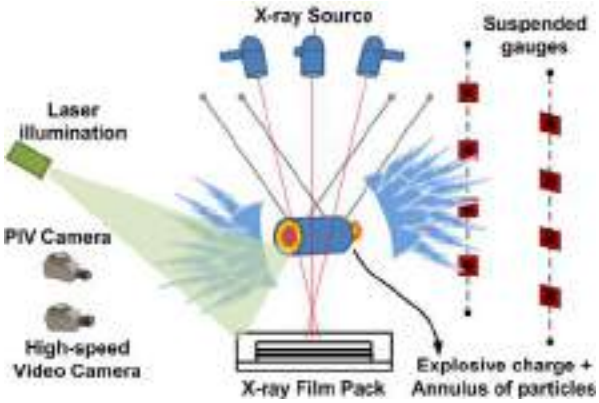
CCMT

CENTER FOR COMPRESSIBLE MULTIPHASE TURBULENCE

AST Review

April 20-21, 2017



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NNSA

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Center for Compressible Multi-Phase Turbulence

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Agenda AST Site Visit April 20-21, 2017

Thursday April 20, 2017

7:45	Van pick up at University Hilton
8:00-9:00	Full Breakfast
	(Review Team and other NNSA personnel will meet in small conference room)
9:00-9:05	Introductions and opening remarks (S. Balachandar, Martin Schulz)
9:05-9:30	Agenda, Review Recommendations, Management, Internships, Educational Impact (Jackson)
9:30-10:30	Overview, Scope and Coupling, Y3 Accomplishments (Balachandar) (RQ 1,2,6)
10:30-10:45	Coffee break
10:45-11:30	Integration of experiments and simulations (Rollin/Diggs) (RQ 2,6)
11:30-11:50	CMT-nek (Jason Hackl) (RQ 4,5,6)
11:50-1:00	Lunch (RT will meet in small conference room)
1:00-1:50	V&V and UQ (Haftka, Park, Kim) (RQ 2,6)
1:50-2:40	Dynamic Load Balancing (Ranka, Banerjee) (RQ 3)
2:45-3:00	Coffee break
3:00-3:50	CS/BE results at scale (Lam, Stitt) (RQ 4,5,6)
4:00-5:15	Lightning Round of Students' Posters/ Poster Session (light refreshments served)
5:15-6:30	RT Caucus
6:30-8:00	Dinner (Faculty, Staff and Visitors; transportation will be provided for all visitors to the University Hilton)

Friday April 21, 2017

7:45	Van pickup at University Hilton
8:00-9:00	Continental Breakfast (RT will meet in small conference room)
9:00-10:30	Overview of Scientific Goals and Accomplishments – I
	Nalini Kumar (Florida; Exascale; 15 mins) David Zwick (Florida; Simulations and CMT-nek; 15 mins) Fred Ouellet (Florida; Simulations and UQ; 15 mins) Yash Mehta (Florida; Physics Microscale and Modelling; 15 mins) Yiming Zhang (Florida; UQ; 15 mins) Carlo Pascoe (Florida; Exascale & FPGA; 15 mins)
10:30-10:45	Coffee Break
10:45-11:15	Overview of Scientific Goals and Accomplishments – II
	Kyle Hughes (Florida; UQ and experiments; 15 mins) Heather Zunino (ASU; expansion of multiphase flows; 15 mins)
11:15-12:15	Center Response to RT Questions (PI Team)
12:15-4:00	Lunch (RT will meet in small conference room)
	Private RT deliberations (small conference room)
	Discussions between Center Management and AST as appropriate (large conference room)
4:00-4:30	RT Summary for Center Management (large conf. room)
4:30	Review ends

Center for Compressible Multiphase Turbulence

AST Review April 20-21, 2017 Attendee List

Faculty

S. Balachandar "Bala"	University of Florida	bala1s@ufl.edu
Rafi Haftka	University of Florida	haftka@ufl.edu
Nam-Ho Kim	University of Florida	nkim@ufl.edu
Herman Lam	University of Florida	hlam@ufl.edu
Sanjay Ranka	University of Florida	ranka@cise.ufl.edu
Greg Stitt	University of Florida	gstitt@ece.ufl.edu
Tom Jackson	University of Florida	tlj@ufl.edu
Siddharth Thakur "ST"	University of Florida	sst@ufl.edu
Bertrand Rollin	Embry-Riddle	rollinb@erau.edu
Donald Littrell	Eglin Air Force Base	donald.littrell@us.af.mil
Angela Diggs	Eglin Air Force Base	angela.diggs.1@us.af.mil
Ju Zhang	Florida Institute of Technology	jzhang@fit.edu

Review Team

Martin Schulz (CS; Chair)	LLNL	schulzm@llnl.gov
Brian Carnes (V&V/UQ)	SNL	bcarnes@sandia.gov
Jeremiah Wilke (CS)	SNL	jjwilke@sandia.gov
Gabe Rockefeller (CS)	LANL	gaber@lanl.gov
Kambiz Salari (Physics)	LLNL	salari1@llnl.gov
Erik Vold (Physics)	LANL	elv@lanl.gov

Others

Jim Costa	Sandia	jecosta@sandia.gov
Fernando Grinstein	LANL	fgrinstein@lanl.gov
Dan Nikkel	LLNL	nikkel1@llnl.gov
Bob Voigt	Leidos/NESD	rvoigt@krellinst.org
Emily Simpson	Leidos/NESD	
Greg Weirs	Sandia	vgweirs@sandia.gov
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Shane Schumacher	Sandia	scschum@sandia.gov

Research Staff

Tania Banerjee	University of Florida	tmishra@cise.ufl.edu
Jason Hackl	University of Florida	jason.hackl@ufl.edu
Chanyoung Park	University of Florida	cy.park@ufl.edu

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Students

Sai Chenna	University of Florida	chenna@hcs.ufl.edu
Paul Crittenden	University of Florida	pcritte@ufl.edu
Brad Durant	University of Florida	neoncrash@ufl.edu
Giselle Fernandez	University of Florida	gisellefernandez@ufl.edu
Mohamed Gadou	University of Florida	mgadou@ufl.edu
Joshua Garno	University of Florida	jgarno@ufl.edu
Trokon Johnson	University of Florida	johnson@hcs.ufl.edu
Kyle Hughes	University of Florida	kylethughes89@ufl.edu
Rahul Koneru	University of Florida	rahul.koneru@ufl.edu
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Goran Marjanovic	University of Florida	gmarjanovic@ufl.edu
Justin Mathew	University of Florida	jmathew03@ufl.edu
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Heather Zunino	Arizona State University	heatherzunino@gmail.com
David Zwick	University of Florida	dpzwick@ufl.edu

Administration Staff

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Financial Staff

Melanie DeProspero	University of Florida	mel7703@ufl.edu

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Agenda, Review Recommendations, Management, Internships, Educational Impact

T.L. Jackson
Technical Manager

AST Meeting Agenda

Thursday

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

Friday

- Overview of Scientific Goals
- Center Response to AST Questions (Balachandar)
- RT Deliberations/Summary

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Review Team Recommendations – 2016

- RQ 1 – Recommendations on Scope
  - Consider simpler experiment for code validation
  - Compaction not yet accounted for
  - Consider contingency plans to meet year 5 goals
- RQ 2 – Recommendations on Experiments/Simulation Coupling
  - Develop and document detailed V&V plan
  - Include more detail on how data from ASU experiment will be extracted
  - V&V experts should work closer with Eglin
- RQ 3 – Recommendations on Dynamic Load Balancing
  - Continue efforts on GPUs and host CPUs
  - Discuss dynamic aspects of load balancing
  - Center should take advantage of lab expertise on load balancing

CCMT 3

Review Team Recommendations – 2016

- RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
  - Adopt rigorous software development and documentation practices
  - Feedback loop between physics and CS/BE efforts
  - More staff with in-depth knowledge on CMT-nek with strong ties to CS
- RQ 5 – Recommendations on Scalability Results
  - Scalability tests for CMT-nek
  - Use existing allocations on Titan & Mira
  - Use testbeds for upcoming machines
- RQ 6 – Additional Recommendations
  - Develop strategy to use lower fidelity runs for hero runs
  - Increase efforts on rigorous code verification for CMT-nek
  - Clarify how microscale results are used at mesoscale subgrid models
  - Scalability of FPGA approach
  - More talks by students

CCMT 4

Review Team Recommendations – 2016

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

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

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Review Team Recommendations – 2016

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

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

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Review Team Recommendations – 2016

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

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

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Review Team Recommendations – 2016

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

- Answer to RQ 4
  - Primarily addressed in BE (Lam, Stitt) and CMT-nek (Hackl) talks
  - http://travis-ci.org/UFCCMT/Nek5000 automated regression testing, Doxygen committed with code, http://github.com/Nek5000/NekDoc
  - Closing the loop: Behavioral Emulation & design-space exploration on CMT-nek
    - Perform large-scale validation (100k+ MPI ranks) on DOE systems (Cab, Vulcan, Titan) and performed predictive simulations to million+ MPI ranks
  - Lectures on CMT-nek formulation and code during Winter Break 2016-2017 for CCMT staff and leadership
  - New staff

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Review Team Recommendations – 2016

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

- Answer to RQ 5
  - Primarily addressed in BE (Lam, Stitt) and Multiphase (David Zwick) talks
  - Scaling studies routinely use 8k to 131k cores on Vulcan
  - New emulation upto 1M cores; significant effort on benchmarking
  - CS uses titan (GPU dev)
  - Large ASU experiment (meso and micro) ongoing on Mira
  - Using Knights Landing (CS/BE)

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Review Team Recommendations – 2016

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

- Answer to RQ 6
  - Primarily addressed by Overview (Bala), Integration (Rollin, Diggs), CMT-nek (Hackl), UQ (Haftka, Park, Kim), BE (Lam, Stitt) talks
  - Multi-fidelity surrogate based strategy has been developed and is being demonstrated with 1D (lower fidelity) and 2D (higher fidelity) mesoscale shock tube simulations
  - CMT-nek comparisons to Rocflu for shock/particle interaction
  - Balachandar will present current approach on coupling microscale to macroscale
  - Scalability of FPGA approach (multi-FPGA scalability projection will be presented)

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Review Team Recommendations – 2016

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

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

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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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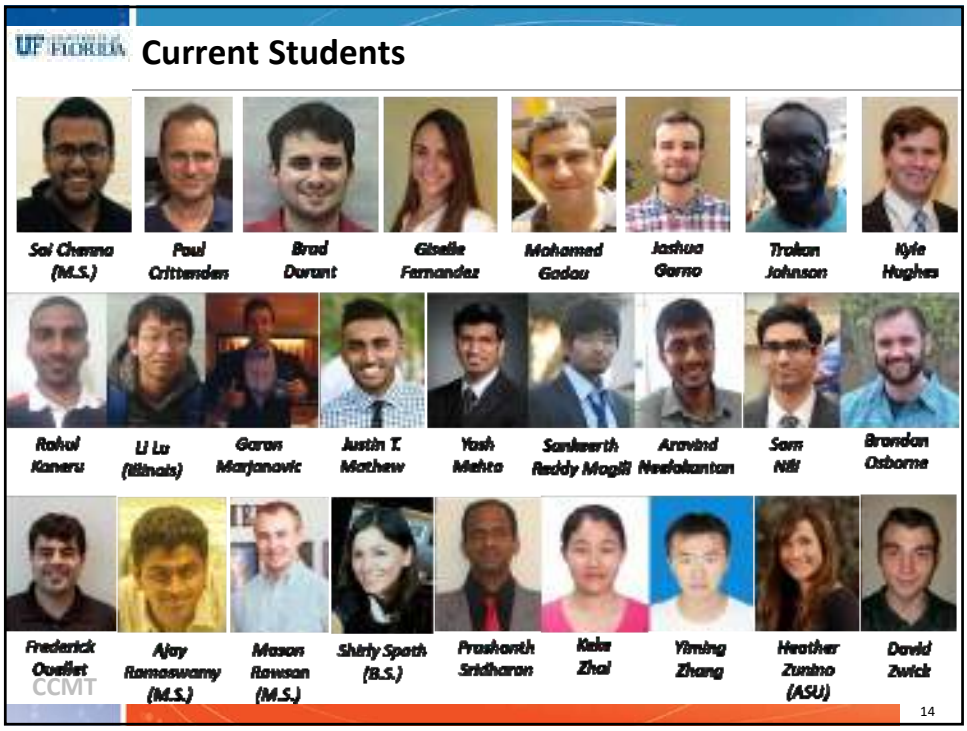
Current Students
Sai Chenna (M.S.)
Paul Crittenden
Brad Durant
Giselle Fernandez
Mohamed Gadou
Joshua Garno
Trakan Johnson
Kyle Hughes
Rahul Kaneru
Li Lu (Illinois)
Goran Marjanovic
Justin T. Mathew
Yash Mehta
Sankeerth Reddy Mogili
Aravind Neelakantan
Sam Nili
Brandon Osborne
Frederick Ouellet
Ajay Ramaswamy (M.S.)
Mason Rawson (M.S.)
Shirly Spath (B.S.)
Prashanth Sridharan
Kelu Zhai
Yiming Zhang
Heather Zunino (ASU)
David Zwick
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Internship Program - Completed

Heather Zunino	LANL	May-Aug, 2014	Dr. Kathy Prestridge
Kevin Cheng	LLNL	May-Aug, 2014	Dr. Maya Gokhale
Nalini Kumar	LLNL	March-Aug, 2015	Dr. James Ang
Christopher Hajas	LLNL	May-Aug, 2015	Dr. Maya Gokhale
Christopher Neal	LLNL	June-Aug, 2015	Dr. Kambiz Salari
Carlo Pascoe	LLNL	June-Aug, 2015	Dr. Maya Gokhale
Giselle Fernandez	Sandia	Oct-Dec, 2015	Drs. Gregory Weirs & Vincent Mousseau
Justin Mathew	LANL	May-Aug,2015	Dr. Nick Hengartner
David Zwick	Sandia	May-Aug, 2016	Drs. John Pott & Kevin Ruggirello
Goran Marjanovic	Sandia	Aug-Nov, 2016	Drs. Paul Crozier & Stefan Domino
Georges Akiki	LANL	May-Aug, 2016	Dr. Marianne Francois

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Internship Program - Planned

Paul Crittenden	LLNL	Spring, 2017	Drs. Kambiz Salari & Sam Schofield
Mohamed Gadou	LANL	Summer, 2017	Dr. Galen Shipman
Yash Mehta	LLNL	Summer, 2017	Dr. Kambiz Salari

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Internship Program – Not Yet Planned

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

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Graduated Students

- Kevin Cheng, MS (2014), Dr. Alan George, ECE
- Hugh Miles, BS (2015), Dr. Greg Stitt, ECE
- Chris Hajas, MS (2015), Dr. Herman Lam, ECE
- Angela Diggs, PhD (2015), Dr. S. Balachandar, MAE
  - Currently employed at Eglin AFB and working with center
- Subbu Annamalai, PhD (2015), Dr. S. Balachandar, MAE
  - Postdoc in center thru March 2017
  - Senior Systems Engineer, Optym, Gainesville FL
- Georges Akiki, PhD (2016), Dr. S. Balachandar, MAE
  - Postdoc in center thru March 2017
  - Postdoctoral Associate, LANL

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Additional Information

- Additional Graduate Program Announcements
  - David Zwick – NSF Fellowship Graduate Program (started Aug 2016)
  - Georges Akiki - MAE Best Dissertation Award (TSFD; May 2017)
  - Chandler Moore – incoming PhD student; NSF Fellowship Graduate Program
- Other metrics (Y1 – Y3)
  - Publications: 82
  - Presentations: 69
- Deep Dive Workshops
  - Exascale & CS Issues, Feb 3-4, 2015, University of Florida
  - Multiphase Physics, Oct 13-14, 2016, Tampa FL
- Center Webpage
  - http://www.eng.ufl.edu/ccmt/

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Educational Programs

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

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Educational Programs under ICE

- Profs. Kim & Haftka
  - Yearly course in Verification, Validation and Uncertainty Quantification
  - A new course started in 2014 in anticipation of CCMT
  - Lessons learned from the research in CCMT are immediately reflected in the course
  - Chanyoung Park, Joo-Ho Choi, Raphael T. Haftka (2014). Teaching a Verification and Validation Course using Simulations and Experiments with Paper Helicopter, *ASME 2014 Verification and Validation Symposium, Las Vegas, NV, May 7-9, 2014*
- Prof. Sanjay Ranka
  - Teaches yearly a specialized course for HPC for computational scientists (as part of the Computational Engineering Certificate)

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Additional Educational Programs

- Prof. S. Balachandar
  - Fall, 2016 – new graduate course on multiphase flows (30 graduate students)
- Profs. Greg Stitt/Herman Lam
  - Discusses exascale challenges and the NGEE work in the reconfigurable computing course (EEL5721/4720) and digital design (EEL4712)
  - Uses the CCMT center as a motivational example in Introduction to Electrical and Computer Engineering (EEL3000)

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Additional Educational Programs

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

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Management: Tasks and Teams

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

Hour time slots	Exascale	CMT-nek	CS	Micro	Macro/ Meso	UQ	Exp
Exascale	X	X	X			X	
CMT-nek	X	X	X	X	X		
CS	X	X	X				
Micro		X		X	X	X	X
Macro/Meso		X		X	X	X	X
UQ	X			X	X	X	X

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

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3rd Annual CCMT Picnic

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Do you have any questions?

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Integration & Accomplishments

S. Balachandar

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Review Team Recommendations – 2016

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

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

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

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

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

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

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Outline

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

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Demonstration Problem

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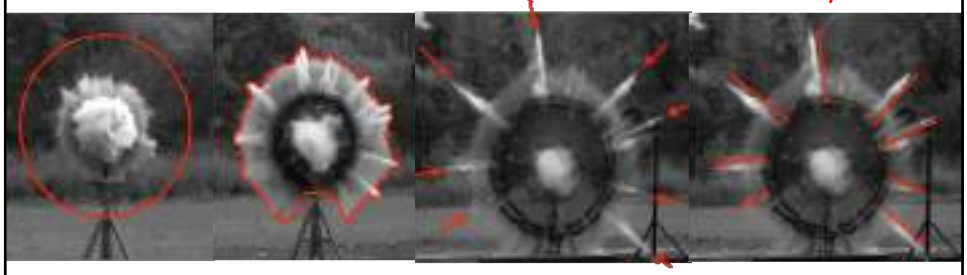
Prediction Metrics

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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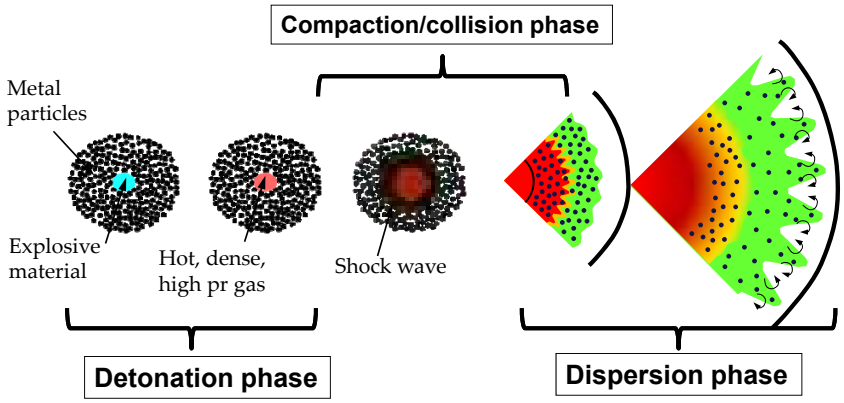
Sequence of Events



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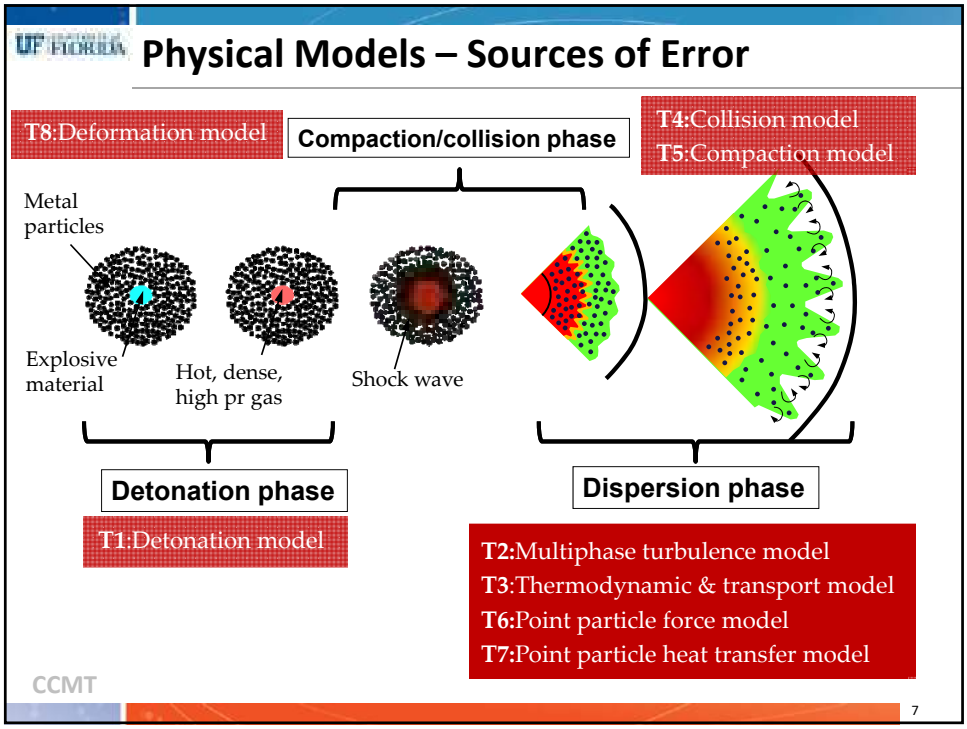
Physical Models – Sources of Error
T8:Deformation model
Compaction/collision phase
T4:Collision model
T5:Compaction model
Metal particles
Explosive material
Hot, dense, high pr gas
Shock wave
Detonation phase
Dispersion phase
T1:Detonation model
T2:Multiphase turbulence model
T3:Thermodynamic & transport model
T6:Point particle force model
T7:Point particle heat transfer model
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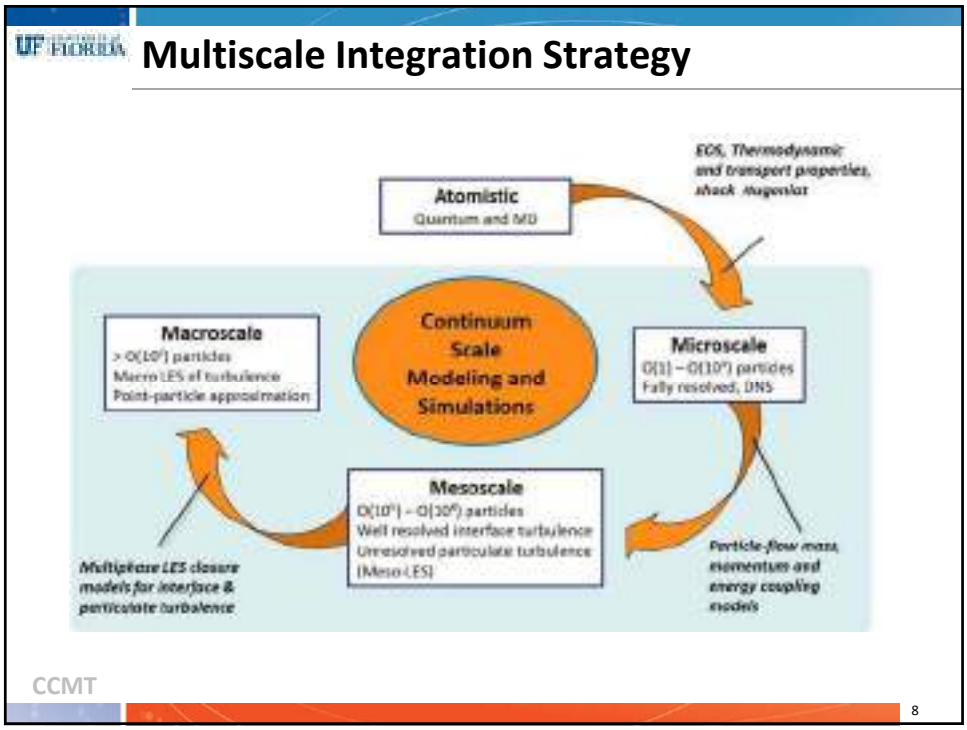
Multiscale Integration Strategy
Atomistic
Quantum and MD
EOS, Thermodynamic and transport properties, shock Hugoniot
Macroscale
> O(10^7) particles
Macro LES of turbulence
Point-particle approximation
Continuum Scale Modeling and Simulations
Microscale
O(1) – O(10^4) particles
Fully resolved, DNS
Mesoscale
O(10^5) – O(10^6) 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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Multiphysics Scope (From Site Visit)

