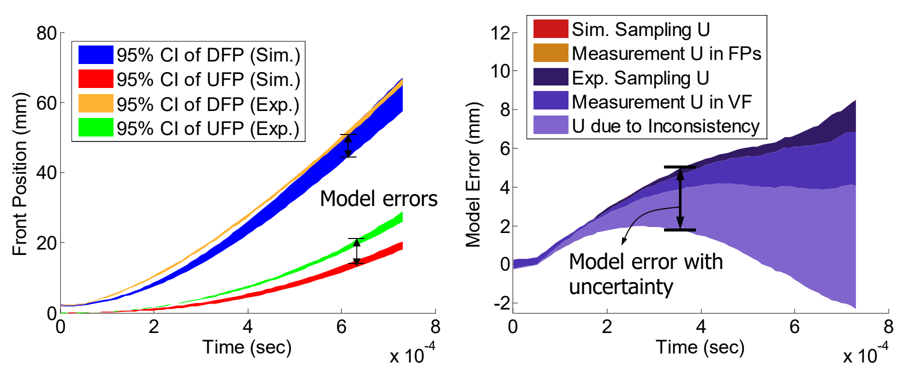
9

Highlights of UQ and UB Results of 1D Sim.



- UQ revealed large uncertainty in the model error estimate
- UB revealed inconsistency between 1D simulation and experiment is the most influential source of uncertainty
- Next step is **uncertainty reduction** and **model error reduction**
- Definition of uncertainty and error presented in the following slides

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10

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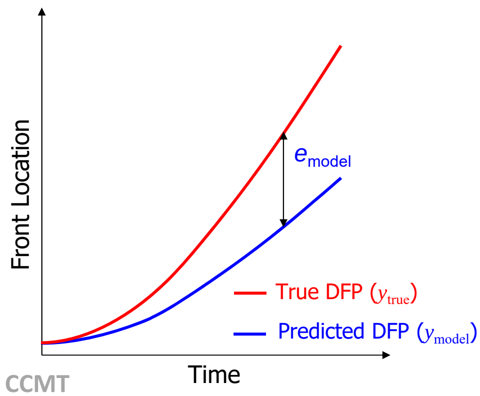
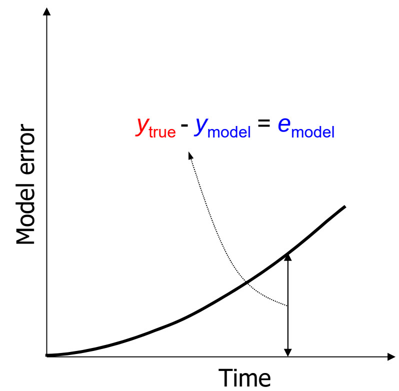
Model Error

- To assess the fidelity of a simulation, model error needs to be estimated
- It is defined as the difference between the true response and the prediction of the simulation





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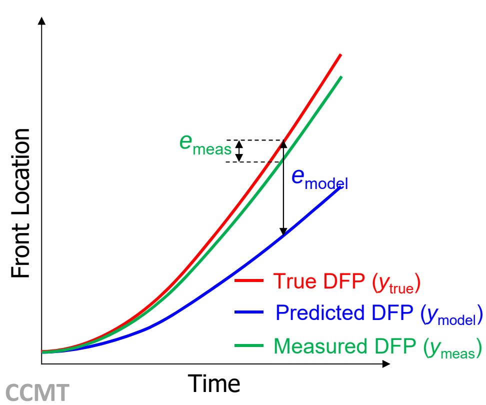
Measurement Error in Model Error Estimate

- We can compare prediction to measurement (not true response)
- Difference between prediction and measurement includes measurement error



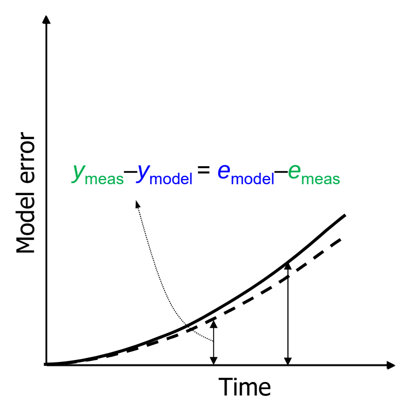


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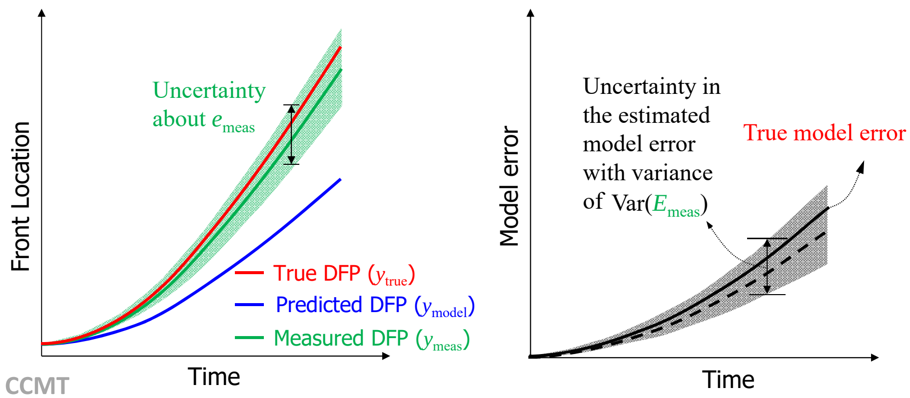
Illustration of Uncertainty in Model Error Est.

- Measurement error is uncertain, and it is modeled as a random variable E_{meas}
- When measurement error is the only source of uncertainty, the variance of the model error estimate is the variance of E_{meas}
- Note that this is an **illustration** not associated with actual results



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13

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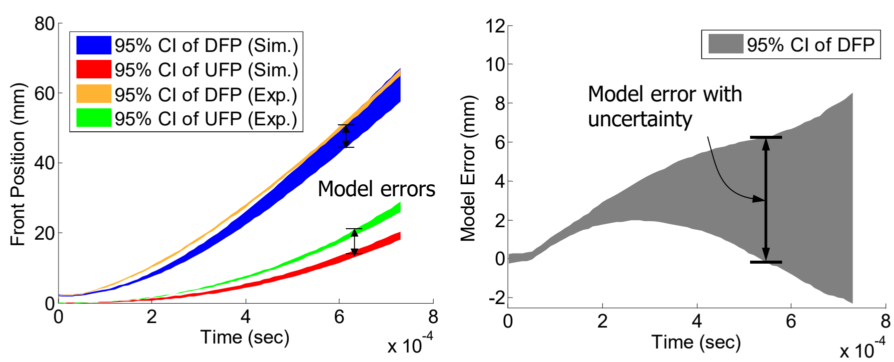
UQ of the 1D Model Error Estimation



- The large uncertainty in the DFP model error estimation makes the estimate less informative (empty success)
- Uncertainty reduction plan was implemented to make the estimate informative (useful failure)

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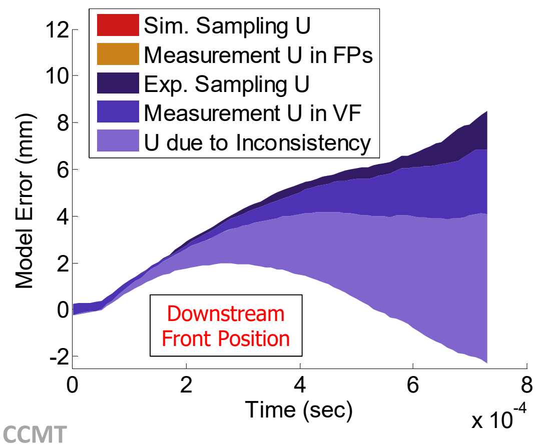
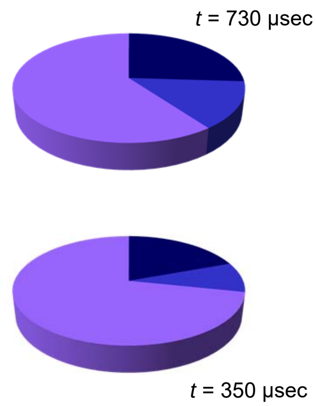
14

UB: Quantifying Sources of U in Error (1D)

- Uncertainty in the model error estimate was decomposed by source using sensitivity index
- Uncertainty due to inconsistency in gap effect is the biggest uncertainty source of 1D prediction





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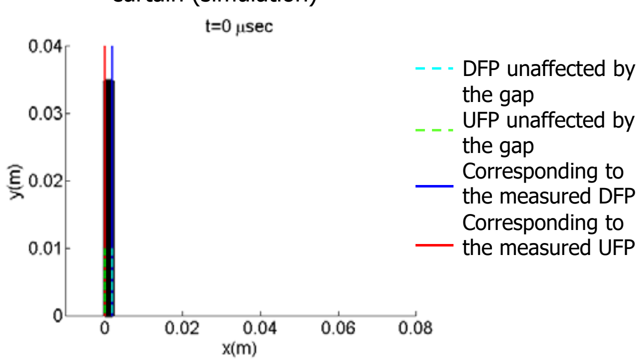
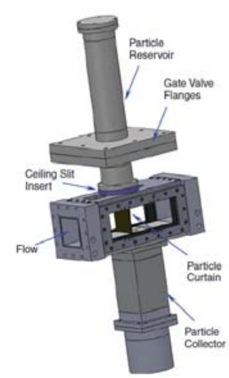
Uncertainty due to Inconsistency in Gap Effect

Top view of the particle curtain (simulation)





- The particle curtain movement is captured through the side window
- Predicted DFP of 1D simulation does not correspond the measured DFP from the experiments

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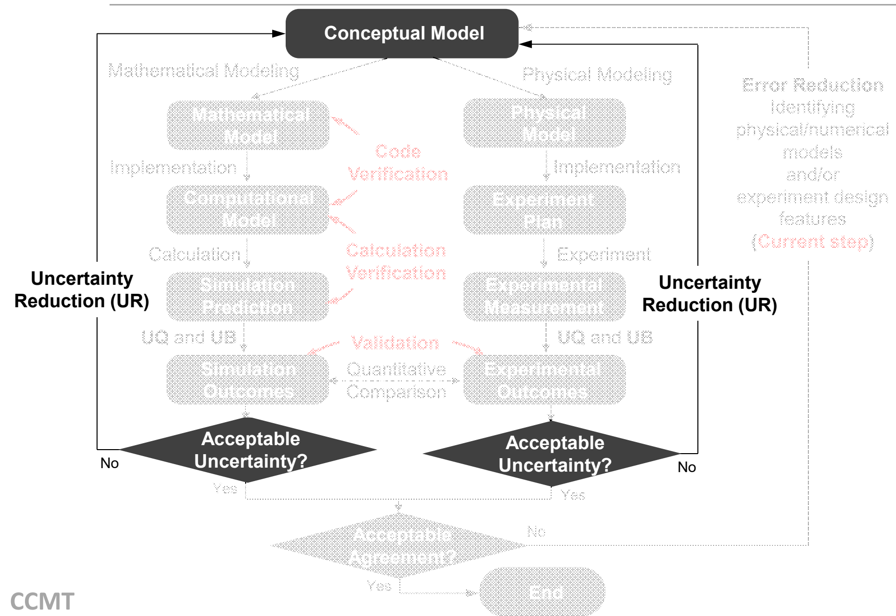
Uncertainty Reduction (First Iteration)



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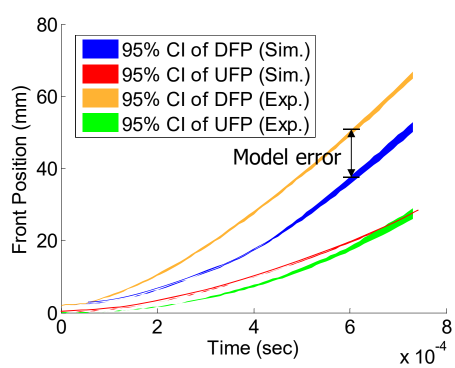
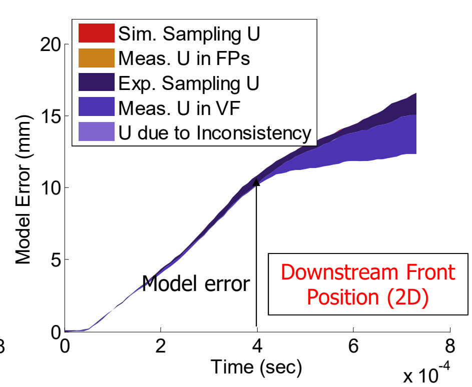
17

UQ and UB of 2D Model Error Estimation

- Predicted DFP of 2D simulation corresponds the measured DFP
- The uncertainty reduction in the model error estimate reveals the large model error





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18

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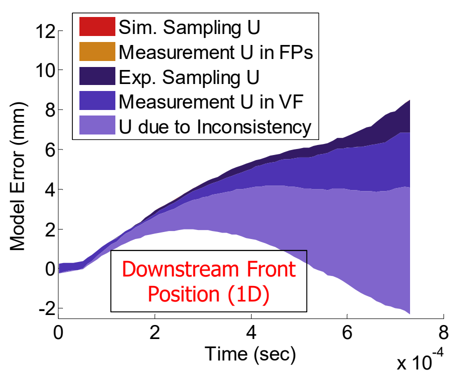
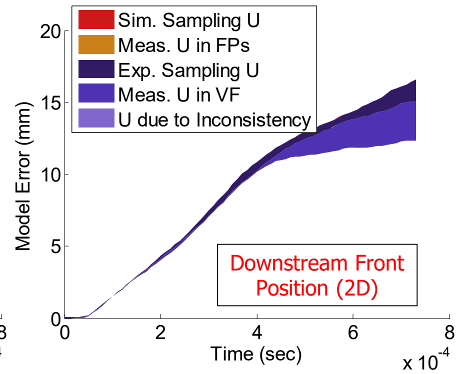
Uncertainty Reduction (1D to 2D)

- 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 error reduction** is needed to improve predictability





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19

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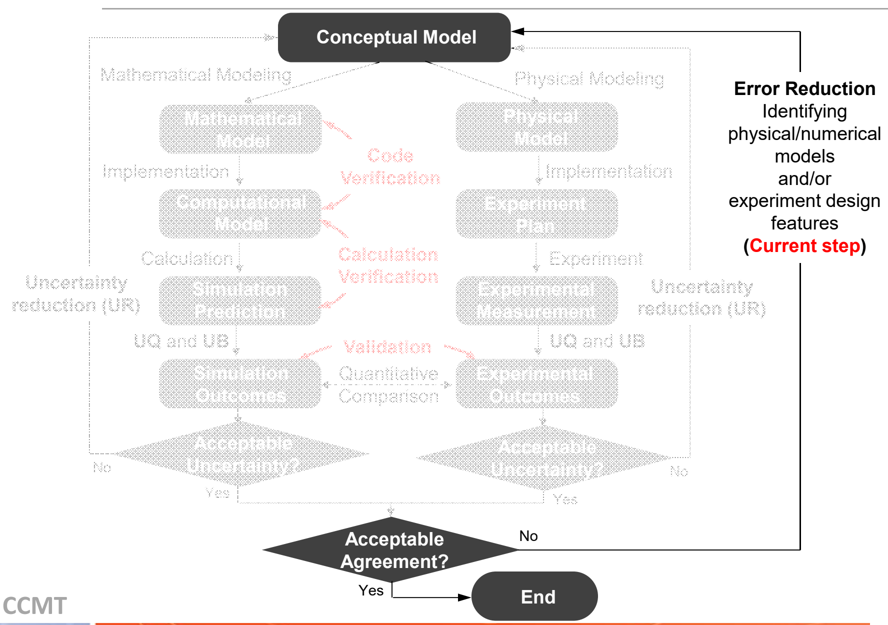
Error Reduction (First Iteration)



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20

Which Models Should be Targeted?

- Errors in the particle force models
  - Prioritizing the particle force models by sensitivity study of particle front positions
- Error in the initial particle volume fraction characterization
  - Studying the effect of initial volume fraction profile

Particle Force Model Errors

- Total force on a particle is the sum of forces

$$F_{\text{calc}} = F_{\text{QS,calc}} + F_{\text{PG,calc}} + F_{\text{AM,calc}} + F_{\text{UV,calc}} + F_{\text{IP,calc}}$$

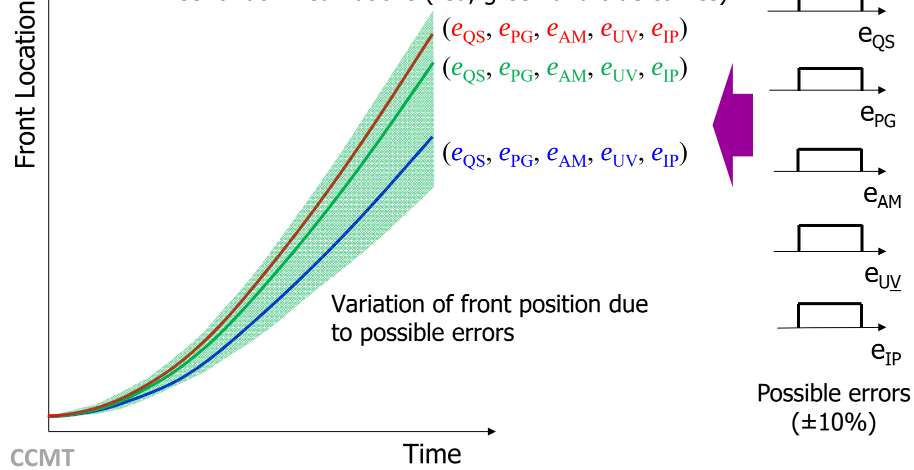
- In terms of unknown errors in force terms, true particle force is

$$F_{\text{true}} = (1\text{-}e_{\text{QS}})F_{\text{QS,calc}} + (1\text{-}e_{\text{PG}})F_{\text{PG,calc}} + (1\text{-}e_{\text{AM}})F_{\text{AM,calc}} + (1\text{-}e_{\text{UV}})F_{\text{UV,calc}} + (1\text{-}e_{\text{IP}})F_{\text{IP,calc}}$$

- Errors are unknown but their ranges can be estimated based on previous experience
- The variation of the front position due to the error ranges shows total **error reduction potential**

Total Error Reduction Potential

- Calculate front positions for randomly generated errors (red, green, blue)
- Variation of front position due to possible errors is obtained to repeat the process
- Three random realizations (red, green and blue curves)



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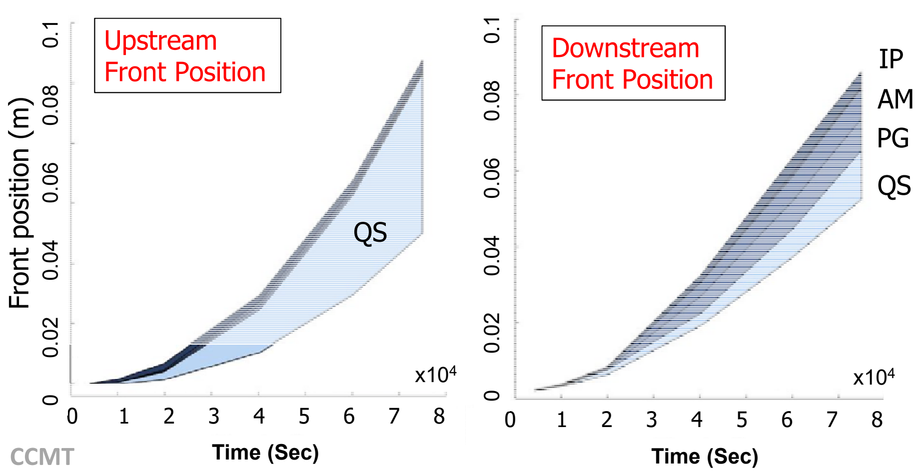
Error Reduction Potentials of Force Models

- Global sensitivity analysis (GSA) quantifies **error reduction potentials** of individual models
- GSA shows chances of large change of front position when one force model is improved



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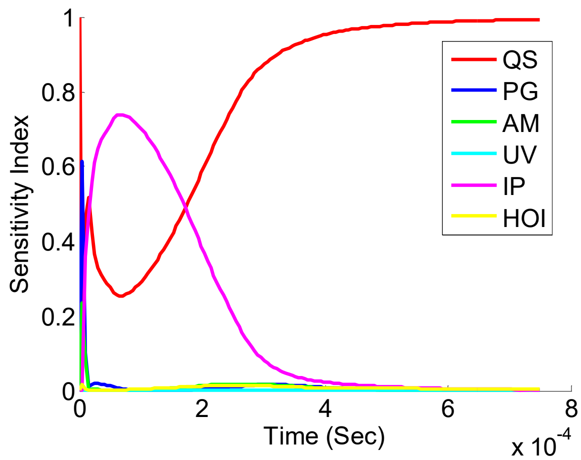
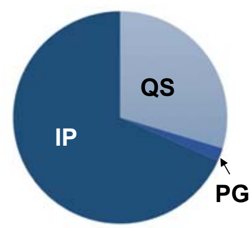
GSA of Upstream Front Position



t=750μs Uncertainty Contribution

t=40μs Uncertainty Contribution



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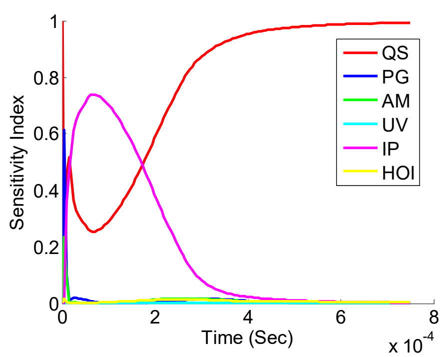
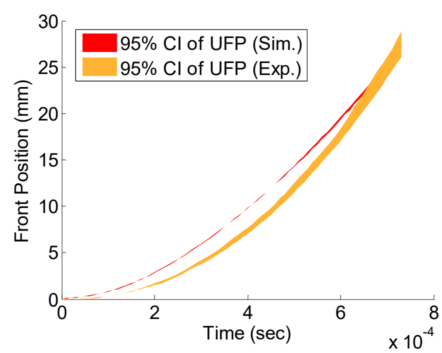
25

GSA of Upstream Front Position





- Error in quasi-steady force likely dominates error at later time
- Effect of inter-particle force decreases as shock develops
- Coupling between errors is negligible

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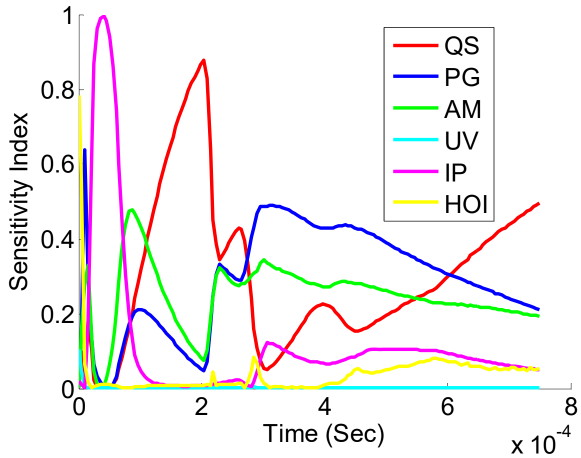
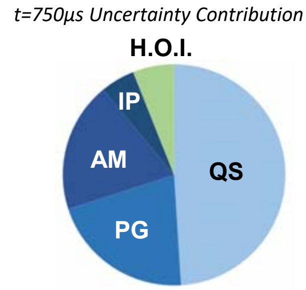
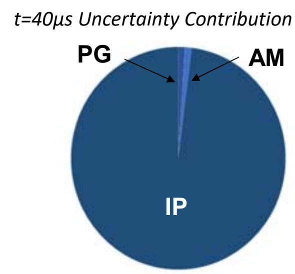
GSA of Downstream Front Position







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27

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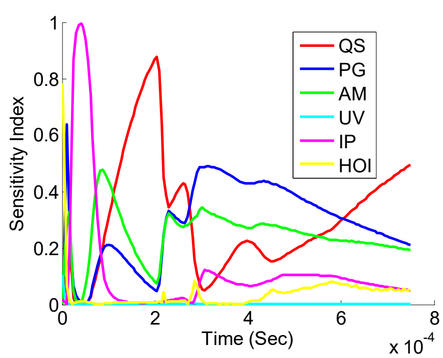
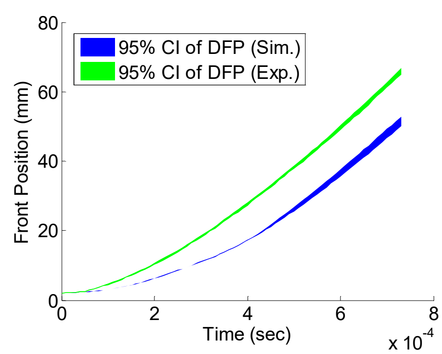
GSA of Downstream Front Position





- Dominant forces change with time
- Inter-particle force is dominant at the very early stage for DFP
- The coupling effect between errors is small

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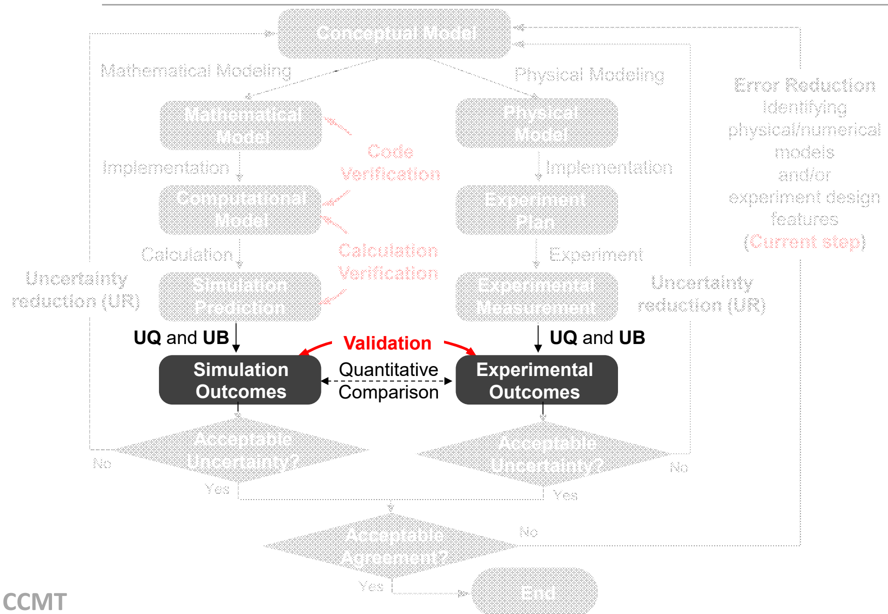
28

Refining UQ and UB (Second Iteration)



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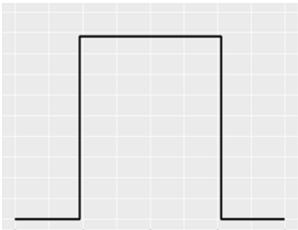
29

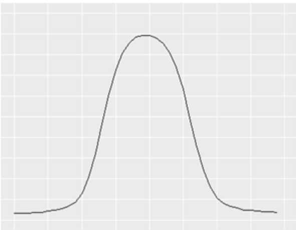
Inconsistency in Initial Volume Fraction Model

- Distribution has to be extracted through image processing
  - X-ray radiography is used for extracting distribution
  - Curtain thickness is extracted from Schlieren images
  - Originally, tophat distribution with curtain thickness from Schlieren and maximum volume fraction from X-ray was used

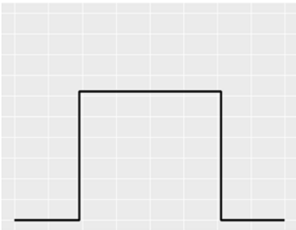
Tophat Distribution with 2 mm width and 21% VF (original model: **inconsistent** shape and **inconsistent** particle mass)



VF Distribution according to X-ray images (**measured distribution**)



Tophat Distribution with 2 mm width and 16% VF (**inconsistent** shape and **consistent** particle mass)



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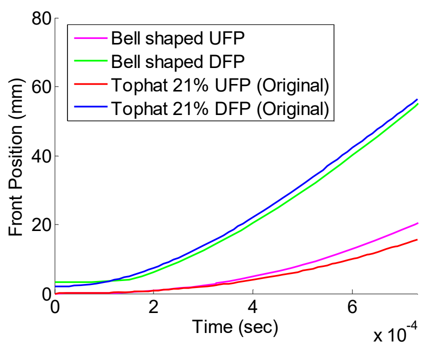
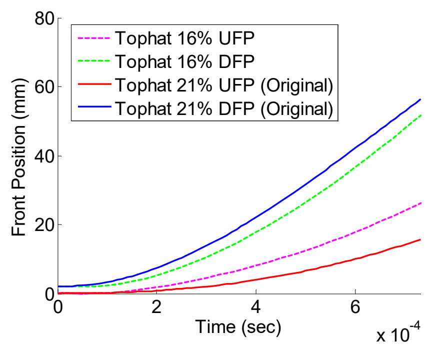
30

Initial Study of the Effect of Initial VF Distr.

- Front positions from the current initial volume fraction model are compared to those from two new distributions
- The effect of initial volume fraction distribution model is not negligible
- Bell shape initial volume fraction model will be used for mesoscale simulations





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31

Processing Data from SNL Experiments

- Schlieren Image processing
  - To extract particle curtain front positions from high-speed schlieren images
- X-ray Image processing
  - To estimate particle volume fraction from radiographs produced by X-ray setup
- **Goal:** Revisit the Schlieren images and X-ray radiographs of the shock tube experiments for rigorous uncertainty quantification of the measurements from the images

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32

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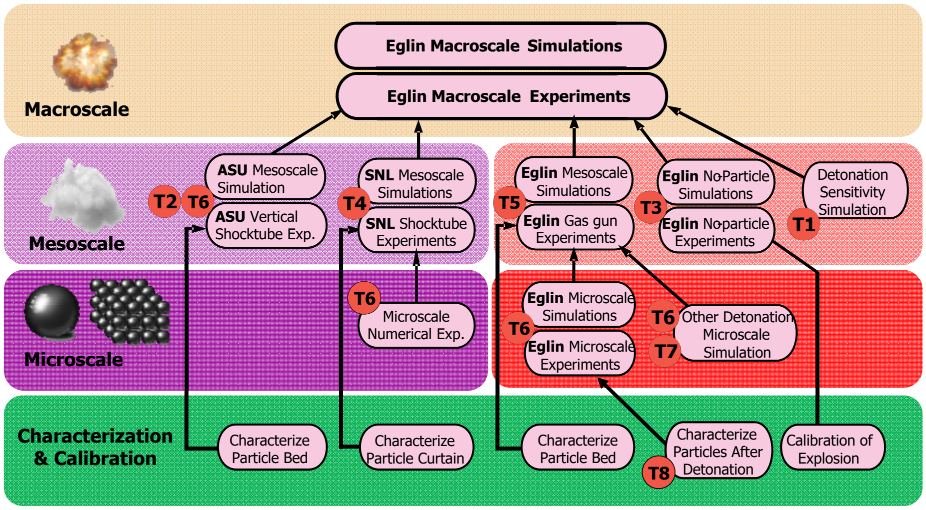
Planned Simulations/Experiments

- Model validation for each scale based on UQ, **uncertainty reduction** and **error reduction** through model improvement



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33

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Influencing Macroscale Eglin Experiment Plan

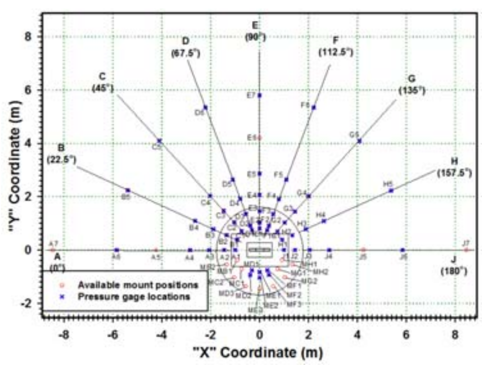

Figure. Locations of 54 pressure transducers (Barreto et al. 2015).

- Instrumentation:
  - 54 pressures probes
  - Momentum traps
  - Three high speed video cameras
  - Possibly linear optical transducers
- Six shots proposed
  - 2 bare charges
  - 1 charge w/tungsten (**notched**)
  - 1 charge w/steel (**notched**)
  - 2 charges w/steel (**un-notched**)

Figure. Picture of charge suspended before a test (Barreto et al. 2015)

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34

Reducing Inconsistency due to Casing

- Experimental planning for reducing **inconsistency** between simulation and experiment concerning casing
- 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
  - No casing separating explosive and particles
  - Notches will be introduced to the casing to attempt to control the failure

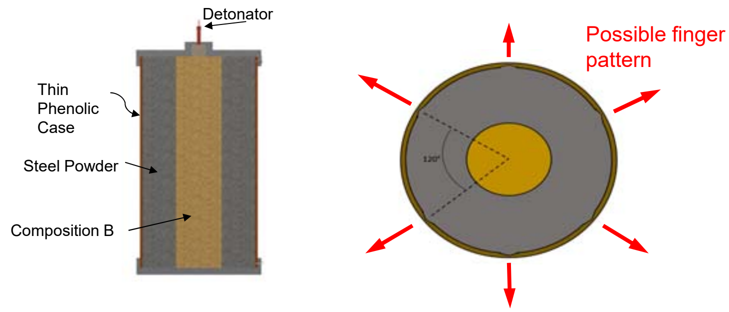

Figure. Schematic of charge cross sections to show attempts to minimize casing influence.

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UQ of Particles

- Reported size range: 75-125 μm
- Size distribution will be obtained with the use of a particle sizer
- SEM images of particles show particles are mostly spherical with some nodular departures

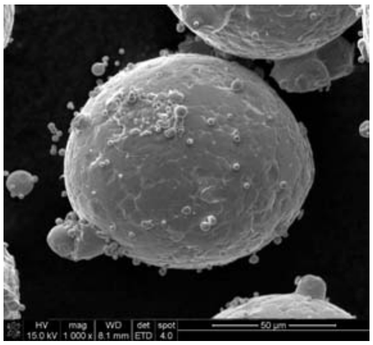

Figure. SEM of single steel particle at 1000x zoom.

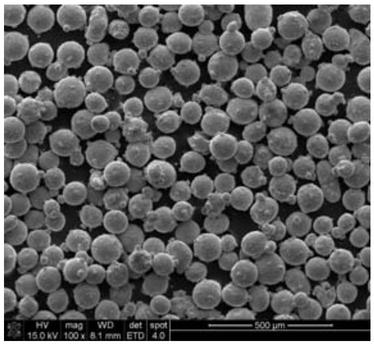

Figure. SEM of several steel particles at 100x zoom.

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Approximating Expensive Simulations

- **Multi-fidelity surrogate**: Approximating an expansive high fidelity simulation behavior by combining a few expensive high fidelity samples and many cheap low fidelity samples
- Studying the benefit of applying Bayesian framework for building a multi-fidelity surrogate
- Finding a simple multi-fidelity surrogate framework equivalent to Bayesian framework
- This technique is used for the collaboration with the **exascale team** to approximate the CMT-bone with CMT-bone-BE and BE emulation
- Will be applied for parametric study and UQ of **heroruns**

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37

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Summary

- Carrying out validation, UQ, UR and ER of the 1D/2D mesoscale simulations
- Modeling gap using 2D simulation is recommended for **reducing uncertainty due to inconsistency**
- GSA indicates quasi steady force model has the highest **model error reduction potential** in terms of the front position
- The influence of inconsistency in original volume fraction model is not ignorable
- Presented the V&V, UQ and UB flowchart
- Planning future experiments and simulations are being influenced by revisiting experience of mesoscale shocktube simulation validation and UQ
- Carrying out a study on Multi-fidelity surrogate for BE emulation development and UQ and parametric study of hero runs

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38

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Do you have any questions?

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Backup Slides

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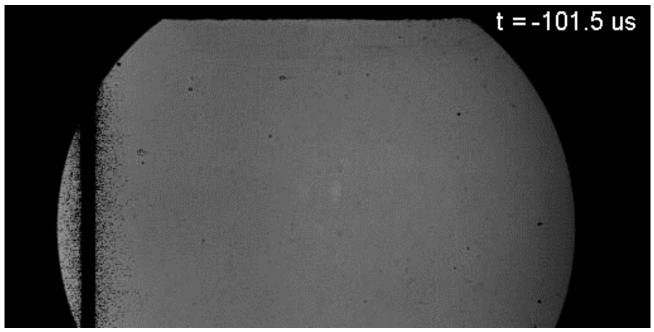
Experimental Schlieren Data

- Replicated post-processing method as described in (Ling et al.) to identify particle front locations from experimental schlieren images.
  - Individual post-processing of each of the four experimental runs allow for variability analysis for front locations throughout the duration of the shock-curtain interaction.



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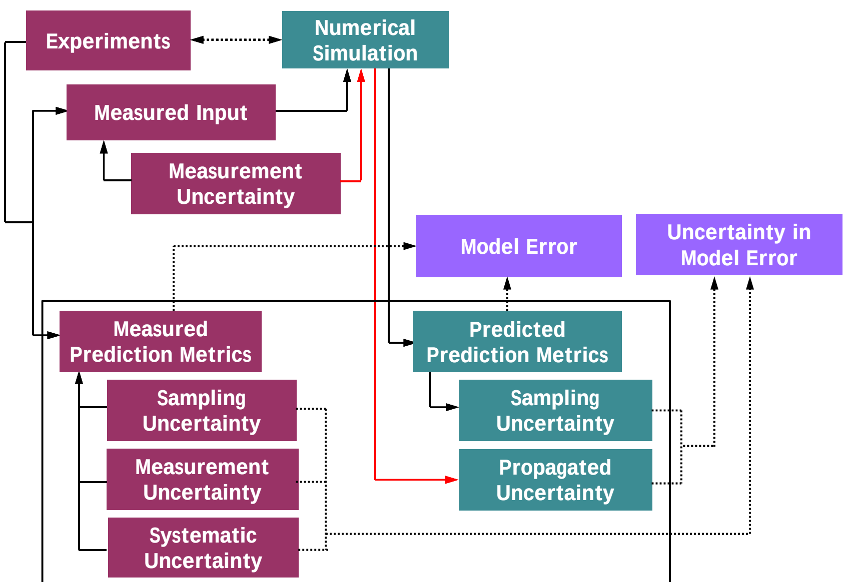
41

Validation and UQ Framework



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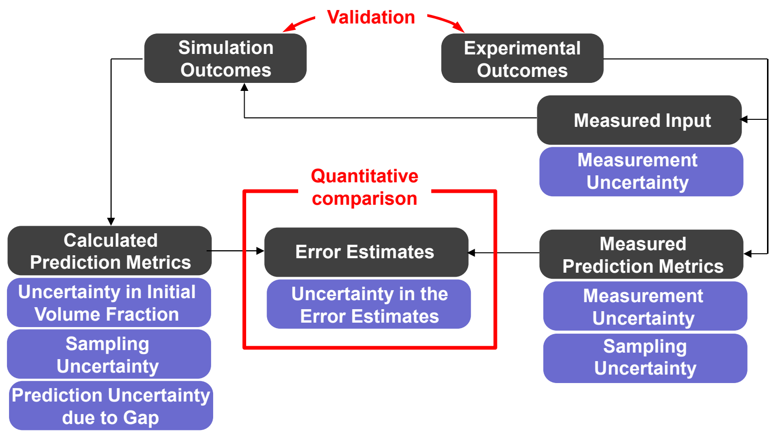
42

Validation and UQ Framework Reassessing



- Validation and UQ plan is implemented using this framework for validation and UQ of the simulations of the Eglin experiments (Kyle Hughes)

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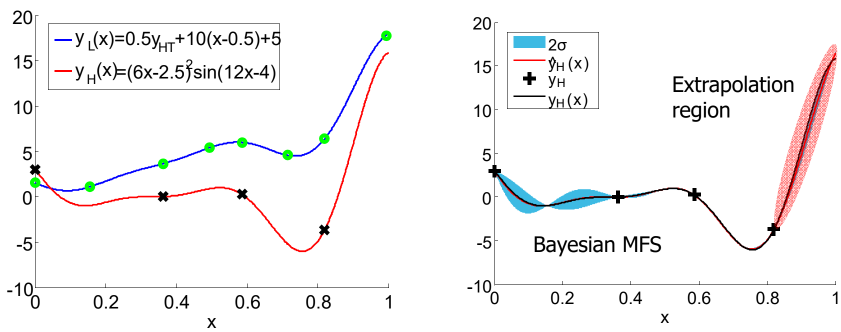
43

Approximating Expensive Simulations



- **Multi-fidelity surrogate:** Predicting an expansive high fidelity model behavior by combining a few expensive high fidelity behavior samples and many cheap low fidelity samples
- This technique is used for the collaboration with the **exascale team** to approximate the CMT-bone
- Will be applied for parametric study and UQ of heroruns

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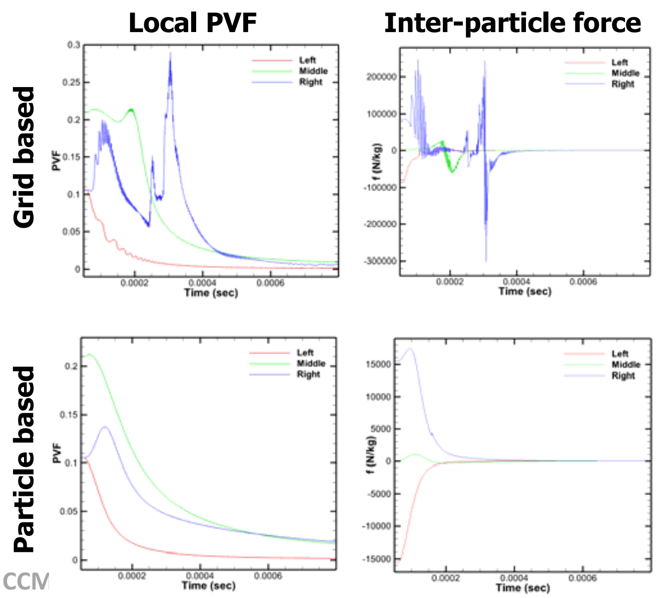
Noise Reduction



- Noise in calculated volume fraction was found in middle particles of 1D simulation
- Particle based volume fraction calculation method was implemented
- Effect of the improvement is being studied

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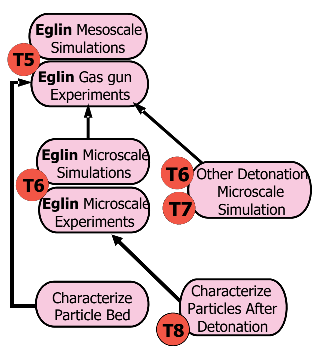
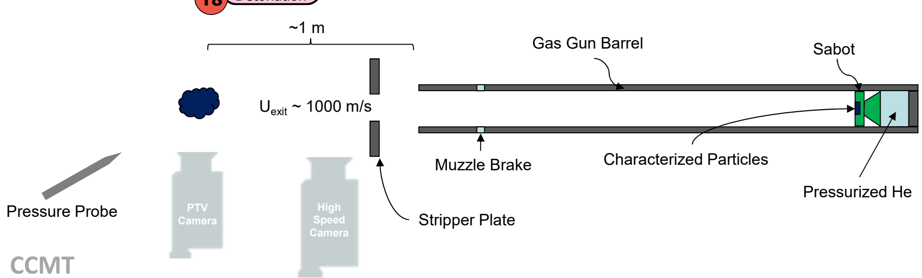
Influence of Simulations on Experiments



- **Motivation:** Instabilities (fingers) observed from the macroscale experiments are currently not well understood
- **Goal:** Identify underlying physics cause the instabilities arise in high speed dispersal of particles without detonation
- Factors that may influence the instabilities:
  - Inhomogeneous volume fraction
  - Wetted vs. dry
  - Particle geometry, etc.