- Our focus will be on
  - Turbulence at the rapidly expanding material front
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities
  - Gas-particle coupling
  - Self-assemble of explosive-driven particles
- Will avoid the following complications
  - Free-shear and wall turbulence (stay away from boundaries)
  - Detonation physics (use simple, well-studied explosives)
  - Fragmentation or atomization physics (avoid casing, liquids)
  - Reactive physics (use non-reactive metal particles)

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Sources of Errors & Uncertainties

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

Key Focus

Advance state-of-the-art

- Multiphase turbulence

- Force coupling model

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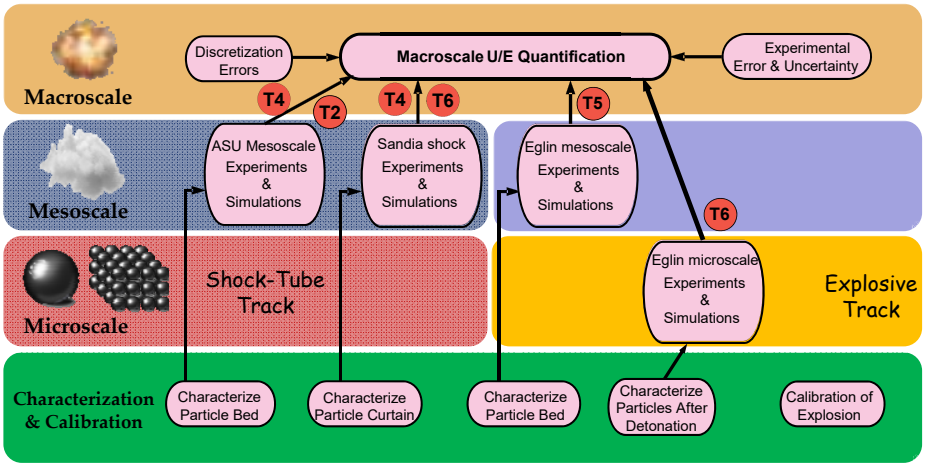
Amendment to Scope

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

- We have added an intermediate configuration that minimizes
  - Compaction effect and associated modeling (T5)
- Revised plan includes
  - Mesoscale and demonstration experiments with lower ϕ
  - Use hollow spheres (thin glass beads)

CCMT 11

Uncertainty Budget – Overall Plan



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

CCMT 12

4 Micro/Meso Campaigns & Target Models

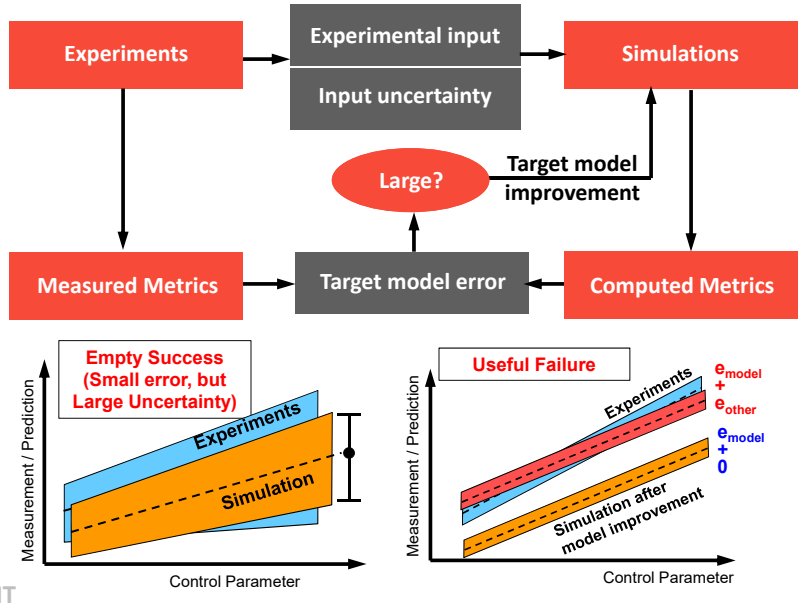
- Sandia shock-tube
  - T6: Force coupling and T4: Particle-particle interaction
- ASU expansion fan
  - T2: Multiphase turbulence and T4: Particle-particle interaction
- Eglin microscale
  - T6: Force coupling
- Eglin mesoscale gas-gun
  - T5: Compaction

↓

- Demonstration problem
  - Yearly hero run

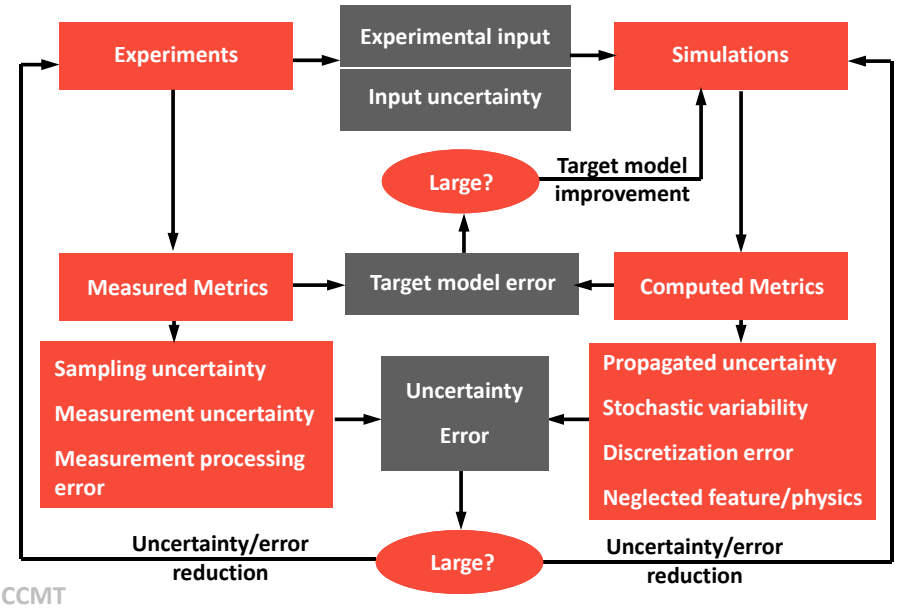
CCMT 13

Uncertainty Budget Workflow



CCMT 14

Uncertainty Budget Workflow



CCMT

15

UB Workflow - Experiment Worksheet

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

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UB Workflow - Experiment Worksheet

- Experimental input
  - Shock properties, particle properties, curtain properties, …
- Input uncertainty
  - Quantified uncertainties in all the above
- Prediction metrics
  - PM1: Shock position, PM2: Upstream and downstream curtain
- Uncertainty & error quantification (UQ)
  - Error in PM1 and PM2 obtained from Schlieren
  - Error in X-ray image particle volume fraction
- Uncertainty & error reduction (UR)
  - Perform new experiments without spanwise gap
  - Improved measurement to reduce volume fraction error

CCMT 17

UB Workflow Simulation Worksheet

- Neglected physics and features
  - …
- Discretization error quantification (UQ)
  - …
- Uncertainty quantification (UQ)
  - …
- Uncertainty reduction efforts (UR)
  - …
- Model form and parameter improvement (MI)
  - …

CCMT 18

UB Workflow Simulation Worksheet

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

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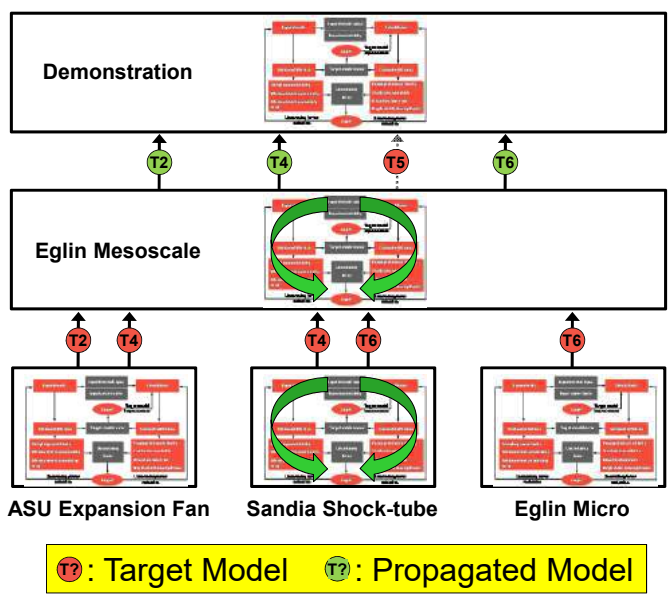
UQ Propagation Across Scale



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20

Other Simulation Efforts

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

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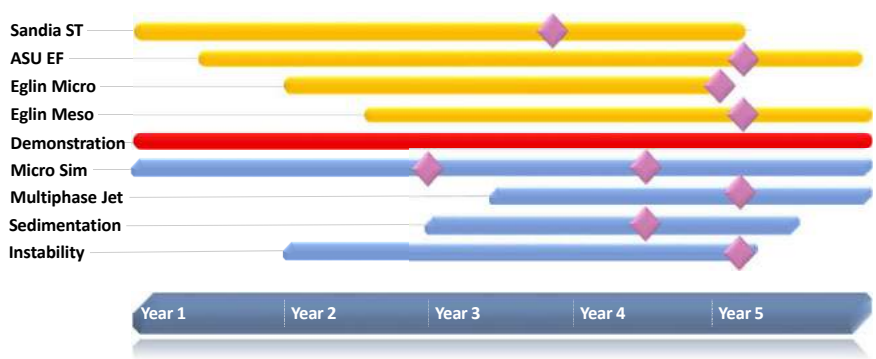
Timeline



: Coupling to Higher Scale

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Essence of Euler-Lagrange Simulation

$$\frac{\partial \mathbf{U}_g}{\partial t} = \mathbf{G}_{inv} + \boldsymbol{G}_{vis} + \boldsymbol{G}_{turb} + \mathbf{f}_{gp} + \mathbf{f}_{ext}$$

$$\mathbf{U}_g = \begin{Bmatrix} \alpha_g \rho_g \\ \alpha_g \rho_g \boldsymbol{u}_g \\ \alpha_g \rho_g E_g \end{Bmatrix}$$

Fluxes (T3)

Turbulence closure (T2)

Detonation source (T1)

Force coupling (T6)
Particle-particle (T4)

$$\frac{d\mathbf{U}_{p,i}}{dt} = \mathbf{f}_{pp} - \mathbf{f}_{gp,i}$$

$$\mathbf{U}_p = \begin{Bmatrix} \rho_p \\ \rho_p \boldsymbol{u}_p \\ \rho_p E_p \end{Bmatrix}$$

Compaction Model (T5)

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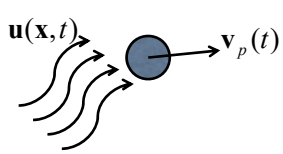
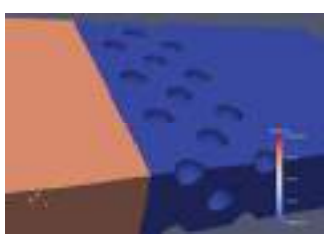
Point-Particle Coupling Models



Commonly used models are based on:

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



But the actual conditions are:

- Strong non-uniformity
- Highly unsteady
- Very large Mach and Reynolds numbers
- Particle-Particle interaction
  - Fluid-mediated
  - Direct collision

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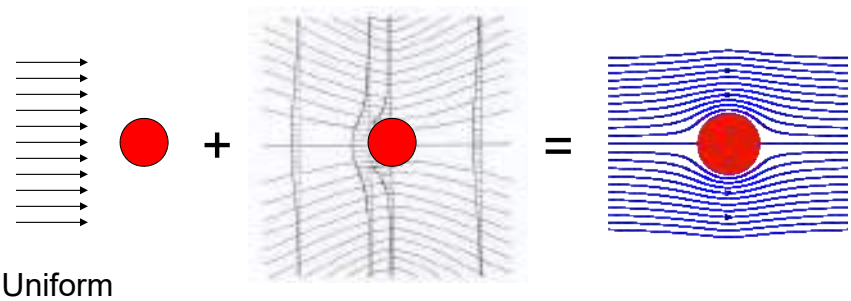
Faxén Theorem (1924)

- Stokes flow (Re = 0 limit)

Undisturbed flow at the particle

$$\text{Stokes Drag} = 3\pi\,\mu\,d\,u$$



Uniform Undisturbed Ambient flow

Perturbation

Stokes flow

Undisturbed flow

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

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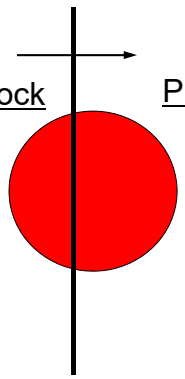
Why We Need Faxén Theorem

- Shock-particle interaction



Post-Shock

p_2
ρ_2
u_2
T_2

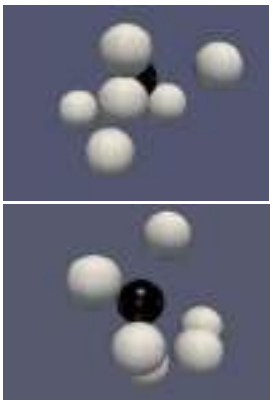
Pre-Shock

p_1
ρ_1
$u_1 = 0$
T_1

?

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

- Flow-mediated particle-particle interaction



A generalized Faxén Theorem has been developed

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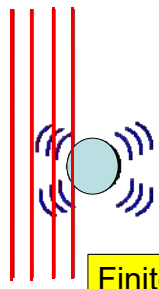
Generalized Faxén Theorem

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

$$m_p \frac{d\mathbf{v}_p}{dt} = F_{gp,i} = \mathbb{V}\,\overline{\rho \frac{D\mathbf{u}}{Dt}}^{V} + 3\pi\mu d\,\overline{\mathbf{u}}^{S} + \mathbb{V}\int_{-\infty}^{t} \left(K_i + K_{vV}\right)\left(\frac{D\overline{\rho\mathbf{u}_r}^{S}}{Dt}\right) d\xi + \mathbb{V}\int_{-\infty}^{t} K_{vS}\left(\frac{D\overline{\rho\mathbf{u}}^{S}}{Dt}\right) d\xi$$



Finite-Particle Force Model

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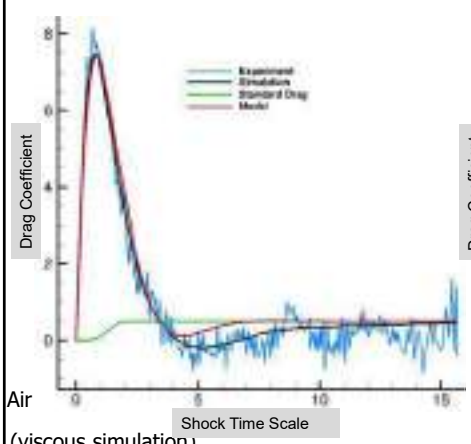
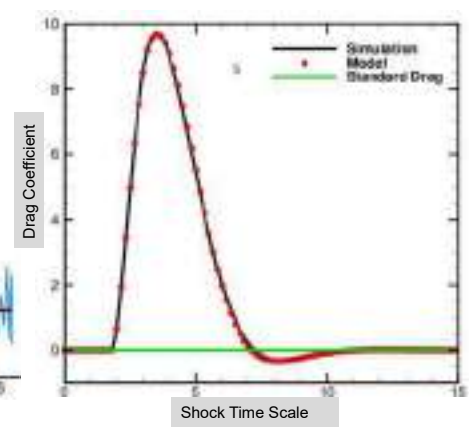
Finite-Size Models for Single Particle



Air
(viscous simulation)



- Fan-Particle Interaction ($M_s = 1.22$)

(inviscid simulation)

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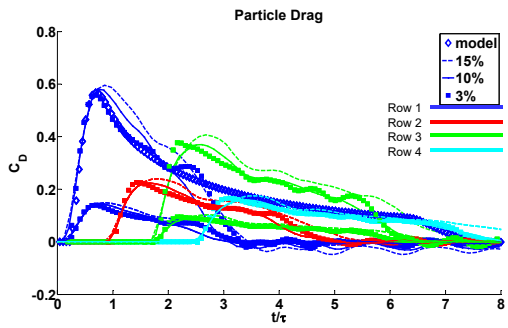
FCC Array of Spheres in An Expansion Fan

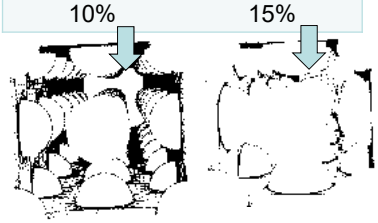
CMT-nek predictions & model dev on Mira

Elements	Spheres	Rows
23424	95	21

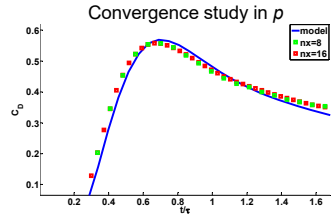


Volume fraction 3%

10% 15%



Convergence study in *p*



Annamalai & Balachandar (2017) *J. Fluid. Mech.* **816**, 381-411

29

Micro-Macro Integration Strategy

1. We have a rigorous theoretical single particle force model
2. From microscale simulations have the best empirical single particle force model at finite Re, Ma
3. Beyond force model – model for particle temperature, pressure
4. Beyond single particle
   - Mean volume fraction effect
   - Systematic inclusion of particle-particle interaction
5. Back effect on gas (modeling of pseudo turbulence)

CCMT - Reynolds stress closure, etc.

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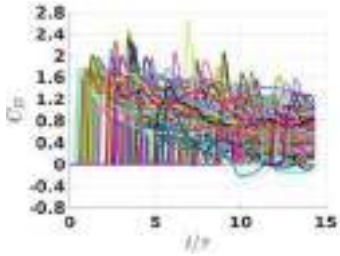
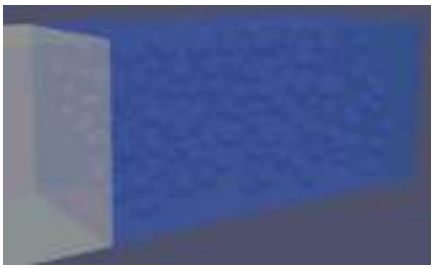
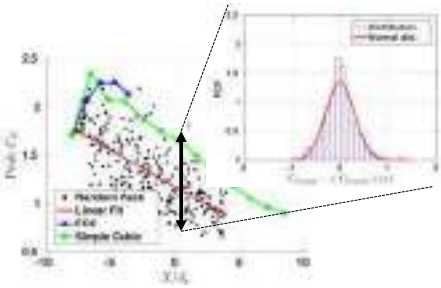
Random Pack – Drag Force

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





Mach 3.0 & 10% Volume Fraction



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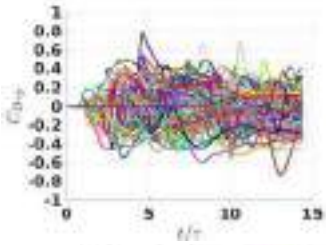
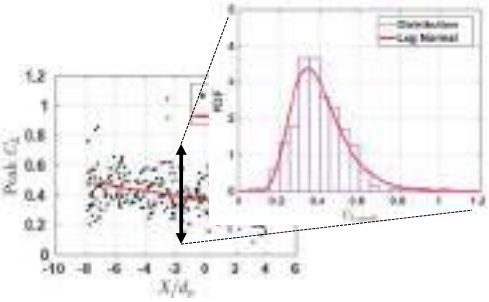
Random Pack – Transverse Force

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



Mach 3.0 & 10% Volume Fraction



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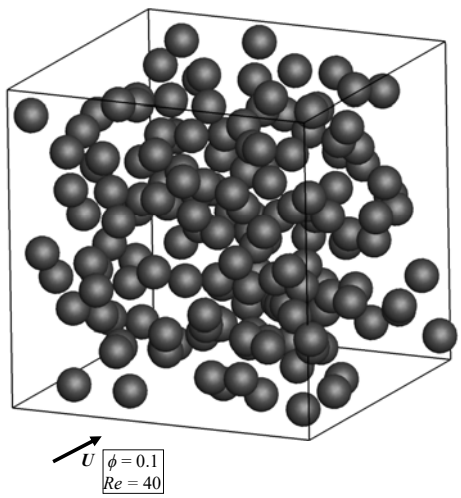
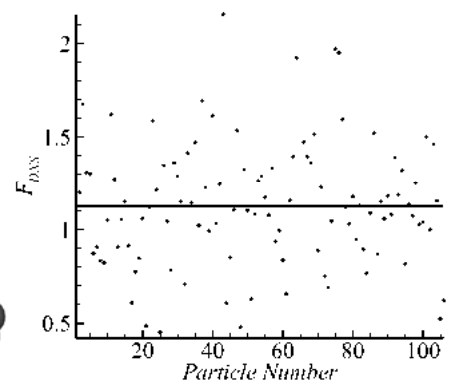
Particle-Particle Interaction (PIEP) Model





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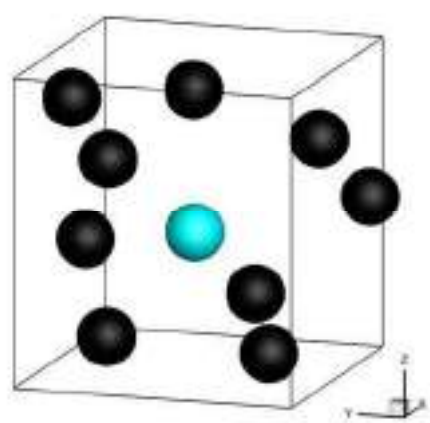
Pairwise Interaction Assumption

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



Undisturbed Velocity:

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

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

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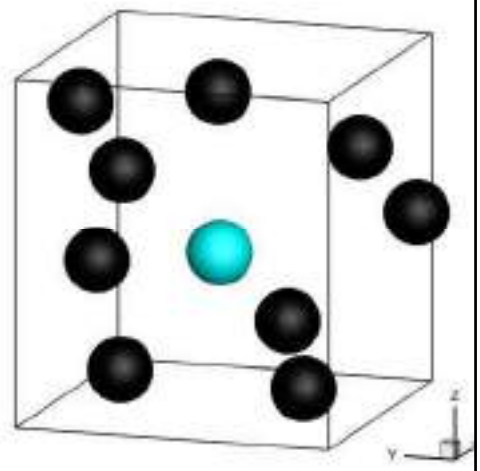
Pairwise Interaction Model

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

Undisturbed Velocity:

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

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



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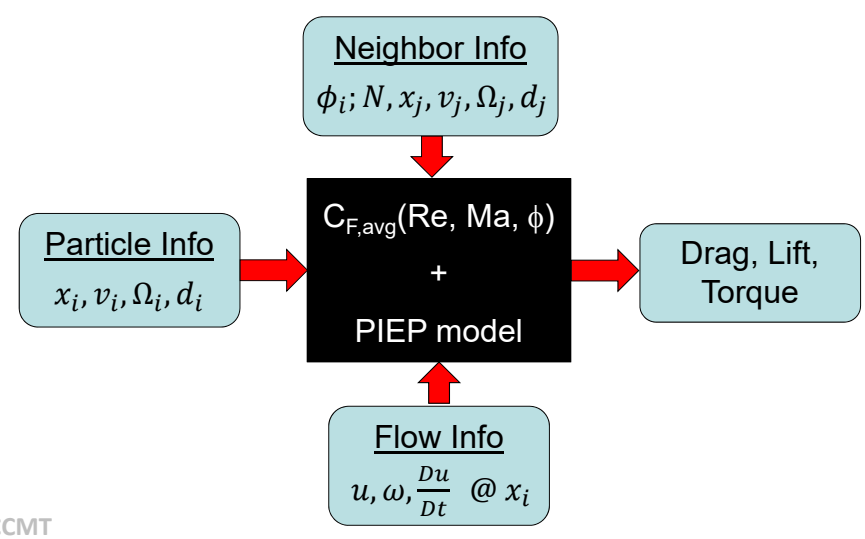
Mesoscale Simulations With PIEP Model

- Matlab and Fortran black boxes with PIEP model



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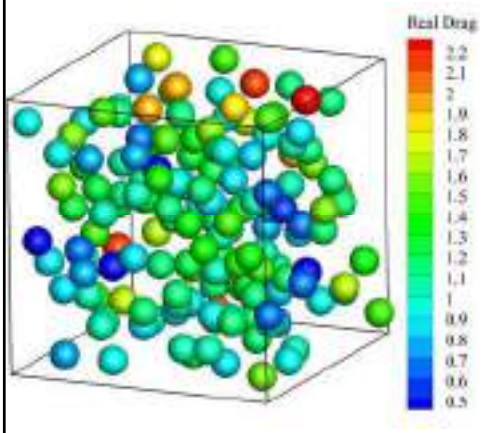
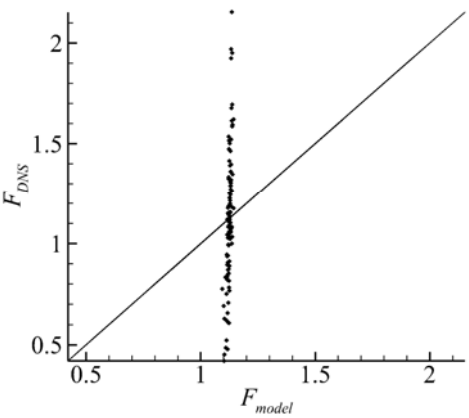
PIEP Model vs DNS (drag)

$R^2 = 0.06$





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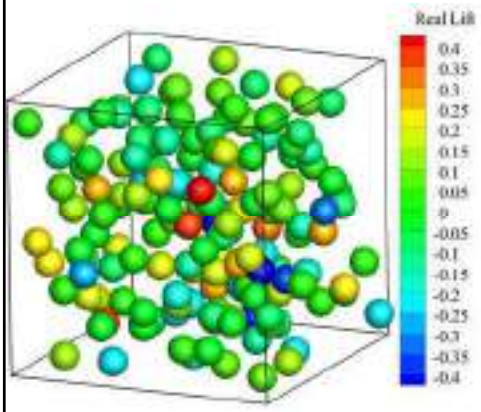
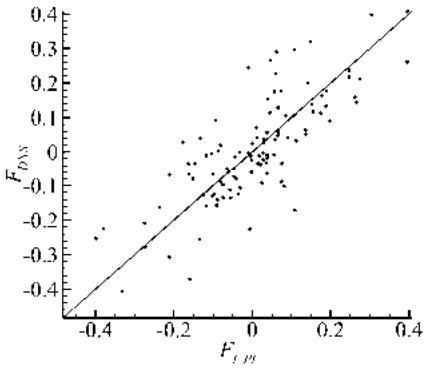
PIEP Model vs DNS (Lift)

$R^2 = 0.60$





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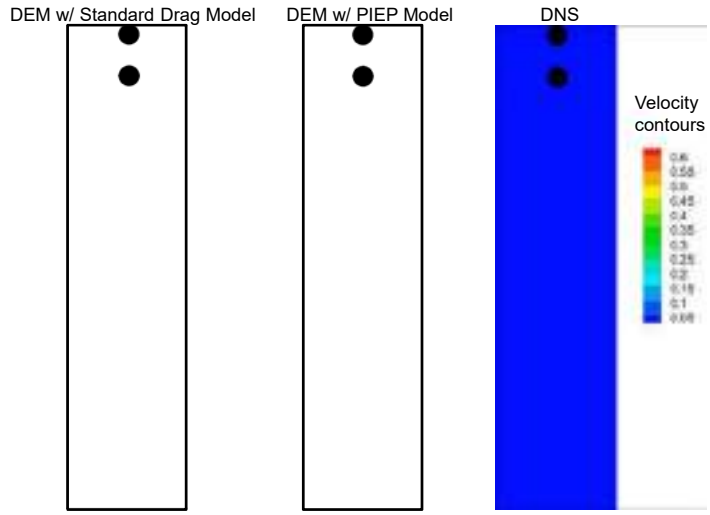
Drafting, Kissing & Tumbling Validation



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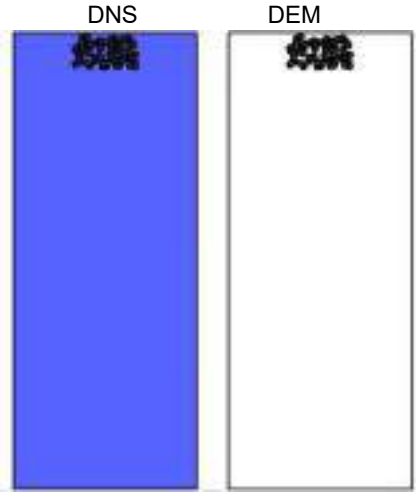
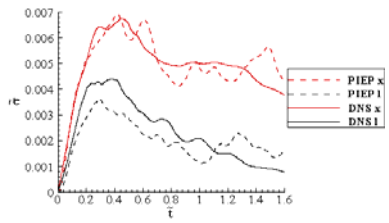
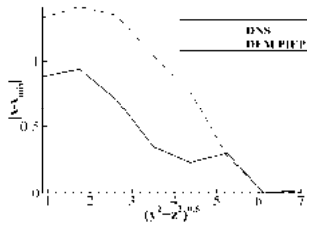
80 Sphere Sedimentation Validation



Velocity Distribution



Height vs radial position



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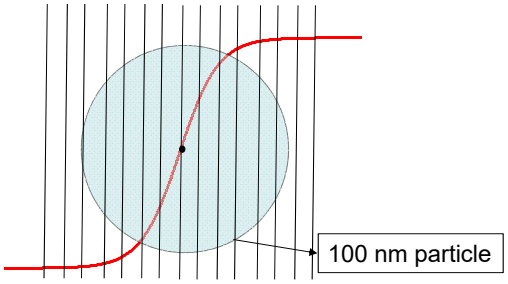
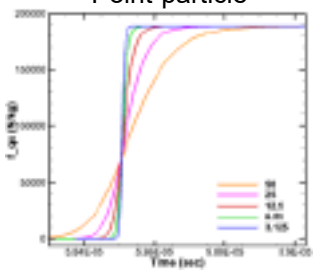
Convergence of Euler-Lagrange Approach

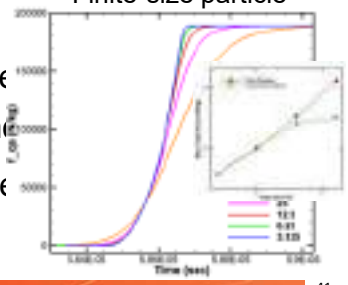
- Shock thickness depends on grid (~10 Δx)



Point-particle



Finite-size particle



- Test case condition
  - Stationary single point particle
  - 1-way coupling
  - Particle diameter: 115 μm
  - Grid size range: 800 to 3.125 μm

With decreasing Δx convergence be
- the shock becomes sharper an
- $\bar{u}^S$ differs from $\bar{u}$ at the particle
- $\bar{u}^S$ depends on gas velocity at

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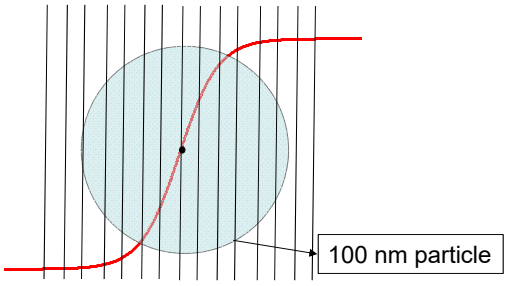
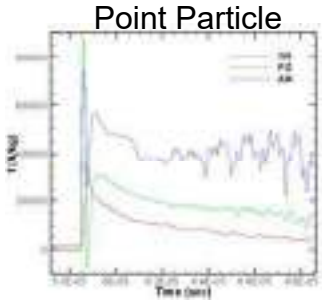
Convergence of Euler-Lagrange Approach

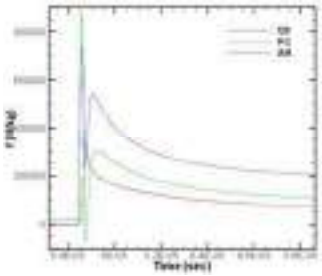
- Shock thickness depends on grid (~10 Δx)



Point Particle



Finite Size Particle



With decreasing Δx only finite size force converges.

Standard EL approach fails!!!

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Y3 Accomplishments

1. Macroscale – Hero Run
2. Mesoscale – CMT-nek simulation of expansion fan
3. Microscale – Shock + Contact
4. Validation experiments & Forensic UQ
5. CMT-nek
6. UQ workflow
7. Design space exploration with Behavioral Emulation
8. Dynamic load balancing of Euler-Lagrange

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1: Demonstration Problem (Macroscale)

Goal

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

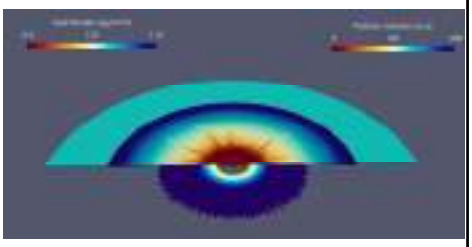
Year 3

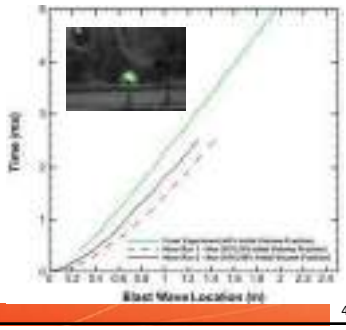
- Use existing code to perform petascale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)
- Develop capabilities for the next hero run: real gas EOS, reactive burn, collision modeling

Presentation

- Bertrand Rollin

3-D demonstration Simulations





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2: Mesoscale Simulations

Goal

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

Year 3

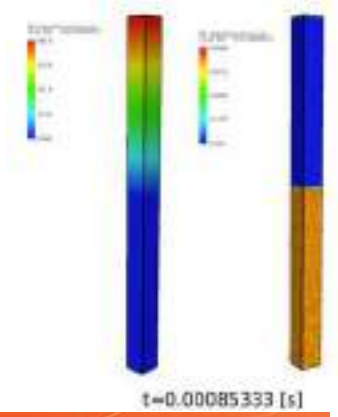
- Scalable 2-way coupled particle capability in CMT-nek
- CMT-nek simulations of ASU experiment
- Incorporating PIEP model into Nek5000 and CMT-nek
- Mesoscale simulations of expansion fan over a bed of particles

Presentation

- David Zwick, Bertrand Rollin

ASU rarefaction experiment

particle properties		
$\rho_p = 25$ [kg/m^3]	N_{elem}	8192
$\Phi_p = 60\%$	Gas DOF	1E6
$D_p = 100$ [μm]	SPL	76
$N_p = 8{,}000{,}000$	MPI ranks	8192



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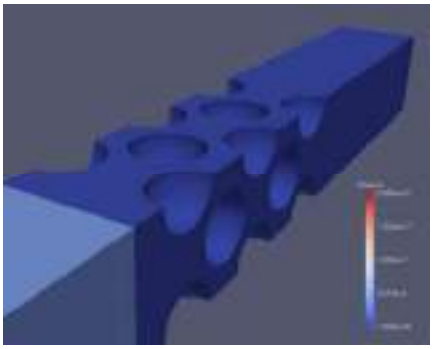
3: Microscale Simulations

Goals

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

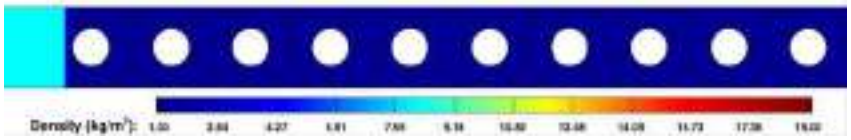


Year 3

- Shock propagation over a structured array
- Shock propagation over a random array
- PIEP model validation & improvement
- Shock + Contact (detonation condition)

Presentation

- Yash Mehta



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4: Validation Experiments

Goals

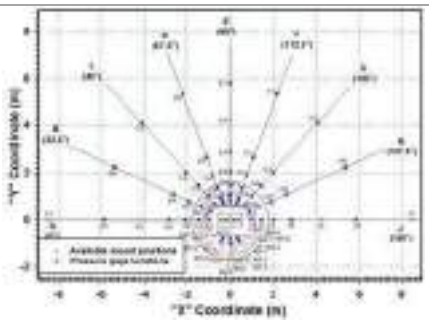
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

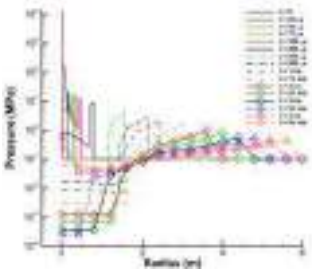
Year 3

- Blast pad experiments at Eglin AFB
- Mesoscale gas-gun experiments at Eglin
- Forensic UQ
- Experimental studies of gas-particle mixtures under sudden expansion at ASU

Presentation

- Angela Diggs, Heather Zunio (ASU) & Kyle Hugh





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4: Validation Experiments

Goals

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- Mesoscale gas-gun experiments at Eglin
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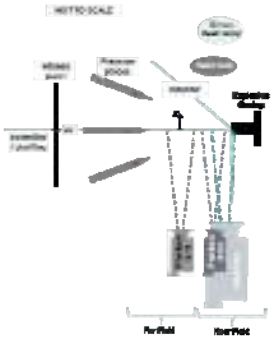
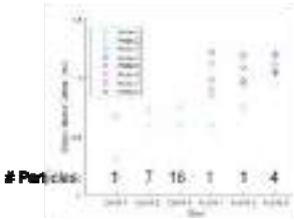
- Experimental studies of gas-particle mixtures under sudden expansion at ASU

Presentation

- Angela Diggs, Heather Zunio (ASU) & Kyle Hugh





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5: CMT-nek Development

Goals

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

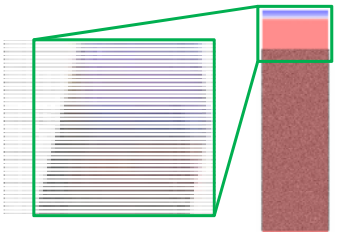
Year 3

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

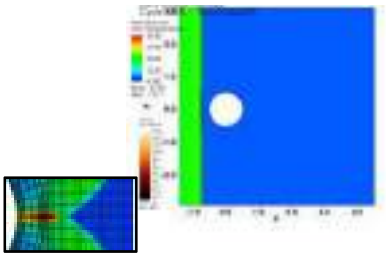
Presentation

- Jason Hackl and David Zwick

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



Mach 3, γ = 1.4, unit gas constant
Color temperature, Pressure contours



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6: UQ Workflow

Goals

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

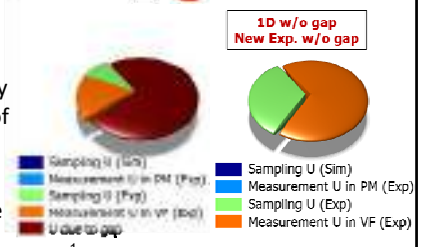
Year 3

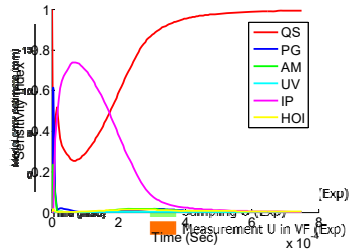
- Identify main uncertainty sources and quantify their contributions to the model uncertainty of the shock tube simulation
- Reduce uncertainty to focus on model error
- UQ and propagation in the context of exascale emulation
- JWL mixture-EOS surrogate for efficient computation

Presentation

- Rafi Haftka, Chanyoung Park, Nam-Ho Kim, Herman Lam, Fred Ouellet, Yiming Zhang

UQ Workflow





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7: Exascale Emulation

Goal

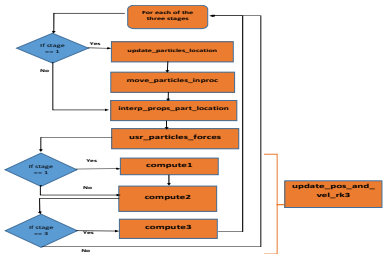
- Develop behavioral emulation (BE) methods and tools to support co-design for algorithmic design-space exploration and optimization of key CMT-bone kernels & applications on future Exascale architectures

Year 3

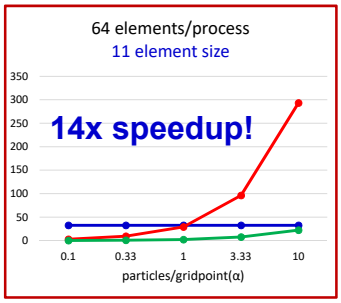
- Enhanced BE methods with network models, interpolation schemes, and benchmarking for CMT-bone AppBEOs
- Performed large-scale experiments on DOE platforms with BE-SST simulator
- Started design space exploration
- Improved throughput and scalability for FPGAs

Presentation

- Herman Lam, Greg Stitt, Nalini Kumar, Carlo Pascoe, Yiming Zhang



Control-flow graph of rk3 algorithm



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8: Dynamic Load Balancing

Goal

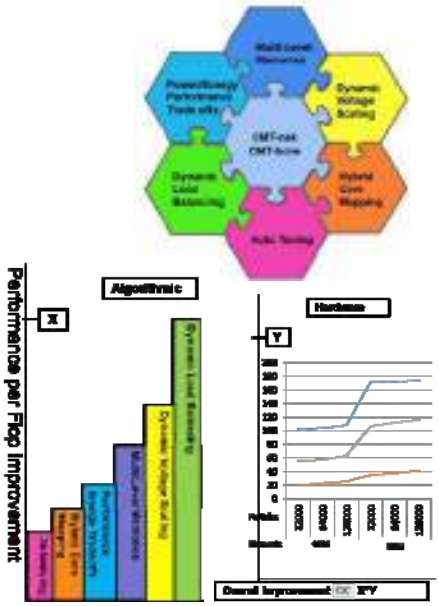
- Derive computationally intensive portions of the CMT-nek code and understand its performance, thermal and energy issues

Year 3

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

Presentation

- Tania Banerjee & Sanjay Ranka



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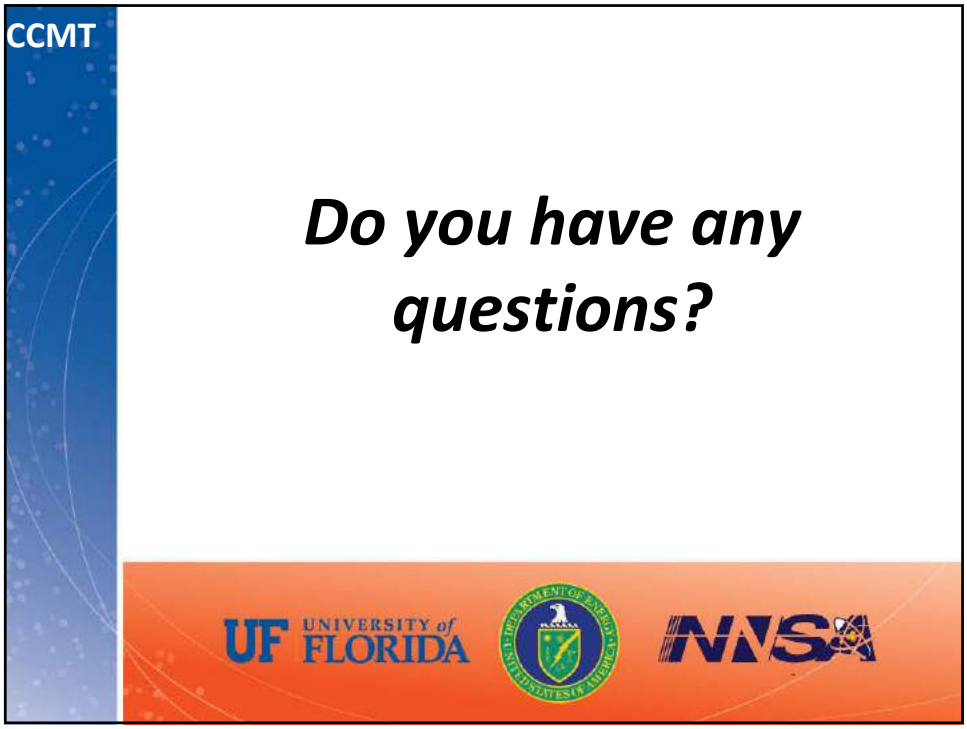
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Do you have any questions?
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NNSA