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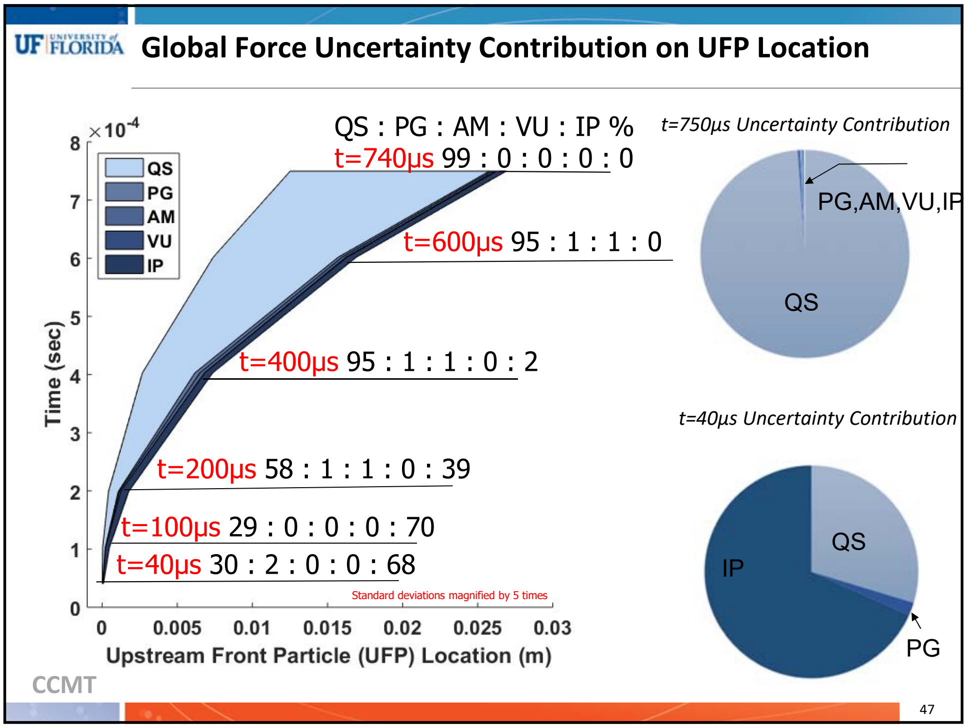
46


Global Force Uncertainty Contribution on UFP Location
QS : PG : AM : VU : IP %
t=740µs 99 : 0 : 0 : 0 : 0
t=600µs 95 : 1 : 1 : 0
t=400µs 95 : 1 : 1 : 0 : 2
t=200µs 58 : 1 : 1 : 0 : 39
t=100µs 29 : 0 : 0 : 0 : 70
t=40µs 30 : 2 : 0 : 0 : 68
Standard deviations magnified by 5 times
QS
PG
AM
VU
IP
×10-4
Time (sec)
Upstream Front Particle (UFP) Location (m)
t=750µs Uncertainty Contribution
PG,AM,VU,IP
QS
t=40µs Uncertainty Contribution
QS
IP
PG
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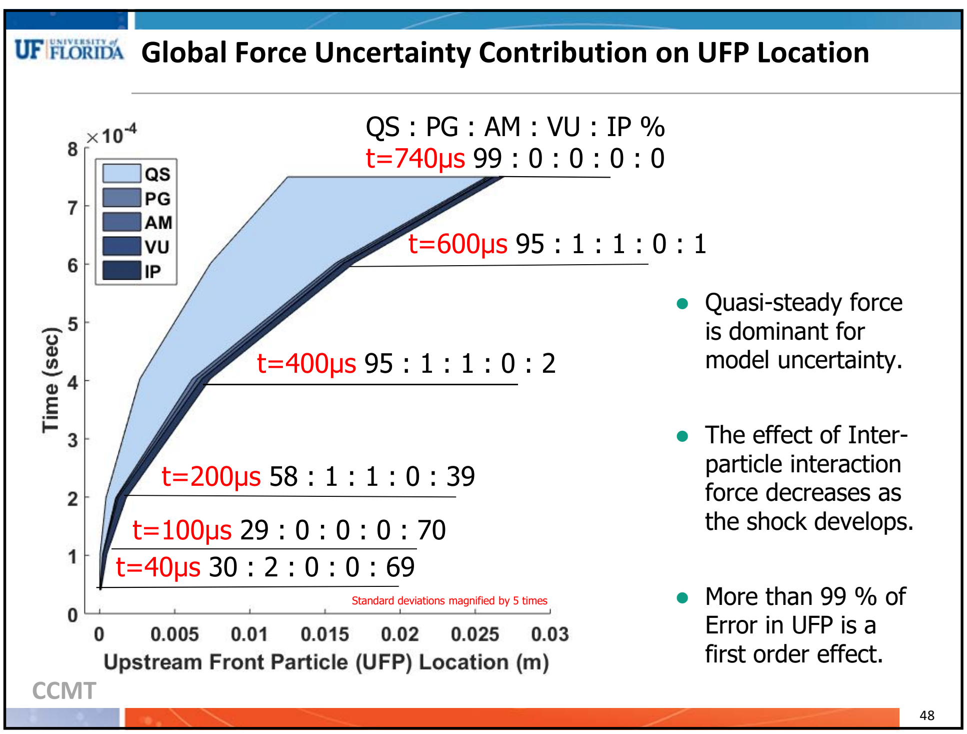
47


Global Force Uncertainty Contribution on UFP Location
QS : PG : AM : VU : IP %
t=740µs 99 : 0 : 0 : 0 : 0
t=600µs 95 : 1 : 1 : 0 : 1
t=400µs 95 : 1 : 1 : 0 : 2
t=200µs 58 : 1 : 1 : 0 : 39
t=100µs 29 : 0 : 0 : 0 : 70
t=40µs 30 : 2 : 0 : 0 : 69
Standard deviations magnified by 5 times
QS
PG
AM
VU
IP
×10-4
Time (sec)
Upstream Front Particle (UFP) Location (m)
Quasi-steady force is dominant for model uncertainty.
The effect of Inter-particle interaction force decreases as the shock develops.
More than 99 % of Error in UFP is a first order effect.
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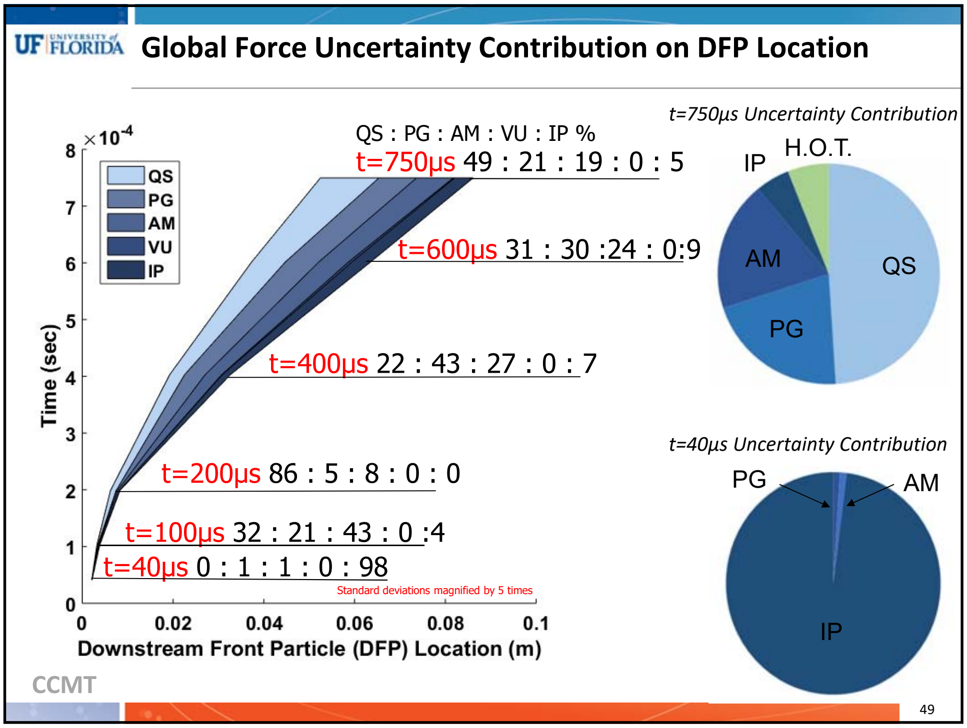
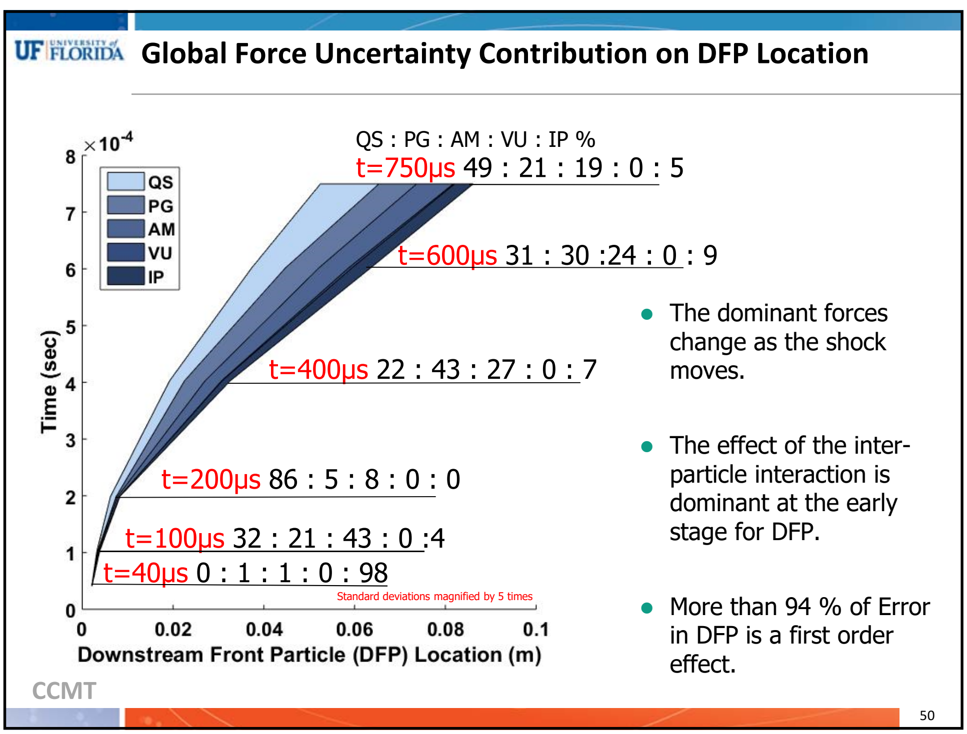
48


UF FLORIDA
Global Force Uncertainty Contribution on DFP Location
QS : PG : AM : VU : IP %
t=750μs 49 : 21 : 19 : 0 : 5
t=600μs 31 : 30 :24 : 0:9
t=400μs 22 : 43 : 27 : 0 : 7
t=200μs 86 : 5 : 8 : 0 : 0
t=100μs 32 : 21 : 43 : 0 :4
t=40μs 0 : 1 : 1 : 0 : 98
Standard deviations magnified by 5 times
QS
PG
AM
VU
IP
×10-4
Time (sec)
Downstream Front Particle (DFP) Location (m)
t=750μs Uncertainty Contribution
H.O.T.
IP
AM
QS
PG
t=40μs Uncertainty Contribution
PG
AM
IP
CCMT
49


UF FLORIDA
Global Force Uncertainty Contribution on DFP Location
QS : PG : AM : VU : IP %
t=750μs 49 : 21 : 19 : 0 : 5
t=600μs 31 : 30 :24 : 0 : 9
t=400μs 22 : 43 : 27 : 0 : 7
t=200μs 86 : 5 : 8 : 0 : 0
t=100μs 32 : 21 : 43 : 0 :4
t=40μs 0 : 1 : 1 : 0 : 98
Standard deviations magnified by 5 times
QS
PG
AM
VU
IP
×10-4
Time (sec)
Downstream Front Particle (DFP) Location (m)
The dominant forces change as the shock moves.
The effect of the inter-particle interaction is dominant at the early stage for DFP.
More than 94 % of Error in DFP is a first order effect.
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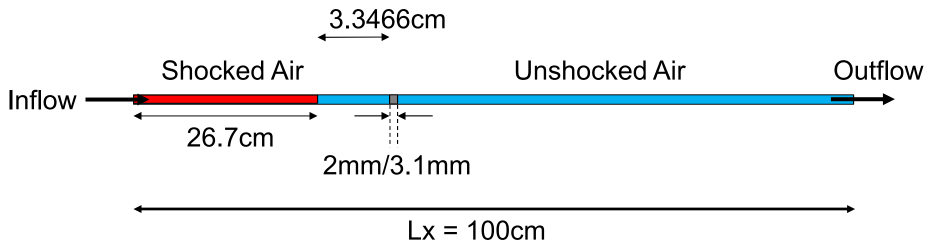
1D Shock Tube Simulations

Not to scale



Description	Value
Start time	5e-5 sec
Final time	80e-5 sec
CFL number	0.8
Time step	1e-7

1D

Numerics: AUSM+up, RK4

Gravity Acceleration: 0

Interpolation Method:
Piece Linear

Special disc. Order: 2

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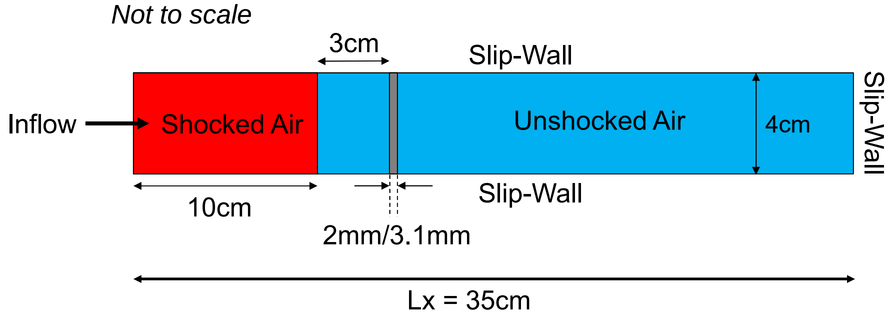
51

2D Shock Tube Simulations

Not to scale



Description	Value
Start time	0 sec
Final time	85e-5 sec
CFL number	1
Initial time step	5e-8

2D

Numerics: AUSM+up, RK3

Gravity Acceleration: 0

Interpolation Method:
Linear

Special disc. Order: 2

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52

Shock Tube Simulations

Air	2D	1D
R ($J.kg^{-1}k^{-1}$)	287	287
c_p ($J.kg^{-1}k^{-1}$)	1004.64	N/A
γ	1.4	1.4
Pr	0.72	0.72

Nitrogen	2D	1D
R ($J.kg^{-1}k^{-1}$)	-	296.8
c_p ($J.kg^{-1}k^{-1}$)	-	N/A
γ	-	1.4
Pr	-	0.69

Shocked Air	2D	1D
Pressure (Pa)	252086	942780
Density ($kg.m^{-3}$)	2.0725	10.7168
Temperature (K)	423.8	296.4
Velocity of air ($m.s^{-1}$)	268.72	268.72
Shock Mach number	1.66	1.66

Unshocked Air		
Pressure (Pa)	82700	82700
Density ($kg.m^{-3}$)	0.972	0.972
Temperature (K)	296.4	296.4

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53

Shocktube Simulations

Particle Related Inputs	2D	1D
Particle Diameter (μm)	115	115
Particle Density ($kg.m^{-3}$)	2500	2520
Particle Initial Temperature (K)	293.15	N/A
Particle Initial Velocity ($m.s^{-1}$)	0.0	0.0
Curtain size	4cm x 2mm x 125μm*	2 mm
Cell size	125x125x125 μm^3	100 μm
Initial volume fraction	19%-23% uniform	19%-23% uniform
# cells in the curtain	5,120	20
# particles used in simulation	600,000	2,000
# computational particles per cell initially	117	100
Super Particle Loading for 20%	4.2E-3	2.65E+5

*Rocflu was initially developed for 3D

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54

Particle Force Model

1D

- Point particle
- Two-way gas particle coupling + inter-particle force
- Inter-particle interaction: Harris and Crighton Model
  - Ps = 2e5 beta = 3 Packed PVF = 0.6

2D

- Point particle
- Two-way gas particle coupling + inter-particle force
- Inter-particle interaction: Harris and Crighton Model
  - Ps = 2e5 beta = 3 Packed PVF = 0.6

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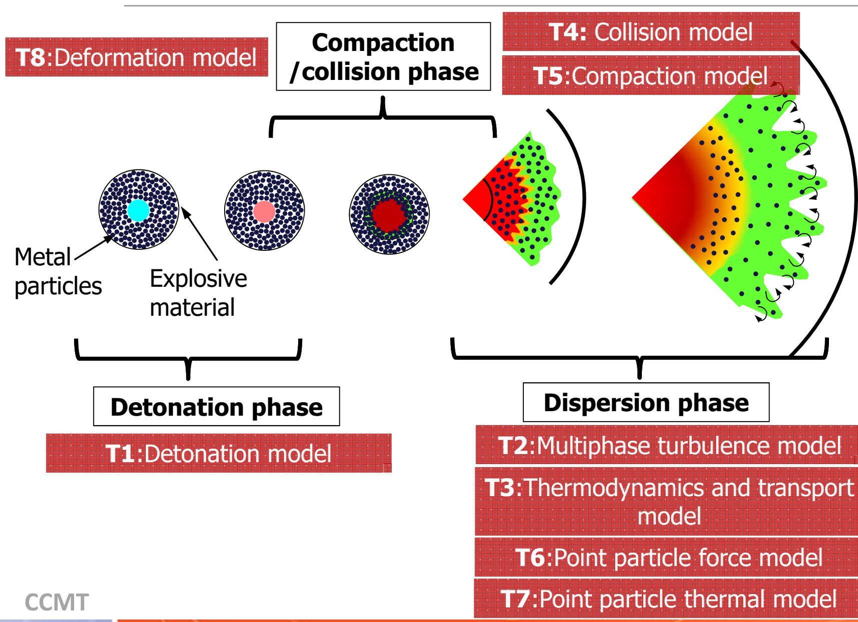
Sequence of Events and Physics Models



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Computer Science

Sanjay Ranka

Computer and Information Science and Engineering

University of Florida

CCMT

Members

Keke Zhai

Mohamed Gadou

Sankeerth Reddy Mogili

Tania Banerjee

Sanjay Ranka

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2

Talk Overview

- CMT-nek
  - Overview
  - CMT-bone validation
- Multi-objective optimization on Hybrid Multiprocessor
  - Multicore Node – Single GPU (similar to Titan)
  - Multicore Node – Multiple GPU
  - KNL
  - DVFS
- Dynamic Load Balancing Framework
  - Colocation of particles with spectral elements
  - Mapping
  - Remapping
- Thermal aware optimization
  - Thermal Setup
  - Static and Dynamic Load Balancing
- Conclusions

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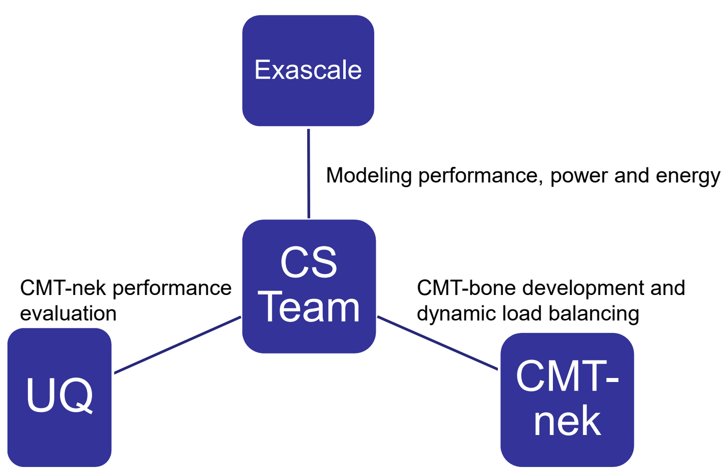
3

Team Interactions



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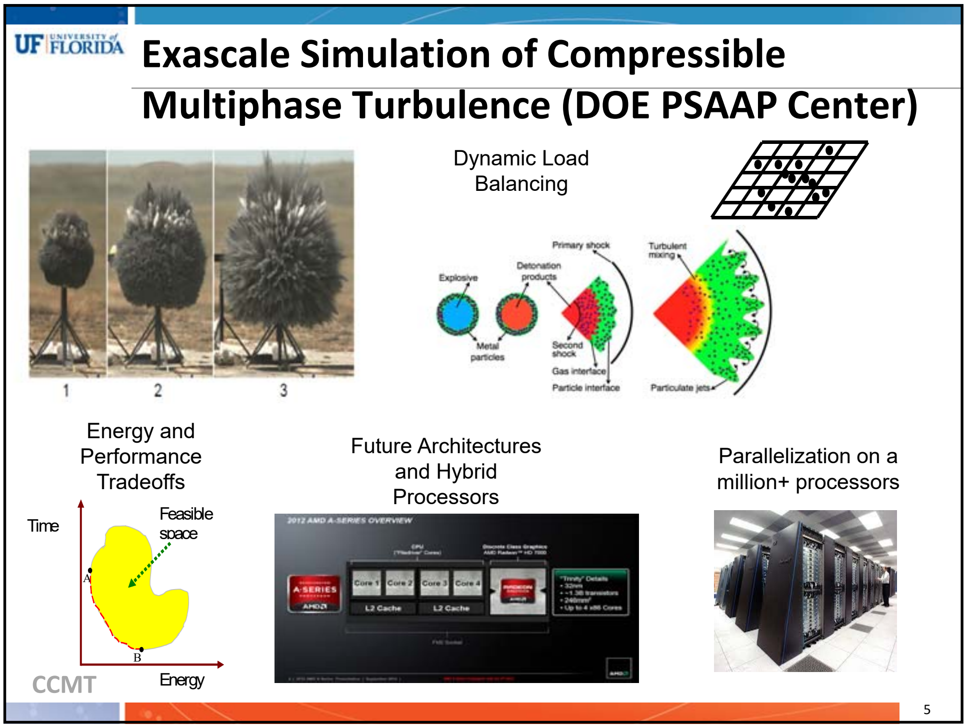
4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Exascale Simulation of Compressible Multiphase Turbulence (DOE PSAAP Center)
1
2
3
Dynamic Load Balancing
Explosive
Metal particles
Detonation products
Primary shock
Second shock
Gas interface
Particle interface
Turbulent mixing
Particulate jets
Energy and Performance Tradeoffs
Time
Feasible space
A
B
Energy
Future Architectures and Hybrid Processors
Core 1
Core 2
Core 3
Core 4
L2 Cache
L2 Cache
Parallelization on a million+ processors
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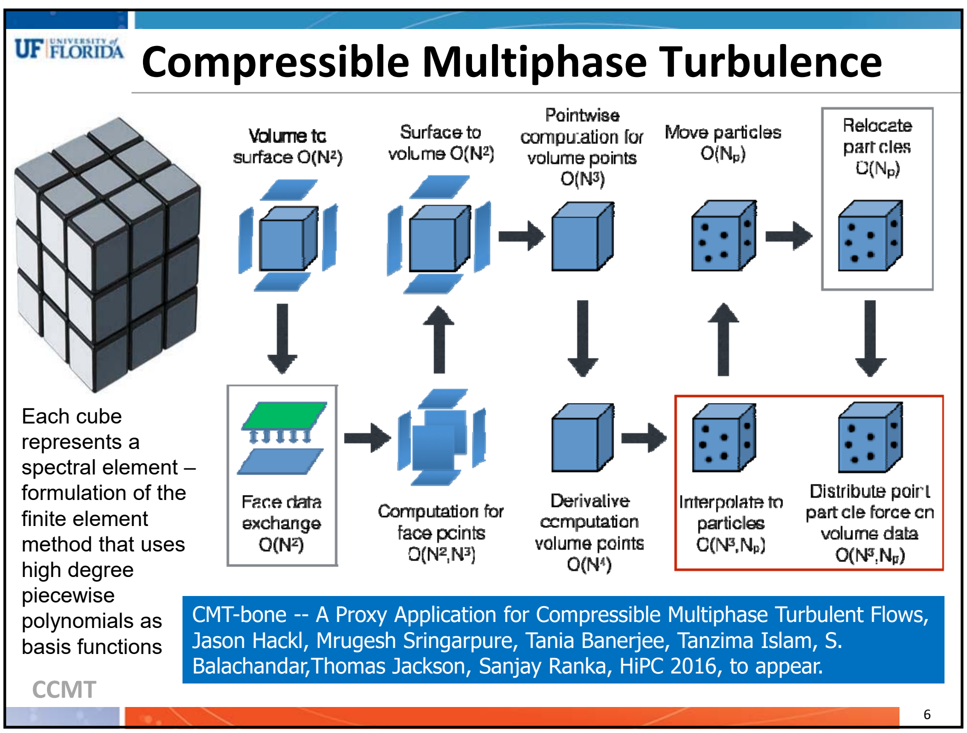
5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Compressible Multiphase Turbulence
Volume to surface O(N²)
Surface to volume O(N²)
Pointwise computation for volume points O(N³)
Move particles O(Np)
Relocate particles O(Np)
Face data exchange O(N²)
Computation for face points O(N²,N³)
Derivative computation volume points O(N⁴)
Interpolate to particles O(N³,Np)
Distribute point particle force on volume data O(N³,Np)
Each cube represents a spectral element – formulation of the finite element method that uses high degree piecewise polynomials as basis functions
CMT-bone -- A Proxy Application for Compressible Multiphase Turbulent Flows, Jason Hackl, Mrugesh Sringarpure, Tania Banerjee, Tanzima Islam, S. Balachandar,Thomas Jackson, Sanjay Ranka, HiPC 2016, to appear.
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Validation of CMT-nek versus CMT-bone

- Four important regions of code were validated separately:
  - Compute intensive section
  - Communication intensive section
  - Point computations
  - Particle processing
- Resources:
- Processors: Varied between 1 though 16 cores (on a single node)

RESOURCE GROUPS FOR INTEL XEON

Resource Group	Intel Xeon
Floating point unit	FP
Branch unit	BR
Prefetch events	PREFETCH
L1 cache	L1
L2 cache	L2
Last level L3 cache	L3
Translation look aside buffer	TLB
Memory	MEM
Remote socket traffic	OFFCORE
PCI express bus	PCIE

WORKLOADS USED IN OUR EXPERIMENTS

Number of Elements	Workload Id	Polynomial Order
512	1	5
	2	7
	3	9
	4	11
	5	13
	6	15
1000	7	5
	8	7
	9	9
	10	11
	11	13
	12	15

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7

Validation of CMT-nek versus CMT-bone

- VERITAS (LLNL)
- A two step process is used for validation
  - Identifies resource utilization of CMT-nek impacting scalability
  - Identifies which of these resource utilization behavior is covered by CMT-bone and how well.
- Tunable Parameters
  - κ determines sparsity of the underlying models
    - Higher κ implies more resources will be included in the model
    - If efficiency loss is explainable using a small set of resources, then a high value of κ can be used to identify higher order bottleneck
  - τ determines model complexity
    - Higher τ implies more PAPI metrics for a resource will be considered in the model
  - Example: κ = 15 and τ = 10 for the compute step

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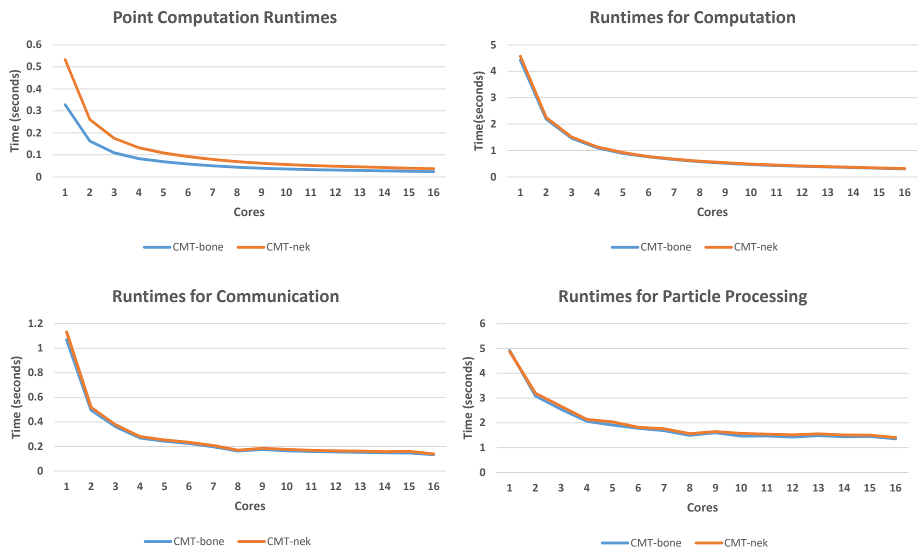
Runtimes



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9

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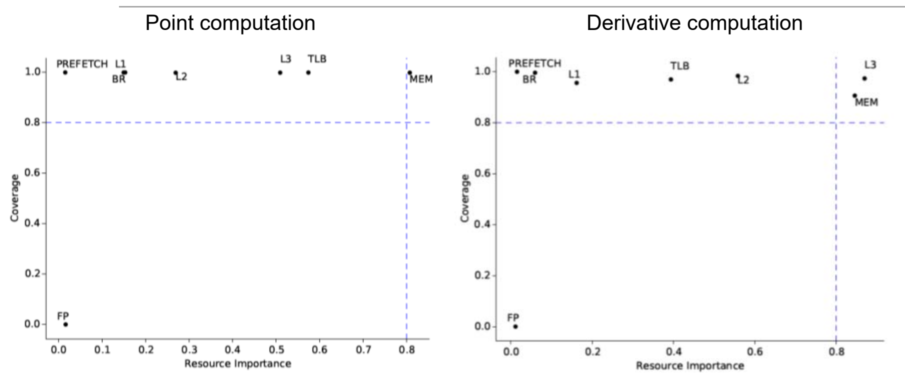
Validation: Computation



- Resource Importance (Higher Values show the resources that are most important in determining performance)
- Coverage = Closeness of CMT-Bone performance vis-à-vis CMT-nek
- Blue lines are thresholds for important resources and good coverage

CMT-bone is a good representation of CMT-nek for computations

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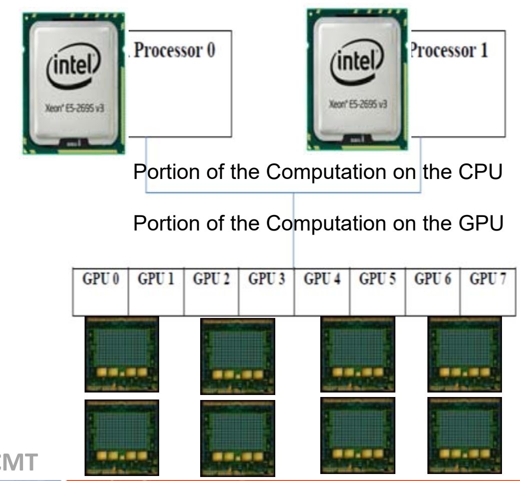
10

Exploring Architectures: System with Multiple GPUs/CPUs

Real Machine – representative of future node architecture



CPU Attribute	Description
Manufacturer	*Intel*
Model	*Xeon™ E5-2695 v2*
Frequency (GHz)	*2.4*
Number of Processors(sockets)	*2*
Number of Cores/Processor(socket)	*12*
Memory(GB)	*768*

GPU Attribute	Description
Manufacturer	*NVIDIA*
Model	*Tesla K40m (Kepler)*
Number of GPUs	*8*
Number of SMs/GPU	*15*
Number of Cores/SM	*192*
Global Memory(GB)	*12*
L2 Cache(KB)	*1536*
Shared Memory/SM (KB)	*48*
L1 cache/SM (KB)	*16*
Number of Registers/SM	*65k*
Peak performance(GFlops)	*1430*

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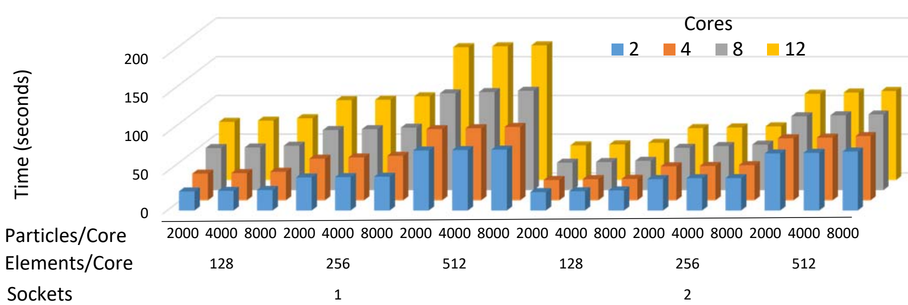
11

CPU Performance



- For a total of 2, 4, 8 and 12 cores distributed over single and dual sockets, the chart shows the time taken to process various problem sizes in terms of number of particles and elements
- When the MPI ranks are distributed on both sockets, processing time improves because each rank gets more shared memory

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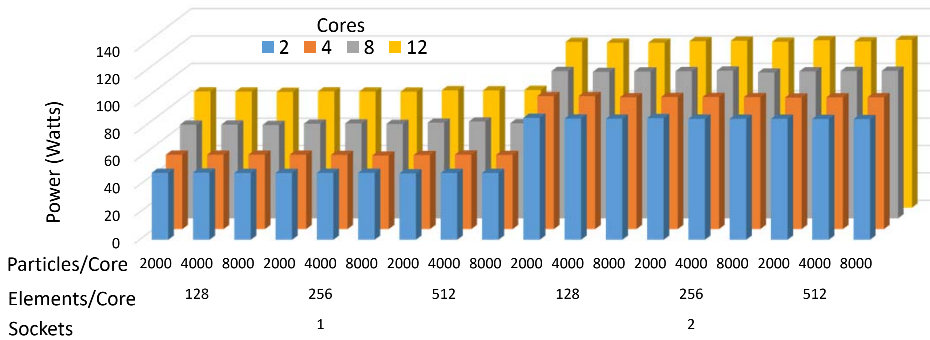
12

CPU Power Consumption



- Power consumption increases approximately twice as both sockets are used
- On the same socket, power consumption depends upon the number of cores used, and in general is not sensitive to application parameters

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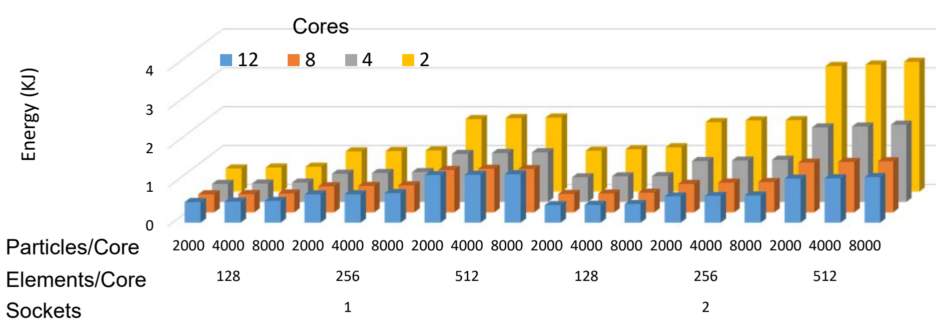
13

CPU Energy Consumption



- CPU energy consumption per core decreases as more cores are used

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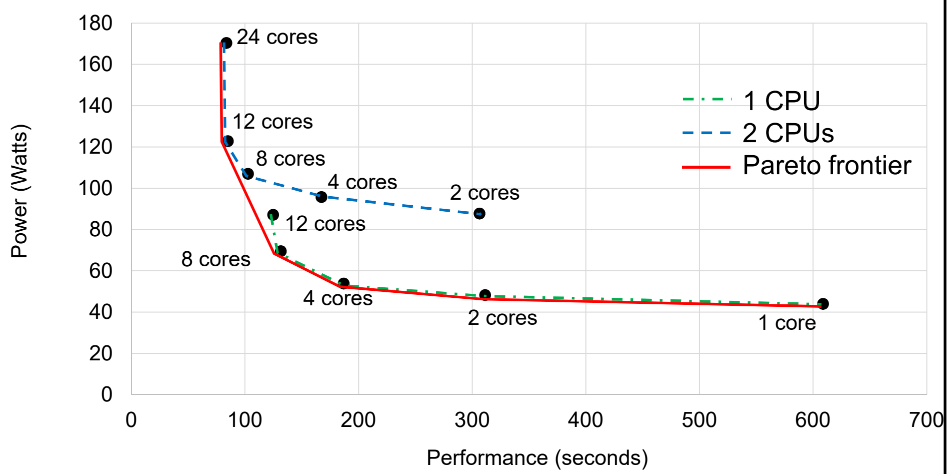
14

CPU Power versus Performance



- CPU power performance tradeoff for processing 4096 elements and 128000 particles
- Useful to operate under a power bound

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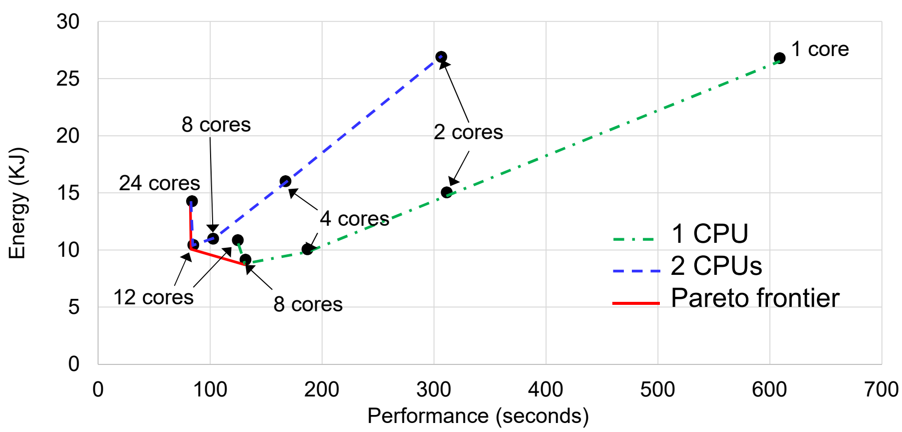
15

CPU Energy versus Performance



- Energy consumption is minimum when 8 cores are used on a single socket
- Best performance is obtained using 12 and 24 cores on dual socket

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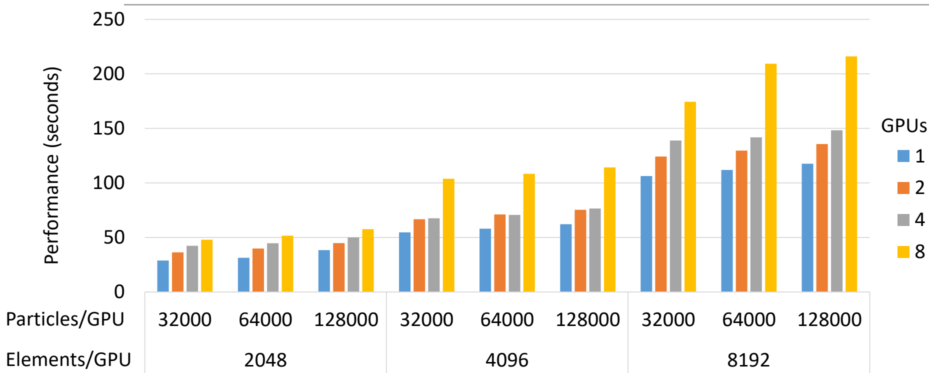
GPU Performance



- Time increases as more GPUs are used due to an increase in communication overhead.

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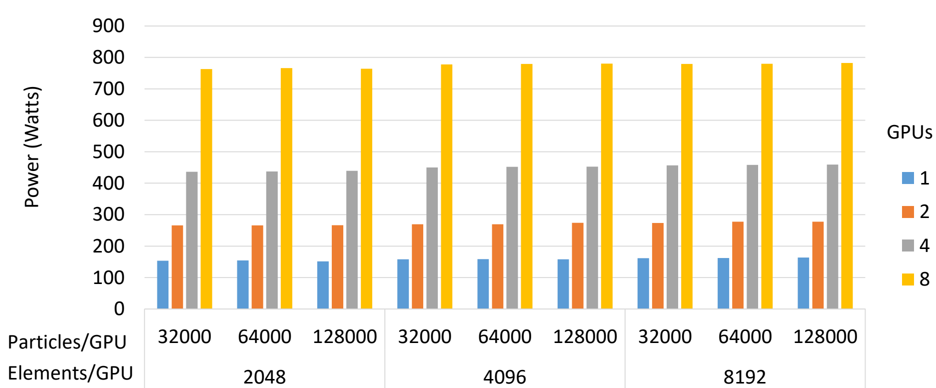
GPU Power Consumption



- GPU power consumption increases proportionally as more GPUs are used

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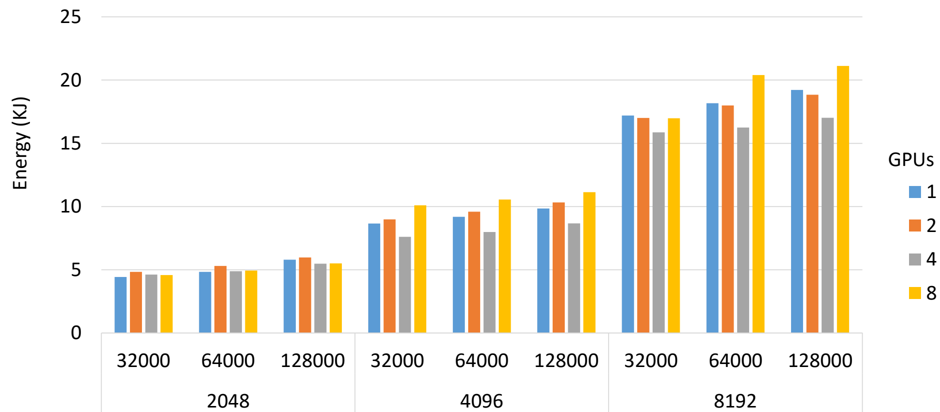
18

GPU Energy Consumption



- Energy consumption

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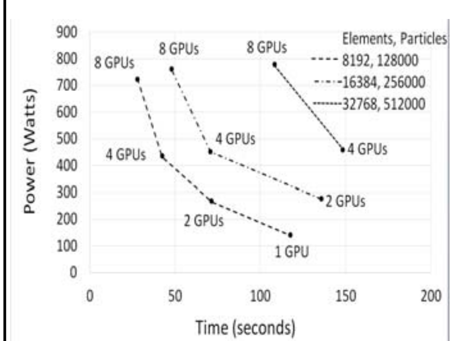
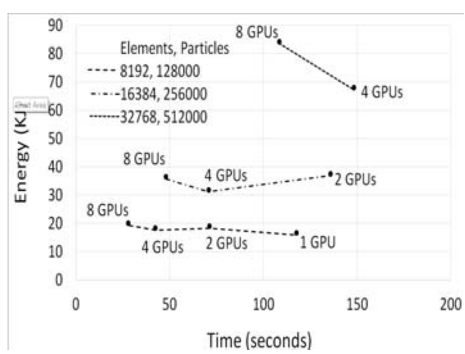
19

GPU Power/Energy versus Performance





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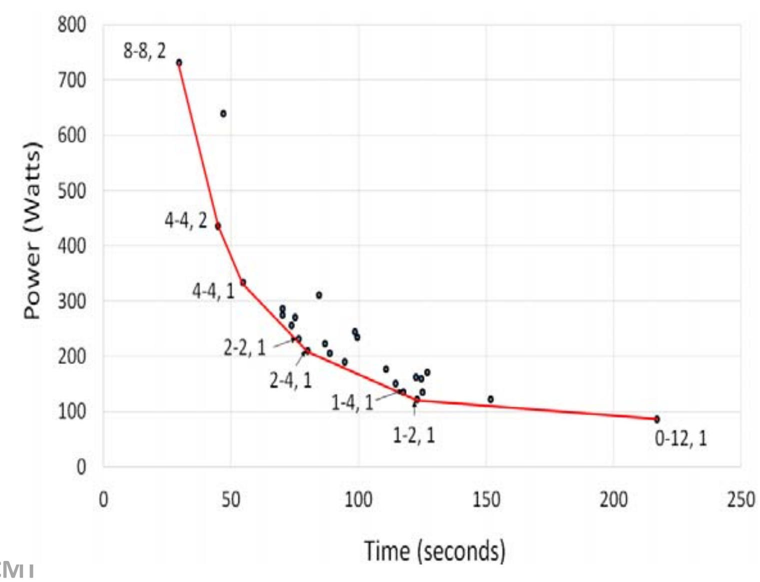
Power versus Performance (Hybrid)



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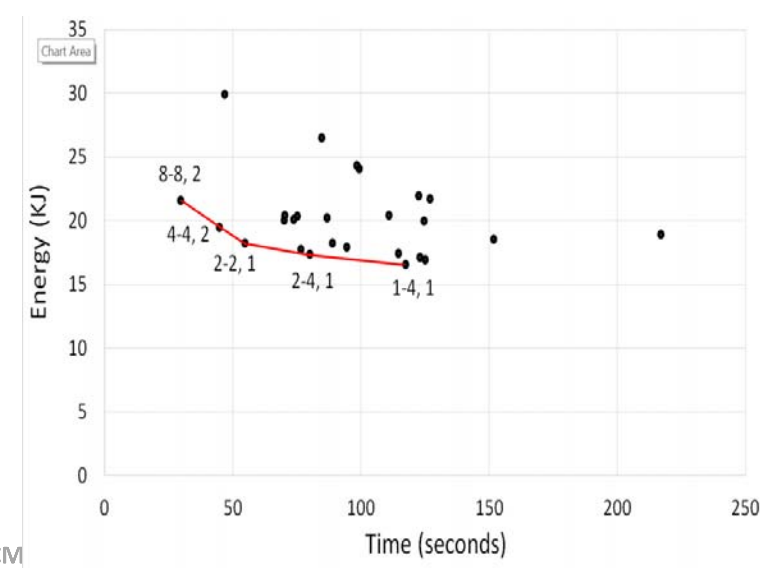
Energy versus Performance (Hybrid)



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22

KNL System Description

Attribute	Description
Chip	2D mesh of 32 Tiles
Cores	2 Cores per Tile, total of 64 Cores on Chip
Node	1 Socket node
Frequency	1.3 GHz
Thermal Design Power	215 Watts
Threads	Hyper threading 4 threads/Core = 256 Threads
Memory(GB)	MCDRAM: 16 in-package DDR4: 384
Transfer rate(GB/s)	MCDRAM: 400+ DDR: 90+
Vector Peak performance	3+ Tflops double precision

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Initial Performance Results

- Globalize usage of OpenMP
- Ensure vectorization is used effectively
- Use MCDRAM – High Bandwidth memory on Intel KNL
- Use Cache tiling to reduce memory access

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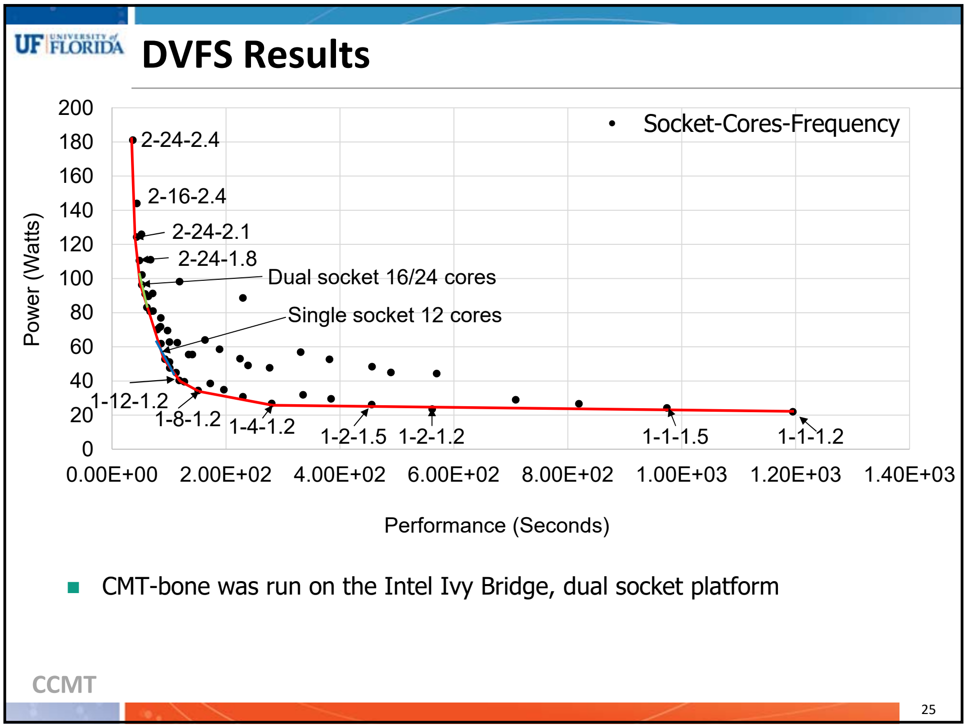
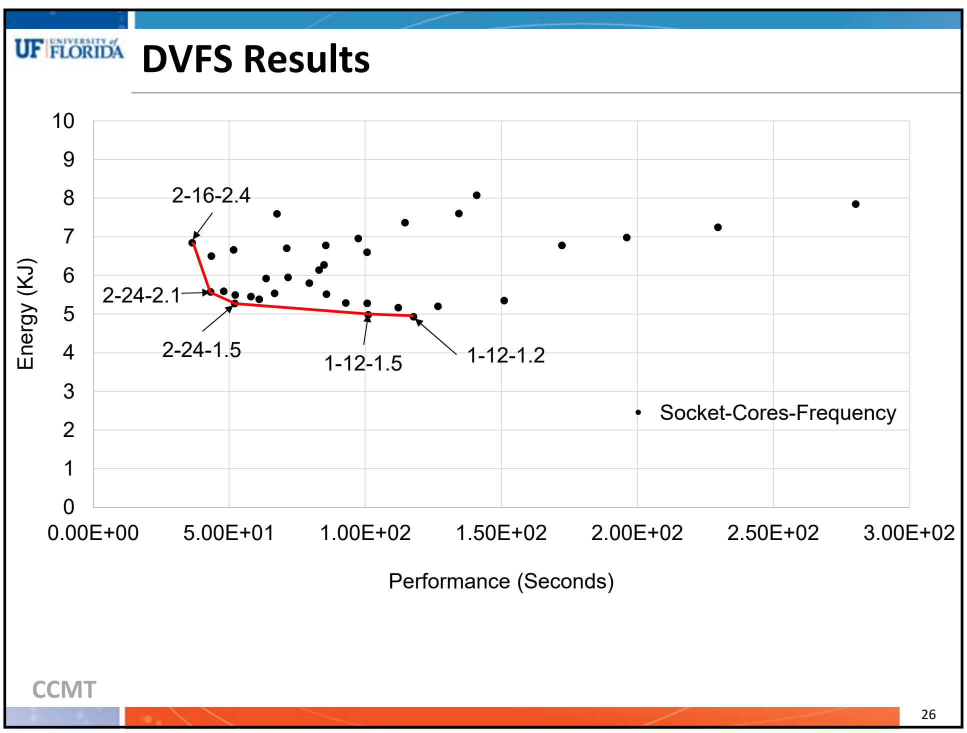

DVFS Results
200
180
160
140
120
100
80
60
40
20
0
Power (Watts)
2-24-2.4
2-16-2.4
2-24-2.1
2-24-1.8
Dual socket 16/24 cores
Single socket 12 cores
1-12-1.2
1-8-1.2
1-4-1.2
1-2-1.5
1-2-1.2
1-1-1.5
1-1-1.2
Socket-Cores-Frequency
0.00E+00
2.00E+02
4.00E+02
6.00E+02
8.00E+02
1.00E+03
1.20E+03
1.40E+03
Performance (Seconds)
CMT-bone was run on the Intel Ivy Bridge, dual socket platform
CCMT
25


DVFS Results
10
9
8
7
6
5
4
3
2
1
0
Energy (KJ)
2-16-2.4
2-24-2.1
2-24-1.5
1-12-1.5
1-12-1.2
Socket-Cores-Frequency
0.00E+00
5.00E+01
1.00E+02
1.50E+02
2.00E+02
2.50E+02
3.00E+02
Performance (Seconds)
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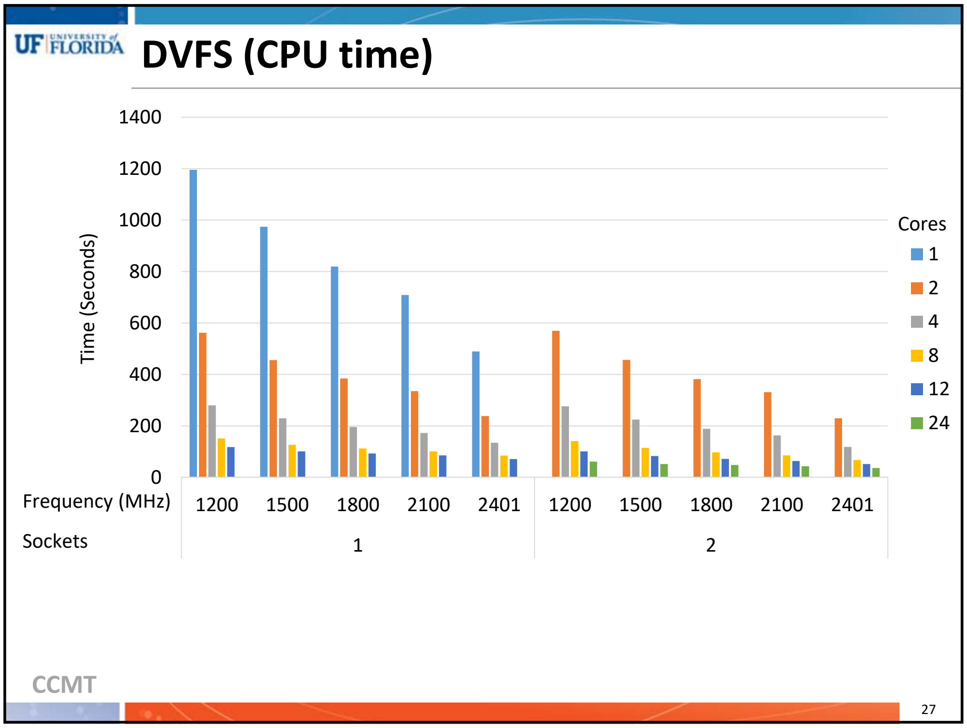
26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DVFS (CPU time)
Time (Seconds)
1400
1200
1000
800
600
400
200
0
Cores
1
2
4
8
12
24
Frequency (MHz)
1200 1500 1800 2100 2401 1200 1500 1800 2100 2401
Sockets
1
2
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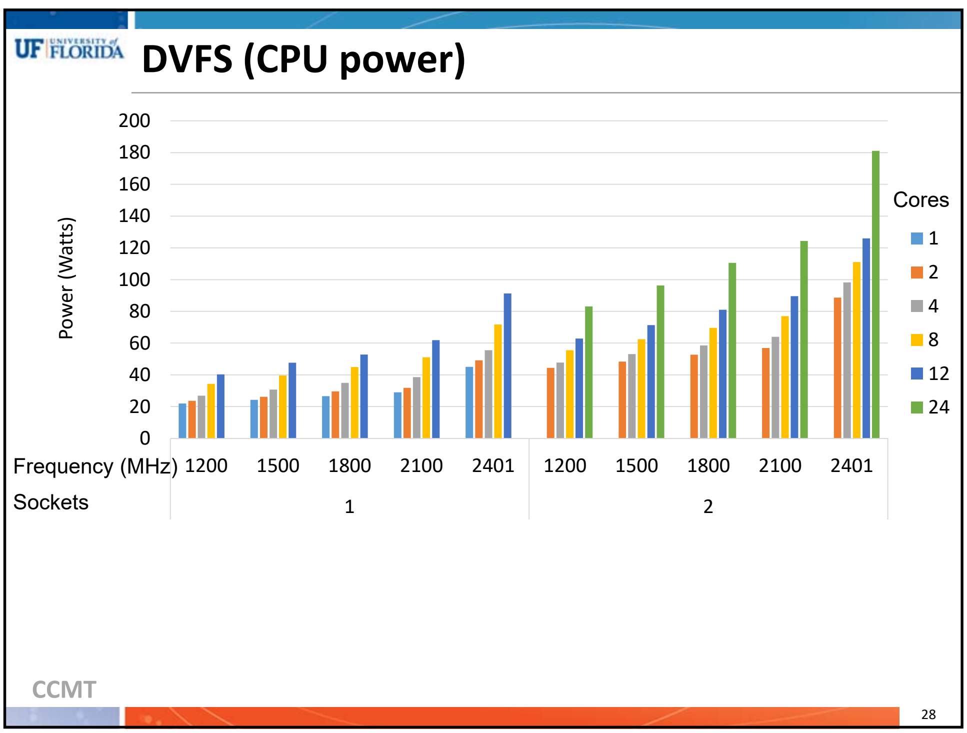
27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DVFS (CPU power)
Power (Watts)
200
180
160
140
120
100
80
60
40
20
0
Cores
1
2
4
8
12
24
Frequency (MHz)
1200 1500 1800 2100 2401 1200 1500 1800 2100 2401
Sockets
1
2
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28

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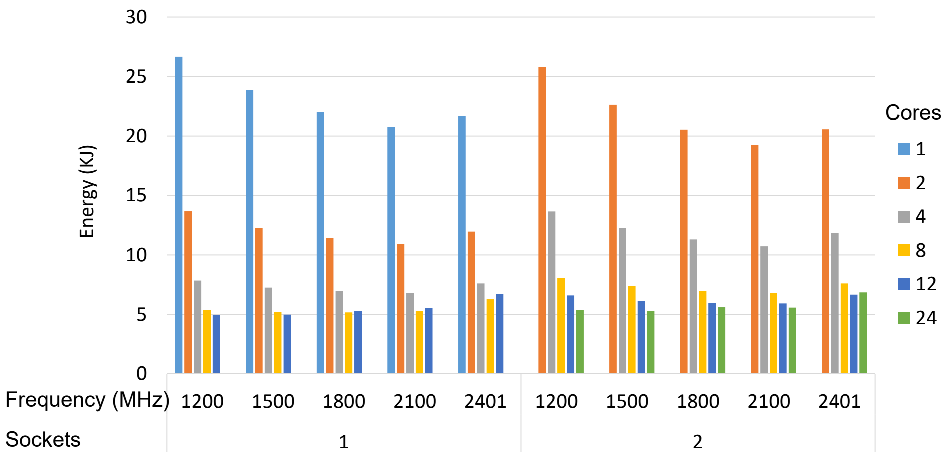
DVFS (CPU Energy)



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29

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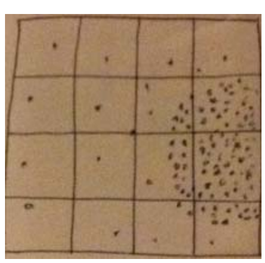
Dynamic Load Balancing

- Divide the elements with particles to different nodes such that they can complete the work in the same amount of time.
- When load balancing is achieved, fewer nodes will be idle during the run time, and thus more work can be done in the same time. And the working efficiency would be maximized.



T=0

T=100

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30

The Mapping Problem

- Mapping the multidimensional elements, particles and face array into one-dimensional index such that the proximity in the multidimensional space is usually maintained
- Various methods
  - Recursive coordinate bisection
  - Hilbert curve
  - Index-based mapping

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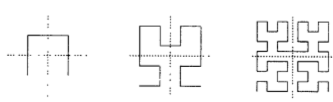
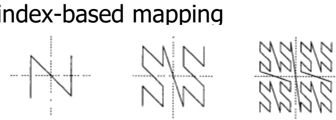
31

The Mapping Problem

- Recursive spectral bisection
  - bisects recursively a given graph along the longest dimension into two subgraphs with approximately equal sizes
- Hilbert curve



- index-based mapping



Ou C W, Gunwani M, Ranka S. Architecture-independent locality-improving transformations of computational graphs embedded in k-dimensions[C]//Proceedings of the 9th international conference on Supercomputing. ACM, 1995: 289-298

Ou C W, Ranka S, Fox G. Fast and parallel mapping algorithms for irregular problems. The Journal of Supercomputing, 1996, 10(2): 119-140.

Tufo H.M., Fischer P.F. Fast parallel direct solvers for coarse grid problems. The Journal of Parallel and Distributed Computing, 61 p. 151-177 (2001)

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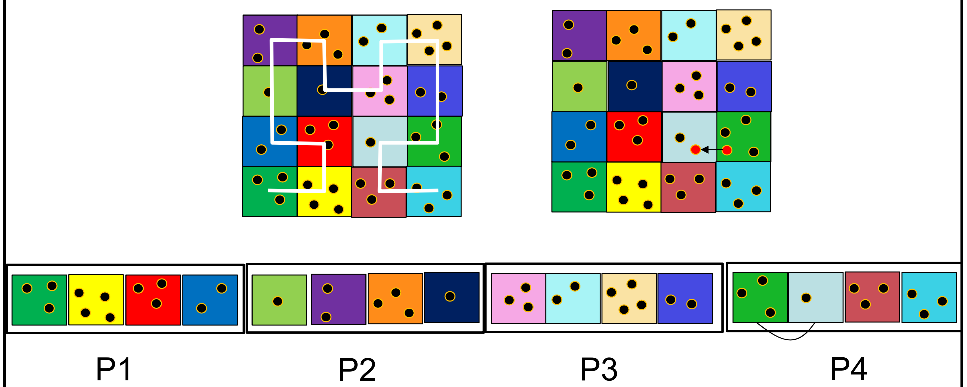
32

Hilbert Curve Demonstration



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33

The Remapping Problem

- Cluster the one-dimensional array into n sections and assign the elements in each section to processors such that the load is nearly balanced
- When the number of particles in each element changes, we have to remap the element array to processors in order to keep the load balanced
- As a result some elements along with their face data and particles will be transferred to other processors

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Implementation status

- Implemented load sensitive element mapping to processors
- Implemented remapping of elements to processors during simulation to balance load

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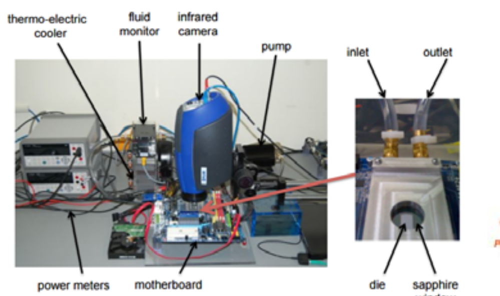
Thermal Aware Optimization

- Setup for temperature measurement



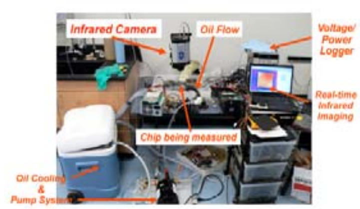


Figure 1. Infrared thermography setup.

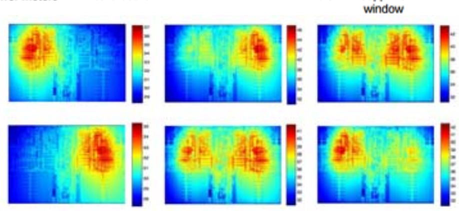


Figure 3.4: Examples of thermal traces of different applications on a dual-core AMD Athlon II.

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36

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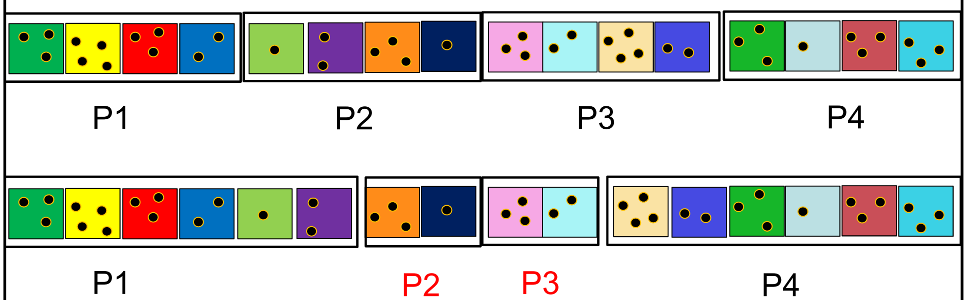
Thermal Optimization

- Perform dynamic load balancing to maintain maximum temperature
- Inner cores that heat up faster would process less load than the outer cores.
- Decision to load balance is made on temperature changes



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37

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Conclusions

1. Developed and Validated CMT-bone.
2. Developed CPU-GPU Implementation for Energy and/or Performance on Hybrid Processors.
3. Performance Evaluation on KNL.
4. Framework for Dynamic Load Balancing of Particles
5. Thermal Setup

1. Tania Banerjee and Sanjay Ranka, Genetic Algorithm based Autotuning Approach for Performance and Energy Optimization, IGSC 2015
2. Tania Banerjee, Mohammed Gadou, Sanjay Ranka, A Genetic Algorithm based Approach for Multi-objective Hardware/Software Co-optimization, Journal of Sustainable Computing, 2016

1. Tania Banerjee, Jason Hackl, Mrugesh Sringarpure,, Tanzima Islam, S. Balachandar, Thomas Jackson, Sanjay Ranka, CMT-bone -- A Proxy Application for Compressible Multiphase Turbulent Flows, HiPC, 2016 (extended version submitted to Journal of Sustainable Computing)
2. Tania Banerjee, Jacob Rabb and Sanjay Ranka, Multi-objective Optimization of Spectral Solvers on Hybrid Multicore Platforms, Journal of Sustainable Computing, 2016
3. Mohammed Gadou, Tania Banerjee, Sanjay Ranka, Multi-objective Optimization of CMT-bone on Hybrid Processors, IGSC 2016.
4. Mohamed Gadou, Tania Banerjee, Sanjay Ranka, Multiobjective optimization of CMT-bone on multiple CPU/GPU systems, submitted to IPDPS 2017

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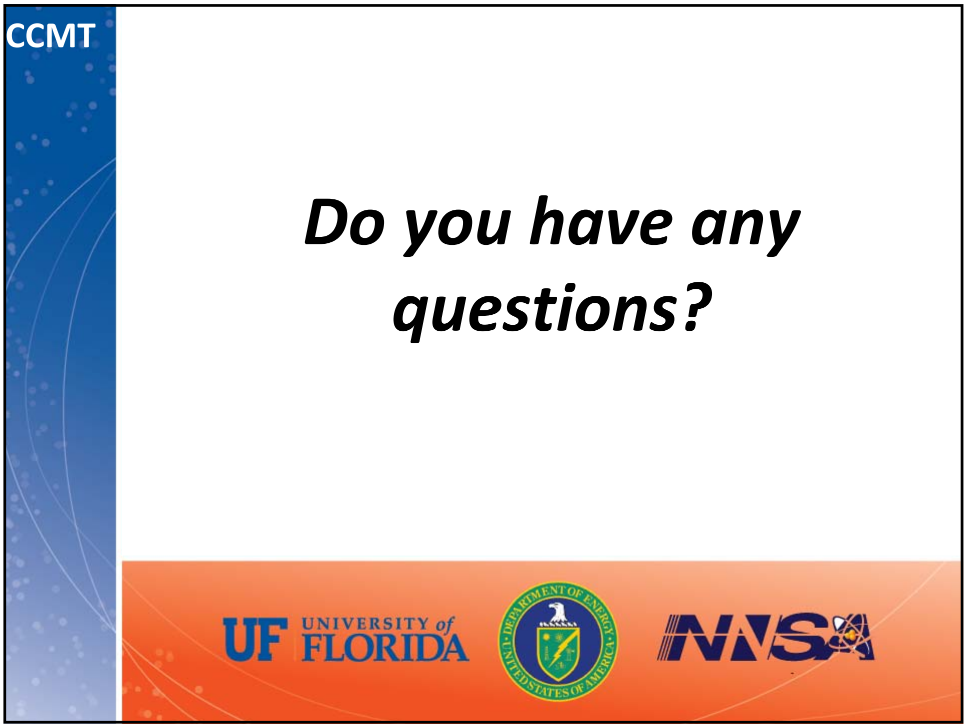
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Do you have any questions?
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DEPARTMENT OF ENERGY
UNITED STATES OF AMERICA
NNSA

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Exascale Behavioral Emulation

Principal Investigators:

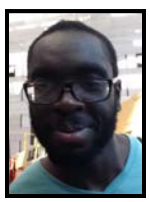
Herman Lam, Greg Stitt

Center for Compressible Multiphase Turbulence (CCMT)

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

Exascale Behavioral Emulation (BE) Students


Sai Chenna
(M.S.)


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.)

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2

Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts & Y3 achievements

- Enhancements to BE methods & tools
  - BE-SST simulator
  - Improved models and methods
  - Performance prediction from BE
- Closing the loop: BE & CMT-nek
- FPGA acceleration of BE

- Summary, conclusions, & future work

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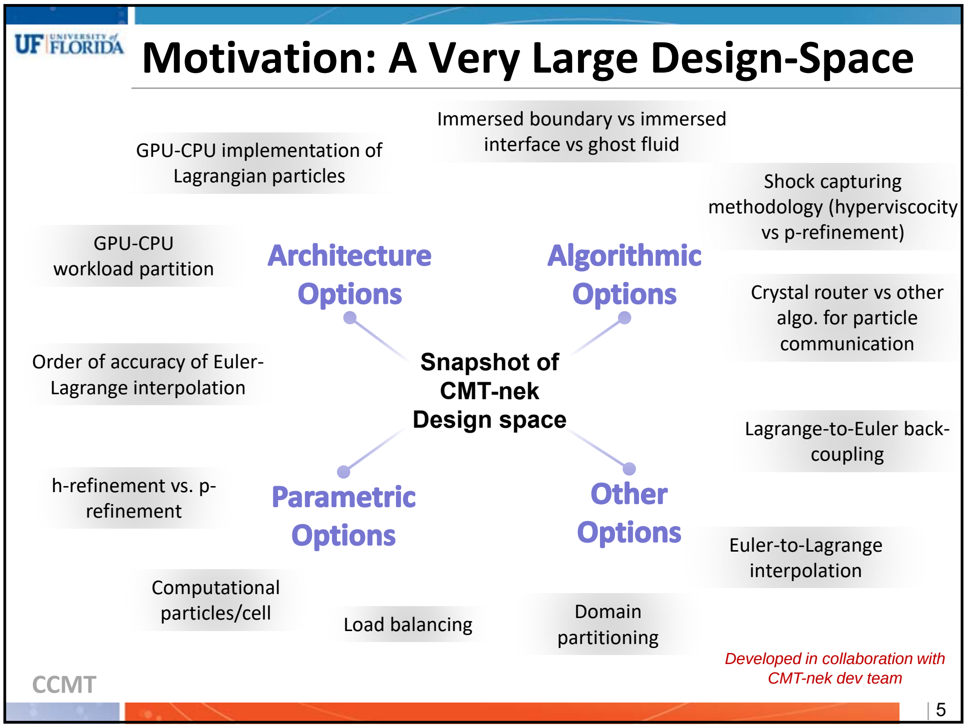
Motivation: A Very Large Design-Space
Immersed boundary vs immersed interface vs ghost fluid
GPU-CPU implementation of Lagrangian particles
Shock capturing methodology (hyperviscocity vs p-refinement)
GPU-CPU workload partition
Architecture Options
Algorithmic Options
Crystal router vs other algo. for particle communication
Order of accuracy of Euler-Lagrange interpolation
Snapshot of CMT-nek Design space
Lagrange-to-Euler back-coupling
h-refinement vs. p-refinement
Parametric Options
Other Options
Euler-to-Lagrange interpolation
Computational particles/cell
Load balancing
Domain partitioning
Developed in collaboration with CMT-nek dev team
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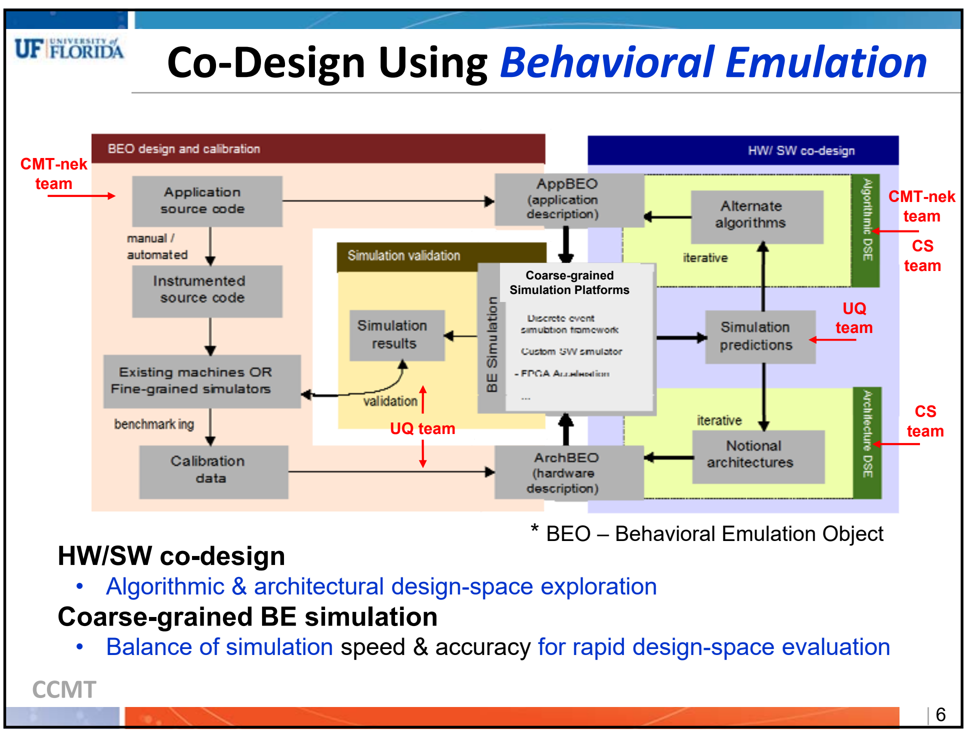
5


Co-Design Using Behavioral Emulation
BEO design and calibration
HW/ SW co-design
CMT-nek team
Application source code
manual / automated
Instrumented source code
Existing machines OR Fine-grained simulators
benchmarking
Calibration data
AppBEO (application description)
Alternate algorithms
iterative
Algorithmic DSE
CMT-nek team
CS team
Simulation validation
Coarse-grained Simulation Platforms
Discrete event simulation framework
Custom SW simulator
BE Simulation
Simulation results
validation
UQ team
Simulation predictions
UQ team
iterative
Notional architectures
Architecture DSE
CS team
ArchBEO (hardware description)
* BEO – Behavioral Emulation Object
HW/SW co-design
• Algorithmic & architectural design-space exploration
Coarse-grained BE simulation
• Balance of simulation speed & accuracy for rapid design-space evaluation
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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:

Methods
- 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)

Tools
- 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 DSE space reduction & UQ (Year 2)

Year 3 Accomplishments:

Methods
- BE method enhancement: network models, interpolation schemes, energy & thermal benchmarking and modeling
- Perform large-scale experiments on DOE systems (Cab, Vulcan, Titan) and simulated 100k+ MPI ranks (working toward million+) on BE-SST
- Closing the loop: Behavioral Emulation & CMT-nek

Tools
- Completed development of v1.0 of SST-based BE simulator
- Investigated dataflow methods to improve throughput & scalability for FPGAs

7

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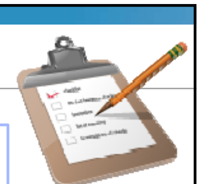
Outline



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1. BE-SST Simulator

- Developed by extending Structural Simulation Toolkit (SST) from SNL
  - Framework for parallel simulations – *for scaling simulations*
  - Supported by developers and vendors that contribute to *model libraries*
  - Flexibility in component design – *useful for designing custom BEOs*

SST Capabilities
- Parallel simulations
- Discrete event simulation
- Clock and event queues
- Network Models
- Component Models

\+

BE Influences
- Software Definitions
- Probabilistic Simulation
- Abstract Network Definitions
- Abstract Hardware Definitions

=

BE-SST
- Parallel discrete event simulation environment
- Distributed component queues
- Software Definitions
- Probabilistic Simulation
- Abstract Network Models
- Abstract Component Models

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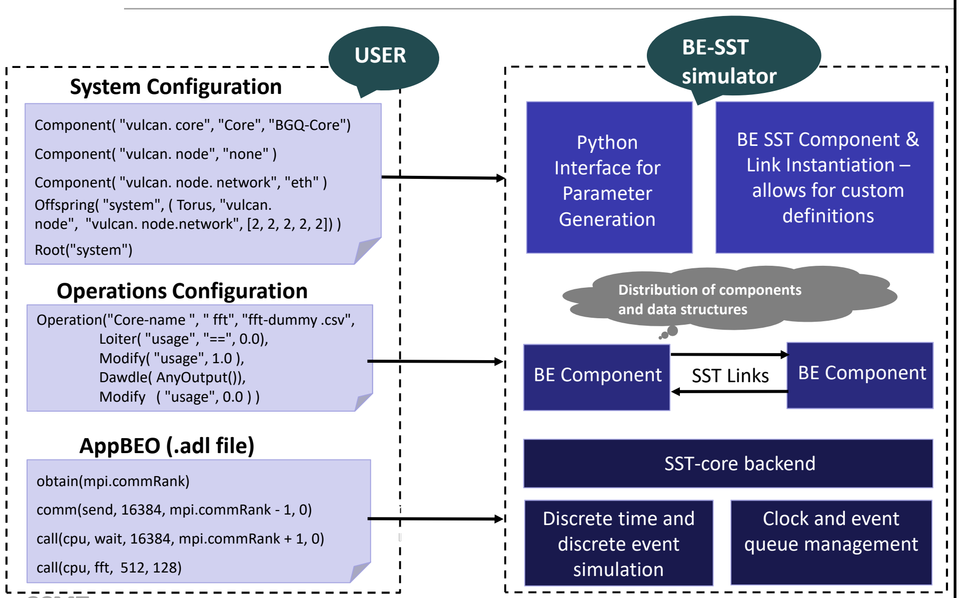
BE-SST v1.0 Features