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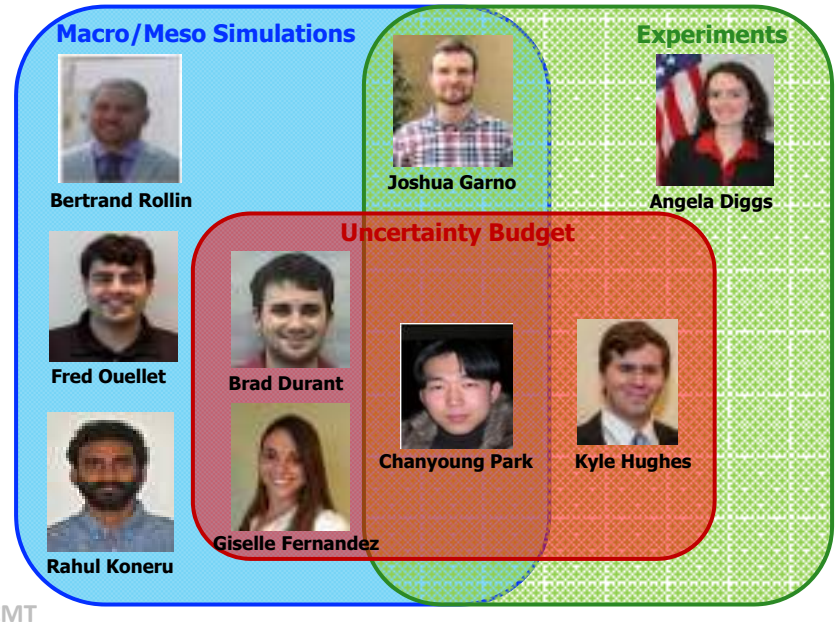
Integration of Experiments and Simulations

Angela Diggs and Bertrand Rollin

UF UNIVERSITY of FLORIDA

Team Members



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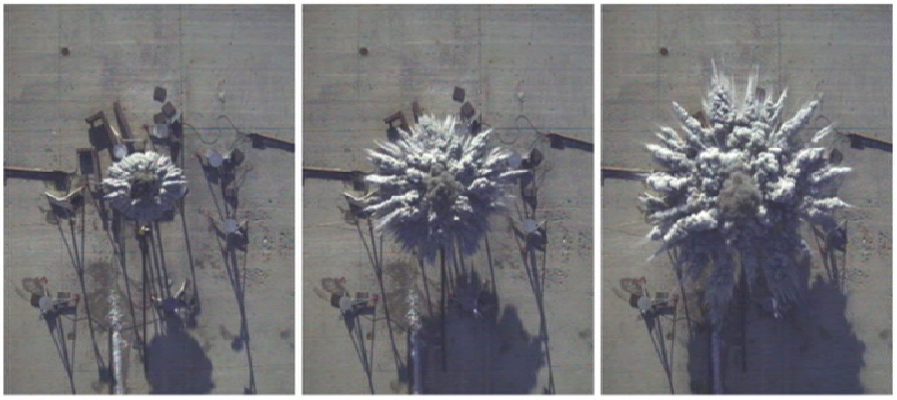
2

Explosive-Driven Particle-Laden Flows



F. Zhang et al. Shock Waves (2015) 25:239–254

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

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3

Review Team Recommendations – 2016

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

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

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

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

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4

Outline

- **Demonstration Problem**
  - Hero Run
  - Eglin's Macroscale Experiment (Blastpad)
- **Model Validation Problems**
  - Eglin's Micro and Mesoscale Experiments
  - SNL's Multiphase Shock Tube

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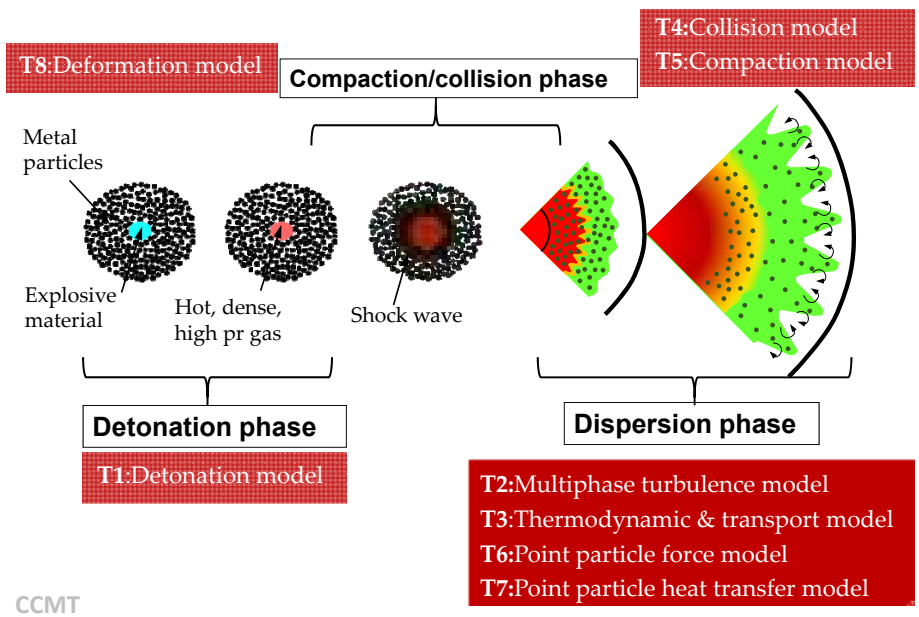
5

Physical Models – Sources of Error



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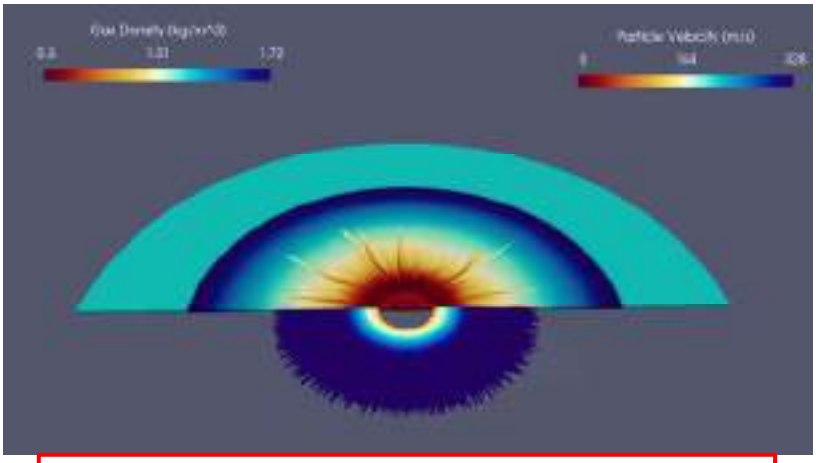
Demonstration Problem: Hero Run 2



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

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Hero Run: Evolution

Properties	Hero Run 1	Hero Run 2	Hero Run 3A	Hero Run 3B	Hero Run 3C	Hero Run 4
Reactive burn	No	No	Yes	Yes	Yes	Yes
Equation of state	Ideal Gas	JWL	JWL	JWL	JWL	JWL
Initial Particle volume fraction	5 %	40 % - Frozen	10 % - Frozen	10 % - Frozen	10 % - Frozen	40 %
Particle bed perturbation	none	none	none	1 mode in azimuthal direction	4 mode in azimuthal direction + white noise	0
No. of computational particles	5 M	5 M	15 M	15 M	15 M	15 M
No. of elements	30 M	30 M	60 M	60 M	60 M	120 M
No. of cores	512	4096	5760	5760	5760	16384

currently running

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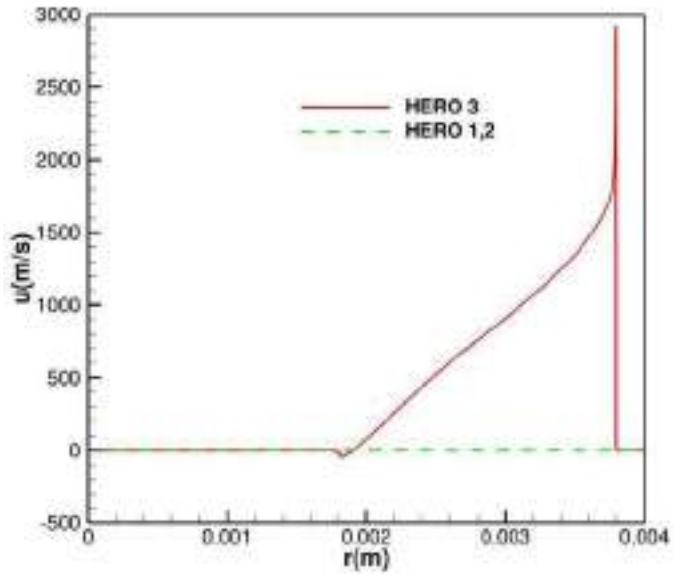
Hero Run 3: Reactive Burn Initial Conditions



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Hero Run 3: Equation of State Model

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.

	One Equation	Iterative method	Multi-fidelity Surrogate
Advantage	- Speed - Algebraic equation	- Accuracy - Problem independent	- Speed - Take account of species equation
Disadvantage	- Uncertainty and error - JWL + ideal gas case only	- May be slow to converge - Computationally expensive	- Uncertainty - Equation of State specific (problem specific)

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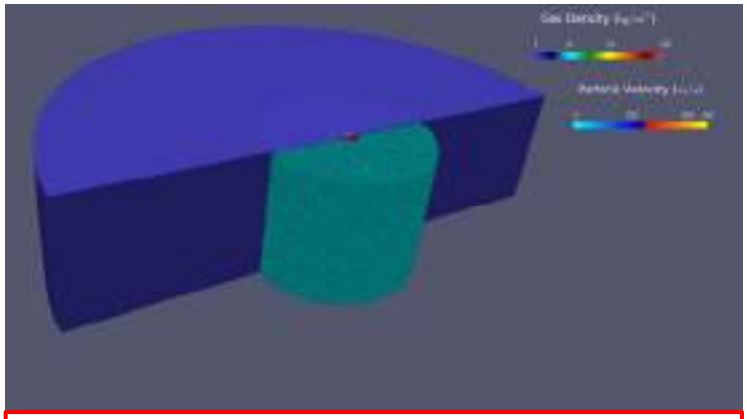
Hero Run 3



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

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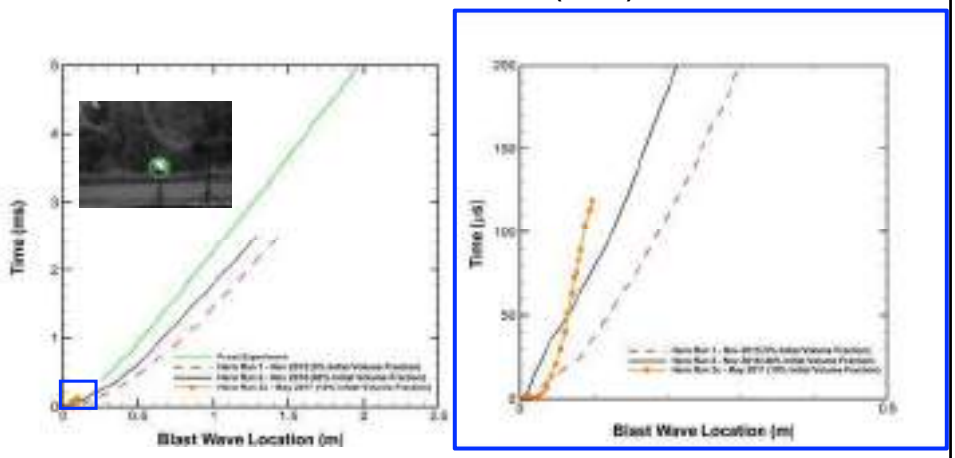
Demonstration Problem: Predictions

Blast Wave Location (PM-1)



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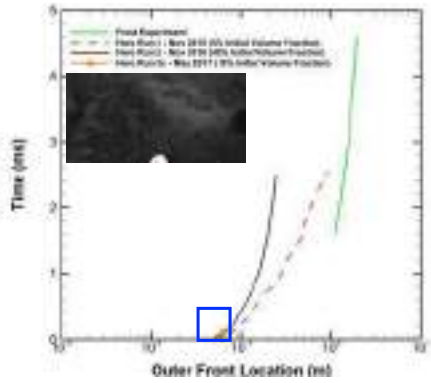
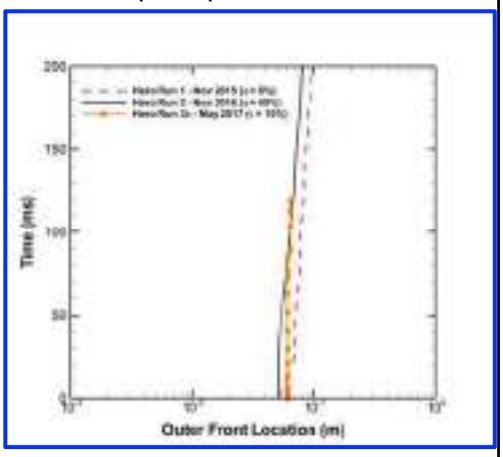
Demonstration Problem: Predictions

Particle Front Location (PM-2)





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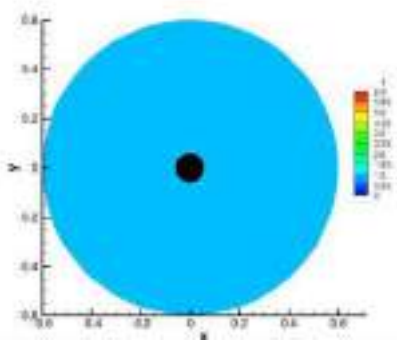
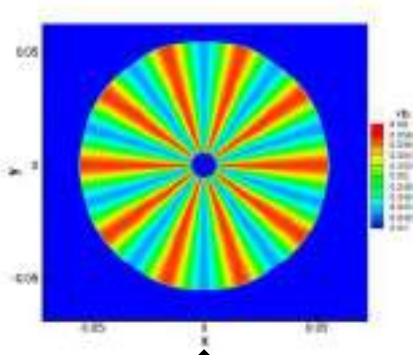
Effect of Initial Particle Volume Faction Distribution

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





Initial perturbation in the particle volume fraction (PVF). It is single mode with wavenumber equal 10, amplitude 0.14 and no phase shift.

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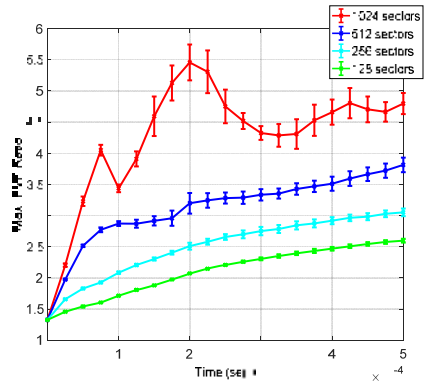
Prediction Metric: Maximum PVF Ratio

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

Schematic of a sector.
We used 1024 sectors

$$Max.PVF\ Ratio = \frac{PVF_M}{PVF_L}$$



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

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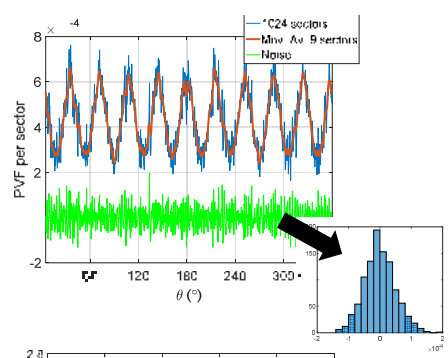
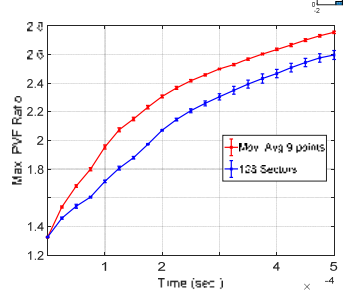
Modal Filtering

- The noise in the data has a normal distribution with mean zero and standard deviation smaller than 6e-5.
- The signal is one order of magnitude bigger than the noise standard deviation for the perturbed case.
- Moving average method will be used as a noise filter in the future optimization process.





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Outline

- **Demonstration Problem**
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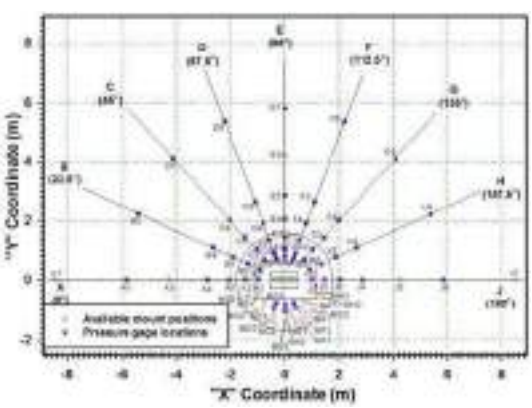
AFRL Blastpad Experimental Setup



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

- Instrumentation:
  - 54 pressures probes
  - Momentum traps (instrumented possible)
  - Four high speed video cameras
  - Linear optical transducers
- Six shots
  - 2 bare charges
  - 1 charge w/tungsten (notched)
  - 1 charge w/steel (notched)
  - 2 charges w/steel (un-notched)

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

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Distribution A. Approved for public release. Distribution unlimited.

18

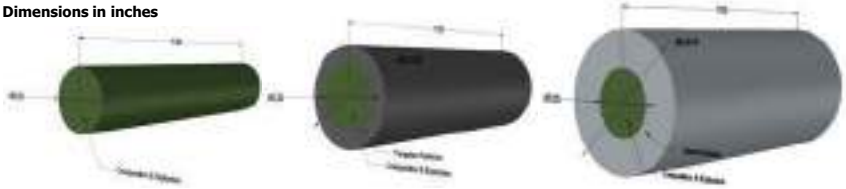
Blastpad Charge Sizing

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

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	226.2	141.375
Particle momentum effects from the detonation of heterogeneous explosives	Frost	435	4350	10
Explosive dispersal of solid particles	Zhang	2400	26000	10.83333

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

Dimensions in inches



a) Bare charge b) Charge w/ tungsten particles c) Charge w/ steel particles

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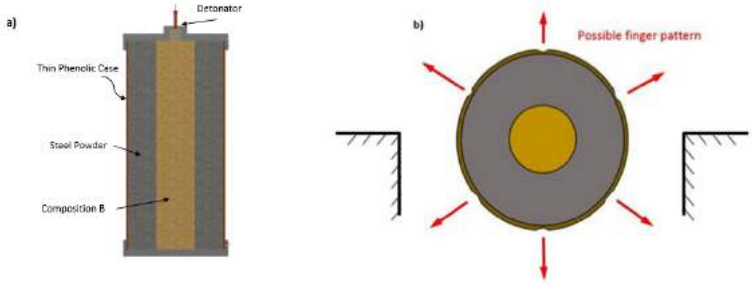
Minimize Case Influence

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



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Distribution A. Approved for public release. Distribution unlimited.

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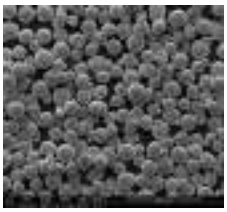
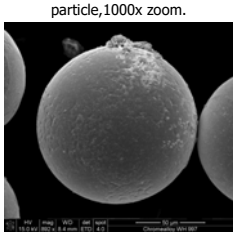
Preliminary Particle Characterization

- Steel Particles
  - Multiple vendors surveyed. Criteria were high particle roundness (sphericity) and narrow particle spread
  - Vendor: Osprey Sandvik
  - Size range (confirmed with particle sizer): 75-125 μm
  - SEM shows mostly spherical particles
- Tungsten Particles
  - Government provided
  - Size range (confirmed with particle sizer): 100-130 μm
  - SEM shows mostly spherical particles

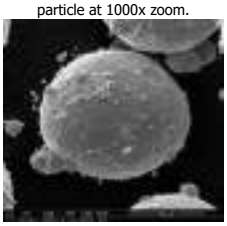
SEM of several steel particles at 100x zoom.



SEM of single tungsten particle,1000x zoom.



SEM of single steel particle at 1000x zoom.