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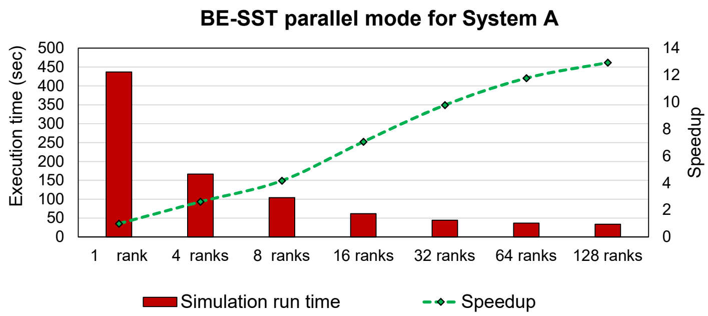
BE-SST Simulator Parallel Performance

- For the simulation of a large system configuration executing CMT-bone-BE, BE-SST demonstrates performance scalability.
  - System A with 32768 cores and 163840 network links in 5D Torus topology [8, 8, 8, 8, 8]



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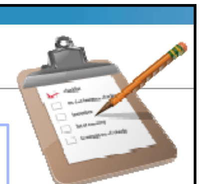
Outline



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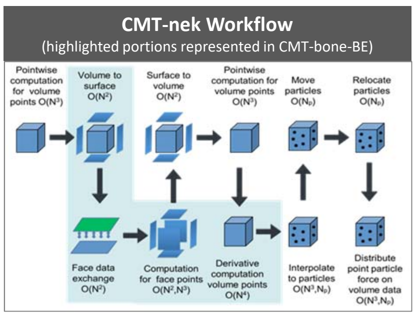
Application Case Study: CMT-bone-BE

- 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** and **modular** that is easy to **modify** and **instrument** for algorithmic DSE



- Computation- & communication-intensive portions of CMT-nek workflow in C & MPI
  - Volume-to-surface data extraction
  - Face data exchange (with neighbors)
  - Derivative computation volume points
- Easier to modify for algorithmic DSE
- 1000 vs 10s of thousands lines of code

* design-space exploration

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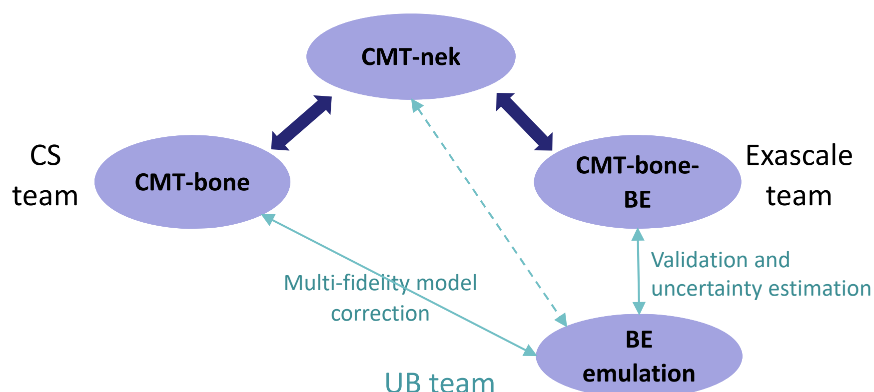
Assessing Behavioral Emulation

w/ UB

- Improve predictions from BE simulation by:
  - Correcting BE simulation to CMT-bone (CMT-nek in future) using a multi-fidelity model
  - Improving interpolation techniques in BEO models



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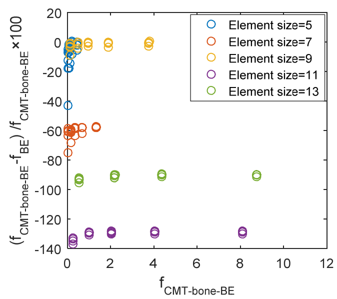
CMT-bone-BE vs BE Emulation

w/ UB

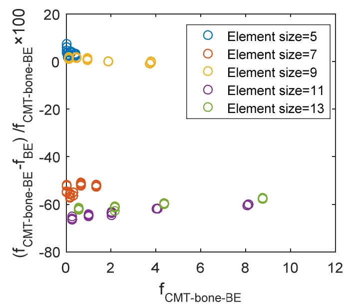
Comparison based on design of experiments

- f_{BE} underestimated $f_{CMT-bone-BE}$ at interpolated configurations
- Discovered that interpolation model is a major source of uncertainty causing jumps between different element size
- As expected, polynomial interpolation gives better results

Percent difference between $f_{CMT-bone-BE}$ and f_{BE}



f_{BE} based on linear interpolation



f_{BE} based on polynomial interpolation

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15

Multi-fidelity Surrogate for Model Correction

w/ UB

- Compare compatibility of different models
  - Fitting CMT-bone and corrected fitting of BE emulation
  - For large problems, low-fidelity BE emulation is cheaper than high fidelity CMT-bone
- Multi-fidelity surrogate for CMT-bone prediction from BE emulation

$$f_{CMT-bone}(x) = \rho\, f_{BE}(x) + \delta(x)$$

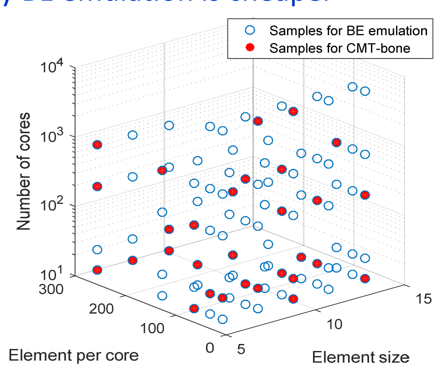

Illustration of samples to develop surrogate models with 30 samples of CMT-bone

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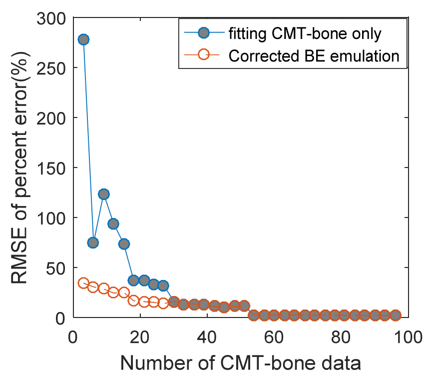
16

Model Correction

w/ UB

Accuracy comparison

- Prediction metric: RMSE* at all samples of CMT-bone
- Multi-fidelity surrogate significantly reduces error for less than 20 data samples, providing a better fit to CMT-bone
- Next, this exercise will be extended to CMT-nek



*RMSE: Root Mean Square Error

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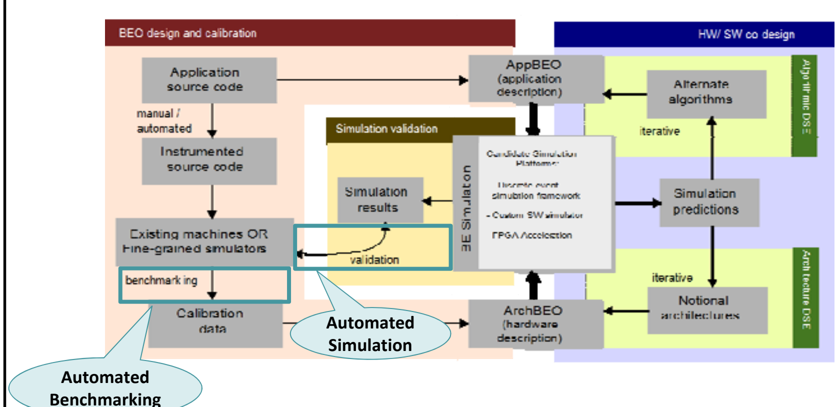
17

BE Framework Automation

- Designed a framework to simplify and automate benchmarking
  - Required for both calibration and validation data collection
  - Job scripts can be generated for different machine/app combinations
  - Easy to extend benchmarking to new applications & systems
- Leveraging similar framework for CMT-nek batch runs as well



18

BE Framework Automation

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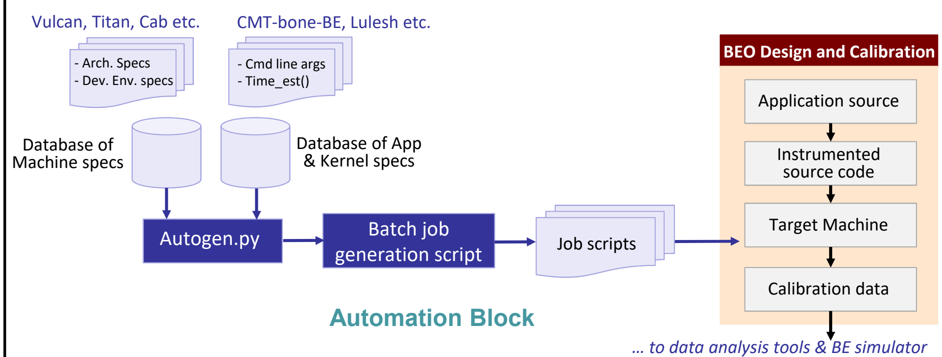

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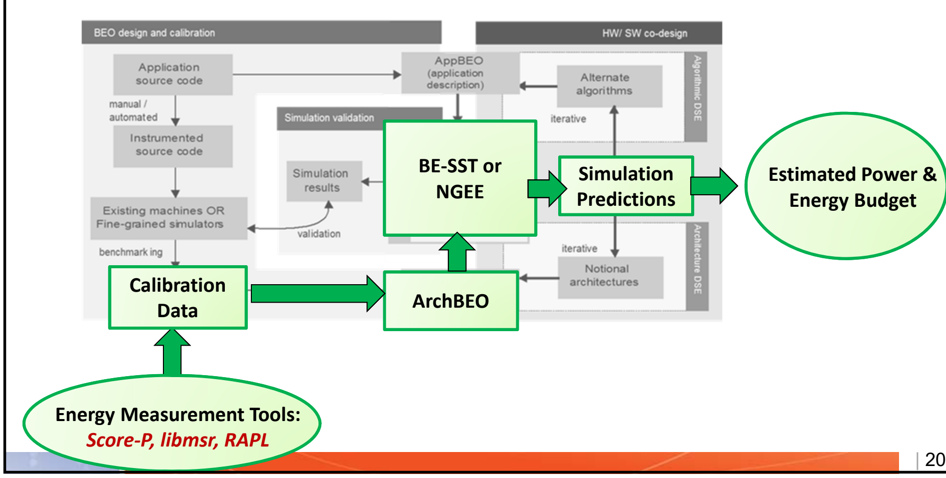
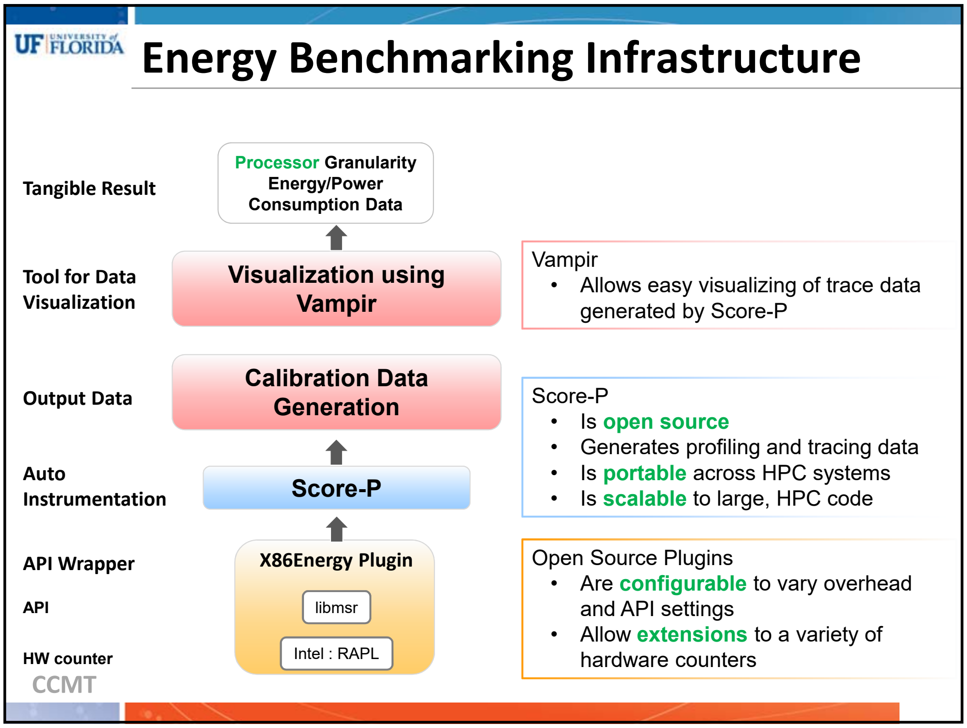
Energy Benchmarking & Modeling

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



| 20


Energy Benchmarking Infrastructure
Tangible Result
Processor Granularity Energy/Power Consumption Data
Tool for Data Visualization
Visualization using Vampir
Vampir
• Allows easy visualizing of trace data generated by Score-P
Output Data
Calibration Data Generation
Score-P
• Is open source
• Generates profiling and tracing data
• Is portable across HPC systems
• Is scalable to large, HPC code
Auto Instrumentation
Score-P
API Wrapper
X86Energy Plugin
API
libmsr
HW counter
Intel : RAPL
Open Source Plugins
• Are configurable to vary overhead and API settings
• Allow extensions to a variety of hardware counters
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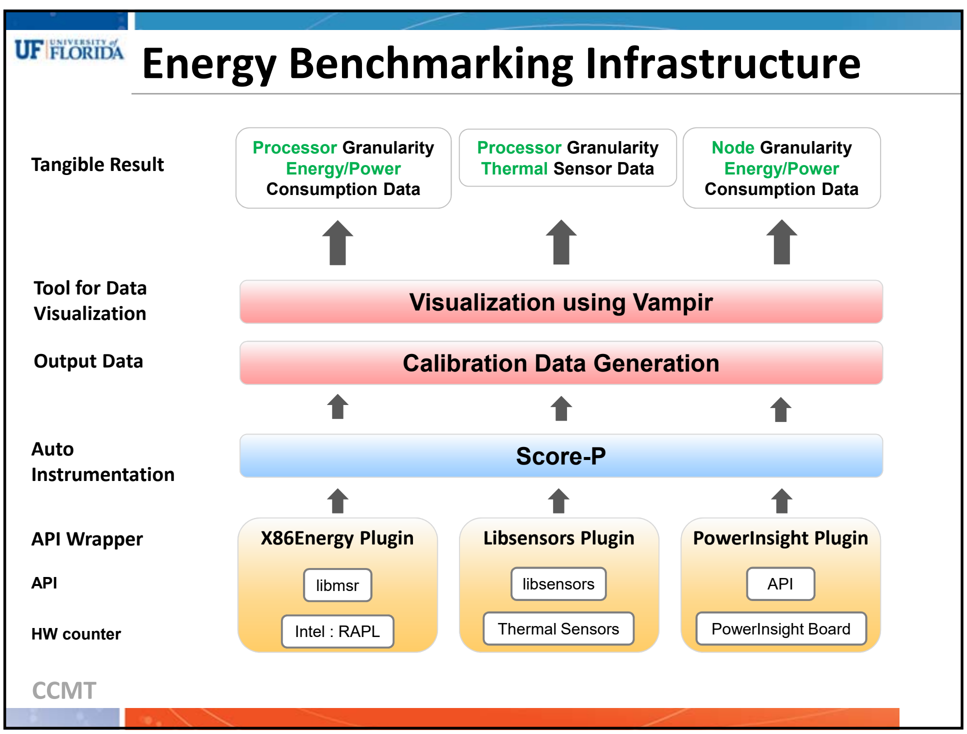
Energy Benchmarking Infrastructure
Tangible Result
Processor Granularity Energy/Power Consumption Data
Processor Granularity Thermal Sensor Data
Node Granularity Energy/Power Consumption Data
Tool for Data Visualization
Visualization using Vampir
Output Data
Calibration Data Generation
Auto Instrumentation
Score-P
API Wrapper
X86Energy Plugin
Libsensors Plugin
PowerInsight Plugin
API
libmsr
libsensors
API
HW counter
Intel : RAPL
Thermal Sensors
PowerInsight Board
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Energy Benchmarking (CS & BE)

- **CS:** Understand performance vs energy trade-offs via benchmarking
  - Single multicore, multi-GPU node
  - Vary hardware configuration - CPU/GPU/core utilization/DVFS
  - Vary software configuration - particles/elements
- **Exascale BE:** Develop energy models for ArchBEOs to enable Behavioral Emulation
  - Extendable approach applicable to HPC system
  - Vary granularity and/or measurement source
    - Processor- and node-level, read frequency, energy/power/thermal sensors, …
  - Vary HPC system and hardware (Intel, IBM, AMD, …)

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Conclusions: BE Model Enhancements

- With UQ team, used multi-fidelity surrogate for BE model correction
- Integrated new interpolation & networking techniques in BE-SST to improve simulation accuracy
- Finalized design of an extendable, scalable, and portable infrastructure for energy benchmarking

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Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts & Y3 achievements

- Enhancements to BE methods & tools
  - BE-SST simulator
  - Improved models and methods
  - Performance prediction from BE
- Closing the loop: BE & CMT-nek
- FPGA acceleration of BE

- Summary, conclusions, & future work

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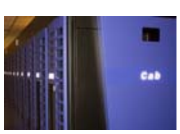
BE simulations of HPC systems

- 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

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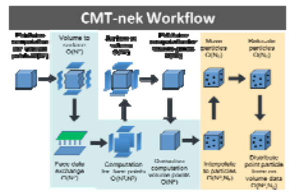
Experiment Setup

- Application case study: CMT-bone-BE (gas solver)
- Application parameters
  - Validation element size: 8,9,13,16,19,21,24
  - Calibration element size: 5,8,9,11,14,17,20,23,25
  - 100 elements/core



- Machine parameters
  - Simulation predictions up to 128k MPI ranks (cores)
  - Simulation validation up to 4k cores
  - Can do both predictions and validations for larger systems
- Monte-Carlo simulations

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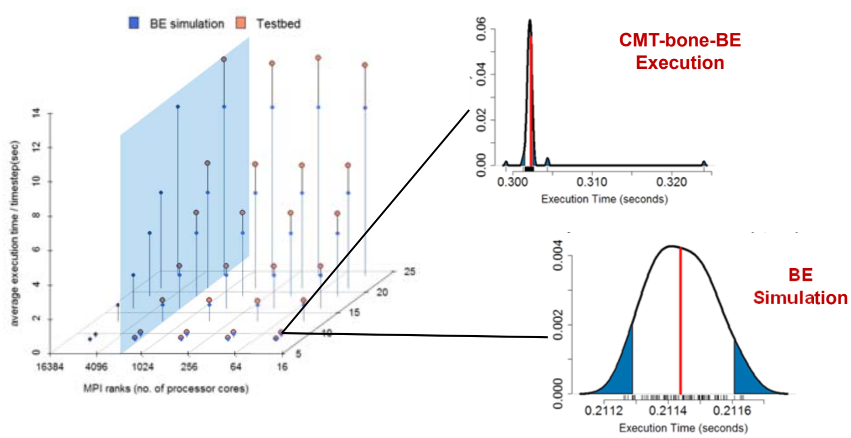
Results: Simulations of Titan



- % error between CMT-bone-BE simulation and execution time is 25%
- This can be attributed to independent microkernel benchmarking vs in-situ benchmarking methods used in the past
- Microkernel benchmarking will be essential for design space exploration studies

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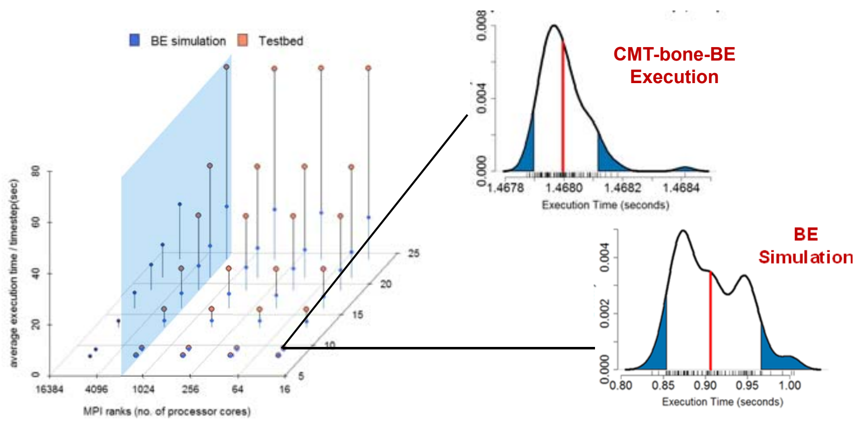
Results: Simulations of Vulcan



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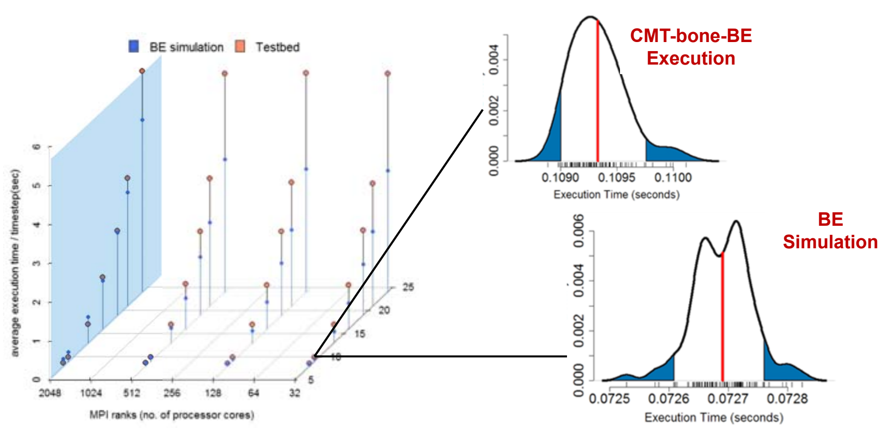
29

Results: Simulations of Cab



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30

Conclusions: Prediction using BE

- Validations up to thousands of MPI ranks
- Demonstrated ability to simulate 100k+ MPI ranks
  - Working on simulation of million+ MPI ranks
- Showcased Monte-Carlo simulation capability in BE

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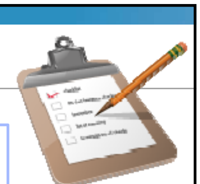
31

Outline



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Very Large Design-Space

Immersed boundary vs immersed interface vs ghost fluid

GPU-CPU implementation of Lagrangian particles

Shock capturing methodology (hyperviscocity vs p-refinement)

GPU-CPU workload partition

Architecture Options

Algorithmic Options

Crystal router vs other algo. for particle communication

Order of accuracy of Euler-Lagrange interpolation

Snapshot of CMT-nek Design space

Lagrange-to-Euler back-coupling

h-refinement vs. p-refinement

Parametric Options

Other Options

Euler-to-Lagrange interpolation

Computational particles/cell

Load balancing

Domain partitioning

Developed in collaboration with CMT-nek dev team

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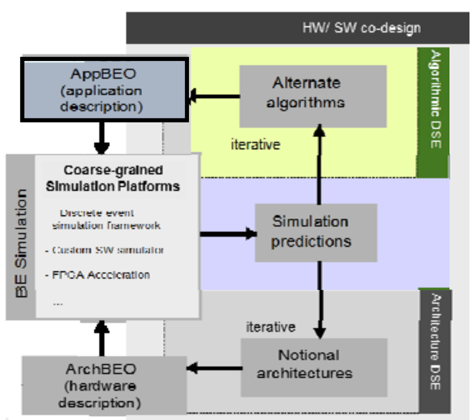
Scope of DSE using BE in Y3

- Goal: Perform algorithmic DSE* to maximize CMT-nek w/particles performance
- Iterative DSE steps:
  1. Identify the most expensive subroutines (DSE candidates)
  2. Modify algorithms for these subroutines
  3. Predict performance
- Use BE predictions to explore performance vs. accuracy tradeoff on the overall CMT-nek code



* Design-Space Exploration

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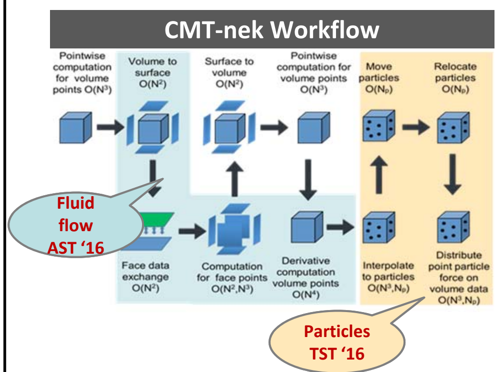
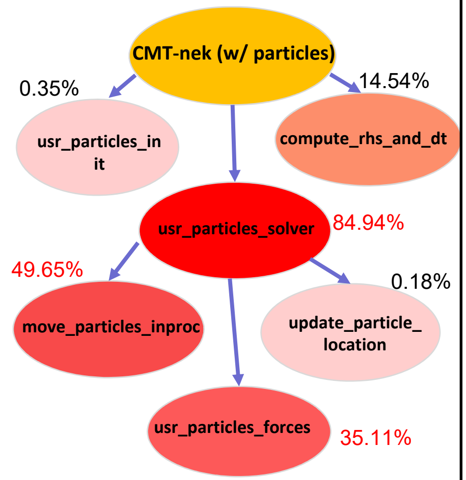
Scope of DSE using BE in Y3

- Extended scope of study from *fluid flow solver to particles solver*





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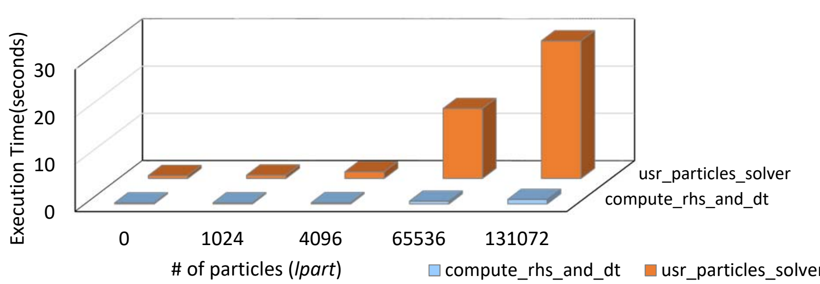
35

Gas vs Particle Subroutines

- Input parameters: # processes: 256

  lpart = # of particles/processor ; lx1 = Element size/resolution (N) ; lelt = # of elements/ processor



- Observations:
  - Gas solver (compute_rhs_and_dt) depends on # of particles (lpart)
  - usr_particle_solver is the most expensive subroutine

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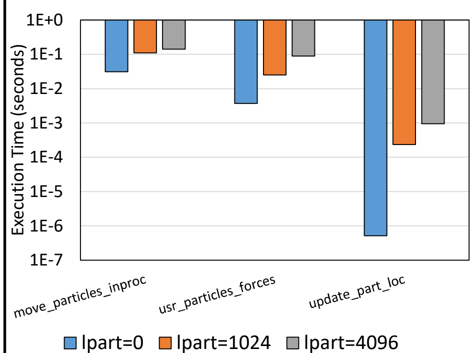
36

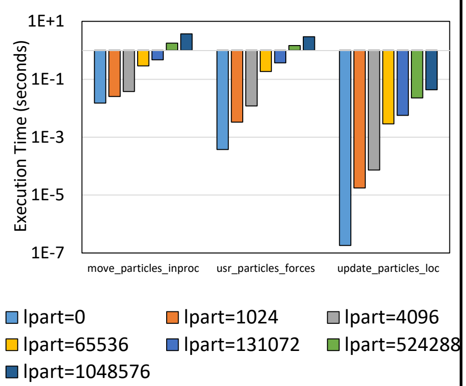
Particle Solver Subroutines

\# processes: 256

On Vulcan (lelt = 8)



On HiPerGator (lelt=8)



- Observations:
  - *move_particles_inproc* and *usr_particles_forces* are the most expensive particle subroutines.
  - *move_particles_inproc* scales better than *usr_particles_forces* with number of particles

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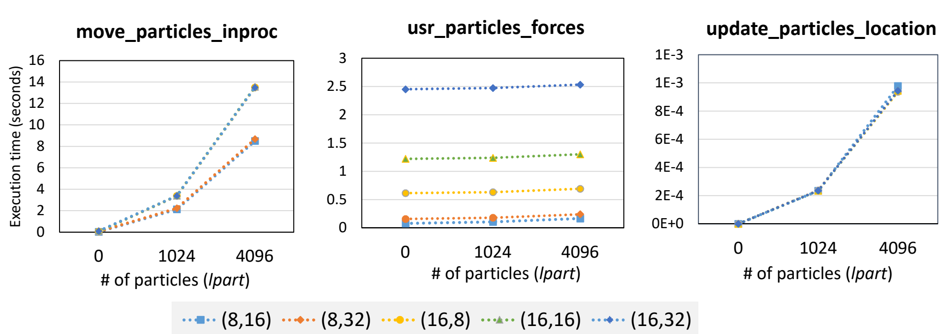
Particle Solver Subroutines *(Vulcan)*

\# processes: 1024



(Element size, number of elements)

Observations:

- *move_particles_inproc* is independent of # of elements per processor (lelt)
- *usr_particles_forces* is primarily dependent on Element size (lx1) and Element count (lelt).
- *update_particles_location* is independent of Element size(lx1) and Element count (lelt).

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Conclusion: Closing the Loop

- Key Observations:
  - Particle solver (*usr_particles_solver*): most expensive stage of CMT-nek
  - *move_particles_inproc and usr_particles_forces:* major particle subroutines
  - *Gas solver:* execution dependent on # of particles
  - *move_particles_inproc:* independent of # of elements
  - *update_particles_location:* independent of lelt and lx1
- Going forward (for Spring AST meeting):
  - Profile different particle distributions
  - Build BE models for particle solver routines
  - Use BE infrastructure & tools to perform algorithmic DSE (predict performance of different algorithms/optimizations)

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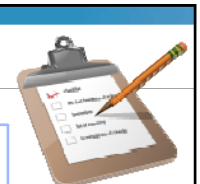
Outline



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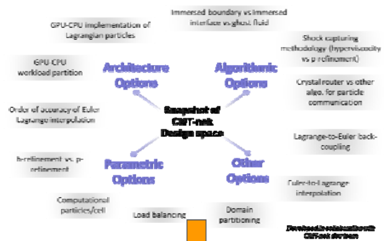
BE Design-Space Exploration



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 Simulator (SW)

~Minutes per simulation

Optimized Design

- **Advantage:** Significantly faster than existing simulators
- **Limitation:** Still not fast enough for DSE of exascale systems
- **Approach:** Use FPGA acceleration to improve exploration

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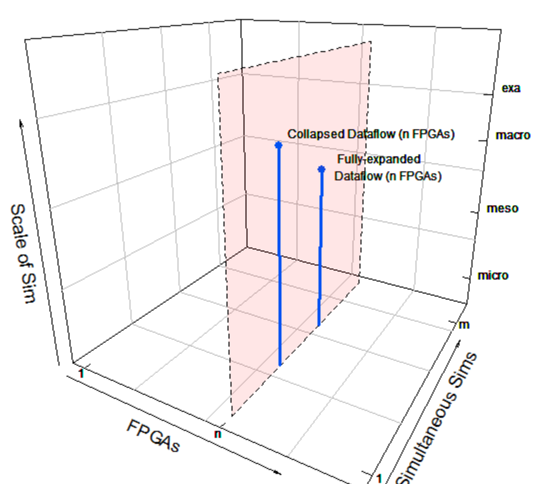
Landscape of FPGA-acceleration Studies



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)*

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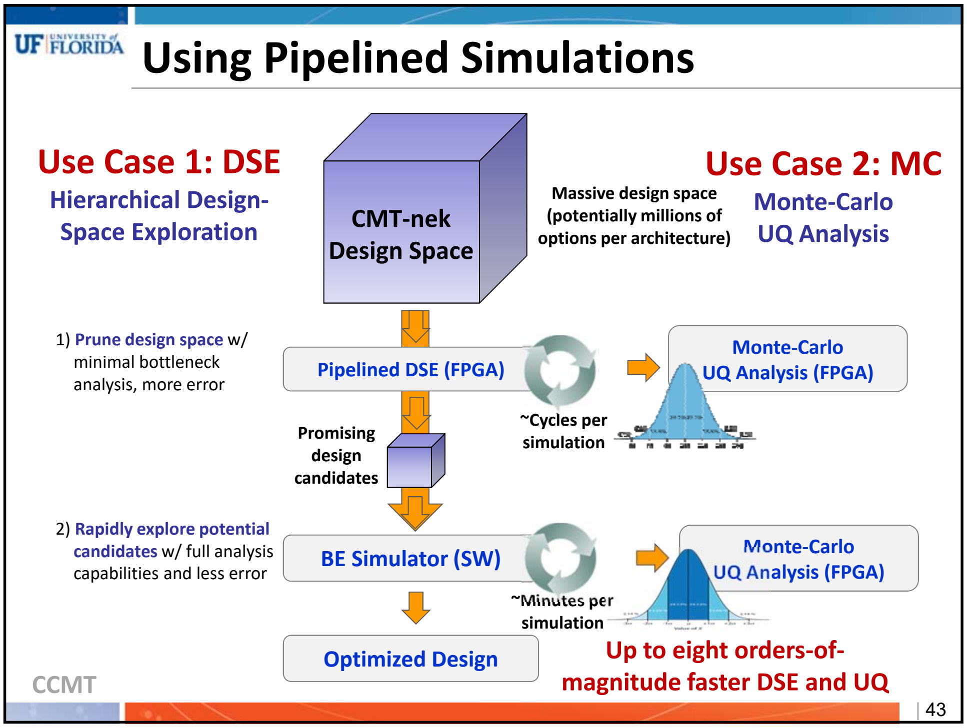
*NGEE: Novo-G Exascale Emulation $^+$DSE: Design-Space Exploration

42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Using Pipelined Simulations
Use Case 1: DSE
Hierarchical Design-Space Exploration
CMT-nek Design Space
Massive design space (potentially millions of options per architecture)
Use Case 2: MC
Monte-Carlo UQ Analysis
1) Prune design space w/ minimal bottleneck analysis, more error
Pipelined DSE (FPGA)
Monte-Carlo UQ Analysis (FPGA)
~Cycles per simulation
Promising design candidates
2) Rapidly explore potential candidates w/ full analysis capabilities and less error
BE Simulator (SW)
Monte-Carlo UQ Analysis (FPGA)
~Minutes per simulation
Optimized Design
Up to eight orders-of-magnitude faster DSE and UQ
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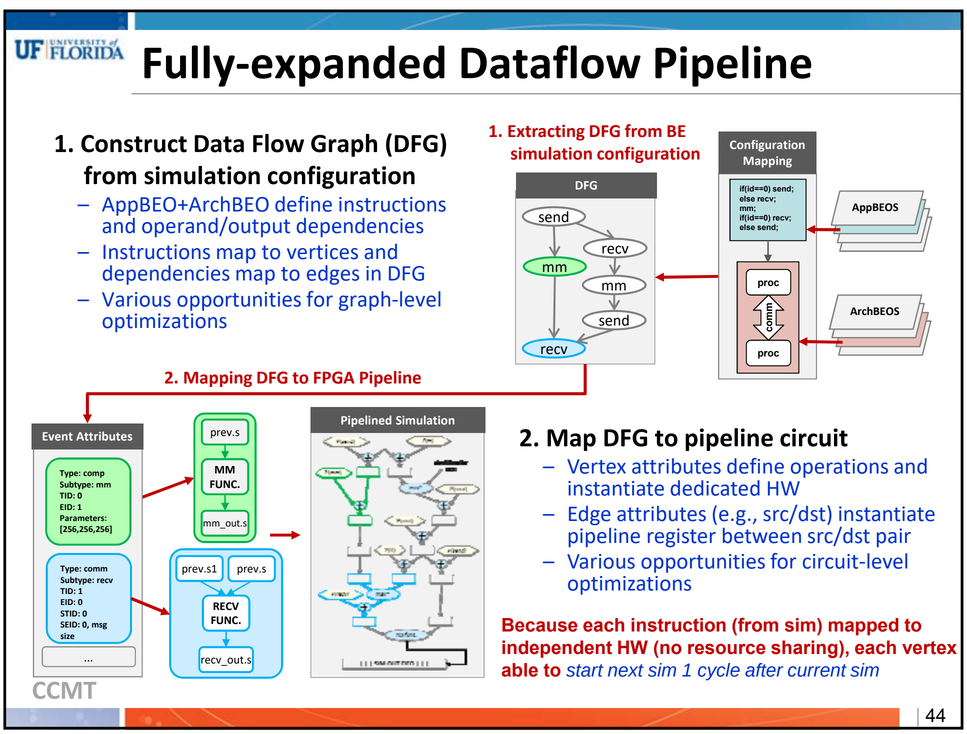
43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Fully-expanded Dataflow Pipeline
1. Construct Data Flow Graph (DFG) from simulation configuration
– AppBEO+ArchBEO define instructions and operand/output dependencies
– Instructions map to vertices and dependencies map to edges in DFG
– Various opportunities for graph-level optimizations
1. Extracting DFG from BE simulation configuration
DFG
send
recv
mm
mm
send
recv
Configuration Mapping
if(id==0) send;
else recv;
mm;
if(id==0) recv;
else send;
proc
comm
proc
AppBEOS
ArchBEOS
2. Mapping DFG to FPGA Pipeline
Event Attributes
Type: comp
Subtype: mm
TID: 0
EID: 1
Parameters: [256,256,256]
Type: comm
Subtype: recv
TID: 1
EID: 0
STID: 0
SEID: 0, msg size
...
prev.s
MM FUNC.
mm_out.s
prev.s1
prev.s
RECV FUNC.
recv_out.s
Pipelined Simulation
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
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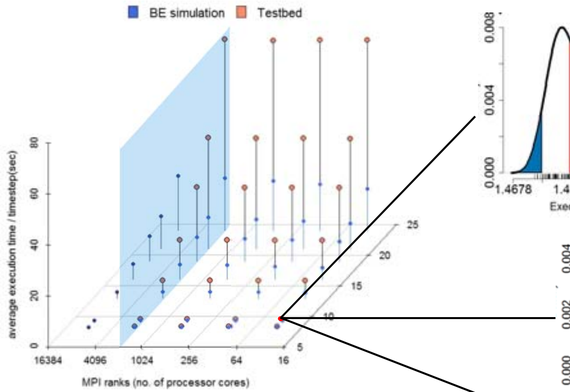
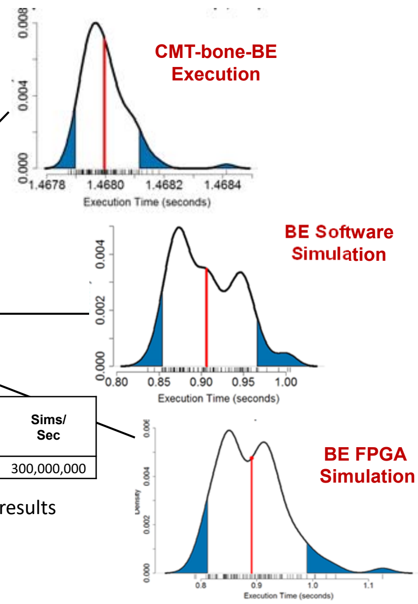
44

Results: Simulations of Vulcan





Num. of MPI Ranks	Num. of Timesteps	Num. of Events	Num. of FPGAs	% Logic Utilization (in ALMs)	FPGA Clk Frequency	Latency to First Output	Sims/ Sec
128	1	6,912	1	58 %	300 MHz	61 Cycles	300,000,000

- BE software and BE FPGA simulations produce similar results
  - Software execution at 1-4 Simulations/second
  - FPGA execution approx. 10^8x faster

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45

Fully-expanded Dataflow Pipeline

Num. of MPI Ranks	Num. of Timesteps	Num. of Events	Num. of FPGAs	% Logic Utilization (in ALMs)	FPGA Clk Frequency	Latency to First Output	Sims/ Sec
128	1	6,912	1	58 %	300 MHz	61 Cycles	300,000,000
128	2	13,824	Currently Cannot Fit in Single FPGA				
128	10	69,120					
128	100	691,200					
32	1	1,728	1	13 %	280 MHz	59	280,000,000
32	2	3,456	1	27 %	335 MHz	113	335,000,000
32	5	8,640	1	76 %	265 MHz	275	265,000,000
32	10	17,280	Currently Cannot Fit in Single FPGA				
32	100	172,800					

- Advantage: very high simulation throughput
- Limitation: doesn't scale well on single FPGA
  - Required resources scale linearly with both MPI Ranks and number of timesteps
- Scaling across multiple FPGAs expected to be ineffective
  - Balanced graph partitioning that limits number of unidirectional links (nondeterminism, longer latency, reduced throughput)

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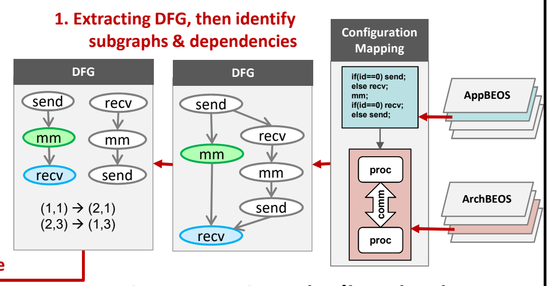
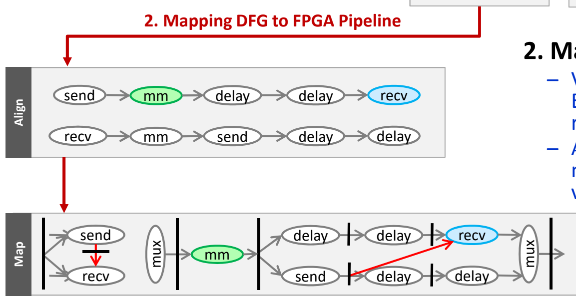
46

Collapsed Dataflow Pipeline

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



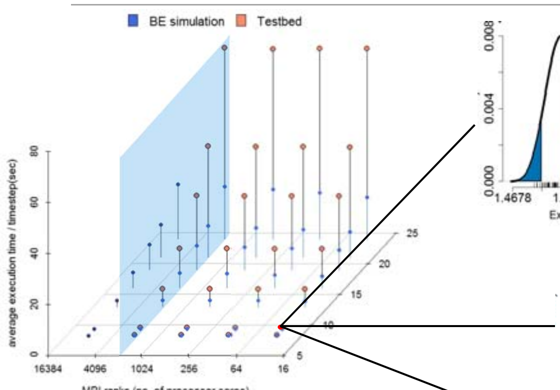


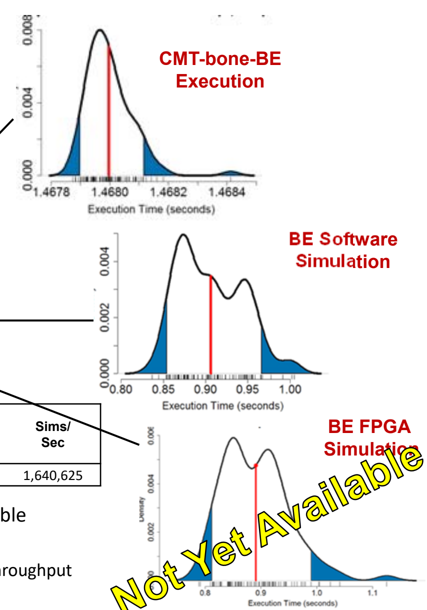
2. Map DFG to pipeline circuit
- Vertex attributes define operations and Edge attributes instantiate pipeline register between src/dst pairs
- Align subgraph traces such that cost is minimized and no dependencies are violated

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*

47

Results: Simulations of Vulcan





Num. of MPI Ranks	Num. of Timesteps	Num. of Events	Num. of FPGAs	% Logic Utilization (in ALMs)	FPGA Clk Frequency	Latency to First Output	Sims/ Sec
128	1	6,912	1	< 1 %	210 MHz	129 Cycles	1,640,625

- Collapsed dataflow pipeline simulations not yet available
  - Resource utilization/timing results only preliminary
  - Demonstrates greater scalability at cost of simulation throughput

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48

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Collapsed Dataflow Pipeline

Num. of MPI Ranks	Num. of Timesteps	Num. of Events	Num. of FPGAs	% Logic Utilization (in ALMs)	FPGA Clk Frequency	Latency to First Output	Sims/ Sec
128	1	6,912	1	< 1 %	210 MHz	129	1,640,625
128	2	13,824	1	< 1%	200 MHz	251	1,562,500
128	5	34,560	1	2 %	220 MHz	617	1,718,750
128	10	69,120	1	3 %	220 MHz	1227	1,718,750
128	100	691,200	1	28 %	200 MHz	12207	1,562,500
128	1000	6,912,000	Currently Cannot Fit in Single FPGA				
32	1	1,728	1	< 1 %	200 MHz	103	6,250,000
32	2	3,456	1	< 1 %	200 MHz	199	6,250,000
32	5	8,640	1	2 %	210 MHz	487	6,562,500
32	10	17,280	1	3 %	210 MHz	967	6,562,500
32	100	172,800	1	28 %	205 MHz	5449	6,406,250
32	1000	1,728,000	Currently Cannot Fit in Single FPGA				
8K	1	442,368	1	1 %	210 MHz	633	25,635
32K	1	1,769,472	1	Still generating configuration files			
128K	1	7,077,888	1				

Preliminary

- Disadvantage: lower simulation throughput
  - But, still more than sufficient for rapid design-space exploration
- Advantage: scales better on single and multiple FPGAs
  - Resources scale linearly with timesteps and sublinearly with MPI Ranks
  - Less inter-FPGA communication

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Conclusion: FPGA Acceleration

- Key Observations:
  - Pipelined simulations can achieve 8 orders of magnitude higher simulation throughput
    - Sacrifices analysis capabilities
  - Full pipelining provides very high throughput, but doesn't scale well
  - Collapsed dataflow approach sacrifices throughput, but improves scalability
- Going forward (for Spring AST meeting):
  - Finalize/verify single-FPGA collapsed dataflow pipeline
  - Scale to many FPGAs
  - Prune design space for CMT-bone-BE w/ particles

CCMT | 50

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Conclusions and Future Work

- BE model & tools enhancements
  - Completed development of v1.0 of SST-based BE simulator
  - Used multi-fidelity surrogate (UQ) for BE model correction
  - Integrated new interpolation & networking techniques
  - Finalized design of an infrastructure for energy benchmarking
  - Perform large-scale experiments on DOE systems and simulated 100k+ MPI ranks (working toward million+) on BE-SST
- Closing the Loop: BE and CMT-nek
  - Profiled CMT-nek to identify its characteristics (e.g., expensive routines, dependencies)
  - Going forward: use BE infrastructure & tools to perform algorithmic DSE (predict performance of different algorithms/optimizations for CMT-nek)
- FPGA accelerated simulations
  - Investigated dataflow methods to improve throughput & scalability for FPGAs
  - Going forward: scale to many FPGAs

CCMT | 51

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Publications:

1. N. Kumar, C. Pascoe, C. Hajas, H. Lam, G. Stitt, and A. George, "Behavioral Emulation for Scalable Design-Space Exploration of Algorithms and Architectures", Workshop on Exascale Multi/Many Core Computing Systems (E-MuCoCoS) at the International Supercomputing Conference (ISC), Frankfurt, Germany, June 19 - 23, 2016.
2. C. Pascoe, N. Kumar, H. Lam, G. Stitt, A. George, "FPGA-Pipelined Discrete-Event Simulations for Accelerated Behavioral Emulation of Extreme-Scale Systems", Workshop on Modeling & Simulation of Systems and Applications (ModSim2016), Seattle, Washington, August 10-12, 2016.

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References:

1. M. Sottile, A. Dakshinamurthy, G. Hendry, and D. Dechev. Semi-automatic extraction of software skeletons for benchmarking large-scale parallel applications. In ACM SIGSIM PADS, May 2013.

2. John Shalf, Dan Quinlan and Curtis Janssen. Rethinking hardware-software co-design for Exa-scale systems. IEEE Computer society, 2011.

3. Damian Dechev, Tae-Hyuk Ahn. Using SST/Macro for Effective Analysis of MPI-Based Applications: Evaluating Large-Scale Genomic Sequence Search. IEEE 2169-3536, 08 July 2013.

4. C. L. Janssen et al. Using simulation to design extreme-scale applications and architectures: programming model exploration. SIGMETRICS Perform. Eval. Rev., 38, 2011.

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Do you have any questions?

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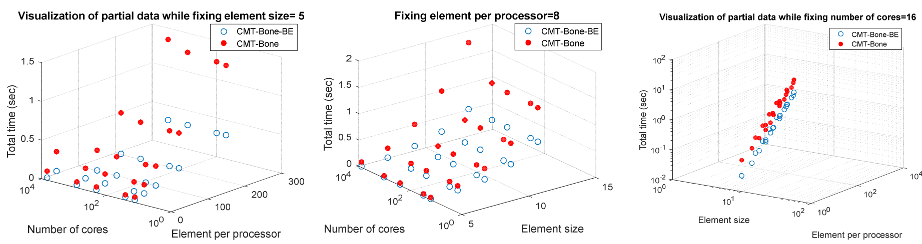
CMT-bone vs CMT-bone-BE

- Test plan for validation between CMT-bone, CMT-bone-BE and BE emulation
  - Element size:5~13
  - Number of cores:16~8192
  - Elements per core:8~256
  - Total execution time at 98 samples, repeated 3 times
  - Negligible experimental variability ~ O (1%)



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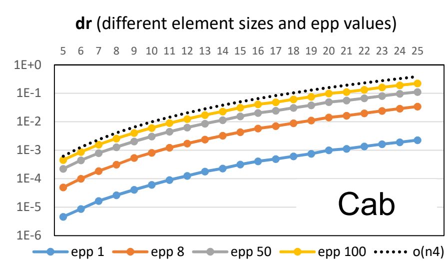
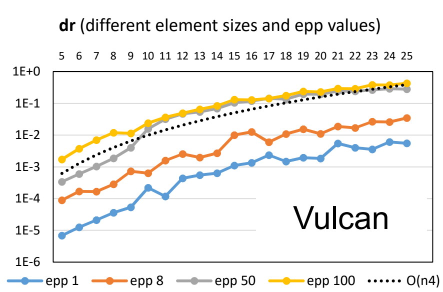
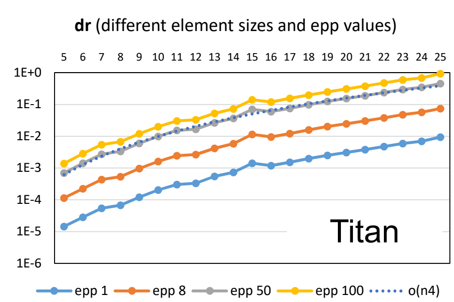
Calibrate dr block







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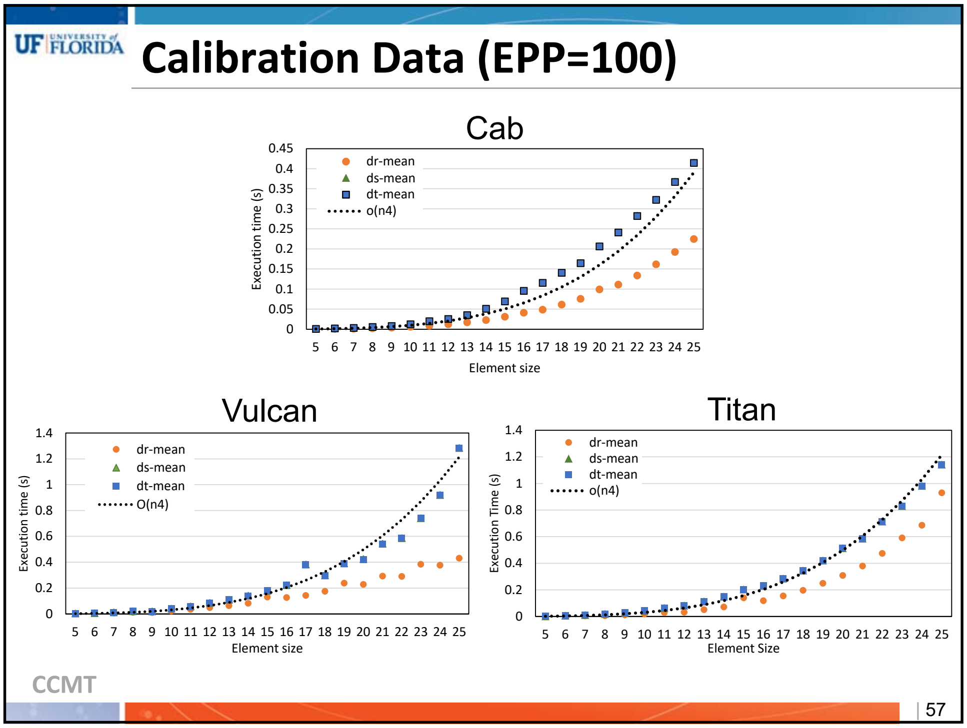
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Calibration Data (EPP=100)
Cab
dr-mean
ds-mean
dt-mean
o(n4)
Execution time (s)
Element size
Vulcan
dr-mean
ds-mean
dt-mean
O(n4)
Execution time (s)
Element size
Titan
dr-mean
ds-mean
dt-mean
o(n4)
Execution Time (s)
Element Size
CCMT
57

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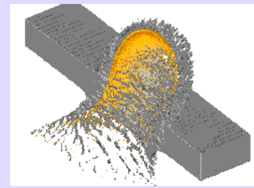
Two-way coupled particles in CTH code

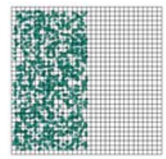
Sandia National Laboratories



dpzwick@ufl.edu

Summer 2016

David Zwick
PhD Student
Mechanical and Aerospace Engineering Department
University of Florida



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Work done

- I worked with the CTH code and developer team
  - Manager: Dr. John Pott (1555)
  - Mentor: Dr. Kevin Ruggirello (1555)
- CTH is a multi-material shock physics code
- The goal was to develop code for Lagrangian particle transport

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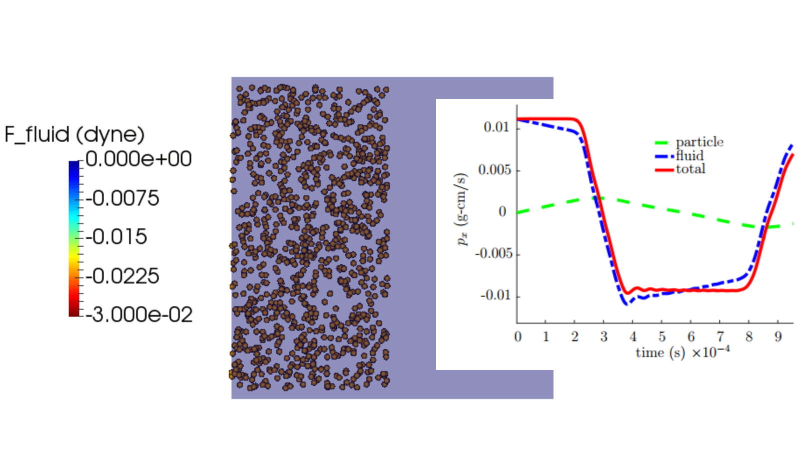
| 2

Results



CCMT | 3

Life in Albuquerque

UNM

Top of Sandia Mountains

Daily drive through Kirtland Air Force Base

Intern day with fellow intern

View from parking lot at Sandia

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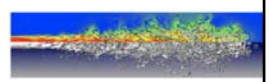
LES modeling in Nalu

Sandia National Laboratories

gmarjanovic@ufl.edu

Fall 2016

Goran Marjanovic
PhD Student
Mechanical and Aerospace Engineering
University of Florida



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The Work

- I worked with the open source code Nalu
  - Manager: Paul Crozier (1541)
  - Mentor: Stefan Domino (1541)
- Nalu is a generalized, unstructured, massively parallel low Mach code
- Implemented internal algorithm to visualize vortex structures and simulated buoyant, free shear flows to validate LES models

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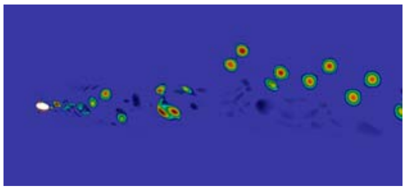
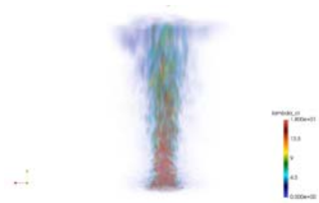
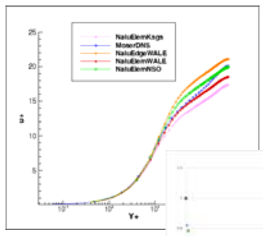
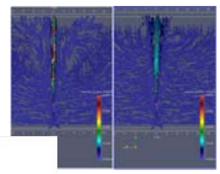
The Work





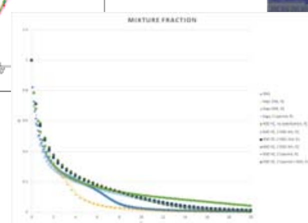




$$\mu_t = \rho \left(C_s \Delta\right)^2 |\tilde{S}|$$

$$\mu_t = C_{\mu_\epsilon} \Delta k^{\mathrm{sgs}\frac{1}{2}}$$

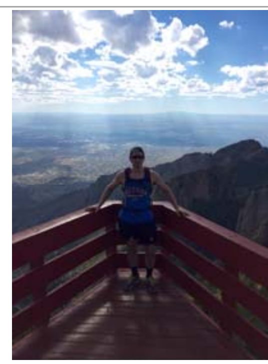
$$-\sum_e \int_\Gamma \nu(\mathbf{R}) g^{ij} \left(\frac{\partial \phi}{\partial x_j} - G_j \phi\right) n_i dS$$



CCMT | 7

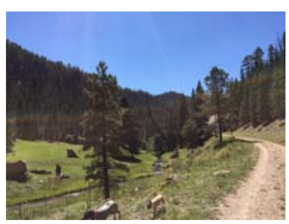
Work-Life Balance

International Balloon Fiesta



Sandia Peak

Sandia Crest



Jemez Hot Springs

Sandia Tramway

Pikes Peak (CO) 14,114 ft

CCMT | 8

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Los Alamos NATIONAL LABORATORY

Internship at Los Alamos National Lab

Georges Akiki
June-August 2016

Department of Mechanical & Aerospace Engineering

UF UNIVERSITY of FLORIDA

NNSA

UF UNIVERSITY of FLORIDA

Advisor

Dr. Marianne Francois

Group Leader,
XCP-4, Methods and Algorithms

Ph.D. in Aerospace Engineering
from the University of Florida
Go Gators

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10

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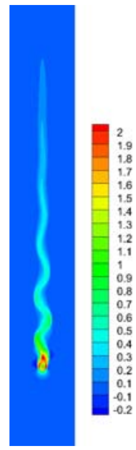
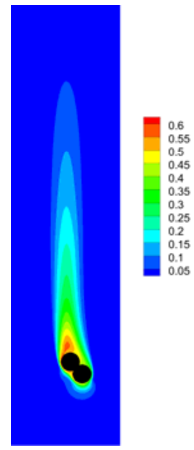
The Work

- DNS simulation of sphere sedimentation using IBM
  - Implementation
  - Validation
- DEM sphere sedimentation simulations
- Implementing IBM in MPI + Open MP code
- Valuable discussions with numerical and experimental experts





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11

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Rich History

Dr. J. Robert Oppenheimer & General Leslie Groves

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12

Life in Los Alamos

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13

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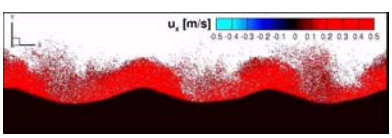
Pairwise Interaction Extended Point-Particle Model

G. Akiki, T. L. Jackson and S. Balachandar
Center for Compressible Multiphase Turbulence
University of Florida

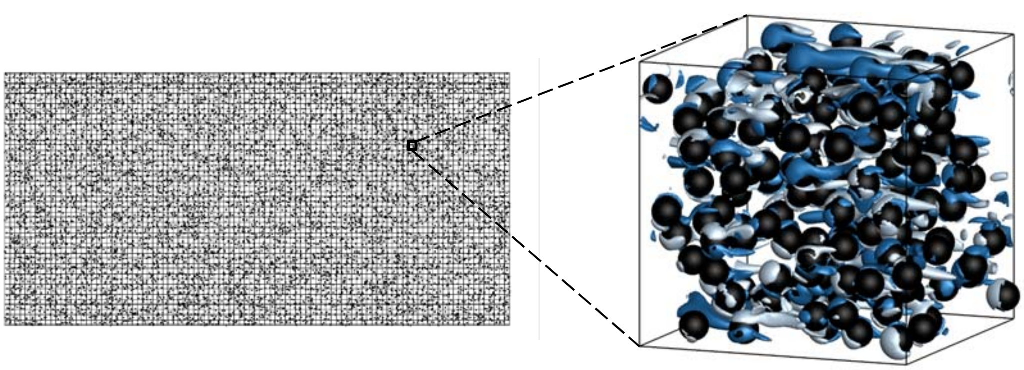
TST Review
Gainesville, Florida, Dec. 1-2, 2016

Point-Particle Model



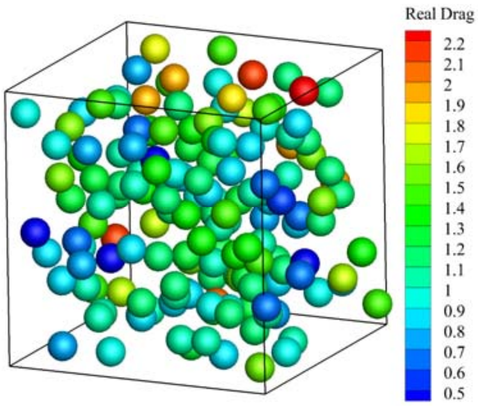
Closure Models obtained at the microscale:
✓ Mean cell velocity
✓ Mean cell volume fraction
→ Mean drag model: $F(\phi, Re)$

- Exact location of particles ?

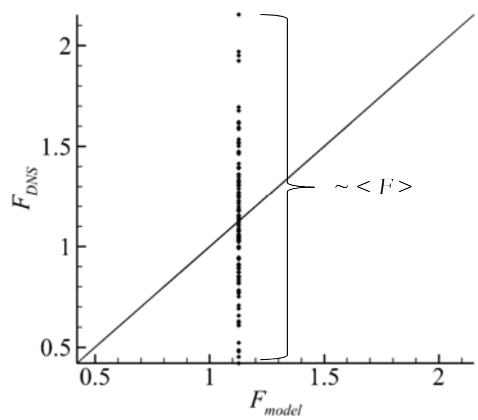


2/24

Goal of Model



$R^2 = 0.00$

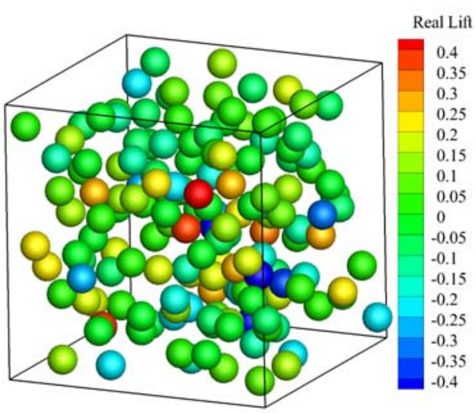


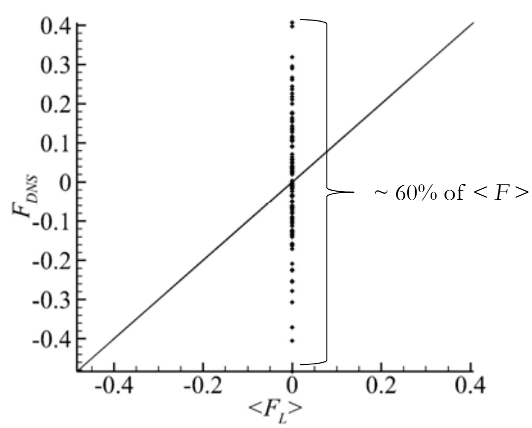
$$R^2 = 1 - \frac{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - F_{model}(n) \right]^2}{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - \langle F_{DNS} \rangle \right]^2}$$

If the model is a fully-resolved DNS simulation!

3/24

Goal of Model





No lift force point-particle model currently in use

4/24

Outline

- Motivation
- Pairwise Interaction Extended Point-particle (PIEP) Model
- PIEP Model in Sedimentation Problem
- Summary and Future Work

Outline

- Motivation
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Pairwise Interaction

Force on a single sphere in a steady non-uniform flow at finite *Re*:

$$\boldsymbol{F} = 3\pi\mu d\boldsymbol{u}_{un}(1+0.15Re^{0.687}) + m_f(1+C_m)\frac{D\boldsymbol{u}_{un}}{Dt} + m_f C_{IL}\boldsymbol{u}_{un}\times\boldsymbol{\omega}_{un}$$

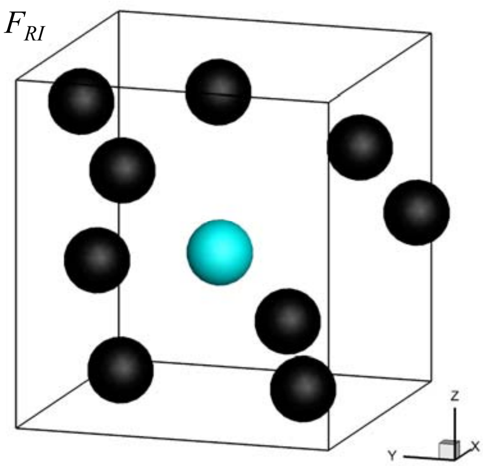
F_{QS} F_{II} F_{RI}

Undisturbed Velocity:

$$\boldsymbol{u}_{un,i}(\boldsymbol{x}_i) = \boldsymbol{u}_{macro}(\boldsymbol{x}_i) + \tilde{\boldsymbol{u}}_{\forall N\to i}(\boldsymbol{x}_i)$$

Pairwise Interaction assumption:

$$\boldsymbol{u}_{un,i}(\boldsymbol{x}_i) \approx \boldsymbol{u}_{macro}(\boldsymbol{x}_i) + \sum_{j=1}^{N-1}\tilde{\boldsymbol{u}}_{j\to i}(\boldsymbol{x}_i)$$



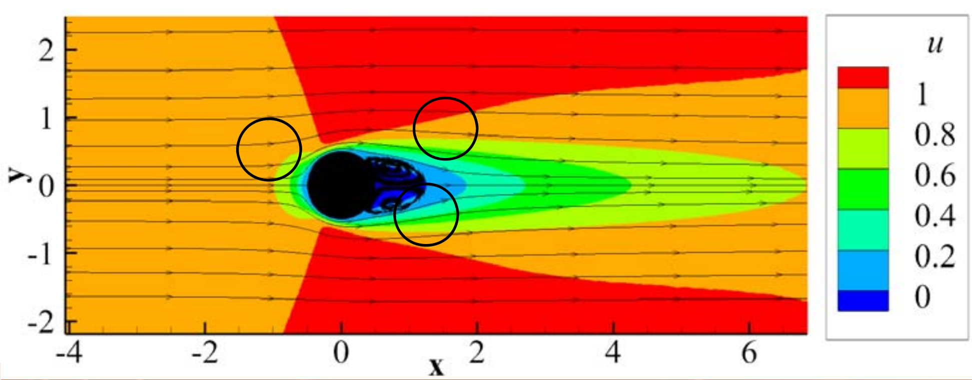
Effect on Neighbor

$$\boldsymbol{F}_{QS} = 3\pi\mu\overline{\left(\boldsymbol{u}_{un}(\boldsymbol{x})\right)}^{S} d\left[1+0.15\left(Re\right)^{0.687}\right]$$

$$\boldsymbol{F}_{II} = (1+C_m)\rho\iiint_{|\boldsymbol{x}-\boldsymbol{x}_i|\le d/2}\frac{D\boldsymbol{u}_{un}(\boldsymbol{x})}{D\hat{t}}d\boldsymbol{x}$$

$$\boldsymbol{F}_{RI} \approx C_{IL}\rho\iiint_{|\boldsymbol{x}-\boldsymbol{x}_i|\le d/2}\left[\boldsymbol{u}_{un}(\boldsymbol{x})\times\boldsymbol{\omega}_{un}(\boldsymbol{x})\right]d\boldsymbol{x}$$

We use the Generalized Faxén's theorem to account for non-uniformity.

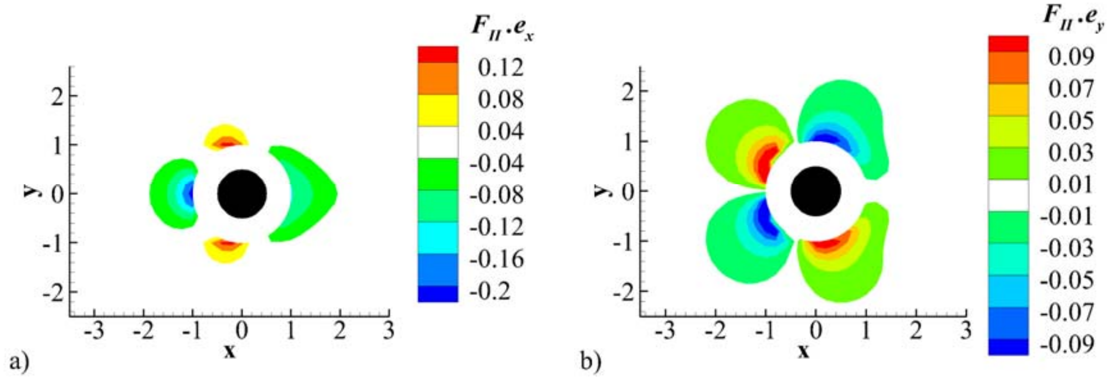


8/24

Irrotational Inviscid Force Mappings

$$\boldsymbol{F}_{II} = (1+C_m)\rho \iint_{|\boldsymbol{x}-\boldsymbol{x}_i|=d/2} \left[\boldsymbol{\tau} - p\boldsymbol{I}(\boldsymbol{x})\right].\boldsymbol{n}dx$$

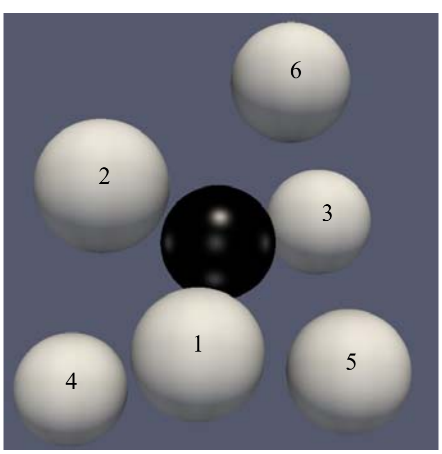
$$F_{II,map} = \iint_{|\boldsymbol{x}-\boldsymbol{x}_i|=d/2} \left[\boldsymbol{\tau} - p\boldsymbol{I}(\boldsymbol{x})\right].\boldsymbol{n}dA$$



Streamwise Force

Lateral Force

Pairwise Interaction Extended Point-Particle (PIEP) Model



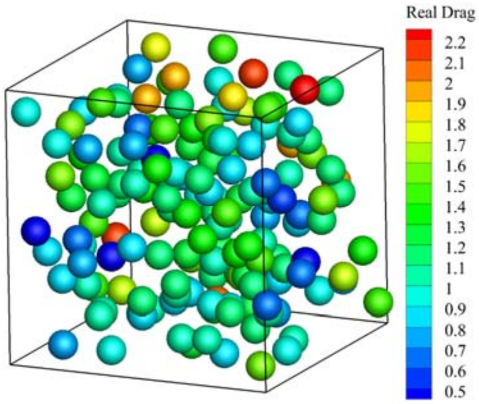
$$\boldsymbol{F}_{QS,PI}(i) = \frac{3\pi}{Re}\left[\sum_{j=1}^{P} \overline{\left(\boldsymbol{u}_{un}(\boldsymbol{x}_i - \boldsymbol{x}_j)\right)}^{S}_{map}\right]\left[1+0.15\left(Re_{surf}(i)\right)^{0.687}\right]$$

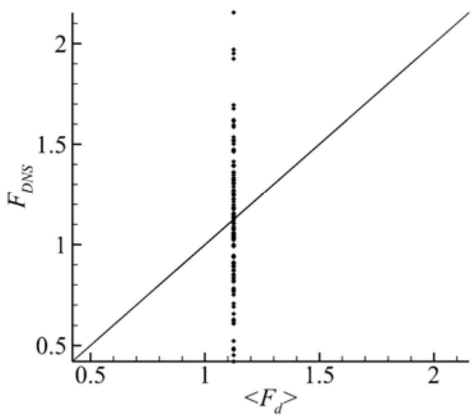
$$\boldsymbol{F}_{II,PI}(i) = (1+C_m)\sum_{j=1}^{P} \boldsymbol{F}_{II}(\boldsymbol{x}_i - \boldsymbol{x}_j)_{map}$$

$$\boldsymbol{F}_{RI,PI}(i) = C_{IL}\left(\sum_{j=1}^{P} \overline{\left(\boldsymbol{u}_{un}(\boldsymbol{x}_i - \boldsymbol{x}_j)\right)}^{V}_{map}\right) \times \left(\sum_{j=1}^{P} \overline{\left(\omega_{un}(\boldsymbol{x}_i - \boldsymbol{x}_j)\right)}^{V}_{map}\right)$$

$$\boxed{\boldsymbol{F}_{PIEP} = \boldsymbol{F}_{QS,PI} + \boldsymbol{F}_{II,PI} + \boldsymbol{F}_{RI,PI}}$$

PIEP vs DNS for drag

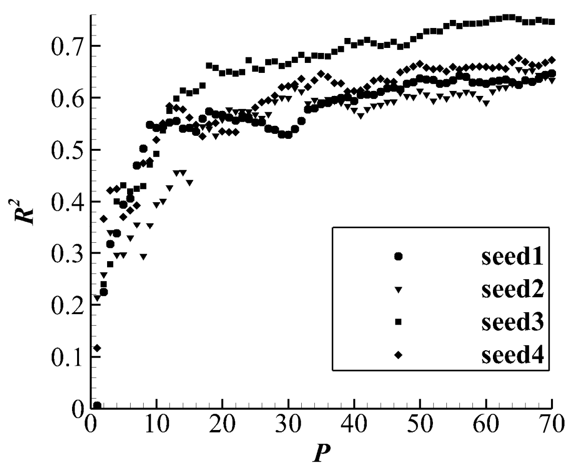




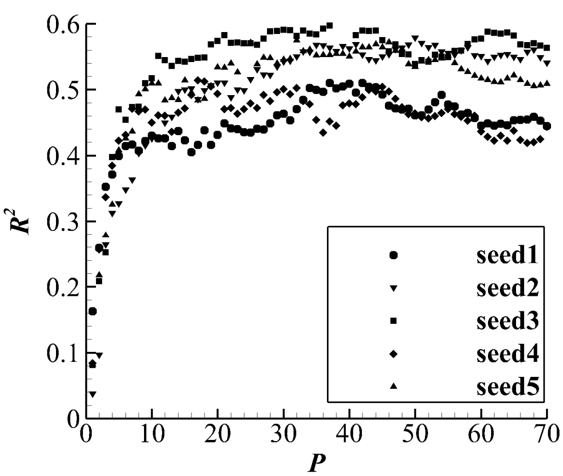
With Quasi-Steady, Irrotational Inviscid and Rotational Inviscid Force Correction

PIEP Using Limited Neighbors

P is the number of neighbors included in the model

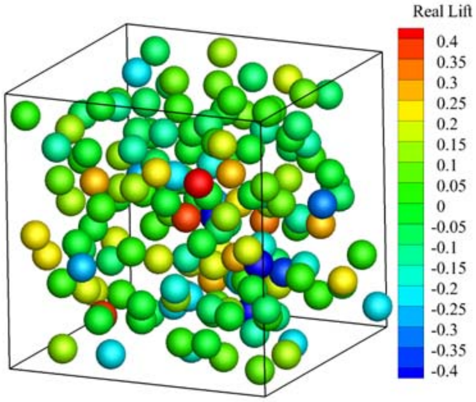


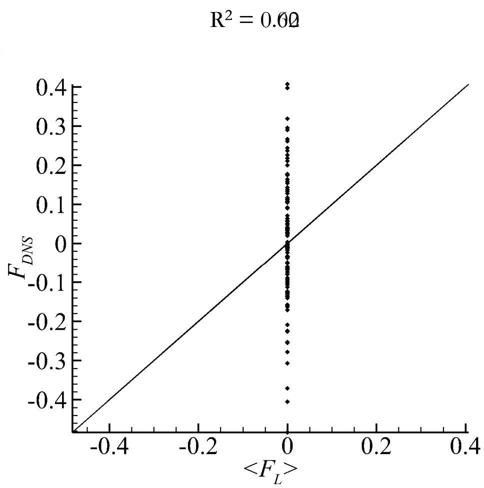
$\phi = 0.1$ $Re = 38$



$\phi = 0.2$ $Re = 16$

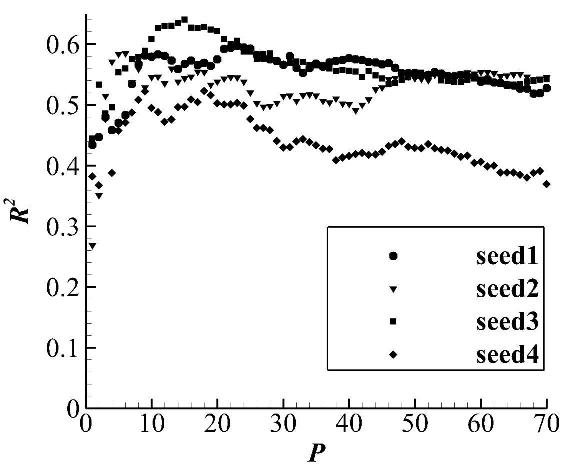
PIEP vs DNS for lift

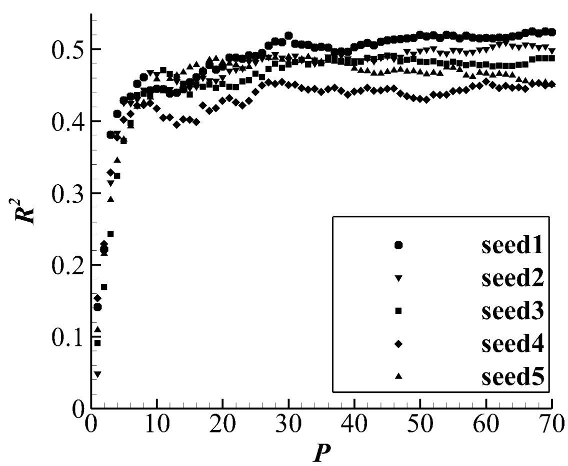




With Quasi-Steady, Irrotational Inviscid, and Rotational Inviscid Force Correction

PIEP Using Limited Neighbors (lift)





Outline

- Motivation
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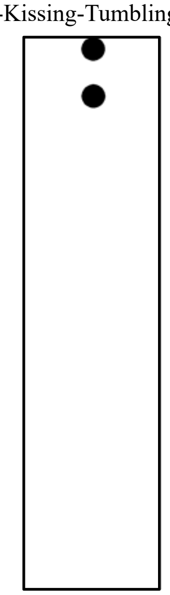
Using PIEP for Sedimentation

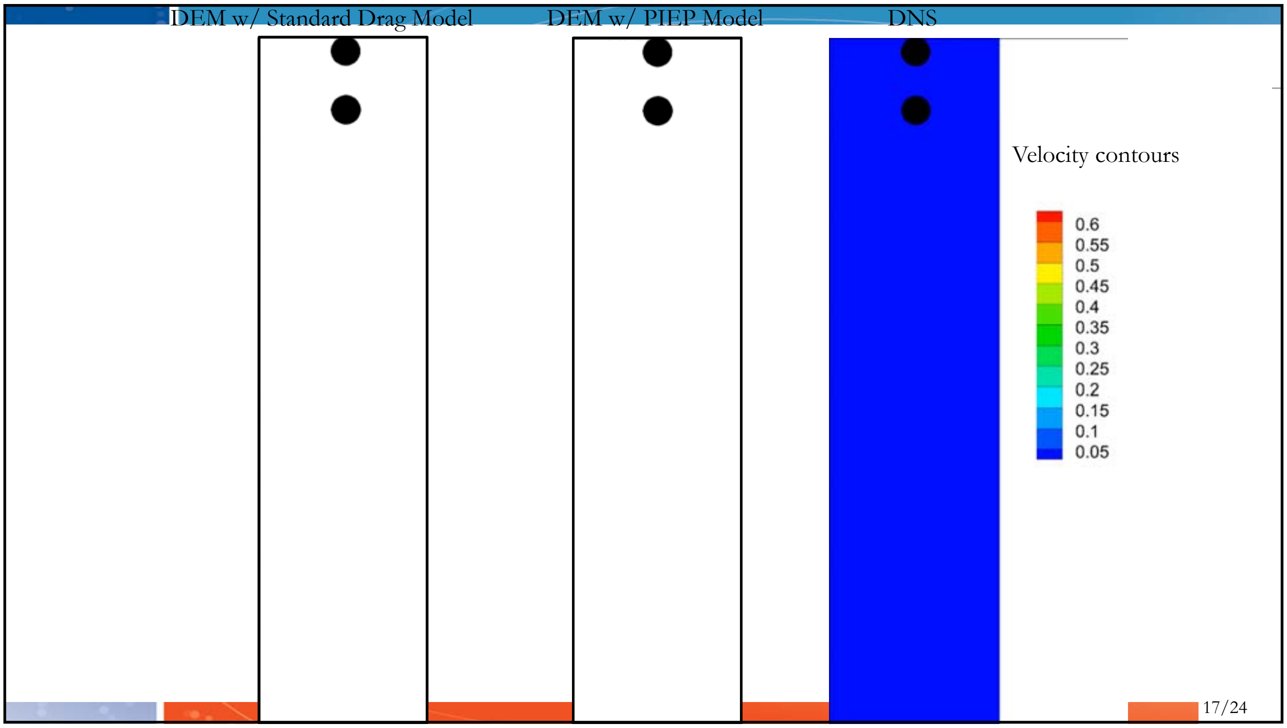
Drafting-Kissing-Tumbling test case



Equations of Motion:

$$\begin{cases} \dfrac{d\tilde{\boldsymbol{x}}_i}{d\tilde{t}} = \tilde{\boldsymbol{v}}_i \\ \tilde{m}_i \dfrac{d\tilde{\boldsymbol{v}}_i}{d\tilde{t}} = (\tilde{m}_i - \tilde{m}_{fi})\,\tilde{\boldsymbol{g}} + \tilde{\boldsymbol{F}}_{hyd,i} + \tilde{\boldsymbol{F}}_{lu,i} + \tilde{\boldsymbol{F}}_{col,i} \\ \tilde{I}_i \dfrac{d\tilde{\boldsymbol{\Omega}}_i}{d\tilde{t}} = \tilde{\boldsymbol{T}}_{hyd,i} + \tilde{\boldsymbol{T}}_{lu,i} + \tilde{\boldsymbol{T}}_{col,i} \end{cases}$$

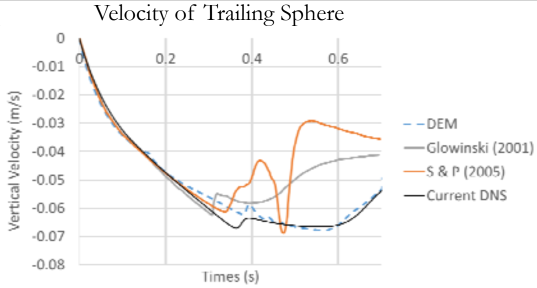
F_{hyd} is obtained using PIEP to account for the position of the second sphere.