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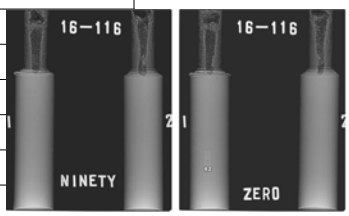
Collaboration: Input Measurement Uncertainty

Input Parameter	Source
Explosive length [mm]	AFRL measurement
Explosive diameter [mm]	AFRL measurement at 5 locations
Explosive density [kg/m^3]	AFRL calculation
Explosive quality	AFRL X-ray
Particle diameter [mm]	CCMT measurement
Particle density [kg/m^3]	CCMT measurement
Particle volume fraction	AFRL calculation
Ambient pressure [kPa]	AFRL weather station
Ambient temperature [C]	AFRL weather station
Probe locations [m]	CCMT measurement



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

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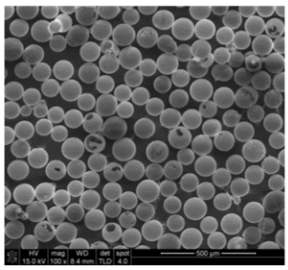
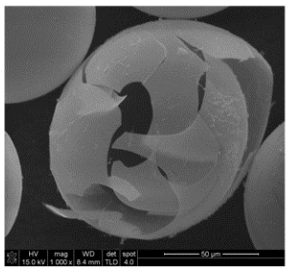
Future Experiments

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

x100 Zoom:



x1000 Zoom:



SEM images of hollow glass microspheres to be crushed when subjected to the shock

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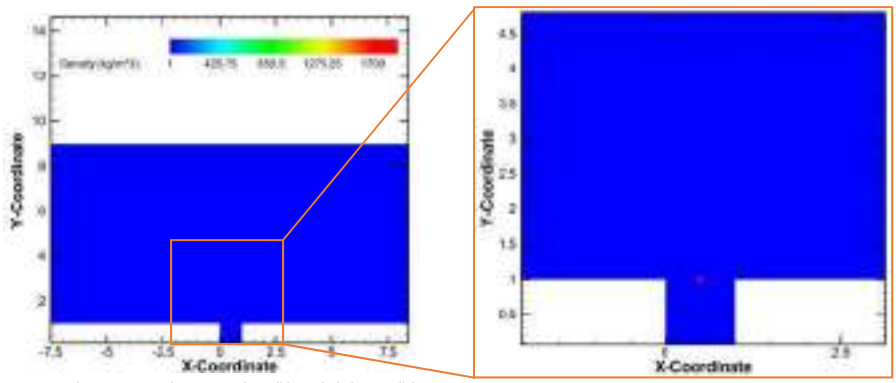
Blastpad Simulation Setup



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

Preliminary Simulation Details:

- 5.16 million cells in two dimensions
- To be run on 1024 cores using LLNL's Quartz machine
- Bottom five boundaries are slipwalls
- Remaining three are outflows
- 65 probes set in locations of experimental sensors

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Blastpad Simulation Parameters

Properties	Comp B	Steel	Tungsten
Diameter	-	100 μm	115 μm
Density	1712 kg/m^3	7660 kg/m^3	15540 kg/m^3
Specific heat	1223.6 J/kg K	510 J/kg K	134 J/kg K
Outer diameter	3.25 in	6.88 in	5.12 in
Depth (thickness)	0.75 in	0.75 in (2 cm)	0.75 in (2 cm)
Energy = (dens x int energy/unit vol)	8.5 GPa (products); 0.662 GPa (unreacted)	-	-
Computational Particles	-	10 M	10 M

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

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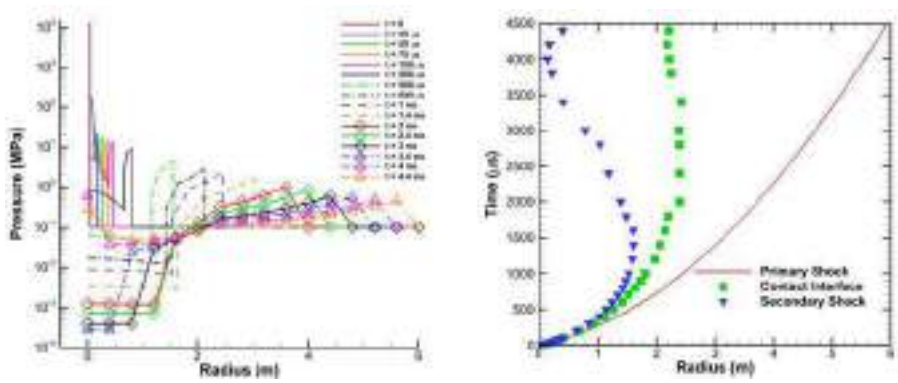
Blastpad Simulation (Bare charge 1d results)



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Outline

- **Demonstration Problem**
  - Hero Run
  - Eglin's Macroscale Experiment (Blastpad)
- **Model Validation Problems**
  - Eglin's Micro and Mesoscale Experiments
  - SNL's Multiphase Shock Tube

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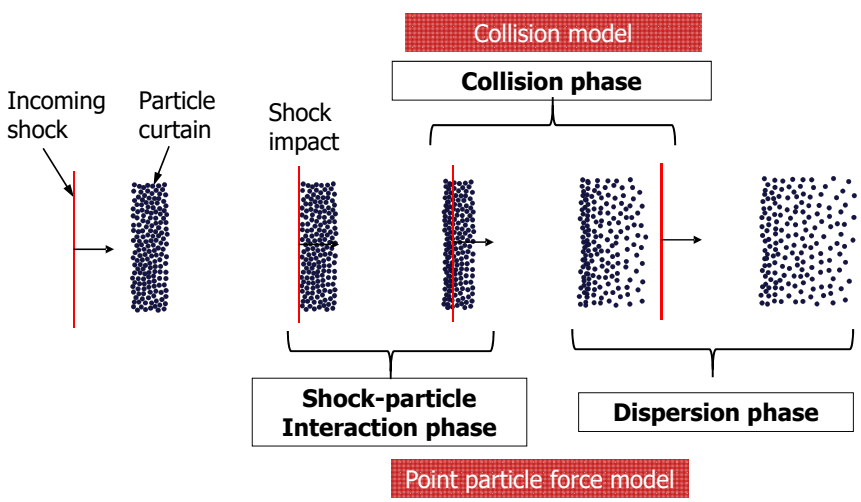
Key Physics



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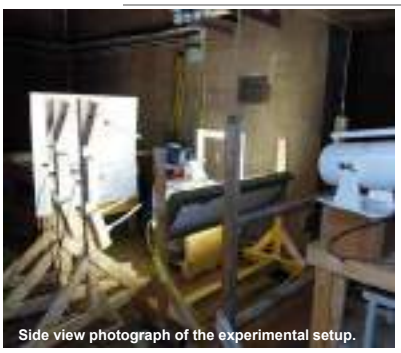
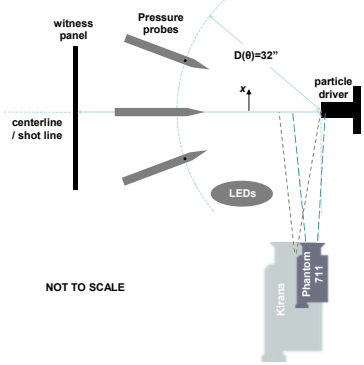
Mesoscale Experiments: November 2015


Side view photograph of the experimental setup.

Overhead schematic of the test set-up.




Loading the tungsten powder.


Sample x-ray.

Summary of 7 mesoscale explosive shots of interest.

Test #	Driver	Particles
Nov15-1	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-2	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-3	RP-2 + 1 N5	0.5 g Tungsten powder
Nov15-4	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-5	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-6	RP-80 + 1 N5	0.5 g Tungsten powder
Nov15-7	RP-80 + 2 N5	0.5 g Tungsten powder

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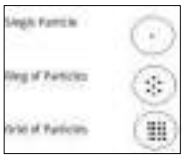
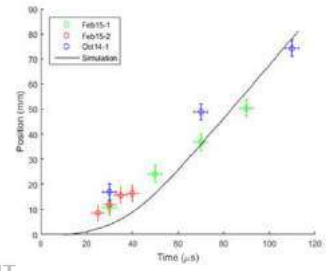
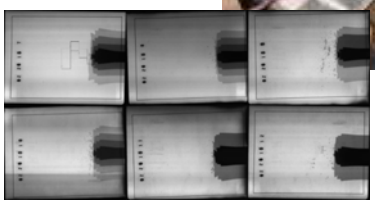
Summary of Microscale Experiments







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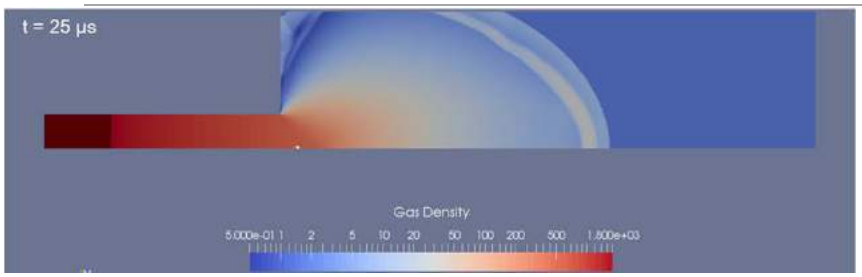
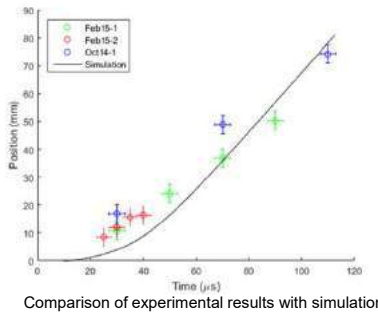
Preliminary Simulation Results





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

Simulation Details:

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

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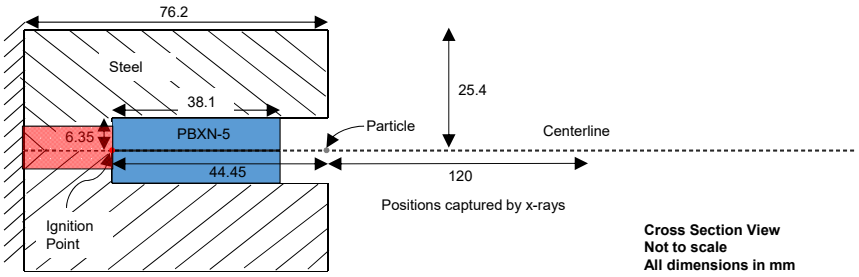
Microscale Simulations Progression

Uncertain Inputs → **Design of Simulation**

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



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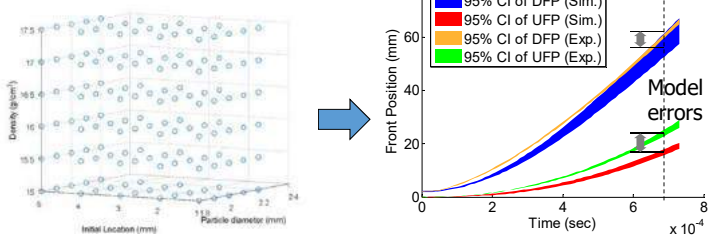
Uncertainty Propagation

Uncertain Inputs
↓
Design of Simulation
↓
Kriging Surrogate
↓
Monte Carlo Sampling
↓
Simulation Prediction Metrics w/ Uncertainty

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



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

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Outline

- **Demonstration Problem**
  - Hero Run
  - Eglin's Blastpad Case
- **Model Validation Problems**
  - Eglin's Micro and Mesoscale Experiments
  - SNL's Multiphase Shock Tube

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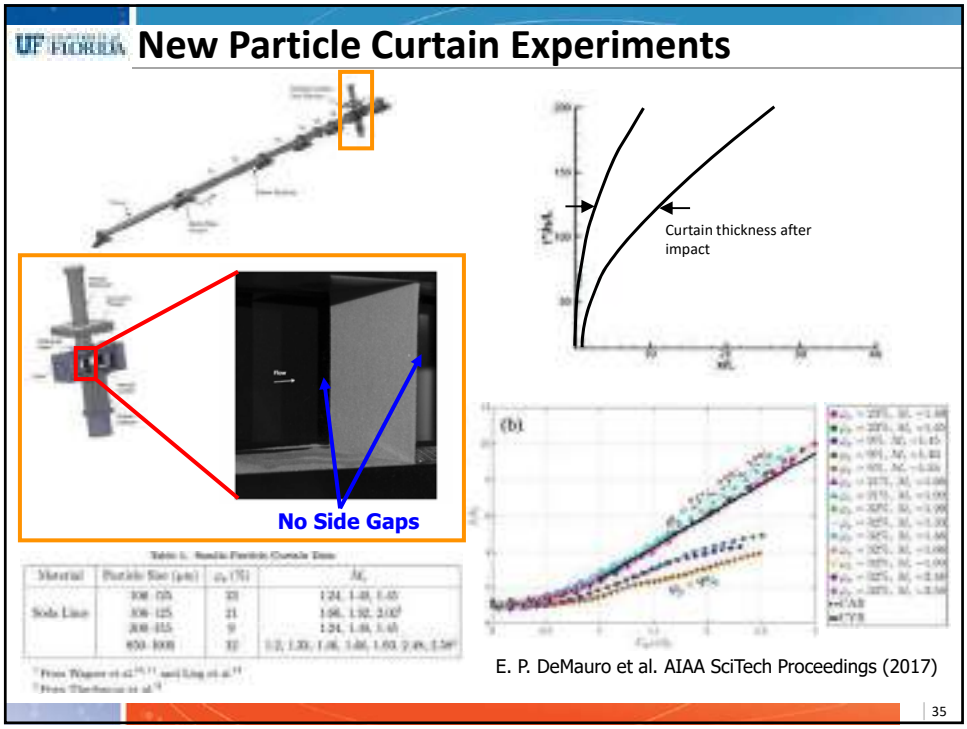
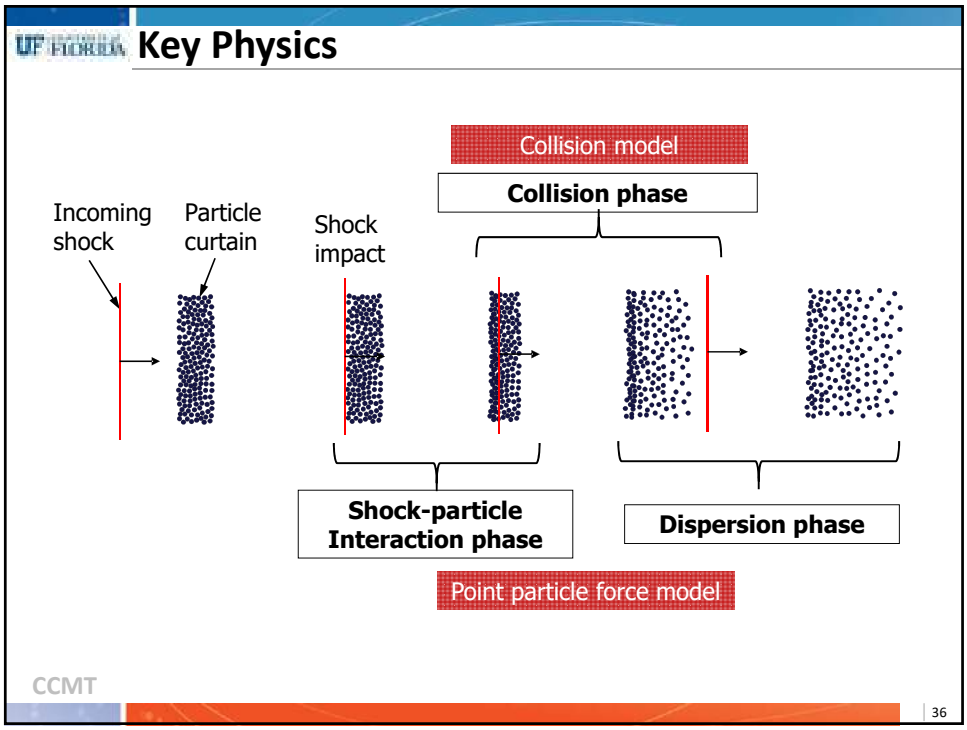

New Particle Curtain Experiments
Curtain thickness after impact
No Side Gaps
(b)
E. P. DeMauro et al. AIAA SciTech Proceedings (2017)
35


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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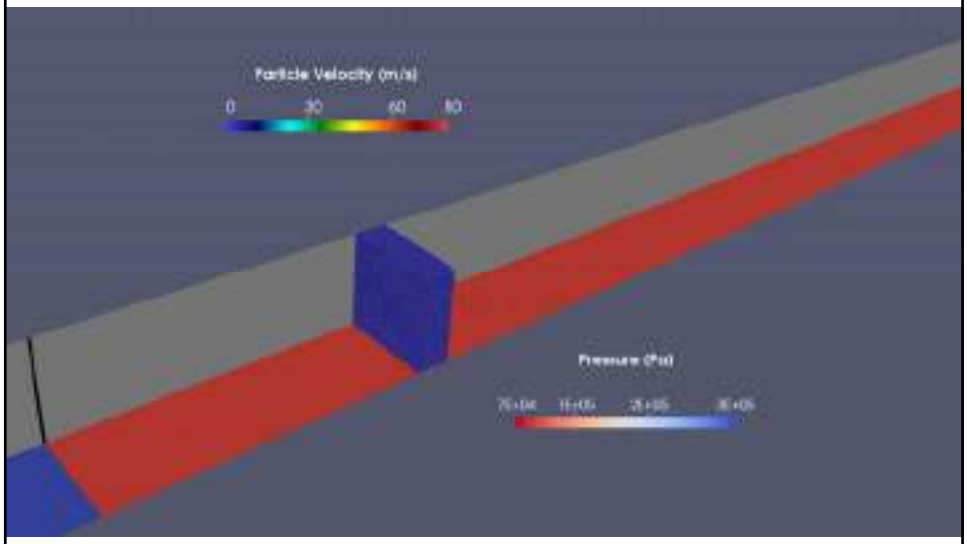
3D Particle Curtain Simulation



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

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Large-Scale Bundle Runs Planning

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

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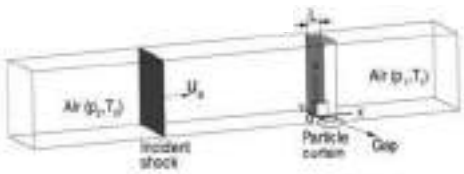
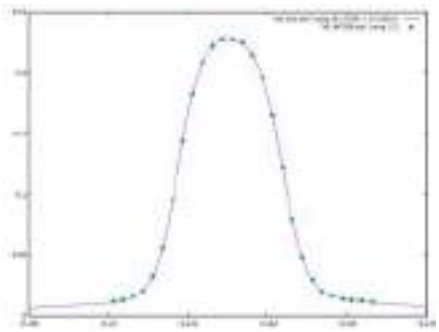
Initial Particle Volume Fraction Study

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



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



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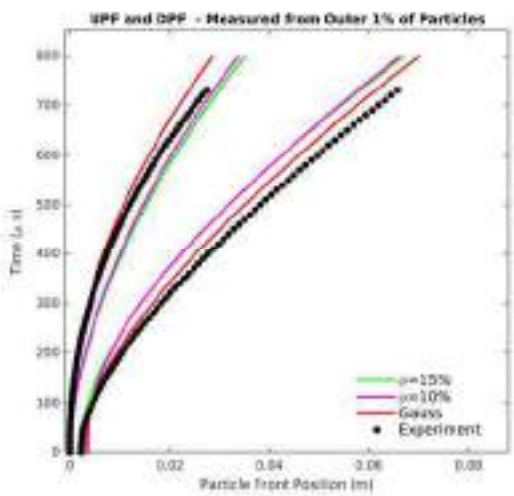
Particle Curtain Initial Volume Fraction Effects



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

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Do you have any questions?
UF UNIVERSITY of FLORIDA
NNSA

CCMT

CMT-nek: A compressible multiphase DGSEM extension to nek5000

Jason F. Hackl

UF UNIVERSITY of FLORIDA

Review Team Recommendations – 2016

- RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
  - Adopt rigorous software development and documentation practices
    - http://travis-ci.org/UFCCMT/Nek5000 automated regression testing, Doxygen committed with code, http://github.com/Nek5000/NekDoc
  - Feedback loop between physics and CS/BE efforts
    - CMT-nek team collaborating with CS & exascale for particle load-balancing; Ongoing application to large simulations of ASU experiment.
  - More staff with in-depth knowledge on CMT-nek with strong ties to CS
    - Lectures on CMT-nek formulation and code during Winter Break 2016-2017 for CCMT staff and leadership.
- RQ 5 – Recommendations on Scalability Results
  - Scalability tests for CMT-nek
    - Only needed for particles; Eulerian code is a trivial subset of nek5000, which already scales well. Production runs and method verification routinely use 8K to 131K cores on vulcan.
  - Use existing allocations on Titan & Mira
    - CS on titan (GPU dev)
    - Large ASU experiment (meso and micro) ongoing on Mira.