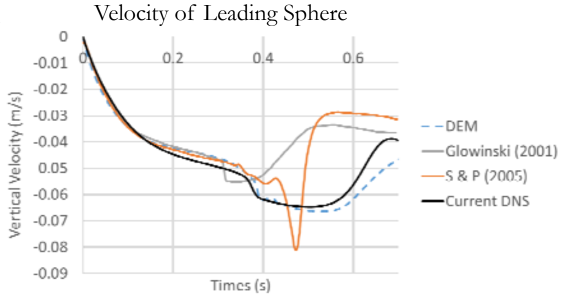
17/24

Vertical Velocity Comparison

Velocity of Trailing Sphere



Velocity of Leading Sphere



Parameters:

$\frac{\rho_p}{\rho_f} = 1.14$

$v = 1\times10^{-6}\ \text{m}^2/\text{s}$

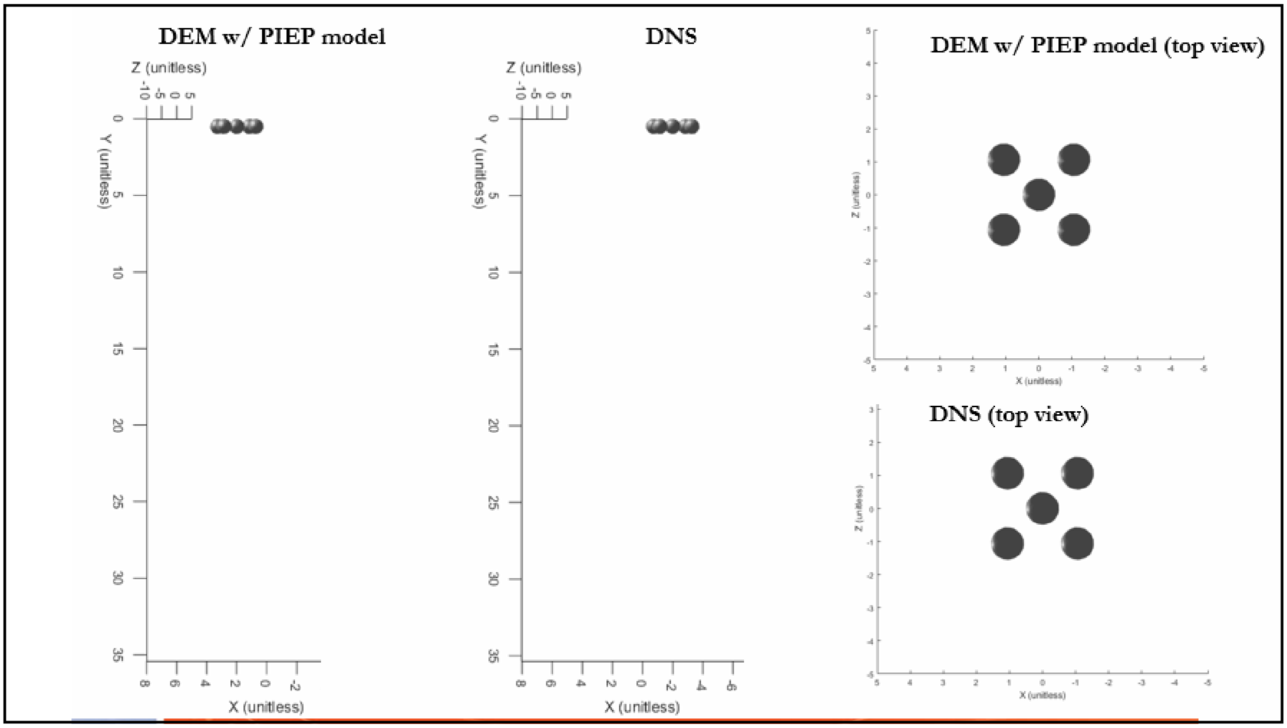
$d = 1/600\ \text{m}$

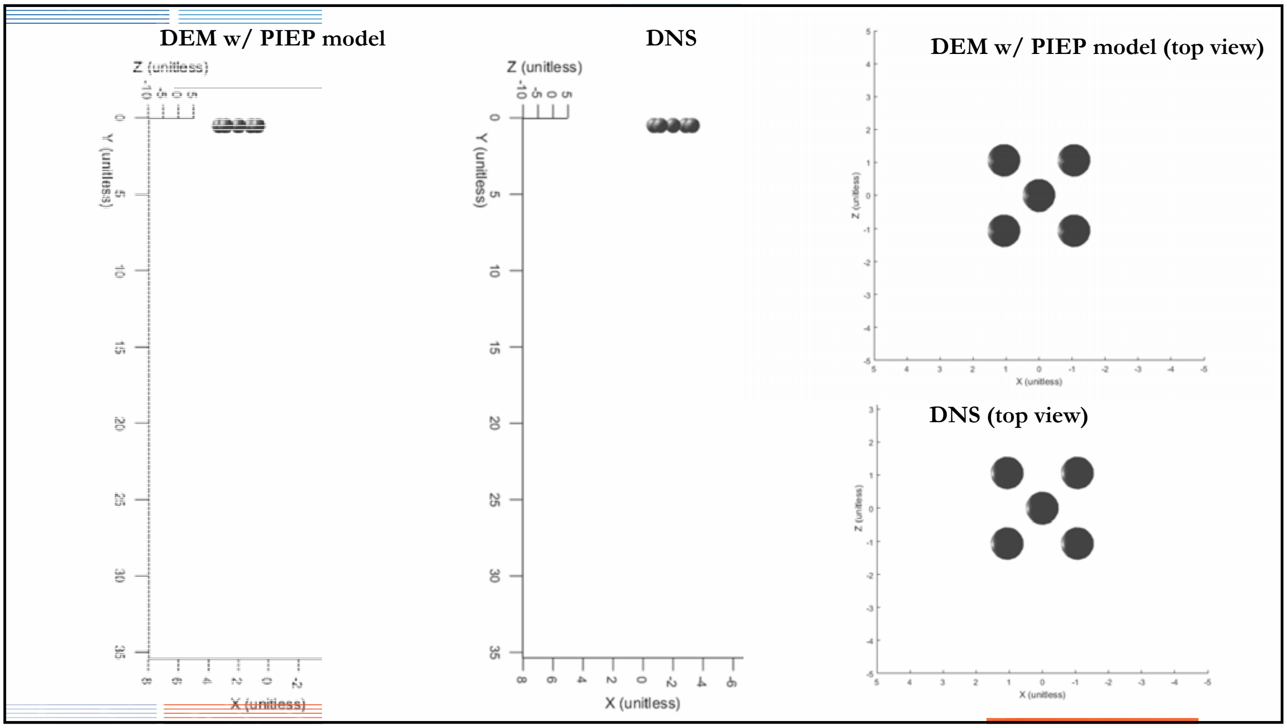
$Re_{p(\max)} \simeq 112$

Other studies running the same case using DNS:

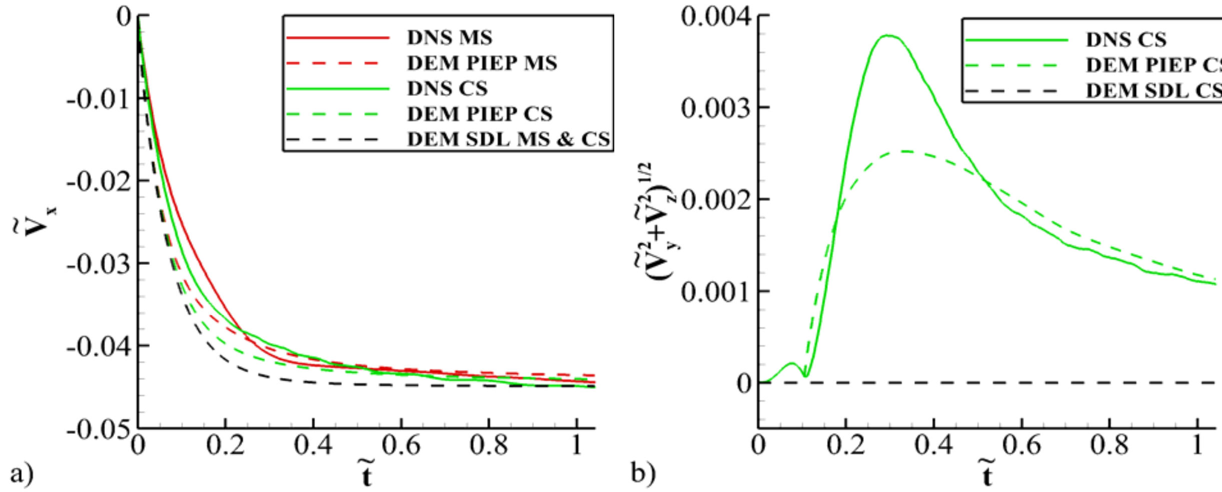
- Glowsinki, JCP 2001
- Sharma & Patankar, JCP 2005

18/24

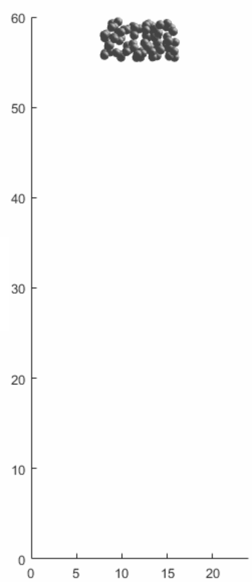

DEM w/ PIEP model
DNS
DEM w/ PIEP model (top view)
DNS (top view)
Z (unitless)
Y (unitless)
X (unitless)


DEM w/ PIEP model
DNS
DEM w/ PIEP model (top view)
DNS (top view)
Z (unitless)
Y (unitless)
X (unitless)

Velocity Comparison

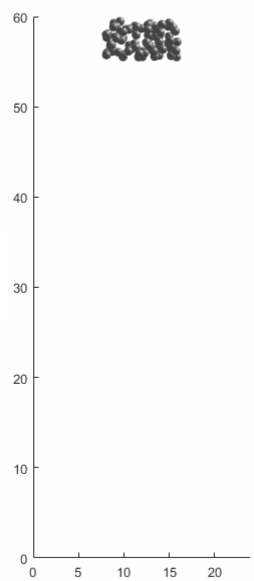


DEM w/PIEP



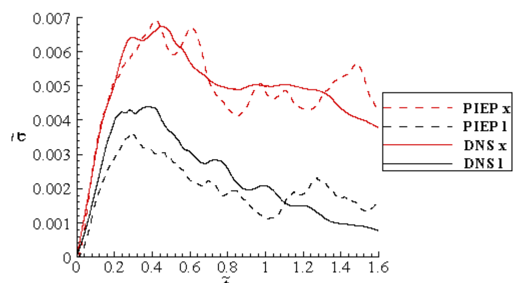
0.5 CPU core hours

DNS

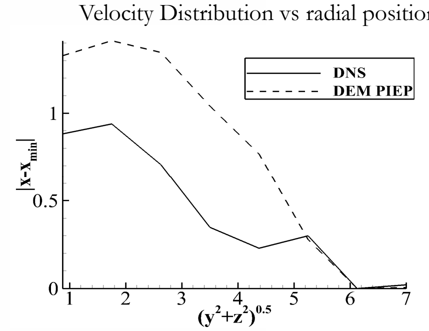


1165 CPU core hours

Velocity Distribution vs time



Velocity Distribution vs radial position



Summary and Future Work

- Quantified the drag and lateral force variations within random arrays of spheres.
  - Standard deviation of the drag distribution is very significant with respect to the mean (~17%-27%).
  - Standard deviation of the lateral force distribution is approximately 14% of the mean drag.
- We developed a model (PIEP) which can approximate the drag and lateral force on each particle using the relative locations of few neighboring particles.
- Demonstrated the capability of PIEP model to simulate complicated particle-particle physics in multiple sphere sedimentation.

Future Work:

- Implementing PIEP model in Eulerian-Lagrangian simulations and compare statistics with classical point-particle models.
- Using PIEP model to explore sedimentation problems with a large number of particles.

Thank you
Questions?

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Experimental Studies of Gas-Particle Mixtures Under Sudden Expansion

Blair Johnson, Ph.D., Heather Zunino
Prof. Ronald Adrian & Prof. Amanda Clarke

School for Engineering of Matter, Transport & Energy
Arizona State University

UF UNIVERSITY of FLORIDA

NNSA

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Previous Research

- Turbulent boundary layers in absence of mean flow
- Characterization of velocity fluctuations, turbulent kinetic energy, energy dissipation rates, integral scales of turbulence, energy spectra
- Parameterization of bed stress with zero mean shear stress

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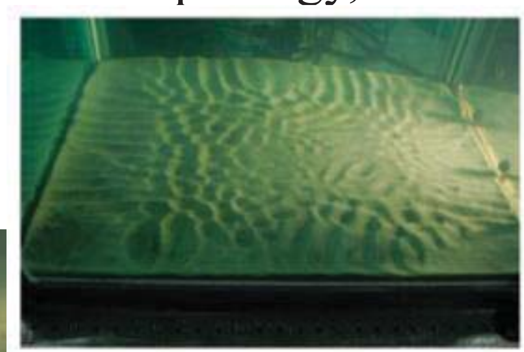
Interaction between turbulence and bed morphology, sediment suspension



Turbulence → Ripples

Ripples → Drag

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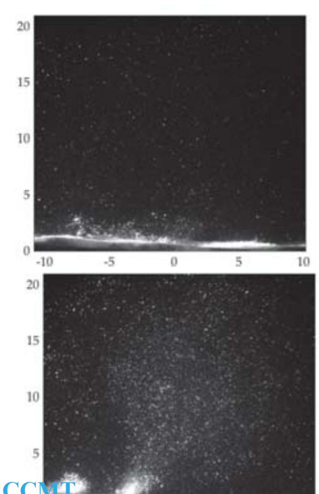
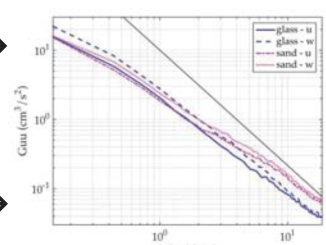
Interaction between turbulence and bed morphology, sediment suspension

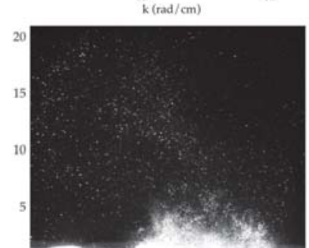


Turbulence → Sediment Suspension

Suspension → Drag?

Suspension → Increased Turbulence!





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  - Image De-warping
  - Fourier Analysis → Cell Frequency
  - Streaks / Void Tracking
  - Particle Image Velocimetry
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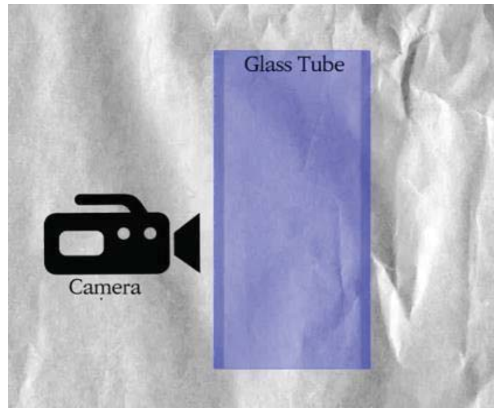
Review Experiment

- Tall glass tube
- Particle bed
  - Ballotini glass spheres (Potters Inc.)
    - 44-88 µm
    - 88-149 µm
    - Typical bed filled to 32 cm depth
- Diaphragm
- High-speed cameras
  - Phantom v641 4-megapixels
    - 1 µs minimum exposure
    - 10,000 fps sampling
    - Constant external illumination
- Parameters: particle size and pressure ratio



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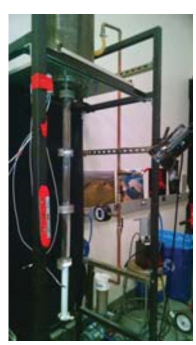
Shock Tube Experimental Setup



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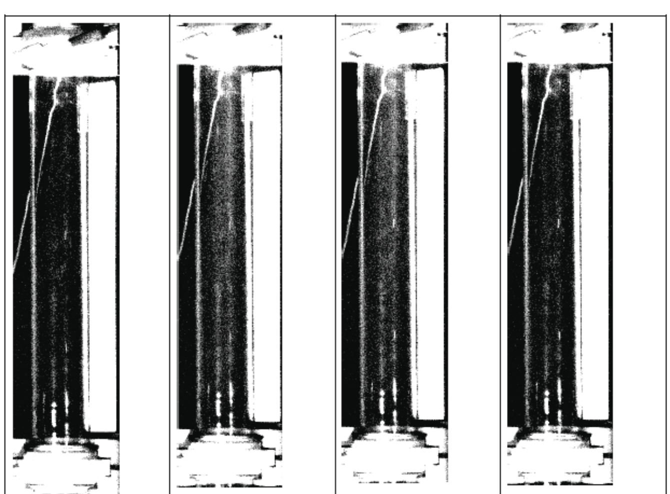
Stages of Decompression: Cloud



t_0 $t_0 + 0.6$ ms t_0 $t_0 + 0.9$ ms t_0 $t_0 + 1.8$ ms

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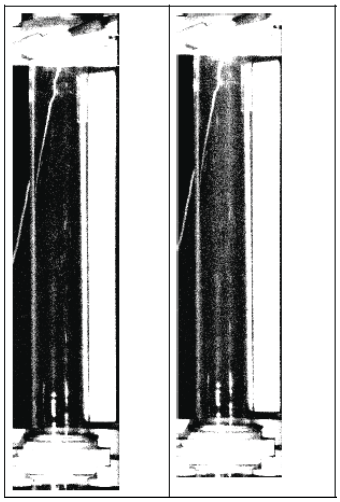
Stages of Decompression: Cloud



t_0 $t_0 + 0.6$ ms

- Water vapor rapidly condenses and freezes
- Observed both with and without particle bed
- Temperature drop of 50K predicted by Bertrand Rollin & simulation team

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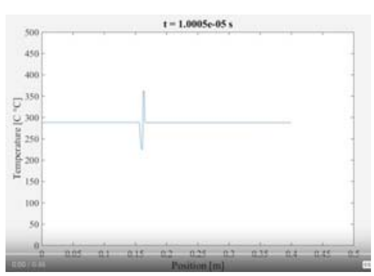
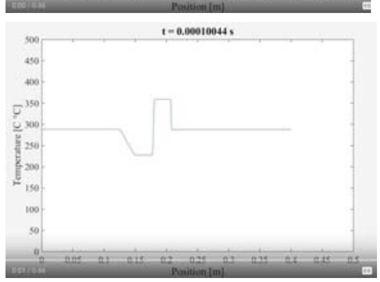
Stages of Decompression: Cloud





- Water vapor rapidly condenses and freezes
- Observed both with and without particle bed
- Temperature drop of 50K predicted by Bertrand Rollin & simulation team
- No instruments presently available to measure this experimentally

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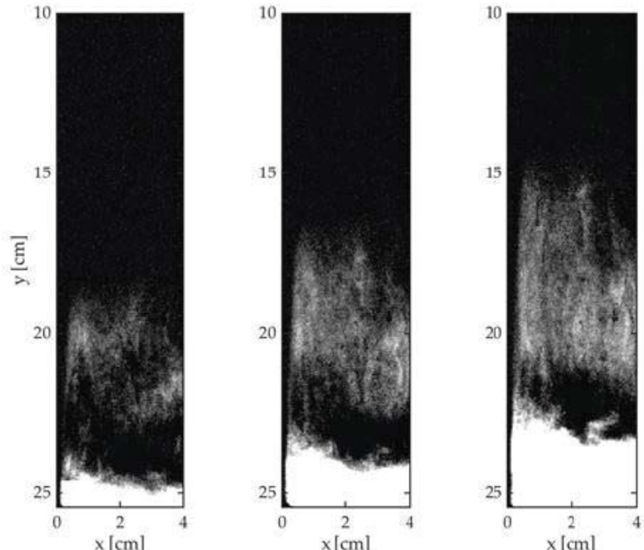
Stages of Decompression: Puff



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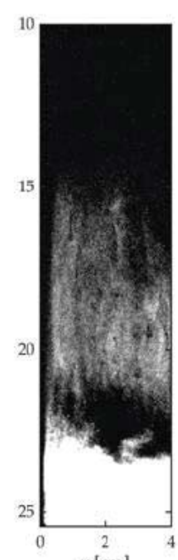
Stages of Decompression: Puff

- Tiny particles / fines
- Rise prior to bed decompression
- Accelerates away from the bed



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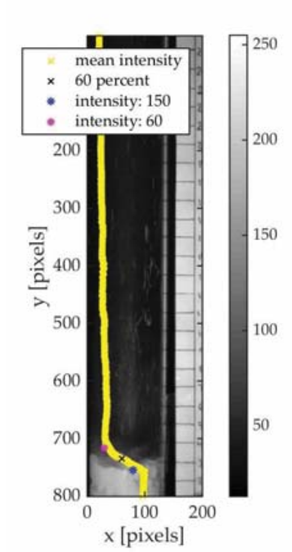
Preliminary Results: Bed Diffusion



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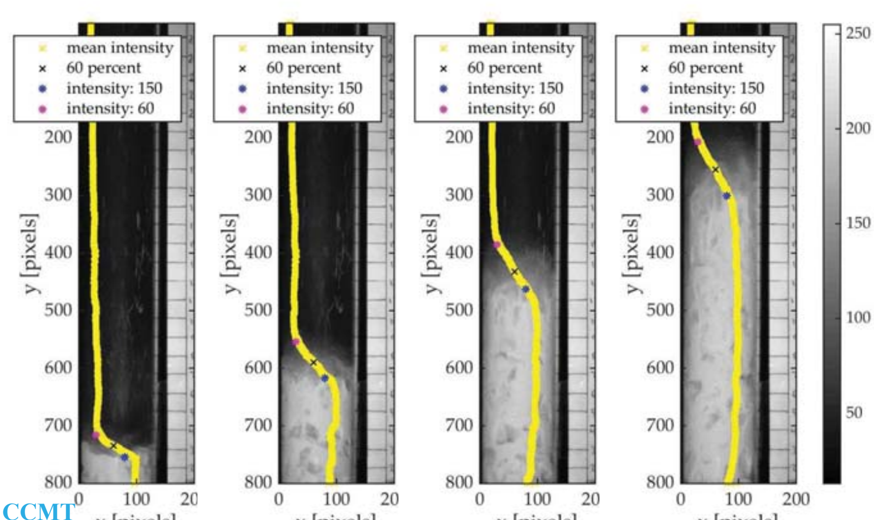

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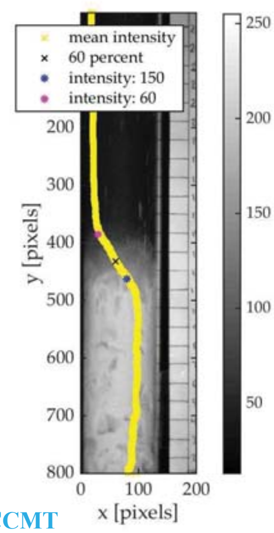

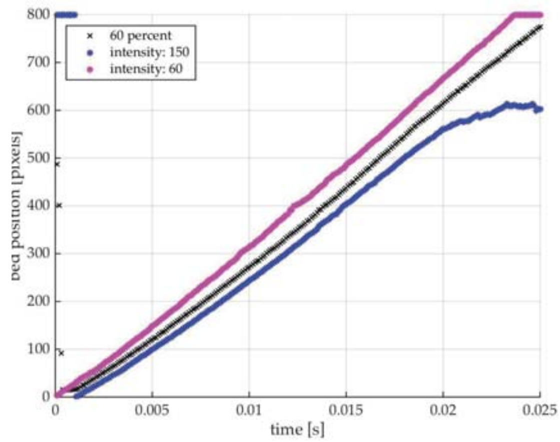

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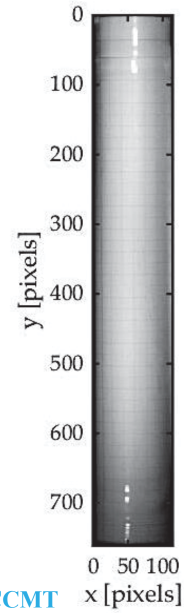
Image De-warping



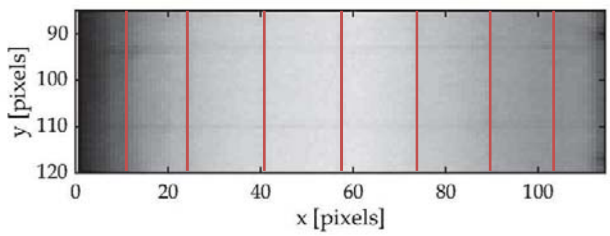


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Image De-warping

- Starting with circle; equally spaced tangential segments:
- Project segments onto straight line:
- Stretch projection into equally-sized segments
- Edges of cylinder not fully visible in photos
- Camera not perfectly centered

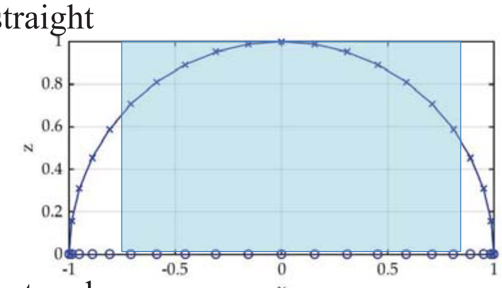

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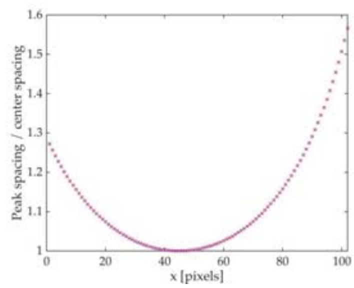
Image De-warping

- Compute image intensity (blue) across width of image
- Identify valleys as grid (pink circles)
- Stretch edges according to ratio relative to center



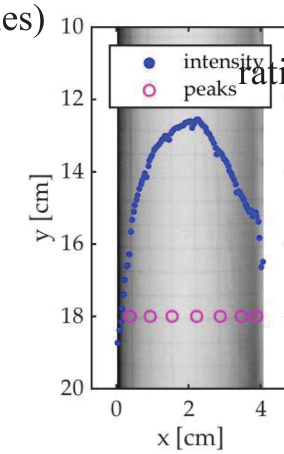


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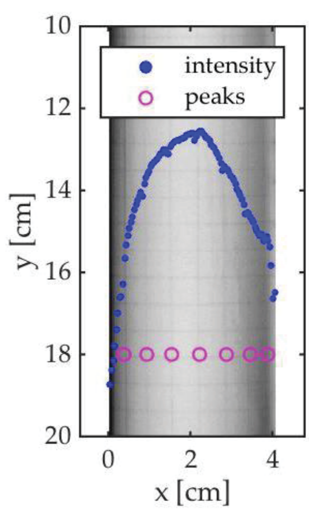
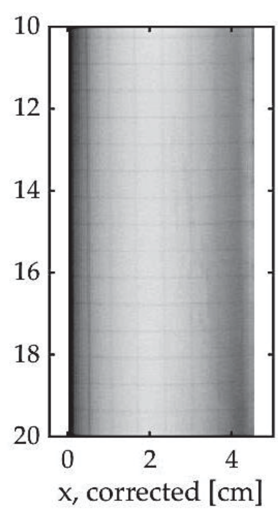
Image De-warping





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Slow Decompression

- Small leak in diaphragm
- Slower pressure drop in particle bed
- Similar features seen when there is a sudden decompression
  - "Boiling"
  - Pattern of cells appears
  - Sinusoidal surface deformation
- Big cells race to the top
  - Highly disruptive
  - Compress or capture smaller cells

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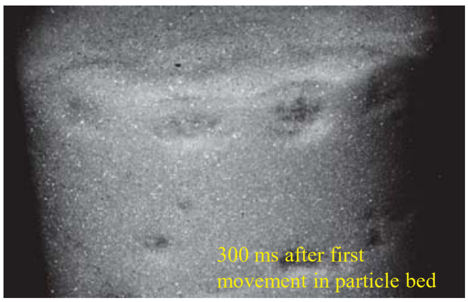
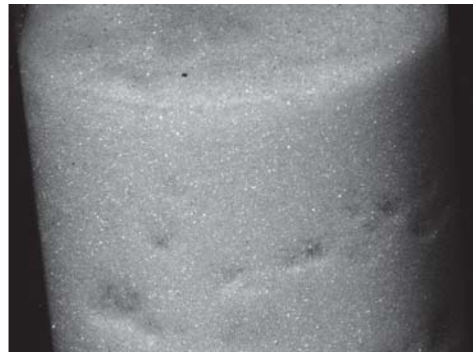
Slow Leak - Rapid Decompression

- Cell structure pattern
  - Immediately formed
  - Relatively uniform
  - Still disturbed by large cells





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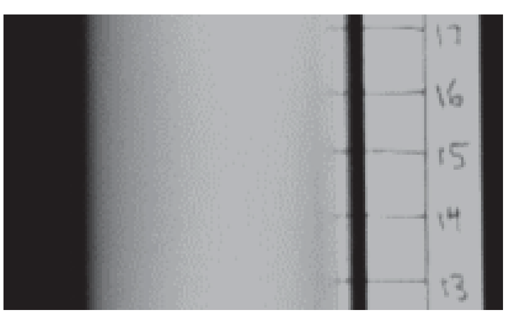
Cell Frequency Comparison



44 – 88 micron particles

88 – 149 micron particles

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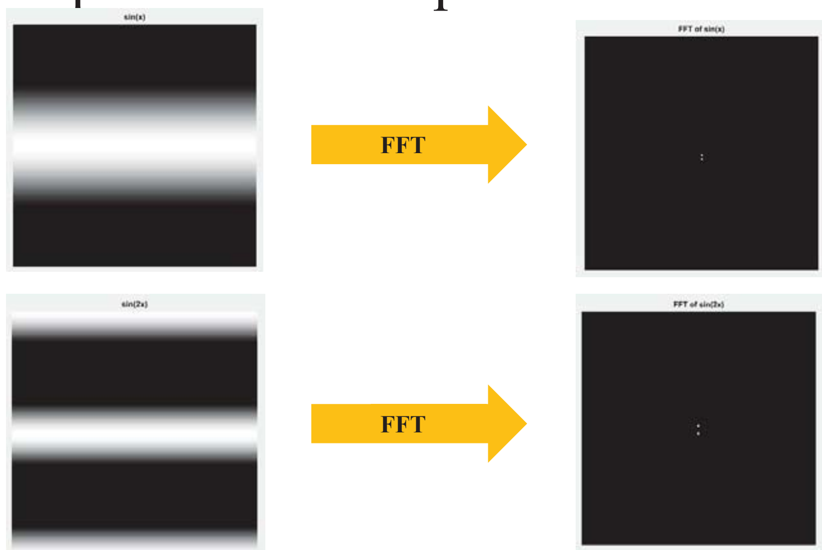
Simple Visual Interpretation of FFT



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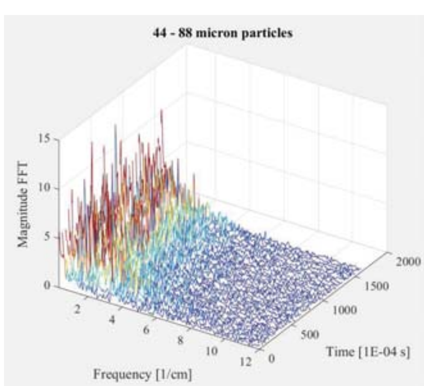
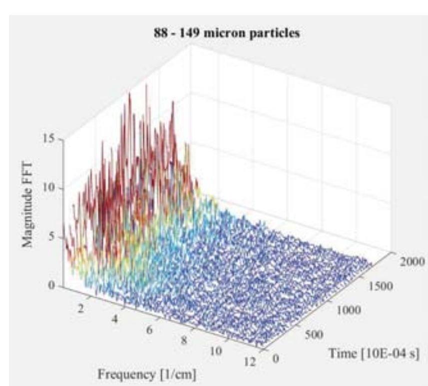
Fourier Analysis – Cell Frequency





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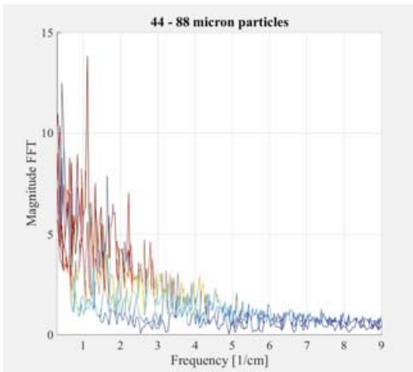

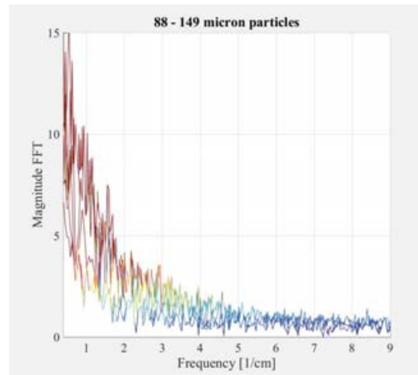

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Conclusions

- When particle bed is decompressed, particle vacant regions appear within the bed
  - Highly irregular pattern appears when the bed is decompressed slowly
  - Semi-regular pattern appears when the bed is rapidly decompressed
- Initially, horizontal cracks appear near the top first and propagate deeper into the bed
- The horizontal cracks then evolve into separated cells
- The pattern associated with these cells and cracks has a dependence on particle size
  - The larger particles yield patterns with longer wavelengths (lower frequencies)
  - The smaller particles yield patterns with shorter wavelengths (higher frequencies)

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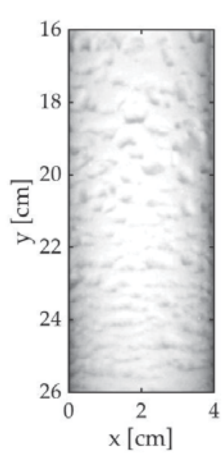
Tracking voids via "Streak" analysis

- Voids typically appear as dark regions
- Track velocity, merging, expansion, etc. of voids



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Tracking voids via “Streak” analysis

- Voids typically appear as dark regions
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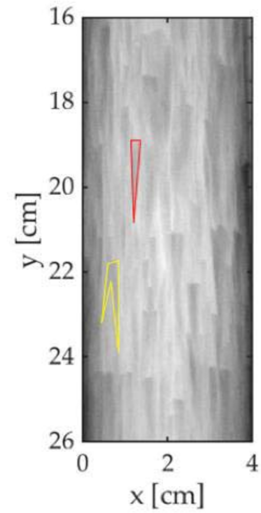
- Compute minimum image intensity across time to construct streak of void paths



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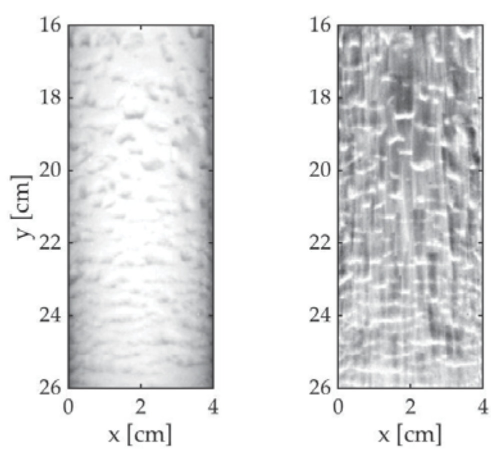

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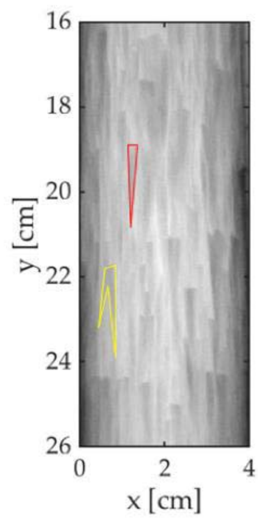

Elapsed time:
5 ms

Average vertical velocity of voids:
~ 400 cm/s

Widen to approximately:
4-5 mm

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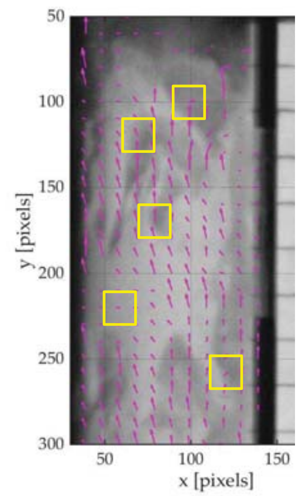
Particle Image Velocimetry (PIV)