CCMT 2

CMT-nek team

Prof. Paul Fischer, UIUC, Argonne

Jason Hackl, UF

David Zwick, UF

Li Lu, UIUC

Brad Durant, UF

Goran Marjanovic, UF

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Accomplishments

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

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Outline

1. Brief review of CMT-nek framework
   a. Discontinuous Galerkin method for gas flow solver
   b. Lagrangian particles and scaling
2. Accomplishments
   – High-order terms and artificial viscosity
   – Particle tracking, 2-way coupling
     • Production rarefaction through particle bed @ meso- and microscale
   – Shock-particle interactions
     • Release for microscale simulation of shocked flows
3. Current and near-future work
   – Shocked mesoscale flows

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Discontinuous Galerkin Spectral Elements

Steps to DGSEM for a conservation law $\frac{\partial U_i}{\partial t} + \nabla \cdot \mathbf{H}_i\left(\mathbf{U}, \nabla \mathbf{U}\right) = R_i$

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 $[-1,1]^d$

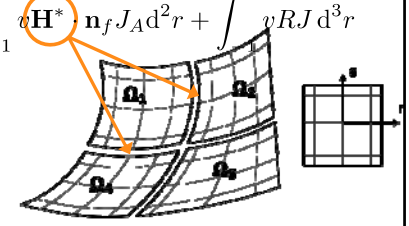
$$\frac{\partial}{\partial x_i} = \frac{\partial r_k}{\partial x_i}\frac{\partial f}{\partial r_k} \approx \left[\mathbf{r}_{k,\mathbf{x}_i}\right]\left[\mathbf{D}_k \mathbf{f}\right]$$

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

Matrix ops within Ω_e

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

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

Discontinuous Galerkin Spectral Elements

Nested tensor products of per-element *N* x *N* matrix operators for…

- Differentiation $\frac{\partial}{\partial x_i} = \frac{\partial r_k}{\partial x_i}\frac{\partial f}{\partial r_k} \approx [\mathbf{r}_{k,\mathbf{x}_i}]\,[\mathbf{D}_k\mathbf{f}]$
- Volume integrals $\int_{\Omega_e} f\,dV$
  (N^3 quadrature points → diagonal mass matrix **B**)
- Surface integrals $\int_{\partial\Omega_e} f$
  (Face restriction **E**, diagonal $\mathbf{B}_A$ on N^2 face points)

$$\sum_{i,j,k=1}^{N} \omega_i\omega_j\omega_k f(r_i,s_j,t_k)J(\mathbf{x}) \to \mathbf{B}\,[\mathbf{f}]$$

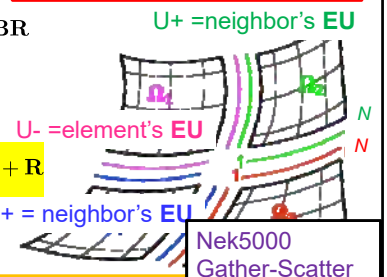
$$\sum_{i,j=1}^{N} \omega_i\omega_j f(r_i,s_j,t_1)J_A(\mathbf{x}) \to \mathbf{B}_A\mathbf{E}\,[\mathbf{f}]$$

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

Equate coefficients of nodal vector of test function **v**
Get semidiscrete system:

$$\left[\frac{\partial\mathbf{U}}{\partial t}\right] = \mathbf{B}^{-1}\mathbf{D}_k^\intercal\mathbf{B}\,[\mathbf{r}_{k,\mathbf{x}_i}]\,[\mathbf{H}_i] - \mathbf{B}^{-1}\mathbf{E}^\intercal\mathbf{B}_A\,[\mathbf{H}^*(\mathbf{E}[\mathbf{U},\nabla\mathbf{U}])] + \mathbf{R}$$

Discretize LHS with explicit TVD RK3



Nek5000
Gather-Scatter
Scales to 10^6
MPI tasks

Fornberg (1998) *A Practical Guide to Pseudospectral Methods.* Cambridge
Lottes & Fischer (2005) *J. Sci. Comp.* **24**(1):45-78 http://nek5000.mcs.anl.gov
Gottlieb & Shu (1998) *Math. Comp.* **67**:73-85

CMT-nek: Convective terms in DGSEM

Euler equations of gas dynamics

i^{th} variable's flux = convective + diffusive

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

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

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

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

Thermodynamic state

Temperature T
Pressure $p(\rho, T)$
Total energy $E = \int c_v T\,dT + \frac{1}{2}u_i u_i$

Conserved variables… to primitive variables… $v = \frac{\rho v}{\rho} = \frac{U_3}{U_1}$

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

- Resolves discontinuous states
- can be any Riemann solver (Advection Upstream Splitting Method)

Liou (1996) "AUSM+" *J. Comp. Phys.*,**129**:362-382

Here, quadrature needs *M* >*N* nodes

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

8

H2

CMT-nek: Entropy viscosity method (EVM)

flux = convective + diffusive

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

Dolejší, V. *Intl. J. Numer. Meth. Fluids* **45**:1083-1106 (2004)

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

Diffusive flux from entropy viscosity (NOT Navier-Stokes)

Mass

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

Momentum

$$H_{i+1,j}^d = -\phi_g\left(\mu_s\rho\sigma_{ij} + \nu_s u_j \frac{\partial\rho}{\partial x_i}\right)$$

Energy

$$\mathbf{H}_{5_i}^d = -\phi_g\left[\mu_s\rho\, u_j\sigma_{ij} + \nu_s\left(\frac{\partial}{\partial x_i}(\rho e) + \frac{1}{2}|\mathbf{u}|^2\frac{\partial\rho}{\partial x_i}\right)\right]$$

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

$$\mathbf{H}^{*d} = \begin{cases} -\mathbf{E}^\intercal\mathbf{B}_A\left[\left(\mathbf{H}_i^d\cdot\mathbf{n}\right)^- - \{\{\mathbf{H}_i^d\cdot\mathbf{n}\}\}\right] \\ +\mathbf{D}_j^\intercal\mathscr{A}_{ij}\mathbf{E}^\intercal\mathbf{B}_A\left[\mathbf{U}^- - \{\{\mathbf{U}\}\}\right][n_i] \end{cases}$$

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

Entropy and its residual

$$s = \log\left(\frac{e^{\frac{1}{\gamma-1}}}{\rho}\right),\ R_s \approx \frac{\partial s}{\partial t} + \nabla\cdot(\mathbf{u}s)$$

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

Tent between maximum @ vertices

Klöckner, Hesthaven & Warburton (2011) *Math. Model. Nat. Phenom.* 6(3):57-83
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

CMT-nek: Lagrangian particles

David Zwick, April 21

Governing equations of ith particle

$$\frac{d\mathbf{X}_p}{dt} = \mathbf{V}_p$$

$$M_p\frac{d\mathbf{V}_p}{dt} = \mathbf{F}_{hyd}(\mathbf{X}_p, \mathbf{V}_p)$$

Particle force from models[1] and gas properties at $\mathbf{X}_p$

- Barycentric interpolation from N^3 GLL grid points

Same Runge Kutta time marching as DGSEM

Back-coupling to gas (e.g. momentum equations)

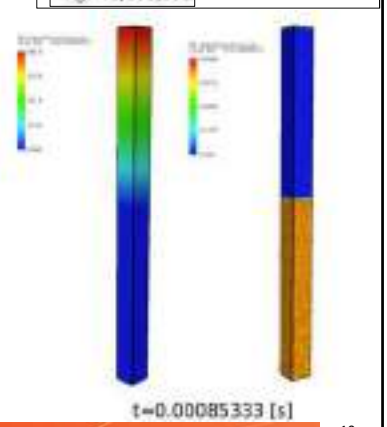
- Gaussian kernel G

$$\phi_g = \sum_{i=1}^{N_p} V_p^{(i)} G(\mathbf{x} - \mathbf{X}_p^{(i)})$$

$$\mathbf{R}(\mathbf{x}) = p\nabla\phi_g - \sum_{i=1}^{N_p}\mathbf{F}_{hyd}^{(i)} G(\mathbf{x} - \mathbf{X}_p^{(i)})$$

ASU rarefaction experiment

particle properties		
$\rho_p = 25$ [kg/m³]	N_{elem}	8192
$\Phi_v = 60\%$	Gas DOF	1E6
$D_p = 100$ [μm]	SPL	76
$N_p = 8{,}000{,}000$	MPI ranks	8192



[1]Ling, Balachandar & Parmar (2016) *Phys. Fluids* **28**, 033304

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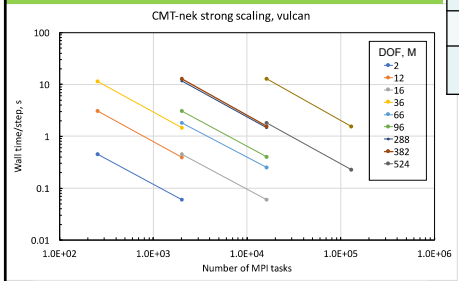
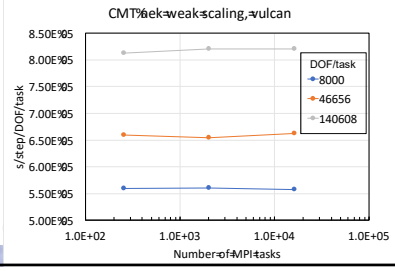
CMT-nek: scaling

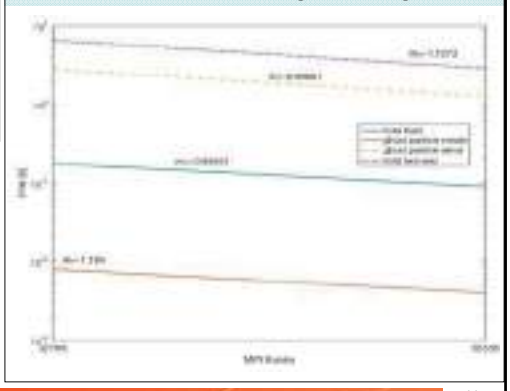
nek5000's guts (F77) & sinews (C, MPI1) gird CMT-nek

Largest values of key parameters so far				
MPI Ranks	$N_{elements}$	Grid points	Particles	Wall time
131,072	4,194,304	250 M	20 B	12 hours
		20.6 B	0	





Particles, Strong Scaling



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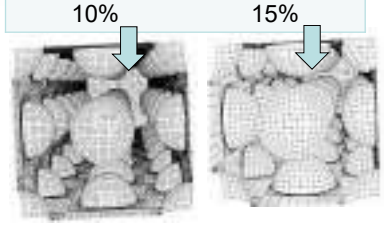
Accomplishments: inviscid sphere array

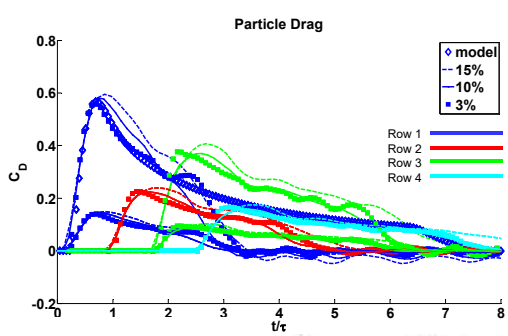
CMT-nek predictions & model dev on Mira

Elements	Spheres	Rows
23424	95	21

Volume fraction 3%

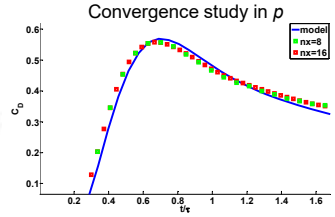
10% 15%





$$F^{GF}(t) = \frac{4}{3}\pi R^3 \rho m \overline{\frac{Du}{Dt}}^{m,V} + 2\pi R^2 \int_{\xi=-\infty}^{t} K_m(t-\xi,M)\left[\frac{D}{D\xi}\overline{(\omega_m)}^{m,S}\right]_{\xi=\xi} d\xi$$

Convergence study in p



Annamalai & Balachandar (2017) *J. Fluid. Mech.* **816**, 381-411

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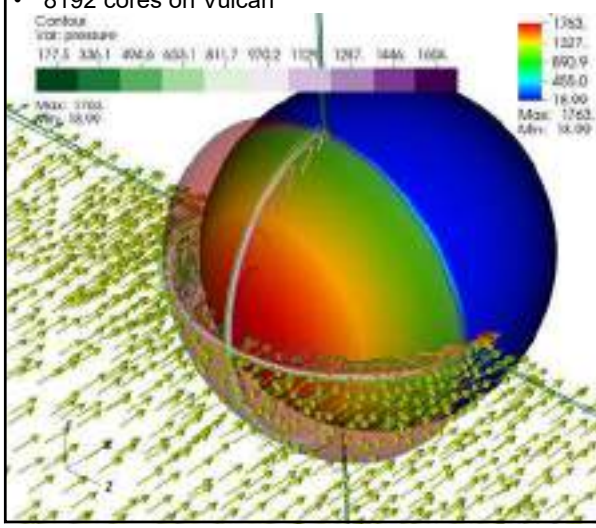
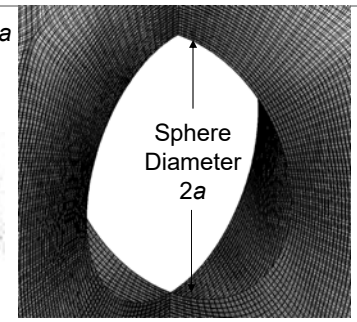
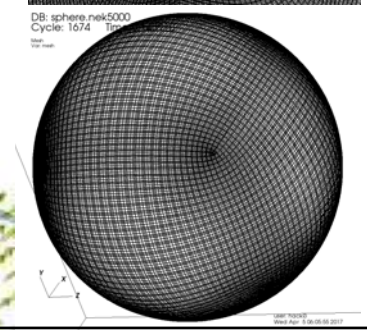
Accomplishments: Mach 3 shock-sphere

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

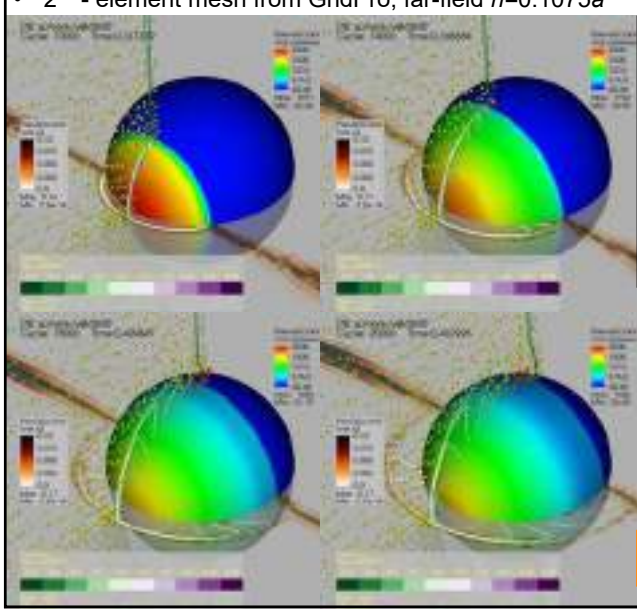






Accomplishments: Mach 3 shock-sphere

- 2^{20} - element mesh from GridPro, far-field h=0.1075a



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

EVM Artificial viscosity
- Localized at shocks
- Scales as[2] h/p

[1]Britain *et al* (1995) *Exp. Fluids* **20**
[2]Perrson & Peraire AIAA 2006-112

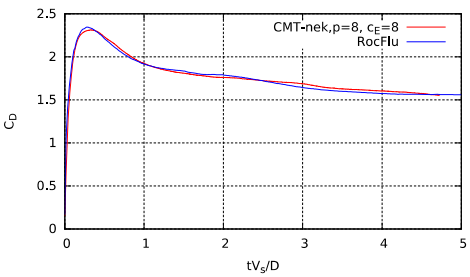
Shock over cylinder: CMT-nek vs RocFlu

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

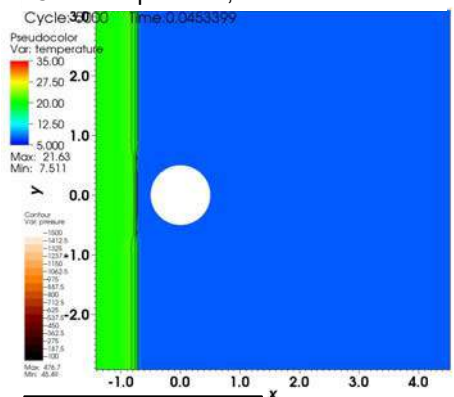
RocFlu
- 300 DOF on cylinder
- 140K DOF in surrounding 2x2 box

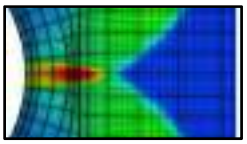
Validation of cylinder drag coefficient

Mehta *et al* (2016) *J. Appl. Phys.* **119**, 104901



Mach 3, γ = 1.4, unit gas constant
Color temperature, Pressure contours





Shock resolution within elements

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Conclusion

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

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

Future Work
- CS feedback; GPU port
- Numerics
  - Implicit time marching
  - Refined smoothing of the viscosity

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Uncertainty Budget

Validation and Uncertainty Reduction

Chanyoung Park, Raphael (Rafi) T. Haftka

Nam-Ho Kim

Department of Mechanical & Aerospace Engineering

UF UNIVERSITY of FLORIDA

Uncertainty Budget Team


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Nam-Ho Kim, PhD


Chanyoung Park, PhD


Kyle Hughes


Sam Nili


Yiming Zhang


Giselle Fernandez


Justin T. Mathew


Shirly Spath (Undergrad)

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

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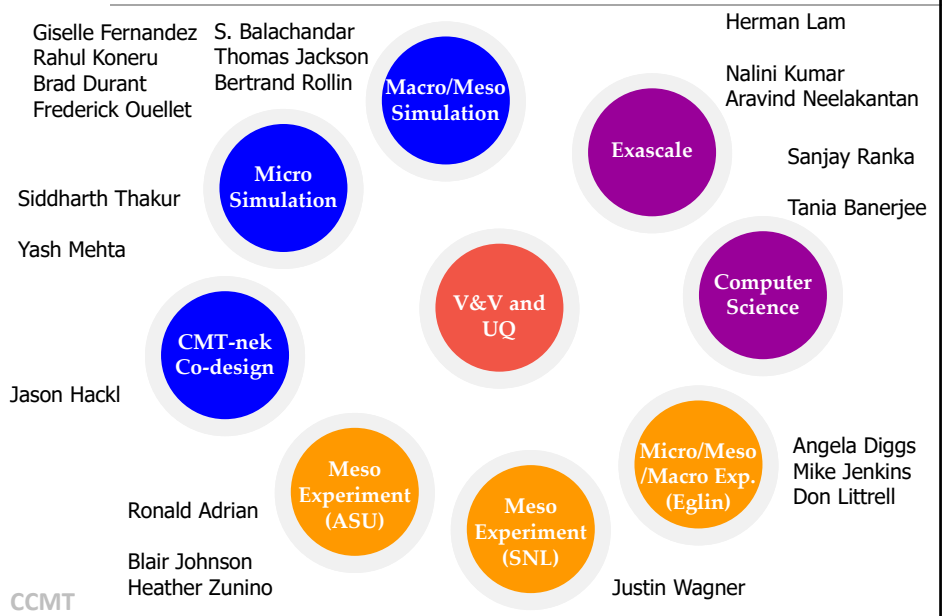
Collaborations



CCMT 3

AST Questions and Answers

- RQ2 – Recommendations on Exp/Sim Coupling
  - Work closer with the team at Eglin

Answer
- How we followed and identified unrecognized uncertainties and realized we are doing forensic UQ

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

Answer
- Sandia shock tube experiments progress
- Eglin mesoscale and macroscale progress

- RQ6 –Additional Recommendations
  - Develop strategy for use of lower fidelity runs to augment the hero runs

Answer
- Multi-fidelity surrogate for exploring parameter space of the Hero runs with an aid of cheap lower fidelity simulation runs
- Multi-fidelity surrogate also for predicting computational times with exascale team.

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Forensic UQ

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

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

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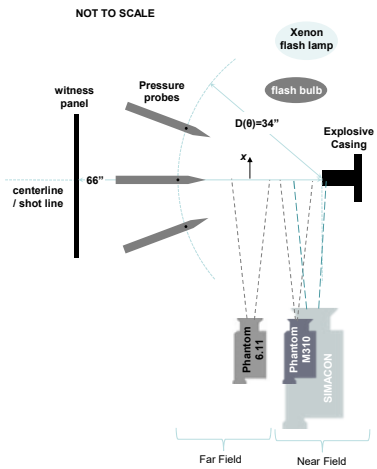
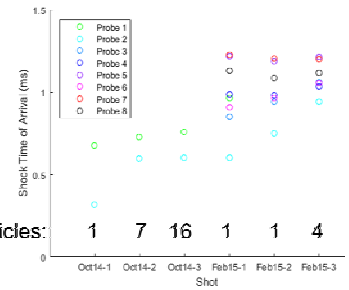
Microscale Experiments: February 2015



Overhead schematic of the test set-up.

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



Particles: 1 7 16 1 1 4

- Surprising evidence that the flow is strongly coupled with particles:
  - Mean shock arrival times increase as the number of particles is increased
- A possible explanation is high volume fraction in the initial plane of the particles:

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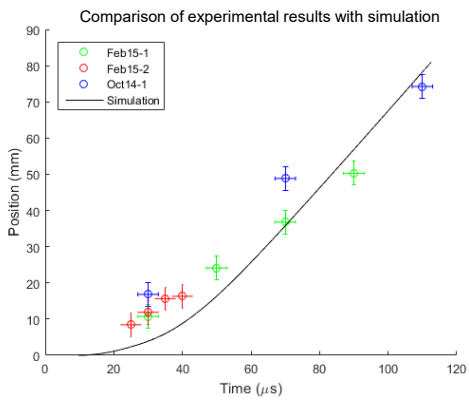
Preliminary Microscale Validation



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

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Lessons Learned from Eglin Microscale Exp

- Kyle Hughes surprised everybody by finding that the small number of particles show significant coupling with the flow
- Uncertainty quantification for validation of even this "simplified" problem required extensive back and forth between UQ, simulation, and experimental teams (~5+ months)
  - Underscores importance of clear communication
  - Written documentation of information source increases rigor
- Start simulation of the problem
  - Simulations are challenging and require a significant ramp-up time
  - Inputs/assumptions can help drive the forensic UQ

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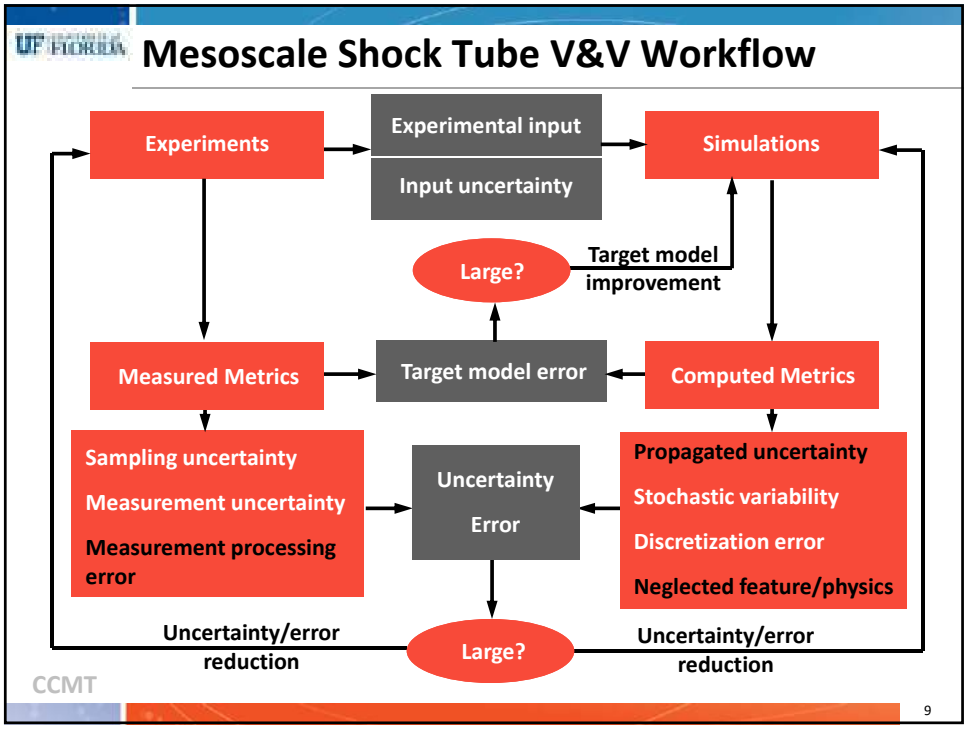
Mesoscale Shock Tube V&V Workflow
Experiments
Experimental input
Input uncertainty
Simulations
Large?
Target model improvement
Measured Metrics
Target model error
Computed Metrics
Sampling uncertainty
Measurement uncertainty
Measurement processing error
Uncertainty
Error
Propagated uncertainty
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
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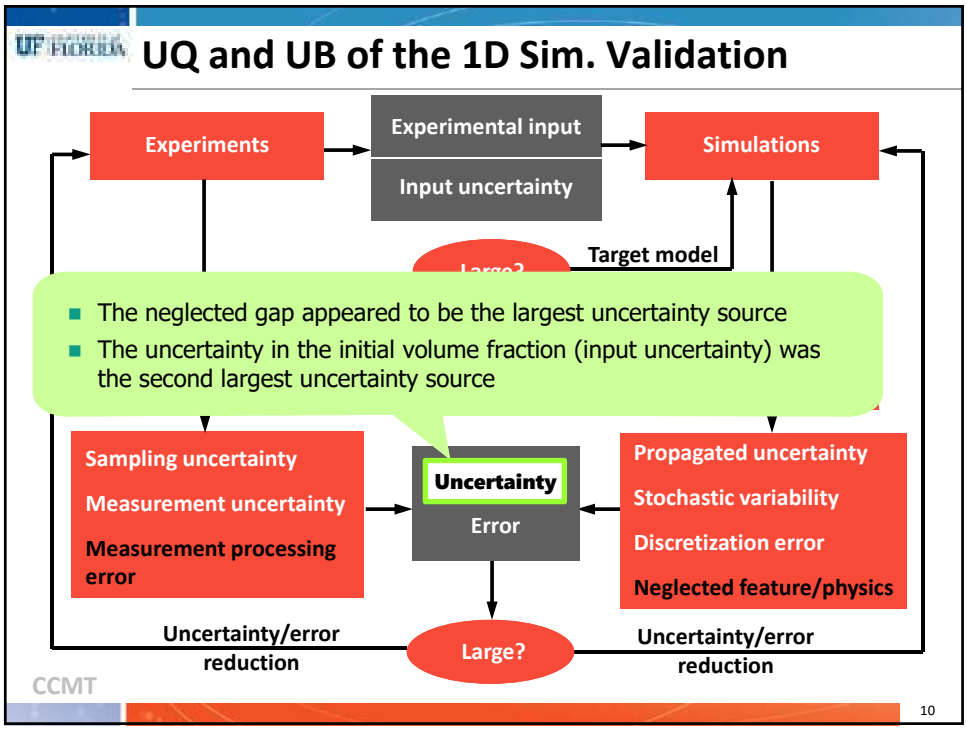
UQ and UB of the 1D Sim. Validation
Experiments
Experimental input
Input uncertainty
Simulations
Target model
The neglected gap appeared to be the largest uncertainty source
The uncertainty in the initial volume fraction (input uncertainty) was the second largest uncertainty source
Sampling uncertainty
Measurement uncertainty
Measurement processing error
Uncertainty
Error
Propagated uncertainty
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
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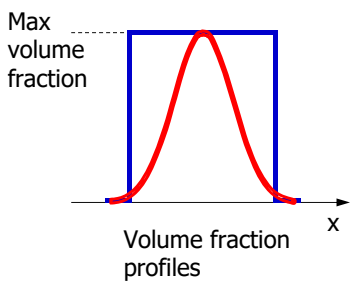
Mesoscale Validation Forensic UQ