- MatPIV: Sub-pixel correlation peak locating algorithm (Liao & Cowen, 2005)
- Δt = 0.3 ms
- Tracking edges, not particles



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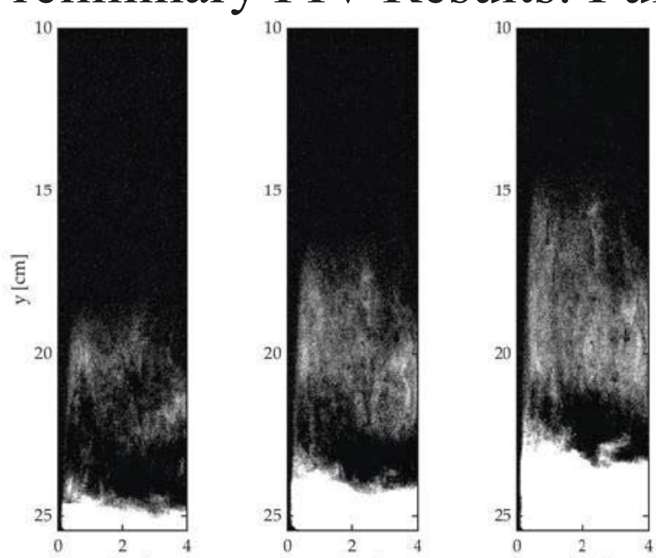
Preliminary PIV Results: Puff



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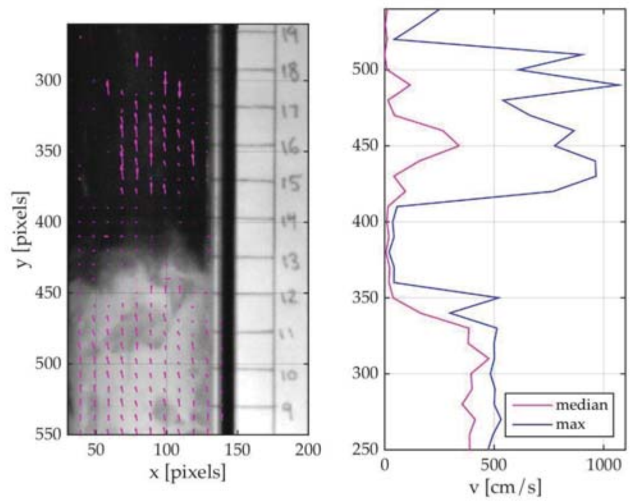

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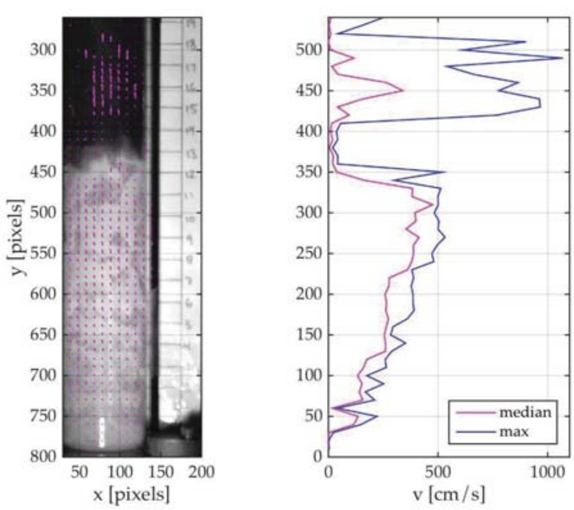

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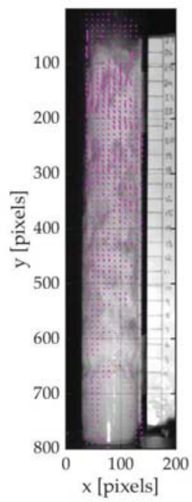
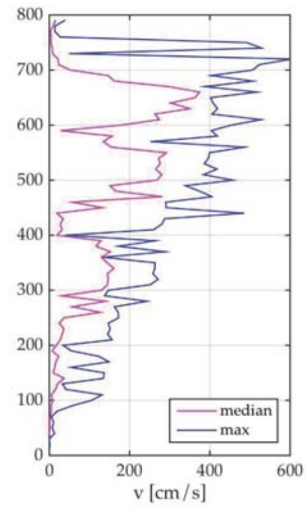
Preliminary PIV Results: Velocity Profile





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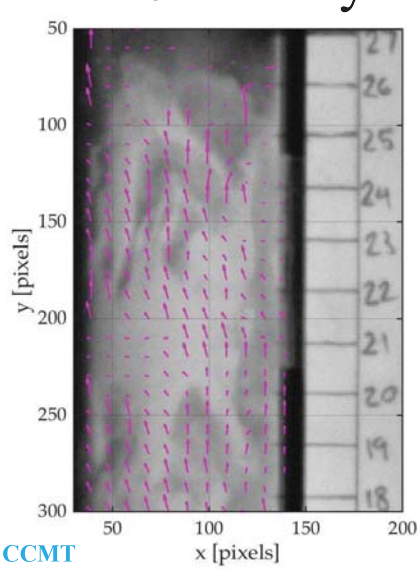
Preliminary PIV Results: Voids



- Lateral motions as voids deform/expand
- Bottoms of voids rise faster than tops of voids
- Better PIV performance at interfaces, dilute regions than smooth particle-filled surfaces

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Upcoming work: PIV of Gas Phase

- Transition to turbulence in compressible gas
- Influence of glass particles on stirring of gas phase
- Determine "viscosity" of both dilute and dense particle phases

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Upcoming work: PIV of Gas Phase

- Nd:YAG double-pulse laser from Litron,
  - 200mJ power
  - 532nm wavelength
- Phantom high speed camera (10-20k fps)
- Gas tracers:
  - 10 µm silver-coated or fluorescent particles
  - smoke
- Differentiate between glass particles and gas tracer particles

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Upcoming work: New Pressure Sensor System

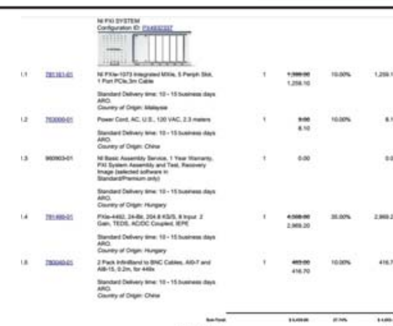
- 8 pressure sensors
  - 15% discount
  - Donated cables
- New DAQ
  - 35% discount
  - Capable of sampling all pressure sensors at 150kHz

Quoted Items

Qty	Model	Description	Delivery	Unit Price	Disc. Price	Extended Net
8	113B28	Platinum Stock Products;High frequency ICP® pressure sensor, 50 psi, 100 mV/psi, 0.218" dia. diaphragm, accel. comp.	Currently In Stock	$590.00	$500.00	$4,000.00
			Subtotals:			$4,000.00

Suggested Accessories

Qty	Model	Description	Delivery	Unit Price	Disc. Price	Extended Net
8	003C10	Low-noise coaxial cable, blue TFE jacket, 10-ft, 10-32 coaxial plug to BNC plug	Currently In Stock	$54.00	$0.00	$0.00
			Subtotals:			$0.00



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Uncertainty Quantification of Eglin Experimental Data

Kyle Hughes
Graduate Student
University of Florida

Angela Diggs
Air Force Research Laboratory
Munitions Directorate
Eglin Air Force Base, Florida

Distribution A. Approved for public release. Distribution unlimited. 96TW-2016-0208.

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Overview

- Validation of simulations requires significant communication between experimentalists and computationalists
- CCMT leadership identified this communication as lacking and added myself (December 2015) to the team and Eglin provided Angela as a point of contact
- Assist with processing of the data from experiments conducted before I was added to the team
- Perform uncertainty quantification of the completed experiments
- Work with Angela to provide any relevant information to the simulation teams
- Assist with planning of future experiments to reduce uncertainty

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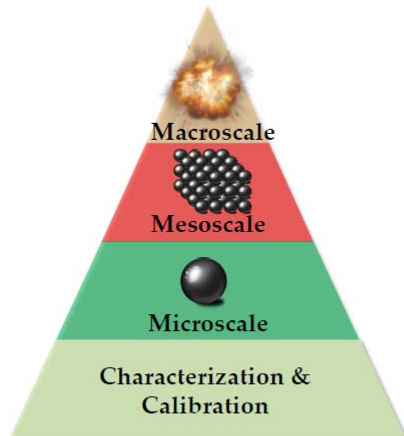
2

Validation Hierarchy

- CCMT employs a physics-based validation hierarchy
- Eglin conducts experiments at all three scales of interest to CCMT
- **Microscale** (O(1-10^4) particles)
  - Validation of microscale drag models
  - Explosive tests conducted October 2014 and February 2015
- **Mesoscale** (O(10^6) particles)
  - Examination of instabilities, volume fraction effects
  - Explosive tests conducted November 2015
  - Gas gun tests in planning stages
- **Macroscale** (O(10^9) particles)
  - Validation of full simulation
  - Explosive tests (AFRL blastpad) in planning stages



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3

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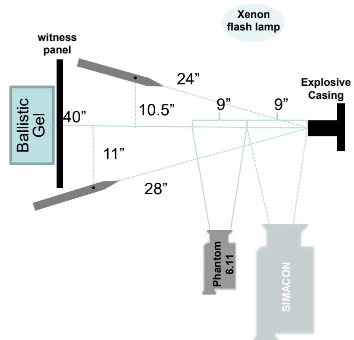
Microscale Experiments

Microscale Experiments: October 2014

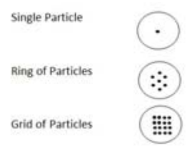
Side view photograph of the experimental setup.



Overhead schematic of the experimental setup.

Summary of test shots performed in October 2014.

Test #	Driver	Particle(s)
Oct14-1	RP-83 + 3 N5	Single (2 mm dia) Tungsten sphere
Oct14-2	RP-83 + 3 N5	Ring of 7 (2 mm dia) Tungsten spheres
Oct14-3	RP-83 + 3 N5	Grid of 16 (2 mm dia) Tungsten spheres



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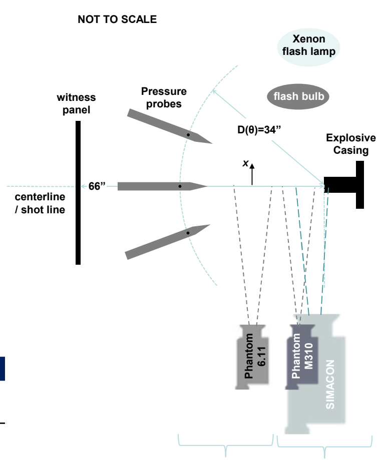
5

Microscale Experiments: February 2015

Side view photograph showing the concave pressure probe array.



Overhead schematic of the test set-up.

Summary of test shots performed in February 2015.

Test #	Driver	Particle(s)
Feb15-7	RP-83 + 3 N5	Single (2mm dia) Tungsten sphere
Feb15-8	RP-83 + 3 N5	Single (2mm dia) Tungsten sphere
Feb15-12	RP-83 + 3 N5	4 (2 mm dia) Tungsten spheres (diamond pattern)

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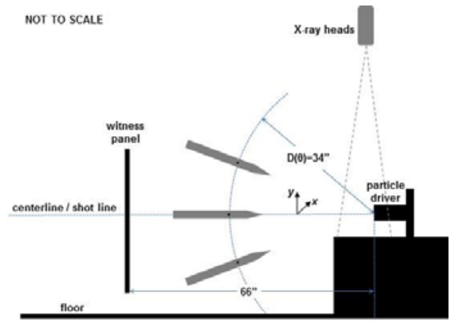
6

Microscale Experiments: February 2015

Photo of the test set-up showing 4 x-ray heads.



Side-view schematic of the test set-up.

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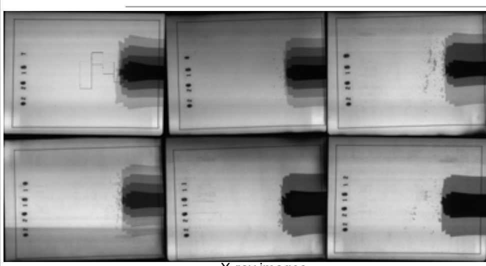
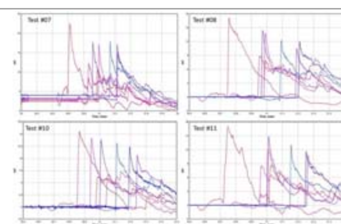
7

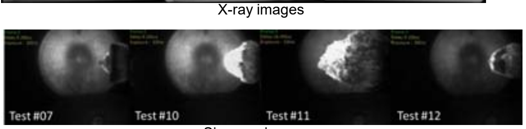
Microscale Experiments: Sample Data



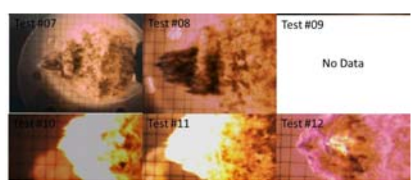
X-ray images



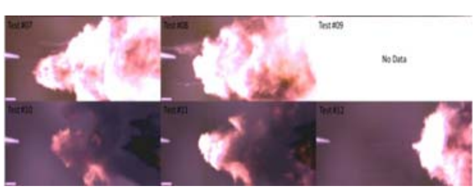
Pressure histories



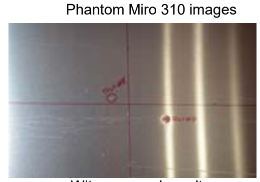
Simacon images



Phantom Miro 310 images



Phantom 6.11 images



Witness panel results

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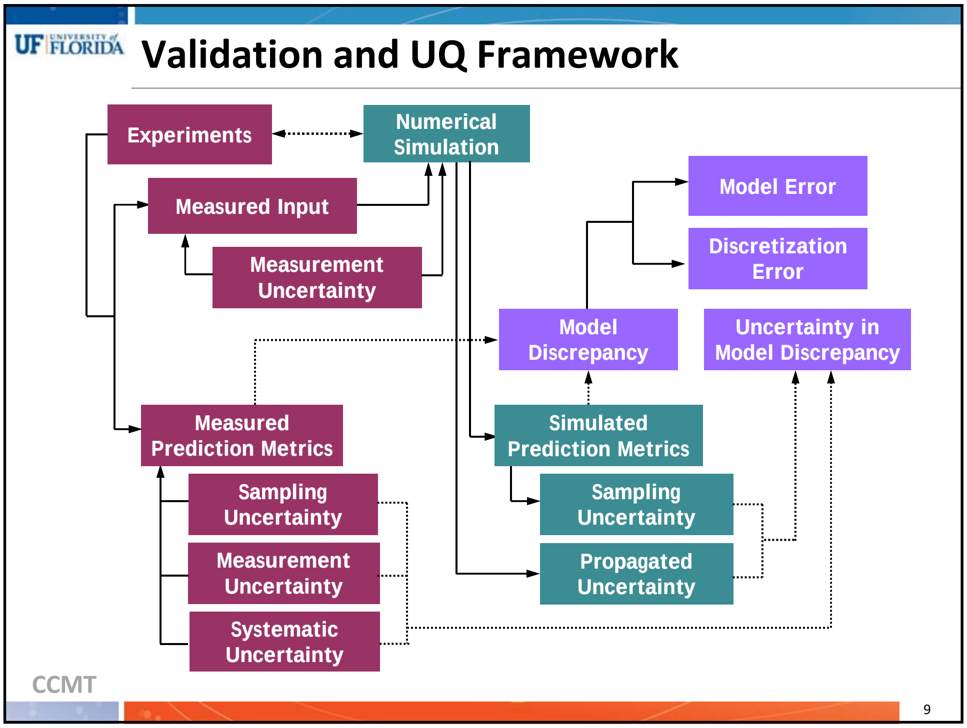
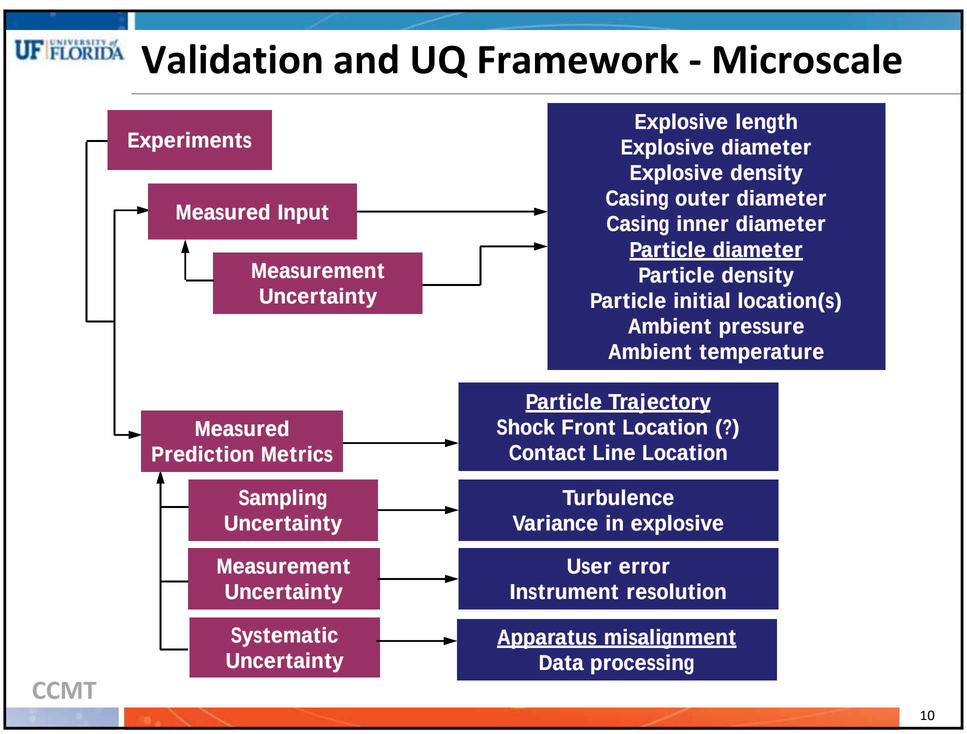
8


Validation and UQ Framework
Experiments
Numerical Simulation
Measured Input
Measurement Uncertainty
Model Error
Discretization Error
Model Discrepancy
Uncertainty in Model Discrepancy
Measured Prediction Metrics
Simulated Prediction Metrics
Sampling Uncertainty
Measurement Uncertainty
Systematic Uncertainty
Sampling Uncertainty
Propagated Uncertainty
CCMT
9


Validation and UQ Framework - Microscale
Experiments
Measured Input
Measurement Uncertainty
Explosive length
Explosive diameter
Explosive density
Casing outer diameter
Casing inner diameter
Particle diameter
Particle density
Particle initial location(s)
Ambient pressure
Ambient temperature
Measured Prediction Metrics
Particle Trajectory
Shock Front Location (?)
Contact Line Location
Sampling Uncertainty
Turbulence
Variance in explosive
Measurement Uncertainty
User error
Instrument resolution
Systematic Uncertainty
Apparatus misalignment
Data processing
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10

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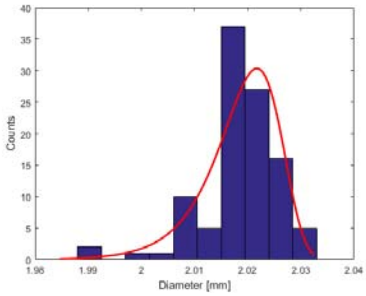
Measurement Uncertainty Quantification: Particle Diameter

- Particle diameter was not measured a priori – previous uncertainty was assumed +/- 10% nominal diameter
- Statistical study of tungsten particles was conducted after the experiments to quantify their uncertainty
- Eglin provided 52 tungsten spheres that were randomly measured by two users

Single particle before detonation



Histograms of particle diameter measurement

Summary statistics for the 52 tungsten particles using micrometers

	Mean [mm]	Stand. Dev. [mm]	Coeffcient of Variation
User 1	2.016	0.0075	0.00370
User 2	2.021	0.0065	0.00321

- Final data shows uncertainty has been **reduced** to 2-3% of nominal diameter compared to prior belief of 10%

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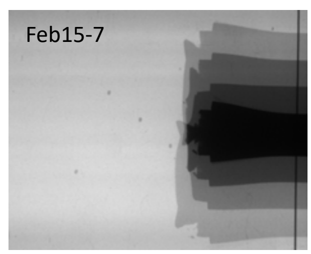
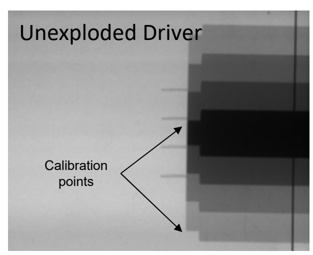
X-Ray Image Calibration

- X-ray calibration is performed through the known dimension of the explosive casing diameter (2")
- The explosion causes significant deformation of the casing
- The X-rays from the unexploded driver are used
- Average of all calibrations is used as it can be difficult to tell which head is which in all shots





Comparison of exploded and unexploded explosive casings.

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12

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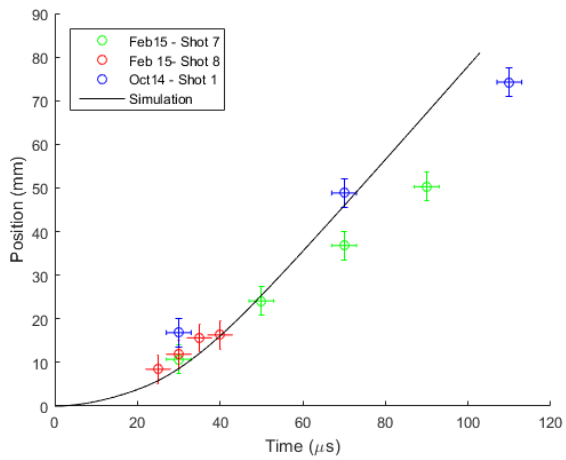
Prediction Metric: Particle Position

- Horizontal error bars are determined from oscilloscope records
- Vertical error bars are determined based on spread in data at repeated times
- Simulation (performed by Josh Garno) is axisymmetric with a single point particle



Validation of simulation with experiment for a single particle.

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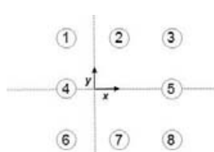
Pressure Probe Setup for Feb15 Experiments

Side view photograph showing the concave pressure probe array.



A schematic of the pressure probe array as viewed from the origin. The crosshair represents the shot line.

- Probes were nominally 34" from the initial position of the particles
- Note that the probes were slightly offset the centerline
- Will use the same numbering for the probes in all plots of the Feb15 tests to be consistent

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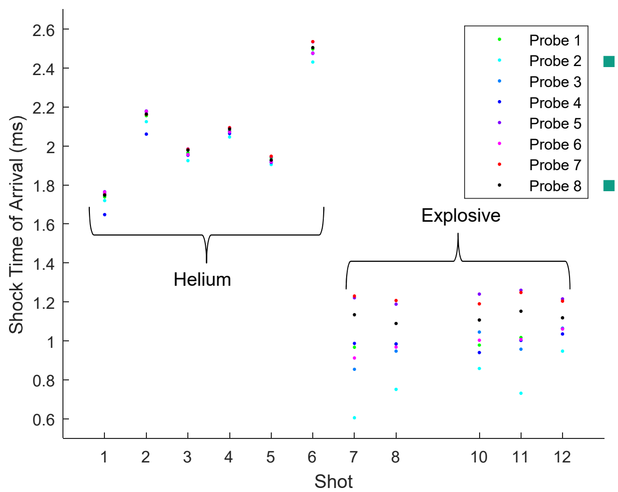
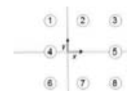
Systematic Uncertainty – Misalignment



Pressure data from February 2015 microscale experiments

- The shock is expected arrive at all probes at approximately the same time
- There is a noticeable order to all explosive shots: Probe 2 always shows the shock arrival first
- A simple correlation analysis was performed for shock time of arrival vs. probe location
  - R^2 = 0.31 for y-location
  - ~31% of the explosive shot variation is explained by y-location



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15

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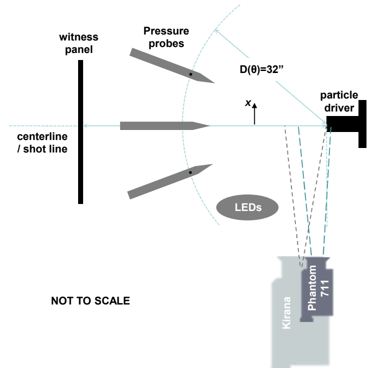
Mesoscale Experiments

Mesoscale Experiments: November 2015

Side view photograph of the experimental setup.



NOT TO SCALE

Overhead schematic of the test set-up.

Summary of mesoscale shots of interest.

Test #	Driver	Particles
Nov15-13	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-15	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-16	RP-2 + 1 N5	0.5 g Tungsten powder
Nov15-17	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-18	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-19	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-21	RP-80 + 2 N5	0.5 g Tungsten powder

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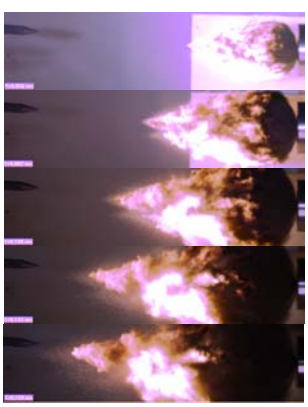
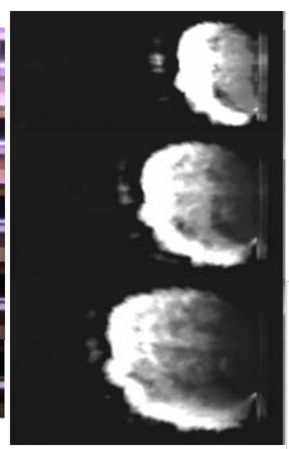
17

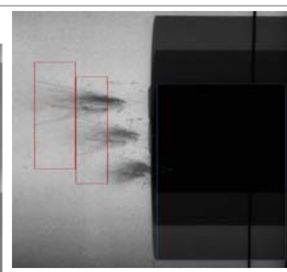
Mesoscale Experiments: Sample Data



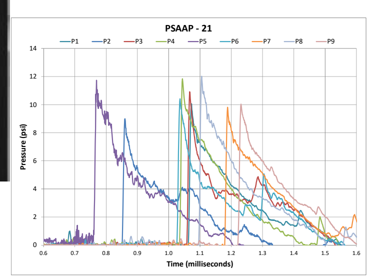
Phantom snapshots



Kirana snapshots



Multiple exposure X-ray image



Pressure histories

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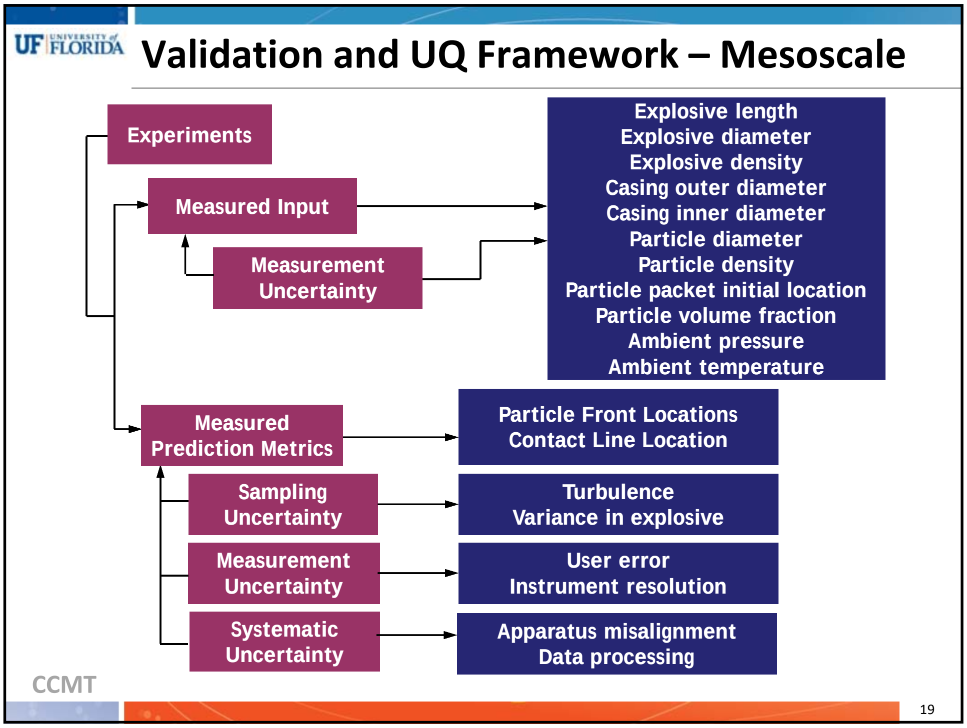
18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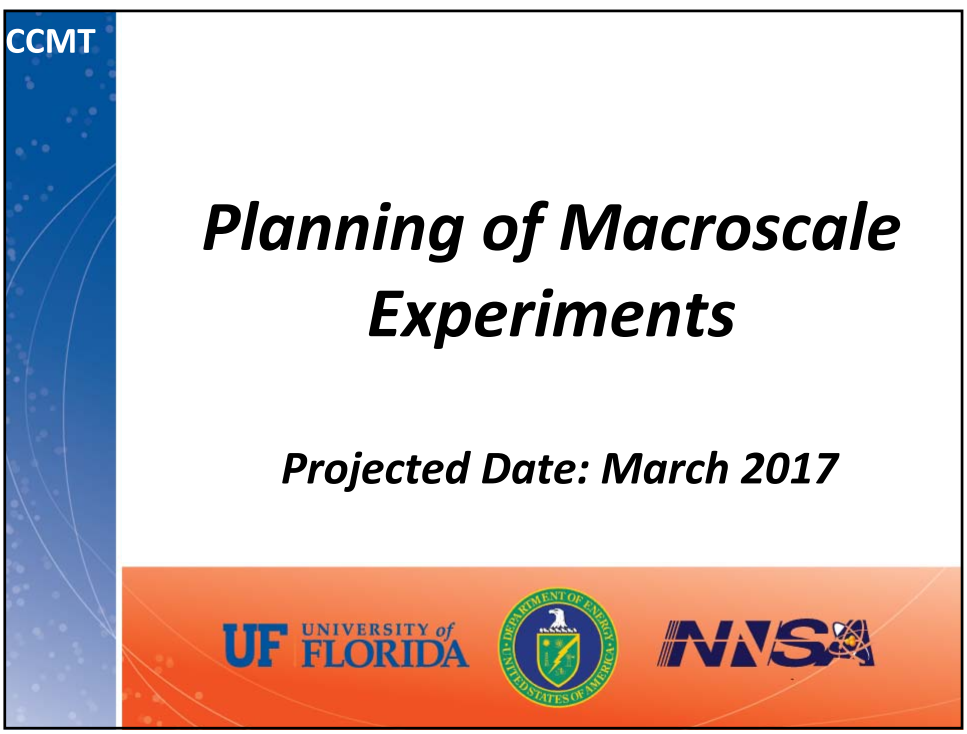
Validation and UQ Framework – Mesoscale
Experiments
Measured Input
Measurement Uncertainty
Explosive length
Explosive diameter
Explosive density
Casing outer diameter
Casing inner diameter
Particle diameter
Particle density
Particle packet initial location
Particle volume fraction
Ambient pressure
Ambient temperature
Measured Prediction Metrics
Particle Front Locations
Contact Line Location
Sampling Uncertainty
Turbulence
Variance in explosive
Measurement Uncertainty
User error
Instrument resolution
Systematic Uncertainty
Apparatus misalignment
Data processing
CCMT
19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Planning of Macroscale Experiments
Projected Date: March 2017
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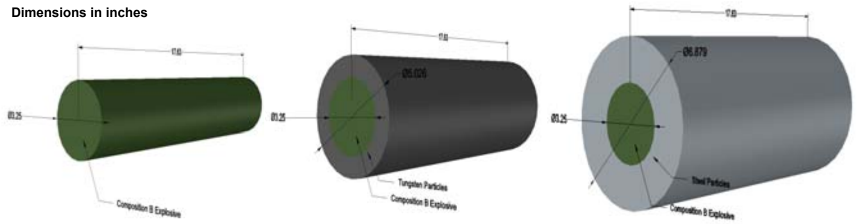
Blastpad Charge Sizing

- 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 instabilities present in their results, M/C ratio of 10 was chosen:

Paper Title	First Author	Charge Mass [g]	Particle Mass [g]	M/C Ratio
Particle jet formation during explosive dispersal of solid particles	Frost	1.6	226	141
Particle momentum effects from the detonation of heterogeneous explosives	Frost	435	4350	10
Explosive dispersal of solid particles	Zhang	2400	26000	10.8

- The charge mass of 3.9 kg is chosen to match legacy data of the AFRL blastpad

Dimensions in inches



Schematics of charge geometries and materials for macroscale experiments.

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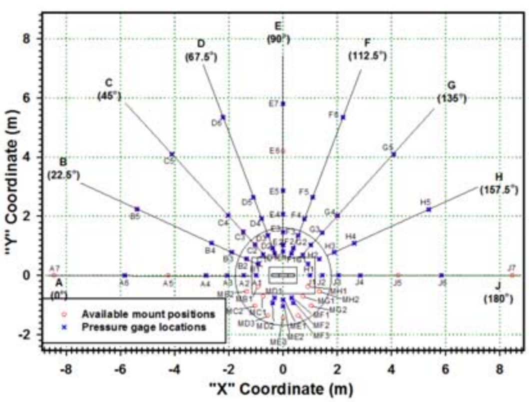
21

AFRL Blastpad Experimental Setup



Locations of 54 pressure transducers [1].

- Instrumentation:
  - 54 pressures probes
  - Momentum traps
  - Three high speed video cameras
  - Possibly linear optical transducers
- Six shots proposed
  - 2 bare charges
  - 1 charge w/tungsten (notched)
  - 1 charge w/steel (notched)
  - 2 charges w/steel (un-notched)

Picture of charge suspended before a test [1].

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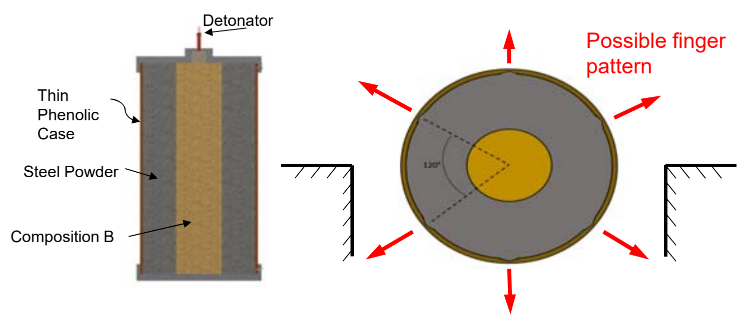
22

Minimizing Casing Influence

- The literature suggests the casing fracture as a possible mechanism for producing the jetting instability [Zhang et al. 2001, Xu et al. 2013]
- To reduce the influence of the casing several 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
  - No casing separating explosive and particles
  - Notches will be introduced to the casing to attempt to control the failure



Schematic of charge cross sections to show attempts to minimize casing influence.

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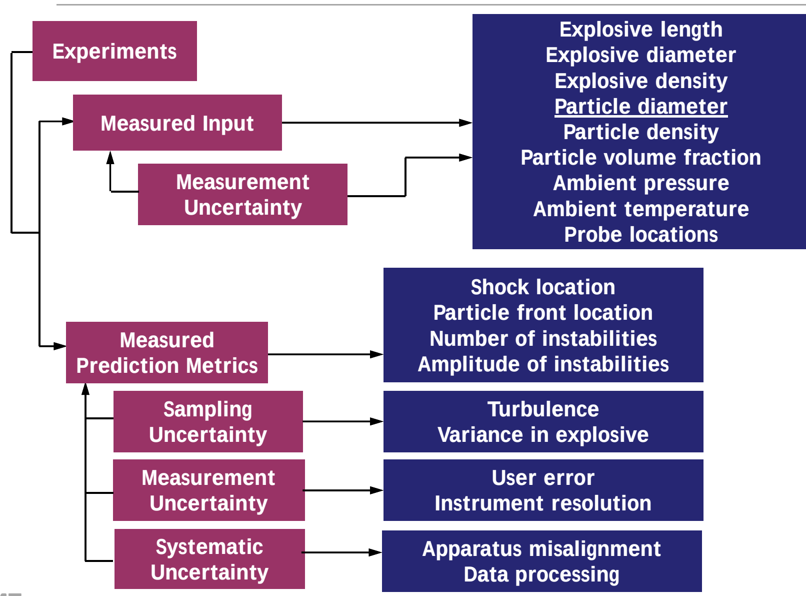
Validation and UQ Framework – Macroscale



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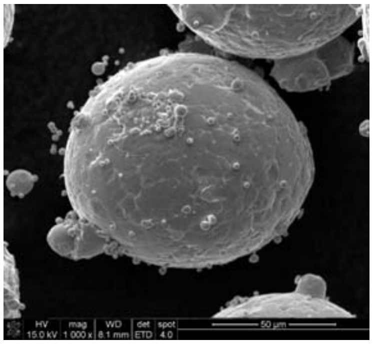
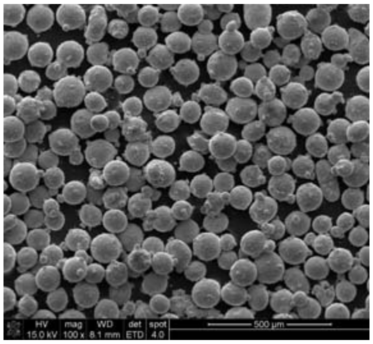
Preliminary Particle Characterization

- Reported size range: 75-125 μm
- Size distribution will need to be confirmed with the use of a particle sizer in future work
- SEM images of particles show particles are mostly spherical with some nodular departures



SEM of single steel particle at 1000x zoom.



SEM of several steel particles at 100x zoom.