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



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

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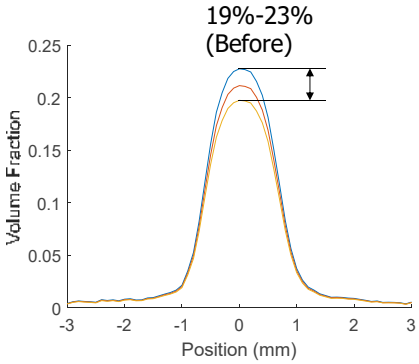
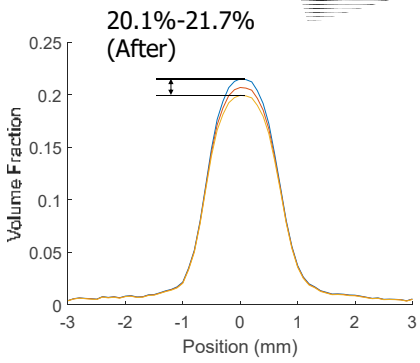
Before and After

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





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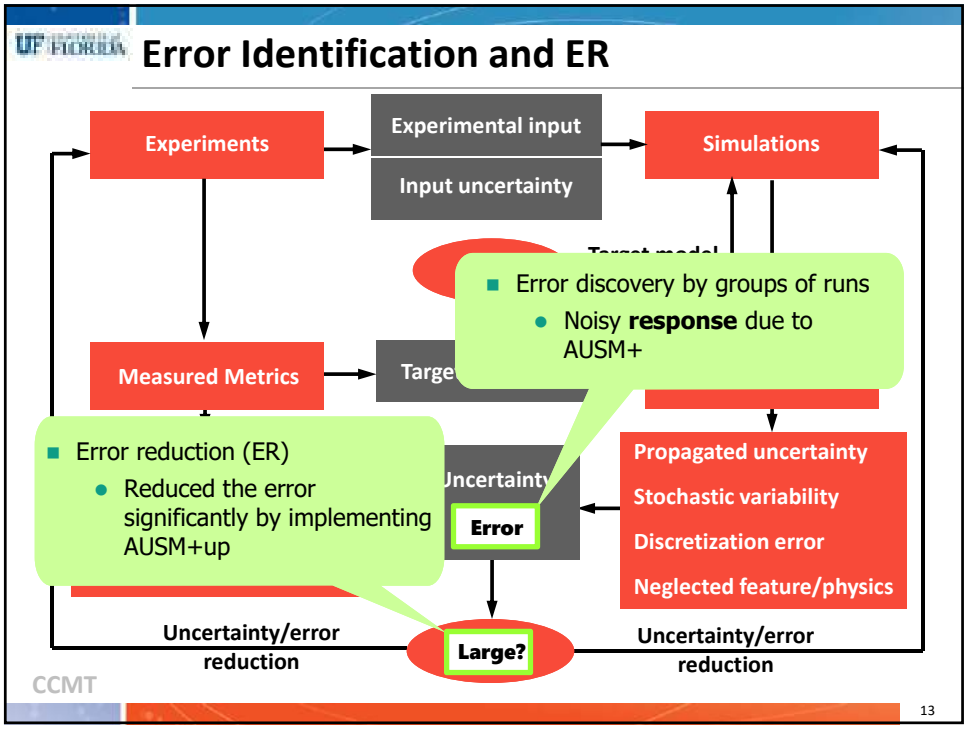
Error Identification and ER
Experiments
Experimental input
Input uncertainty
Simulations
Measured Metrics
Error discovery by groups of runs
Noisy **response** due to AUSM+
Error reduction (ER)
Reduced the error significantly by implementing AUSM+up
Error
Propagated uncertainty
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
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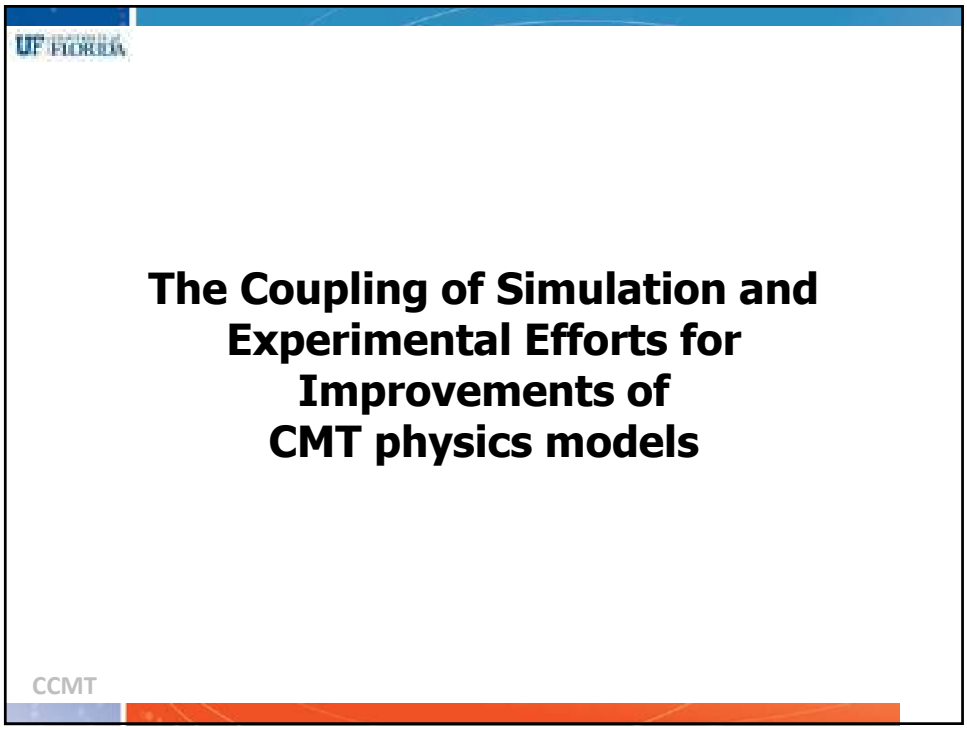
The Coupling of Simulation and Experimental Efforts for Improvements of CMT physics models
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V&V Plan With UR and ER for Improvements

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

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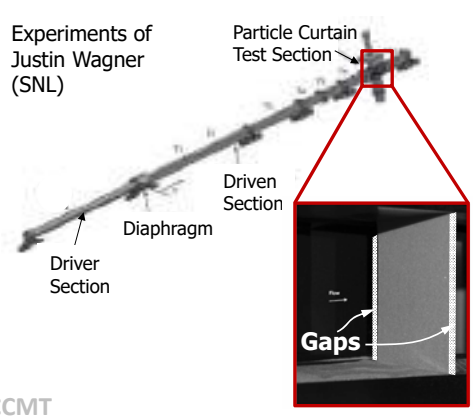
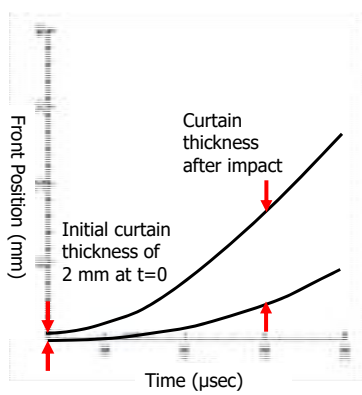
Shock Tube Experiment

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





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Key Uncertainties and Prediction Metrics

- Key uncertainties (highest 6 out of 24)

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

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

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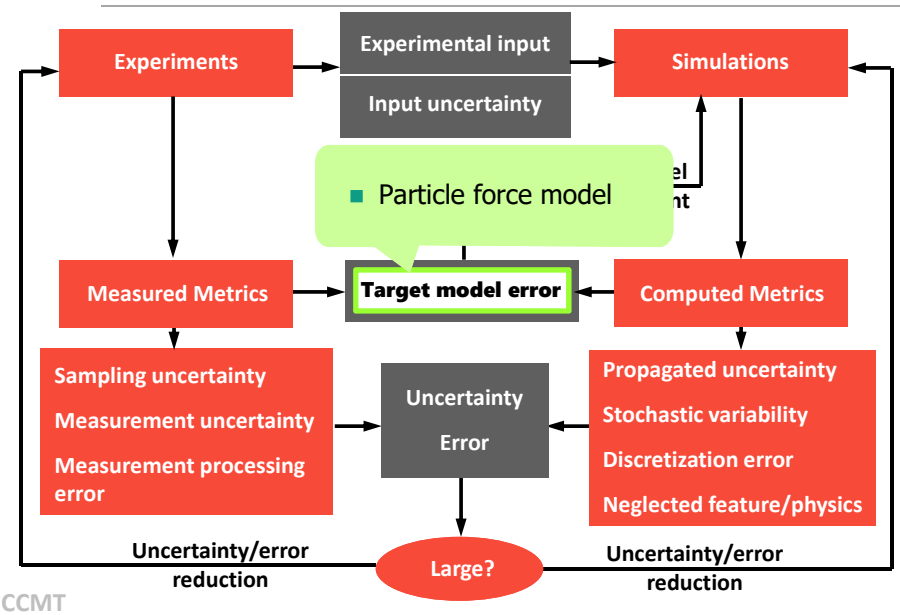
Target Modeling Setting



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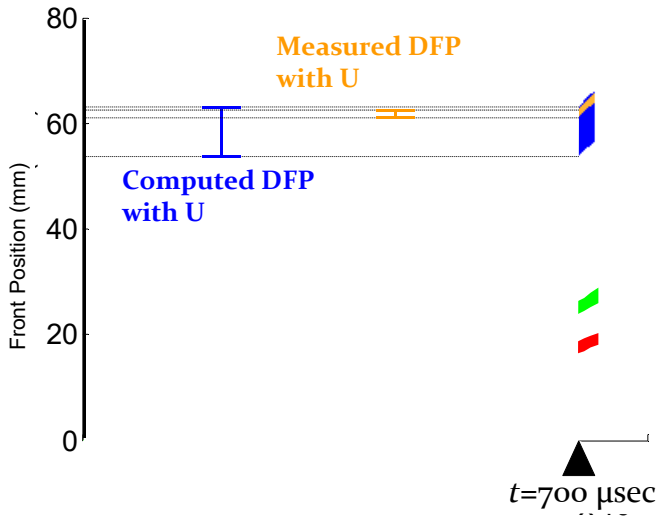
Highlights of 1D Shock Tube Sim. (Before UR)

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



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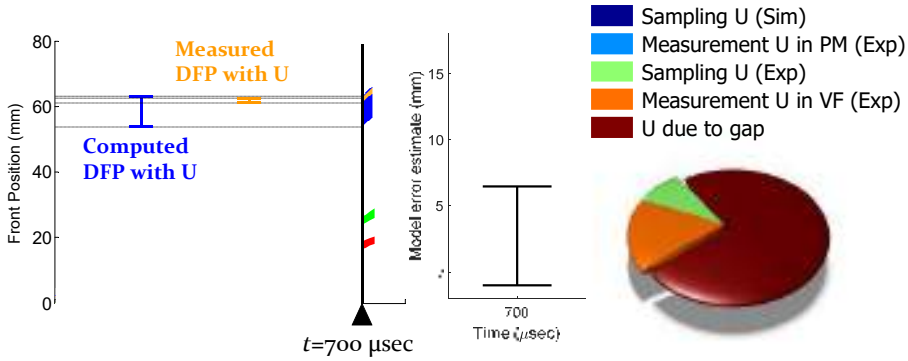
Highlights of 1D Shock Tube Sim. (Before UR)



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

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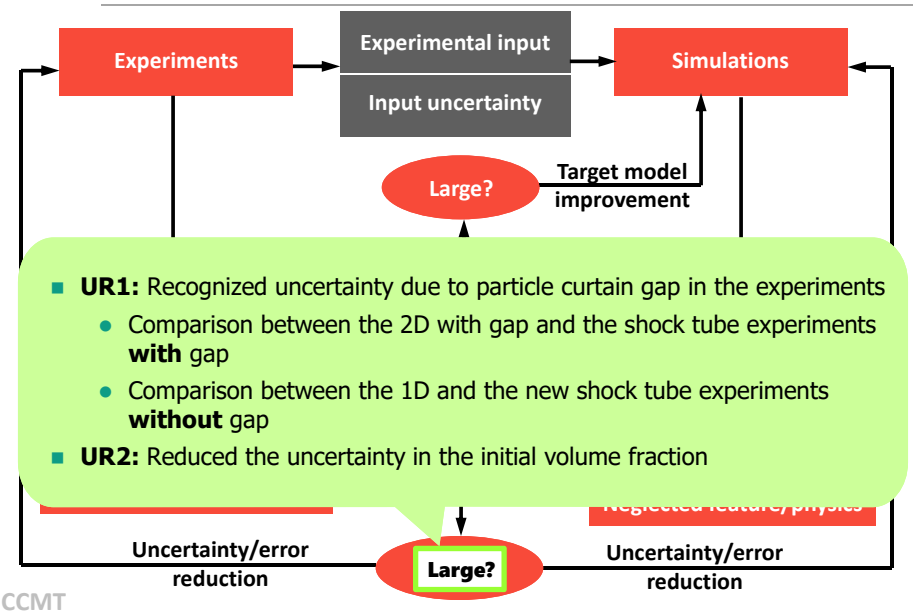
Uncertainty Reduction (UR)



- **UR1:** Recognized uncertainty due to particle curtain gap in the experiments
  - Comparison between the 2D with gap and the shock tube experiments **with** gap
  - Comparison between the 1D and the new shock tube experiments **without** gap
- **UR2:** Reduced the uncertainty in the initial volume fraction

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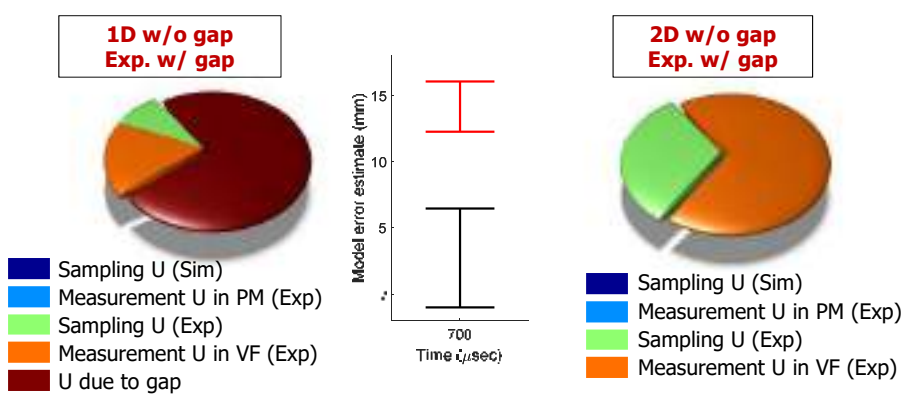
UR1 – Option1: 2D Simulation With Gap

- Predicted DFP of 2D simulation (Rahul Koneru) corresponding the measured DFP
- Uncertainty due to inconsistency of the 1D simulation due to missing gap effect was reduced by modeling gap through 2D simulation
- The uncertainty reduction revealed that model improvement is needed



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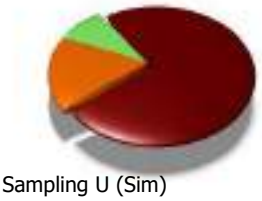
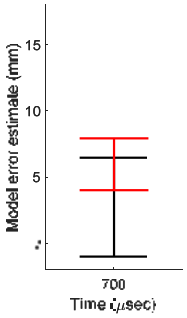
UR1 – Option2: Removing Gap from the Exp.

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

1D w/o gap
Exp. w/ gap



- Sampling U (Sim)
- Measurement U in PM (Exp)
- Sampling U (Exp)
- Measurement U in VF (Exp)
- U due to gap



1D w/o gap
New Exp. w/o gap

- Sampling U (Sim)
- Measurement U in PM (Exp)
- Sampling U (Exp)
- Measurement U in VF (Exp)

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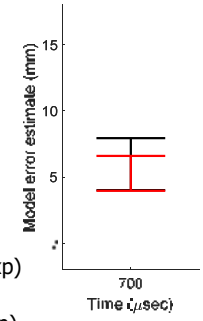
UR2: Reducing Uncertainty in Init. VF

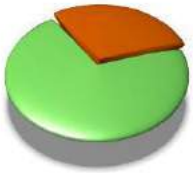
- Preliminary UQ on initial VF was conservative including data noise in the uncertainty of the initial VF calculation
- Estimated uncertainty in initial VF estimated at 19%-23%
- Revised UQ (Justin Mathew and Chanyoung Park) filters out data noise and considers uncertainty in the measurement processing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

1D w/o gap
New Exp. w/o gap

- Sampling U (Sim)
- Measurement U in PM (Exp)
- Sampling U (Exp)
- Measurement U in VF (Exp)

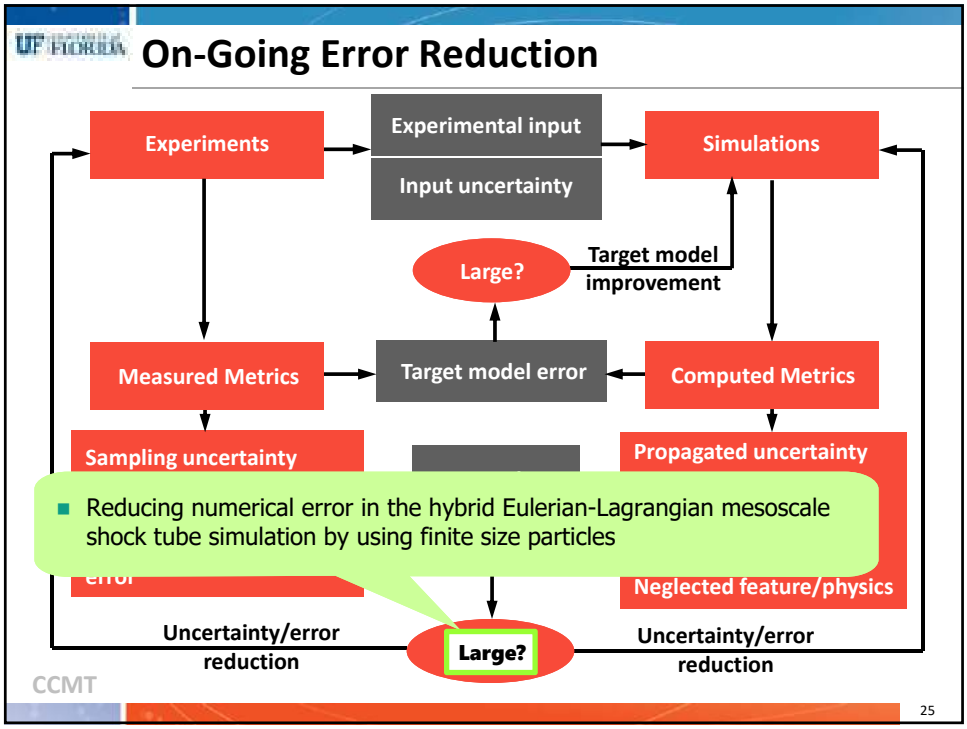


1D with reduced
initial VF



- Sampling U (Sim)
- Measurement U in PM (Exp)
- Sampling U (Exp)
- Measurement U in VF (Exp)