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Qualitative Uncertainty Reduction Discussion

- The expense of the explosive charges places a strict constraint on the number of tests available for the macroscale experiments
- Two of these tests are required to be bare charges to "ring out" the test setup
  - These two tests plus the legacy data will act as three tests to validate the reactive burn simulation
- Initially two tests each were planned for tungsten and steel
  - The desire to reduce the large sampling uncertainty led to the conversion of one of the tungsten shots to steel
- Casing as a mechanism for instability was a major concern and steps were taken to minimize it
  - Small sample size prevented us from performing a factorial design with or without the notching
- Characterization of the experimental inputs is being performed, such as particle diameter and density, to reduce these uncertainties a priori

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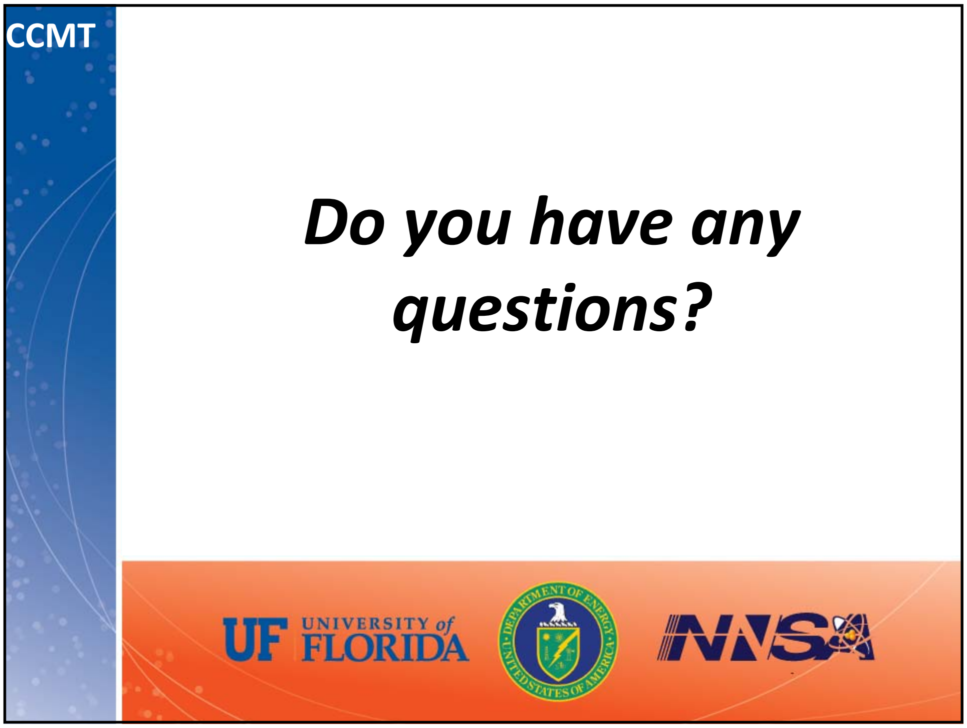
CCMT
Do you have any questions?
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CMT-nek progress

Center for Compressible Multiphase Turbulence
Tri-Lab Services Team Review

December 2, 2016

Jason Hackl
David Zwick

UF UNIVERSITY of FLORIDA

NNSA

UF UNIVERSITY of FLORIDA

CMT-nek team

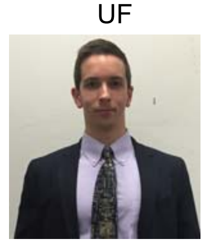
Prof. Paul Fischer, UIUC

Jason Hackl, UF

David Zwick, UF

Li Lu, UIUC

Brad Durant, UF



Goran Marjanovic, UF

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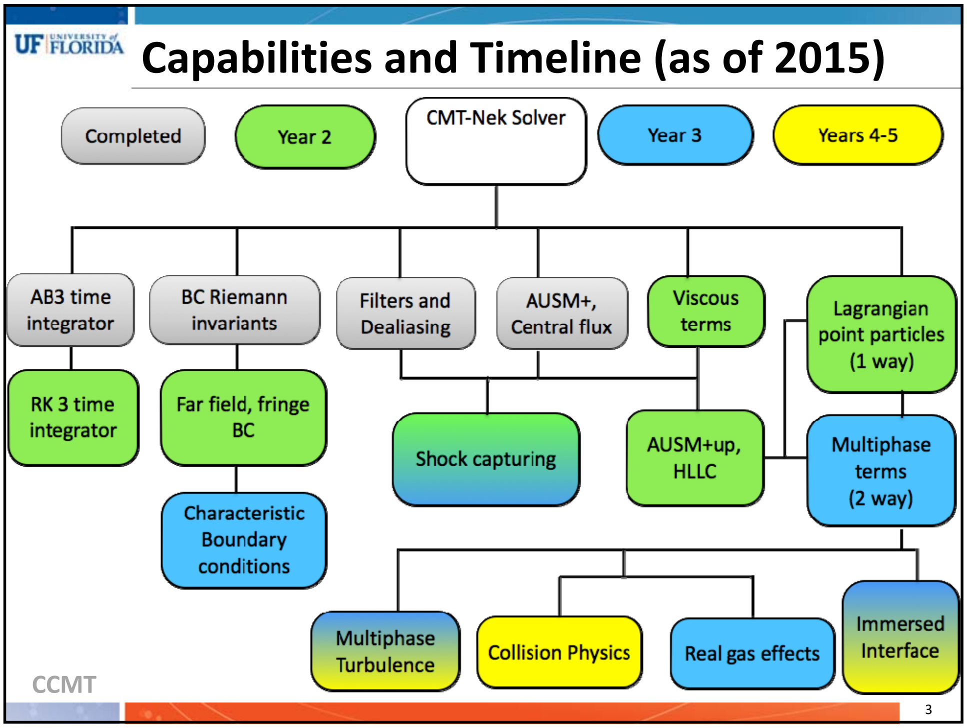
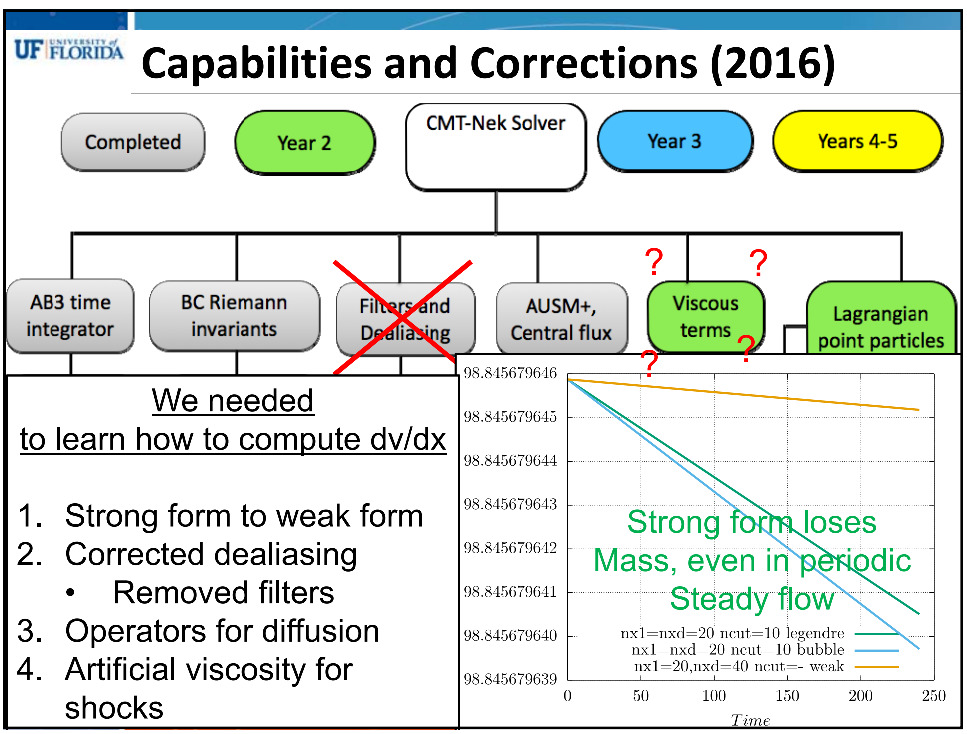
2



Capabilities and Timeline (as of 2015)
Completed
Year 2
CMT-Nek Solver
Year 3
Years 4-5
AB3 time integrator
BC Riemann invariants
Filters and Dealiasing
AUSM+, Central flux
Viscous terms
Lagrangian point particles (1 way)
RK 3 time integrator
Far field, fringe BC
Shock capturing
AUSM+up, HLLC
Multiphase terms (2 way)
Characteristic Boundary conditions
Multiphase Turbulence
Collision Physics
Real gas effects
Immersed Interface
CCMT
3



Capabilities and Corrections (2016)
Completed
Year 2
CMT-Nek Solver
Year 3
Years 4-5
AB3 time integrator
BC Riemann invariants
Filters and Dealiasing
AUSM+, Central flux
Viscous terms
Lagrangian point particles
?
We needed
to learn how to compute dv/dx
1. Strong form to weak form
2. Corrected dealiasing
• Removed filters
3. Operators for diffusion
4. Artificial viscosity for shocks
98.845679646
98.845679645
98.845679644
98.845679643
98.845679642
98.845679641
98.845679640
98.845679639
0
50
100
150
200
250
Time
Strong form loses Mass, even in periodic Steady flow
nx1=nxd=20 ncut=10 legendre
nx1=nxd=20 ncut=10 bubble
nx1=20,nxd=40 ncut=- weak

Outline

- CMT-nek hydrodynamics (improved capabilities)
  - Discontinuous Galerkin spectral element method (DGSEM)
  - 2016 inviscid results
  - Implementation for compressible Navier-Stokes and Euler equations + entropy viscosity method (EVM)
- Current capabilities
- CMT-nek particles
  - Formulation
- Particles+Hydro=Multiphase

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Discontinuous Galerkin spectral element

$$\frac{\partial U_i}{\partial t} + \nabla \cdot \mathbf{H}_i(\mathbf{U}, \nabla \mathbf{U}) = R_i$$

*i*th variable's flux = convective + diffusive

$$\mathbf{H}_i = \mathbf{H}_i^c(\mathbf{U}) + \mathbf{H}_i^d(\mathbf{U}, \nabla \mathbf{U})$$

1. Inner product with test function *v*
2. Integrate by parts on hexahedral Ω_e
3. Numerical flux $\mathbf{H}^*$ in surface integral
   - Weak boundary conditions
   - Couples elements together
4. Isoparametrically map Ω_e to $[-1,1]^d$

$$\frac{\partial}{\partial x_i} = \frac{\partial r_k}{\partial x_i}\frac{\partial f}{\partial r_k} \approx [\mathbf{r}_{k,\mathbf{x}_i}][\mathbf{D}_k \mathbf{f}]$$

Matrix ops within Ω_e

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

$$\int_{-1}^{1} v \frac{\partial U}{\partial t} J\, \mathrm{d}^3 r = \int_{-1}^{1} \frac{\partial r_k}{\partial x_j}\frac{\partial v}{\partial r_k} H_j\, J\, \mathrm{d}^3 r - \sum_{f=1}^{6}\int_{-1}^{1} v\mathbf{H}^* \cdot \mathbf{n}_f J_A \mathrm{d}^2 r + \int_{-1}^{1} vRJ\, \mathrm{d}^3 r$$

5. Approximate integrals with quadrature
6. Approximate *U* & *v* with Lagrange polynomials
   - *N* Gauss-Legendre-Lobatto (GLL) nodes
   - Nested tensor product ~ $O(N^4) < N^3 \times N^3$

     N x *N* matrices applied N^2 times

Ronquist and Patera (1987) *Intl. J. Numerical Methods Engrg.* **24**, 2273-2299
Deville, Fischer and Mund (2002) *Higher-Order Methods for Incomp. Flows* Cambridge
Dolejší & Feistauer(2015) *Discontinuous Galerkin Method:Analysis & Applications to Compressible Flow*. Springer

CMT-nek: Convective terms in DGSEM

$$\int_{-1}^{1} v \frac{\partial U}{\partial t} J\,\mathrm{d}^3 r = \int_{-1}^{1} \frac{\partial r_k}{\partial x_j}\frac{\partial v}{\partial r_k} H_j\, J\,\mathrm{d}^3 r - \sum_{f=1}^{6}\int_{-1}^{1} v\mathbf{H}^* \cdot \mathbf{n}_f J_A \mathrm{d}^2 r + \int_{-1}^{1} vRJ\,\mathrm{d}^3 r$$

$$\mathbf{v}^\mathsf{T}\mathbf{B}\left[\frac{\partial \mathbf{U}}{\partial t}\right] = \mathbf{v}^\mathsf{T}\mathbf{D}_k^\mathsf{T}\mathbf{B}\left[\mathbf{r}_{k,\mathbf{x}_i}\right]\left[\mathbf{H}_i\right] - \mathbf{v}^\mathsf{T}\mathbf{E}^\mathsf{T}\mathbf{B}_A\left[\mathbf{H}_i^* n_i\right] + \mathbf{v}^\mathsf{T}\mathbf{B}\mathbf{R}$$

Volume fractions of ***g***as…

$\phi_g \equiv 1 - \phi_p$

$\phi_p \equiv \lim_{V \to 0} \frac{V_p}{V}$

…and ***p***articles

$$\mathbf{U} \equiv \phi_g \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix}$$

Convective fluxes of

Mass

$\mathbf{H}_c = (U_2, U_3, U_4)^\mathsf{T}$

Thermodynamic state

Temperature T

Pressure $p(\rho, T)$

Total energy $E = \int c_v T\, dT + \frac{1}{2} u_i u_i$

Momentum

$$\mathbf{H}_2^c = \phi_g \begin{bmatrix} (\rho u)u + p \\ (\rho u)v \\ (\rho u)w \end{bmatrix}, \mathbf{H}_3^c = \phi_g \begin{bmatrix} (\rho u)u \\ (\rho u)v + p \\ (\rho u)w \end{bmatrix}, \mathbf{H}_4^c = \phi_g \begin{bmatrix} (\rho u)u \\ (\rho u)v \\ (\rho u)w + p \end{bmatrix}$$

Energy

$$\mathbf{H}_5^c = \phi_g (\rho E + p) \begin{bmatrix} u \\ v \\ w \end{bmatrix}$$

Conserved variables…

to primitive variables… $v = \frac{\rho v}{\rho} = \frac{U_3}{U_1}$ to fluxes in the **Euler equations of gas dyn.**

7

CMT-nek: Convective terms in DGSEM

Convective terms: $\text{RHS}_c = \mathbf{v}^\mathsf{T}\mathbf{D}_k^\mathsf{T}\mathbf{B}\left[\mathbf{r}_{k,\mathbf{x}_i}\right]\left[\mathbf{H}_i^c\right] - \mathbf{v}^\mathsf{T}\mathbf{E}^\mathsf{T}\mathbf{B}_A\left[\mathbf{H}_i^{c*}(\mathbf{E}\mathbf{U})n_i\right] + \mathbf{v}^\mathsf{T}\mathbf{B}\mathbf{R}$

$\mathbf{v}^\mathsf{T}\mathbf{D}_k^\mathsf{T}\mathbf{B}\left[\mathbf{r}_{k,\mathbf{x}_i}\right]\left[U_j\right]\left[u_i\right]$

$\mathbb{P}^{N-1}$ $\mathbb{P}^{N-1}$ $\mathbb{P}^{N-1}$

- Integrand has polynomial degree > 3(N-1)
- GLL quadrature needs more than *N* nodes
- *M* x *N* matrix *I* interpolates onto *M* = 3(*N*-1)/2 Gauss-Legendre points to "dealias" RHS_c

$$\mathbf{v}^\mathsf{T}\mathcal{I}^\mathsf{T}\mathbf{D}_{M,k}^\mathsf{T}\mathbf{B}_M\left(\left[\mathcal{I}\mathbf{r}_{k,\mathbf{x}_i}\right]\left[\mathcal{I}U_j\right]\left[\mathcal{I}u_i\right] + \left[\mathcal{I}p\right]\delta_{ij}\right)$$

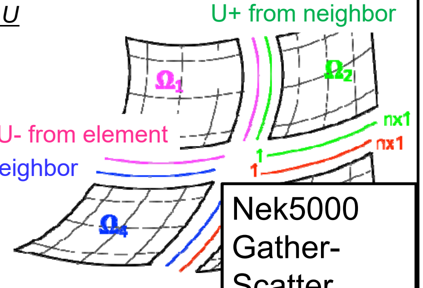
Restriction operator **E** on *U*

Upwind numerical flux $\mathbf{H}^*_c$

- Function of primitive variables ($p^{+,-}$, $\boldsymbol{u}^{+,-}$,…)
- can be any Riemann solver (Advection Upstream Splitting (AUSM))

Boundary conditions weakly imposed

- Dirichlet: prescribe U^+
- Neumann: prescribe flux



Nek5000 Gather-Scatter

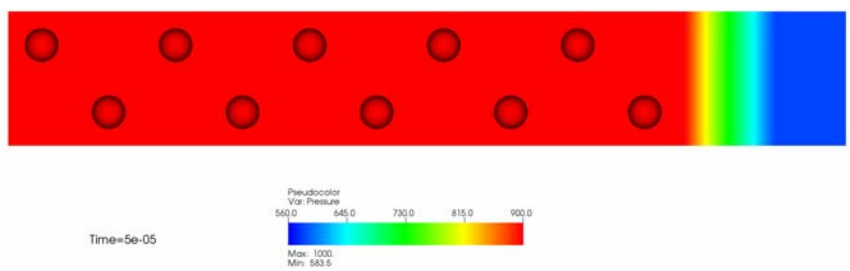
Liou (1996) "AUSM+" *J. Comp. Phys.*, **129**:362-382
Fornberg (1998) *A Practical Guide to Pseudospectral Methods.* Cambridge
Jiao *et al* (2003) "*Roccom*: An object-oriented, data-centric…" Proc. 17th Ann. Int. Conf. Supercomp. ACM 358-68
Lottes & Fischer (2005) *J. Sci. Comp.* **24**(1):45-78 http://nek5000.mcs.anl.gov

Inviscid rarefaction flow over spheres

Dealias restricted surface terms
Equate coefficients of $\mathbf{v}^\intercal$

Right-hand-side for fully explicit RK3

$$\left[\frac{\partial \mathbf{U}}{\partial t}\right] = \mathbf{B}^{-1}\left[\mathcal{I}^\intercal \mathbf{D}^\intercal_{M,k}\mathbf{B}_M\mathcal{I}\left[\mathbf{r}_{k,\mathbf{x}_i}\right]\left[\mathbf{H}_i^c\left(\mathcal{I}\mathbf{U}\right)\right] - \mathbf{E}^\intercal\mathcal{I}_A^\intercal\mathbf{B}_{M,A}\left[\mathbf{H}_i^{c*}\left(\mathcal{I}\left[\mathbf{E}\mathbf{U}\right]\right)\right]\left[\mathcal{I}_A n_i\right]\right]$$



Simulations of smooth inviscid flows

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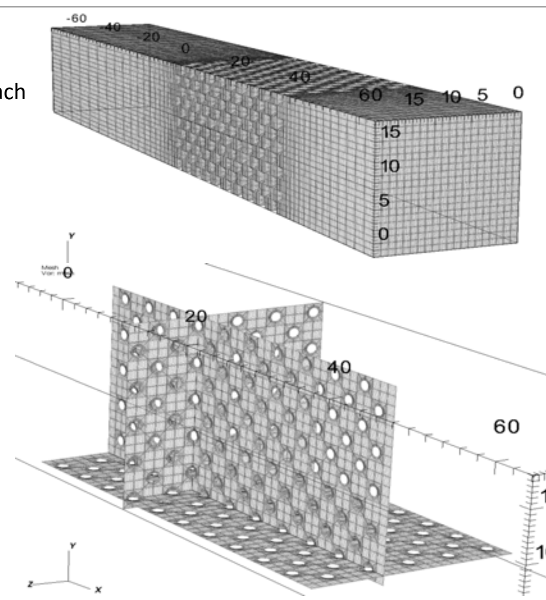
9

Inviscid rarefaction flow over spheres

- 1,000 spheres of unit diameter
  - 20 layers of 50 spheres each
  - 24 elements per sphere
  - 17,496 grid points per sphere
- 134x20x20 domain
- 69,200 elements with a polynomial order of 8
- 50,446,800 degrees of freedom
- 768 MPI ranks on Mustang
- 90 elements per core
- 50,000 core hours



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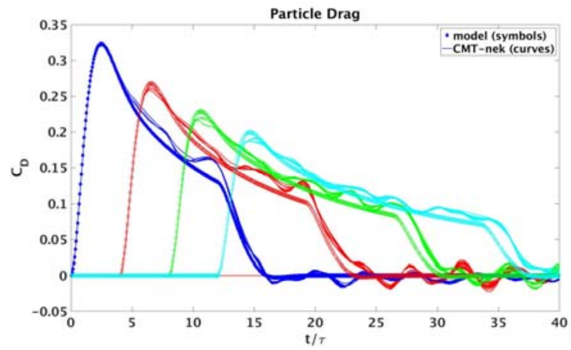
10

Inviscid rarefaction flow over spheres

$$\mathbf{F}^{\mathrm{GF}}(t) = \frac{4}{3}\pi R^3 \overline{\rho^{\mathrm{un}} \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t}^{\mathrm{un}}}^{V} + 4\pi R^3 \int_{\tilde{\xi}=-\infty}^{\tilde{t}} K_{\mathrm{iu}}(\tilde{t}-\tilde{\xi}; M) \left[\frac{\mathrm{D}}{\mathrm{D}t} \overline{(\rho \mathbf{u}_r)^{\mathrm{un}}}^{S} \right]_{\tilde{t}=\tilde{\xi}} \mathrm{d}\tilde{\xi}$$

(undisturbed/pressure gradient force) (added mass/inviscid unsteady force)



Annamalai S, Balachandar S. Generalized Faxen's Theorem for Time-domain Force on a Sphere in Unsteady Viscous Compressible Flows. *Journal of Fluid Mechanics.* Submitted, under review.

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11

CMT-nek: Diffusive terms in DGSEM

flux = convective + diffusive

$$\mathbf{H}_i = \mathbf{H}_i^c(\mathbf{U}) + \mathbf{H}_i^d(\mathbf{U}, \nabla\mathbf{U})$$

Entropy residual $\dfrac{\partial s}{\partial t} + \nabla \cdot (\mathbf{u}s) =: R_s$

Diffusive flux of…

Mass

$$\mathbf{H}_1^d = -\phi_g \kappa_s \nabla\rho$$

Momentum

$$H_{i+1,j}^d = -\phi_g \left(\tau_{ij}^s + \kappa_s u_i \frac{\partial\rho}{\partial x_j} \right)$$

$$\tau_{ij}^s = \mu_s \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

due to **entropy viscosity**

$$\mu_* = c_E h(\mathbf{x})^2 \frac{|R_s|}{||s - \langle s \rangle||_\infty}$$

$$\mu\mathrm{max} \equiv \frac{1}{2} h(\mathbf{x}) \max_{\Omega_e}(|\mathbf{u}| + c)$$

$$\mu_s = \min(\mu_*, \mu\mathrm{max})$$

Artificial viscosity calibrated (tuneables c_E, P) to avoid spurious 2nd-Law violations

- Artificial stress tensor (**NOT** Navier-Stokes)

Energy

$$\mathbf{H}_{5,j}^d = -\phi_g \left[\kappa_s \left(\frac{\partial}{\partial x_j}(\rho e) + \frac{1}{2}|\mathbf{u}|^2 \frac{\partial\rho}{\partial x_j} \right) + \mu_s \rho\, u_i \tau_{ij}^s \right]^j, \quad \kappa_s = \mathcal{P}\mu_s,\ \mathcal{P} \approx \frac{1}{4}$$

Zingan *et al* (2013) "Implementation of entropy viscosity method…" *Comput. Meth. Appl. Mech. Eng.* **253**:479-490
Guermond & Popov (2014) "Viscous regularization of Euler eqn and entropy principles" *J. Appl. Math.* **74**:284-305
Guermond, Popov & Tomov (2016) *Comput. Meth. Appl. Mech. Eng.* **300**:402-426

CMT-nek: Diffusive terms in DGSEM

Quasi-linear flux Jacobian *A*

Primal form

Dolejší, V. *Intl. J. Numer. Meth. Fluids* **45**:1083-1106 (2004)
Hartmann & Houston (2008) *J. Comp. Phys.* **227**:9670-9685

$\Gamma \equiv \bigcup_e \partial\Omega_e$

Jump $[\![u]\!] \equiv u^- \mathbf{n}^- + u^+ \mathbf{n}^+$

average $\{\{u\}\} \equiv \frac{1}{2}\left(u^- + u^+\right)$

$$H_{ij}^d = \mathscr{A}_{ijkl} \frac{\partial U_k}{\partial x_l}$$

Arnold *et al* (2002) *SIAM J. Numer. Analysis* **39**:1749-1779

Weighted resid, int by parts → primal form → DGSEM ops

$$\int_{\Omega_e} v \nabla \cdot \mathbf{H}_i^d \, dV \rightarrow I_{KU} - I_{GU} + I_{G^\intercal U}$$

$$I_{GU} = \int_\Gamma \{\{\mathscr{A}\,\nabla \mathbf{U}\}\} \cdot [\![v]\!] \, dA \rightarrow \mathbf{v}^\intercal \mathbf{E}^\intercal \mathbf{B}_A \left[\left(\mathbf{H}_i^d \cdot \mathbf{n}\right)^- - \{\{\mathbf{H}_i^d \cdot \mathbf{n}\}\}\right]$$

$$I_{G^\intercal U} = \int_\Gamma \{\{\mathscr{A}^\intercal \nabla v\}\} \cdot [\![\mathbf{U}]\!] \, dA \rightarrow \mathbf{v}^\intercal \mathbf{D}_j^\intercal \mathscr{A}_{ij} \mathbf{E}^\intercal \mathbf{B}_A \left[\mathbf{U}^- - \{\{\mathbf{U}\}\}\right] [n_i]$$

$$I_{KU} = \int_{\Omega_e} (\nabla v) \cdot \mathbf{H}_i^d \, dV \rightarrow \mathbf{v}^\intercal \mathbf{D}_k^\intercal \mathbf{B} \left[\mathbf{r}_{k,\mathbf{x}_i}\right] \mathbf{H}_i^d$$

Baumann & Oden (1999) *Comput. Methods Appl. Math. Engrg.* **175**:311-341

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13

CMT-nek: final form of DGSEM

Equate coefficients of $\mathbf{v}^\intercal$

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

$$\left[\frac{\partial \mathbf{U}}{\partial t}\right] = \mathbf{B}^{-1}\left[\mathcal{I}^\intercal \mathbf{D}_{M,k}^\intercal \mathbf{B}_M \mathcal{I}\left[\mathbf{r}_{k,\mathbf{x}_i}\right]\left[\mathbf{H}_i^c\left(\mathcal{I}\mathbf{U}\right)\right] + I_{KU}\right]$$

$$-\mathbf{B}^{-1}\left[\mathbf{E}^\intercal \mathcal{I}_A^\intercal \mathbf{B}_{M,A}\left[\mathbf{H}_i^{c*}\left(\mathcal{I}\left[\mathbf{E}\mathbf{U}\right]\right)\right]\left[\mathcal{I}_A n_i\right] + I_{GU} - I_{G^\intercal U}\right]$$

Surface: O($N_{elem}M^2$)

Right-hand-side for fully explicit RK3 = Surface ops + Volume ops; **diffusion number *D***

Gottlieb & Shu (1998) *Math. Comp.* **67**:73-85
Bannerjee *et al* (2016) *HiPC.* submitted

$$D = \frac{\mu \Delta t}{h^2}, \; D \ll 1$$

Mass matrix is diagonal; all other matrices are block-diagonal

- Locality, scaling

Diagonal mass matrix means LHS inner product is ***not*** exactly Integrated ("variational crime")

- Tensor-nesting saves M^2 factor in cost of volume operations
- Correction technique (Teukolsky (2014) arXiv:1412.2276v1)

14

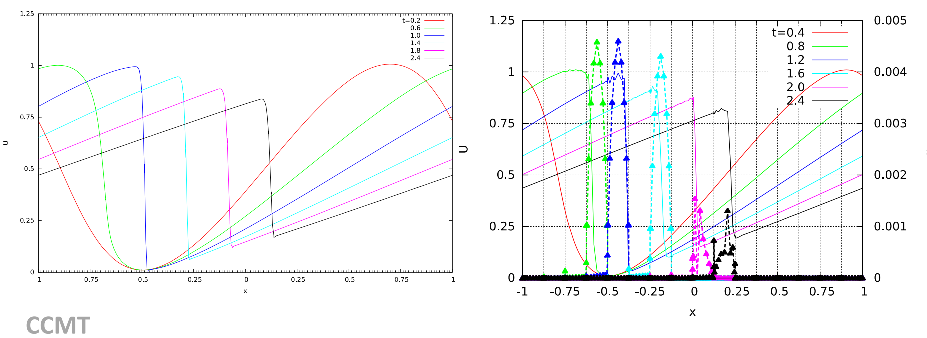
Shocks are coming soon!!!

Catching up to a rapidly evolving field; as usual, SEM is neglected

- Evaluating compressible Navier-Stokes fluxes and validating viscous solver against exact solutions
- Entropy residual is poorly understood at high polynomial order

EVM works with 1D Burgers! $\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{H}(U) = \nabla \cdot (\nu_s \nabla U)\,,\ \mathbf{H} \equiv \frac{1}{2} U^2$

160 elements, nx=3 | 16 elements, nx=11



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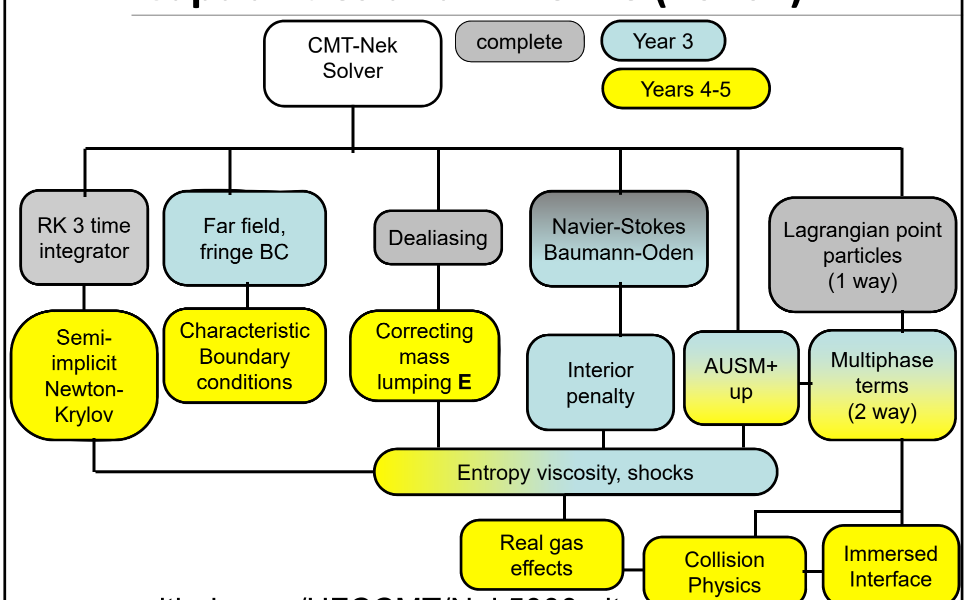
Capabilities and Timeline (2016+)



CCMT github.com/UFCCMT/Nek5000.git 16

Meso/macroscale approach in CMT-nek

- Previous results for fully-resolved microscale simulations
- Meso/macroscale problem will require billions of particles
  - Euler-Lagrange approach
- Applications
  - Frost experiment, Eglin blast pad experiment
  - ASU Experiment, SNL MST experiment
  - Eglin gas gun experiment

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Euler-Lagrange approach in CMT-nek

- Interpolate gas properties to particles
  - Spectral accuracy
- Move particles according to Newton's laws
  - Particle-particle interaction (detect neighbors & collisions)
  - As particles move inter-processor data communication
- Feed force back to the gas
  - Each particle influences a Gaussian envelope
    - Each element influenced by "ghost" particles that are just outside
    - Each particle can influence the gas in at most eight elements

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Particles: Past, present, and future

	Nek5000 (past)	CMT-nek (present)	CMT-nek (future)
Interpolation	• Standard Lagrange	• Barycentric Lagrange	• Barycentric Lagrange
Time integration	• BDF/EXT	• RK3	• RK3
Force models	• Stokes drag	• Improved models	• Volume fractions • Extended point particle models
Coupling	• 1-way	• 1-way	• 2-way
Restart	• No restart	• Restart	• Restart
Boundary conditions	• Periodic	• Periodic • Inflow/outflow	• Periodic • Inflow/outflow
I/O	• Serial	• Parallel	• Parallel
Data residency	• Remote	• Local	• Load balanced

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19

1-way particles: physics

- Governing equation of particle motion (1-way coupled):

$$m_p \frac{\partial \vec{v}}{\partial t} = \vec{F}_{qs} + \vec{F}_{un} + \vec{F}_{iu}$$

- Quasi-steady force:

$$\vec{F}_{qs} = S(\vec{u} - \vec{v})C_D \qquad S = \frac{Re_p m_p}{24\tau_p}$$

- Undisturbed force:

$$\vec{F}_{un} = m_g \frac{D\vec{u}}{Dt}$$

- Inviscid unsteady force

$$\vec{F}_{iu} = \frac{1}{2} V_p \left(\rho_g \frac{D\vec{u}}{Dt} - \frac{\partial \rho_g \vec{v}}{\partial t} \right) C_M$$

Finite Mach and Reynolds number corrections:

$$C_D(Re_p, M_p)$$

$$C_M(M_p)$$

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20

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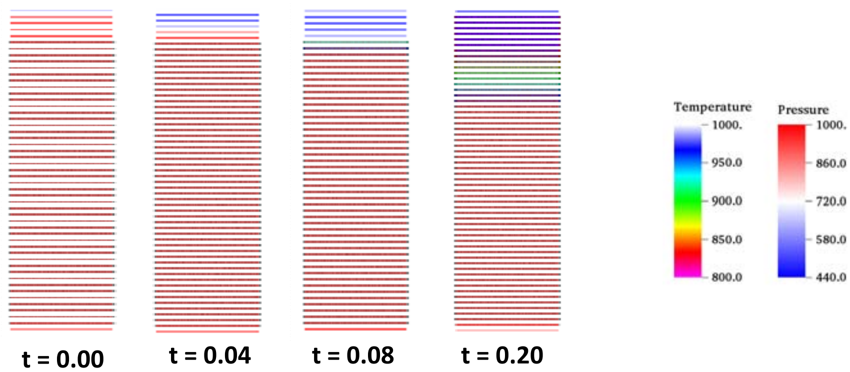
Demonstration: Particles in rarefaction

MPI Ranks	Spectral Elements	Grid points	Particles	Solve time
131k	131k	250 million	20 billion	12 hours



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21

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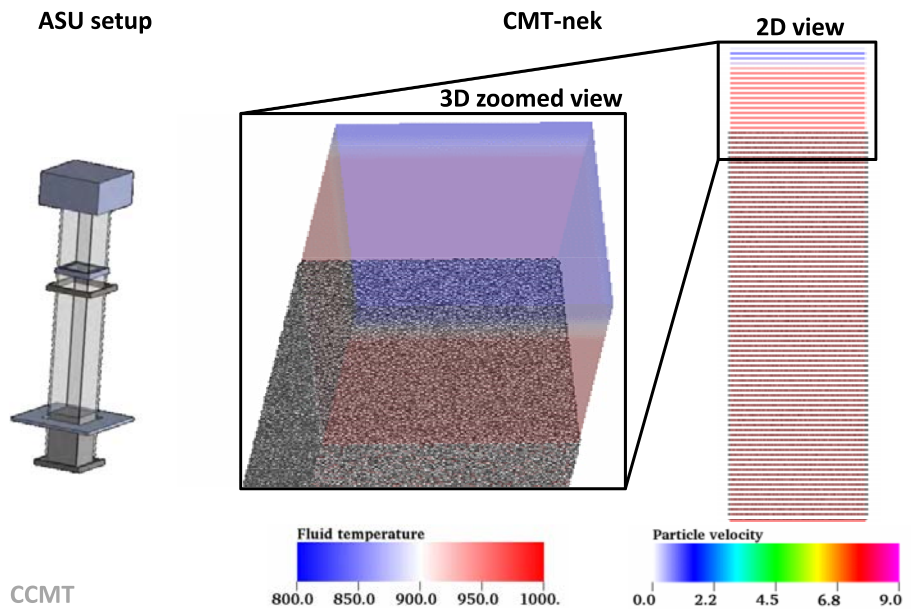
Macroscale: ASU and CMT-nek



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22

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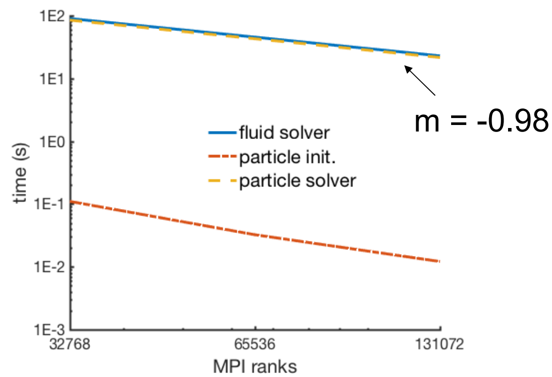
Particles in rarefaction strong scaling

MPI Ranks	Spectral Elements	Grid points	Particles	Solve time
32k, 65k, 131k	524k	905 million	905 million	11 hours



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*Times are total time per time step per MPI rank

23

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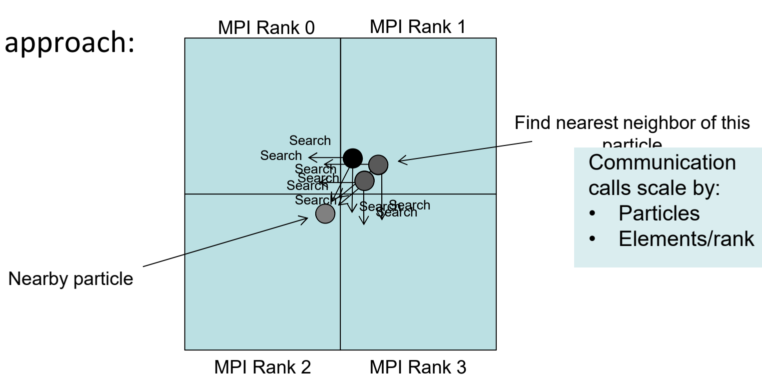
Need for Ghost Particles

Each particle’s influence extends beyond its element/MPI-rank:

- Back coupling with gas in a Gaussian envelope
- Nearest neighbors for local volume fraction
- Nearest neighbors for particle-particle interaction

Naïve approach:



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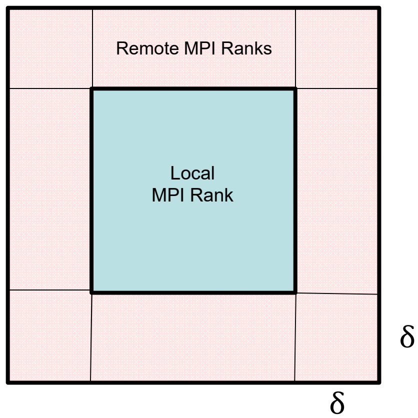
24

Ghost particle approach

Ghost particle approach:

- A list of nearby particles is kept for each processor
- A given processor will know what particles are within nearby regions



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25

Ghost particle algorithm

Idea:

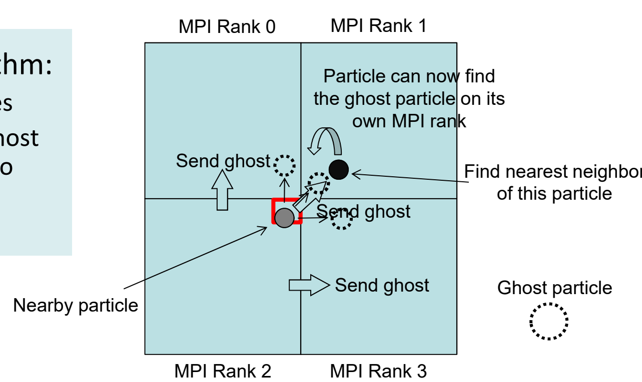
- If a particle is near a MPI rank edge, it will create a copy of itself called a ghost particle
- <u>Sending</u> perspective rather than <u>receiving</u> perspective

Ghost particle algorithm:

1. Create ghost particles
2. Find processor for ghost particles to be sent to
3. Send ghost particles

Communication calls scale by:

- Elements/rank



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26

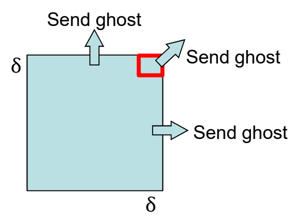
Ghost particle scaling

Scalability of algorithm:

- We consider a test case that is a 3D periodic box
- Particles are randomly distributed in domain and advected by uniform gas flow

MPI Ranks	Spectral Elements	Polynomial	Grid points	Particles	Time steps
100 - 1000	8000	5	1 million	1 million	100

- The distance δ is varied



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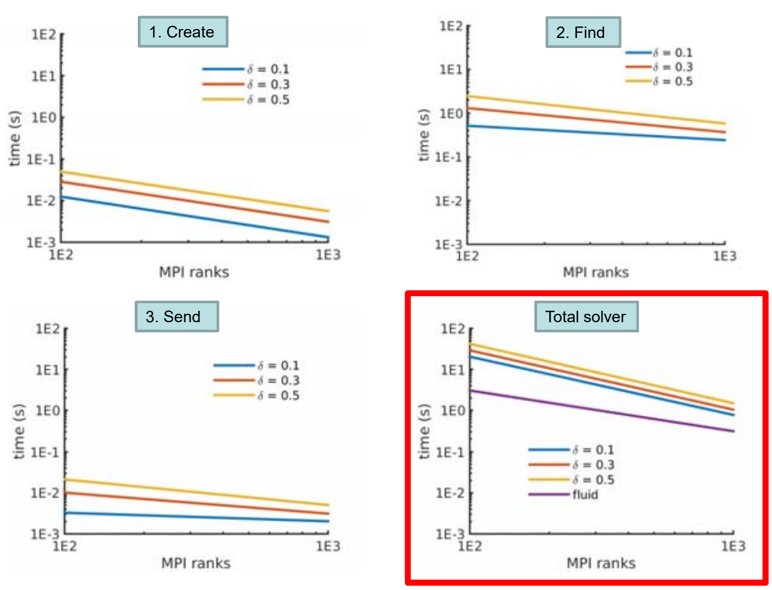
27

Ghost particle strong scaling



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*Times are total time per time step per MPI rank

28

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Summary of Euler-Lagrange progress

- 1-way coupling
  - Particles in rarefaction
  - Demonstrate current physics
- 2-way coupling
  - Ghost particle algorithm will not be a show-stopper in macroscale simulation
  - Necessary for back-coupling

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29

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Do you have any questions?

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