24


On-Going Error Reduction
Experiments
Experimental input
Input uncertainty
Simulations
Large?
Target model improvement
Measured Metrics
Target model error
Computed Metrics
Sampling uncertainty
Propagated uncertainty
Reducing numerical error in the hybrid Eulerian-Lagrangian mesoscale shock tube simulation by using finite size particles
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
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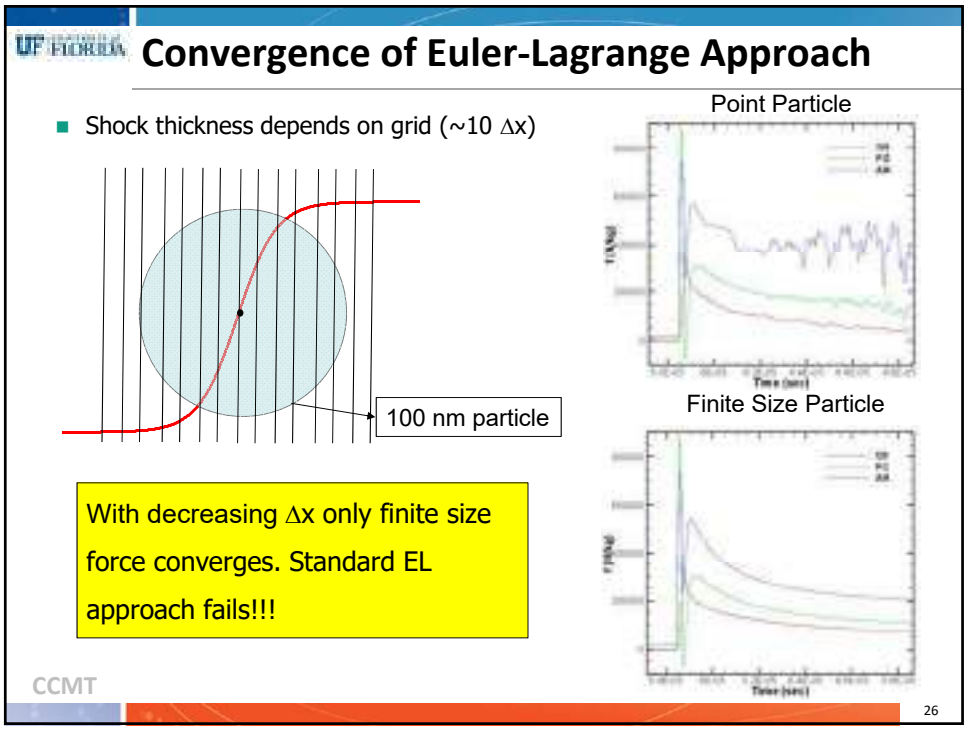
Convergence of Euler-Lagrange Approach
Shock thickness depends on grid (~10 Δx)
100 nm particle
With decreasing Δx only finite size force converges. Standard EL approach fails!!!
Point Particle
Finite Size Particle
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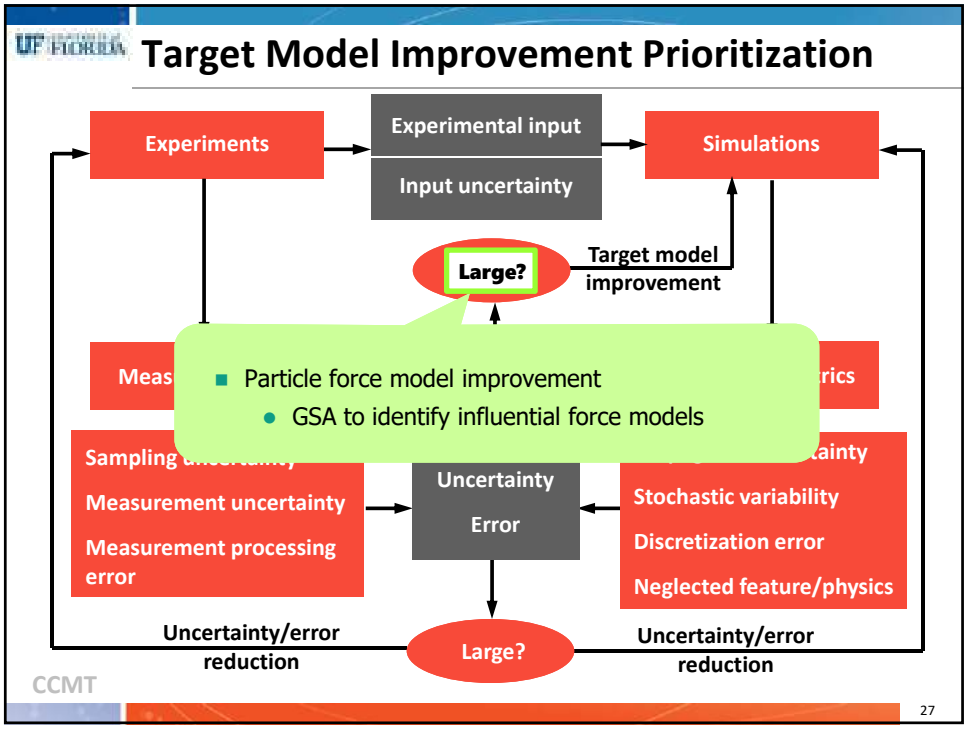
Target Model Improvement Prioritization
Experiments
Experimental input
Input uncertainty
Simulations
Large?
Target model improvement
Particle force model improvement
GSA to identify influential force models
Measurement uncertainty
Measurement processing error
Uncertainty
Error
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
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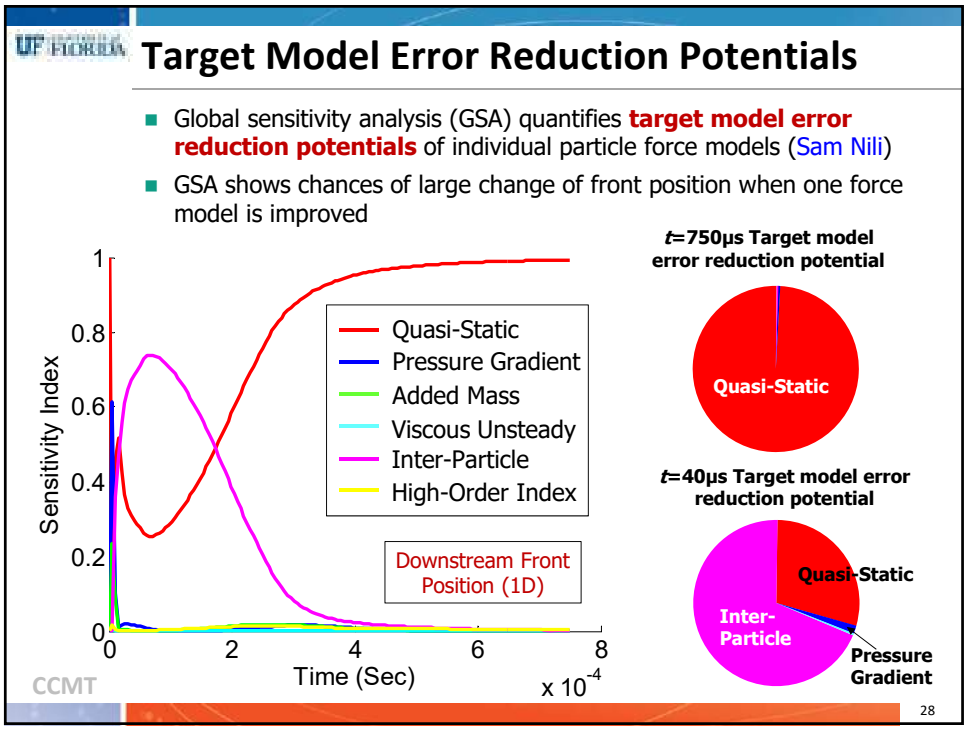
Target Model Error Reduction Potentials
Global sensitivity analysis (GSA) quantifies target model error reduction potentials of individual particle force models (Sam Nili)
GSA shows chances of large change of front position when one force model is improved
Sensitivity Index
Time (Sec)
x 10^-4
Quasi-Static
Pressure Gradient
Added Mass
Viscous Unsteady
Inter-Particle
High-Order Index
Downstream Front Position (1D)
t=750μs Target model error reduction potential
Quasi-Static
t=40μs Target model error reduction potential
Quasi-Static
Inter-Particle
Pressure Gradient
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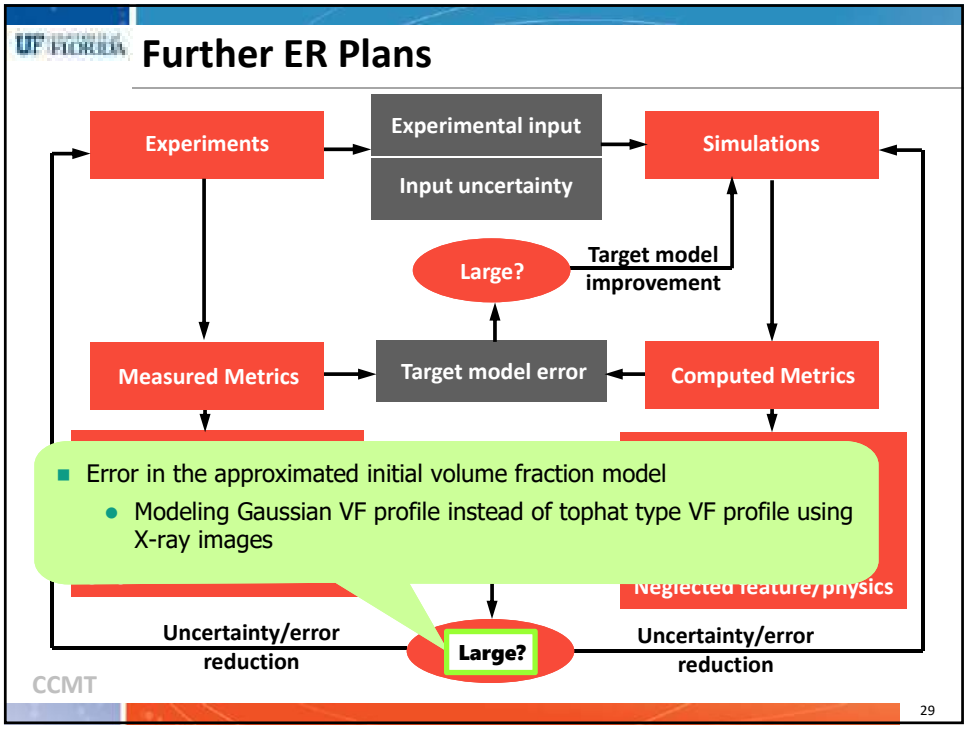
Further ER Plans
Experiments
Experimental input
Input uncertainty
Simulations
Large?
Target model improvement
Measured Metrics
Target model error
Computed Metrics
Error in the approximated initial volume fraction model
Modeling Gaussian VF profile instead of tophat type VF profile using X-ray images
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
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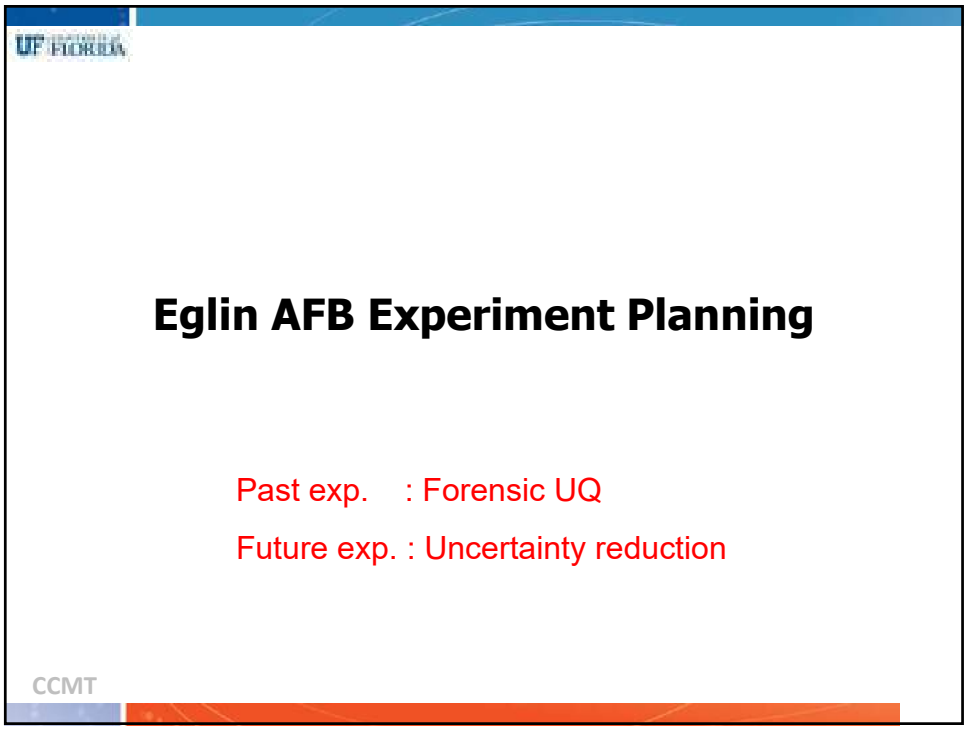
Eglin AFB Experiment Planning
Past exp. : Forensic UQ
Future exp. : Uncertainty reduction
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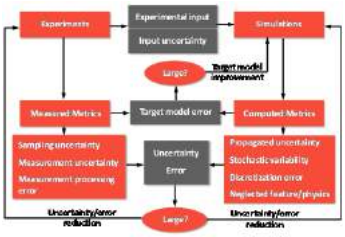
Summary of Eglin Experiments

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



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

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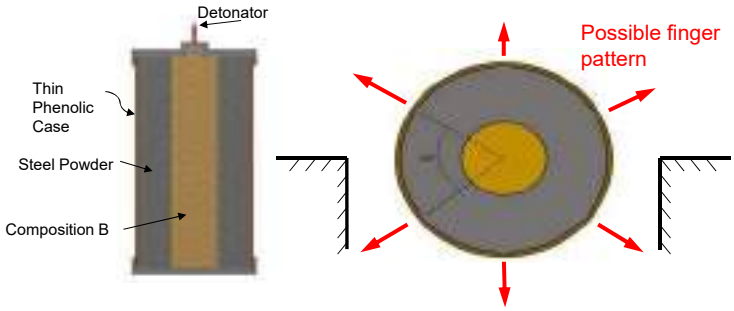
Ex: Casing Design for UR

- Casing fracture can be a possible cause of jet formation [Zhang et al. 2001, Xu et al. 2013]
- In order to minimize/control the casing effect, two measures were taken:
  - Thin phenolic tubing (3/16") was chosen for the outer casing with a failure energy estimated to be 0.06% of the energy of the explosive
  - Notches will be introduced to the casing to attempt to control the failure



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

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Multi-Fidelity Surrogate Model for Augmenting the Hero Runs in Order to Explore Parameter Space

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RQ 6 – Additional Recommendations

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

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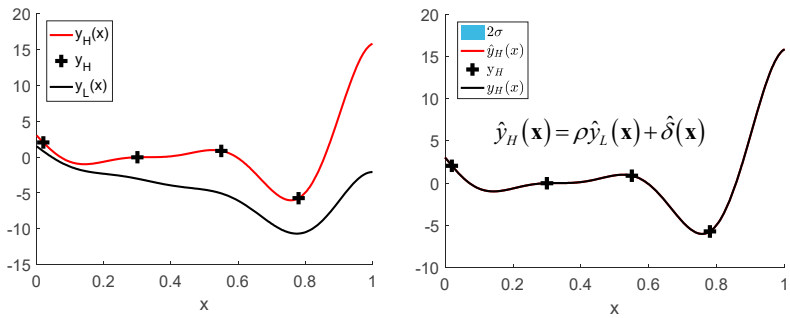
Multi-Fidelity Surrogate



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

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1D/2D/3D Mesoscale Simulation Runs

- Comparison between mesoscale 1D/2D/3D simulations and the new SNL experiments with a **non-tophat** initial VF profile
  - Chanyoung and Justin (UB team) / Brad (Physics team)
  - Modeling initial VF profile model using **Beta distribution**
  - Expected outputs: particle front positions at time t
  - Runs for
    - 5 different Mach numbers: 1.24, 1.40, 1.45, 1.66, 1.92
    - Initial volume fractions
    - Random initial particle locations
    - 2 beta distribution parameters
    - Curtain thickness
  - Required **18000** Simulation runs (full factorial design): **5** (Mach numbers) **x16** (initial volume fractions) **x5** (random initial particle locations) **x5** (curtain thickness) **x9** (two beta distribution parameters)
  - Required subset of 1D simulation runs for 2D and 3D and **multi-fidelity model prediction** will be applied

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Data Extraction from the Experiments

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RQ 2 – Recommendations on Coupling

- The plan should include how data will be extracted from the experiments
  - For example, how are the PIs planning to extract velocity fluctuation measurements in the ASU experiments, etc.
  - The PIs should consider ways to explain structural details within the particle bed and document ways to characterize the impact of wall contribution to void structure.
  - RQ 2 – Recommendations on Experiments/Simulation Coupling

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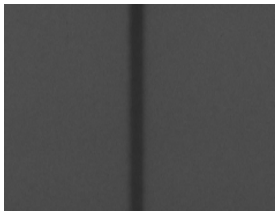
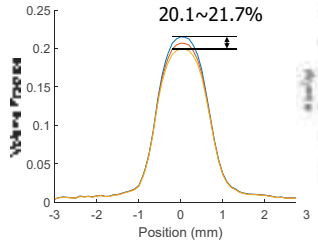
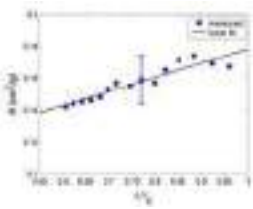
Data Extraction from Shock Tube Experiment



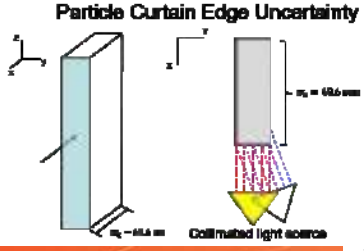




Calibration exp.

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

Particle Curtain Edge Uncertainty



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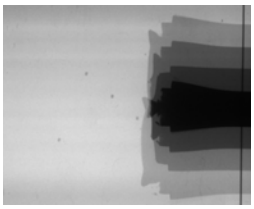
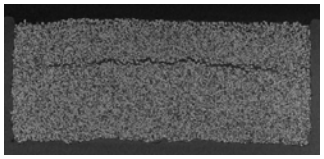
Data Extraction from Eglin Experiments

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

Simacon image of the Eglin microscale experiment



Multiple exposure x-ray of single particle



CT scans of particle packet for the Eglin mesoscale gas gun experiment

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

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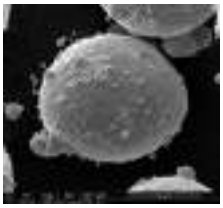
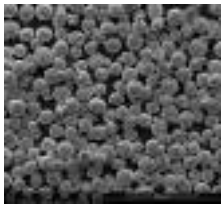
Data Extraction from Eglin Experiments

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

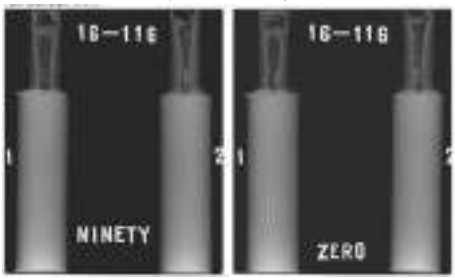


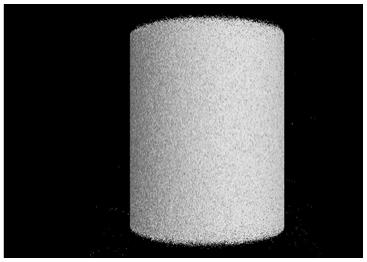
SEM of single steel particle at 1000x zoom.



SEM of several steel particles at 100x zoom.

Comp B x-rays for different angles





Steel mock CT scan

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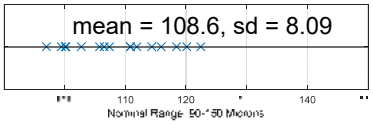
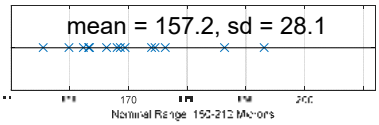
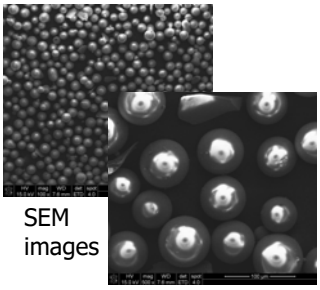
Data Extraction from ASU Shock Tube

- SEM shows particle diameters tending to the lower end of nominal ranges

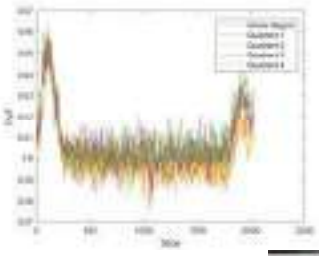


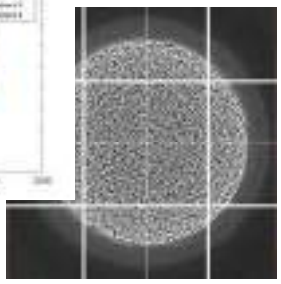


- CT scan-based volume fraction measurement
- Working on UQ in particle bed locations



SEM images





CT-scan for volume fraction

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Lessons Learned in Year 3

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

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Summary

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

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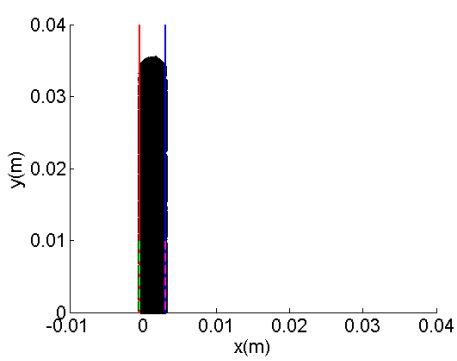
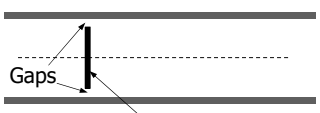
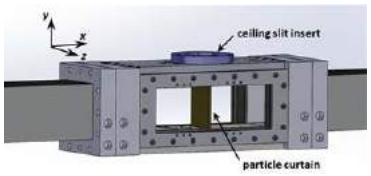
Do you have any questions?

Influence of Gap on Front Position (PM)



Top view of the test section





- Front positions were obtained from schileren images that capture the side view of the **entire** particle curtain
- 2D half particle curtain model with 99000 particles (**Top view**)
- Approximately 0-10% measurement bias in measured downstream front positions

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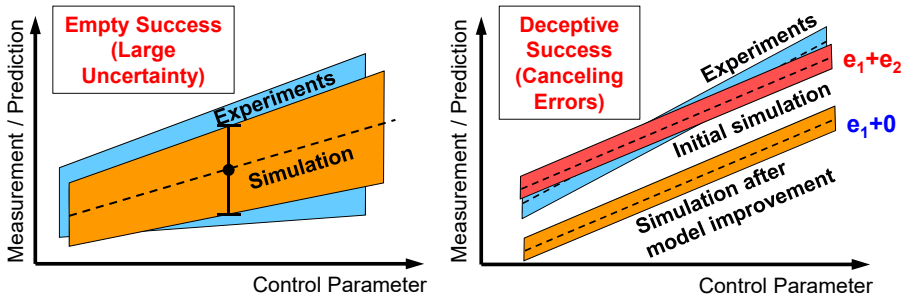
What are Our Criteria for Success?



- Reducing uncertainty in model error estimate (UR)
  - Large uncertainty prevents observation of model error
  - Will require substantial uncertainty reduction
  - Hidden model error due to canceling errors
  - Identify models where refinement matters and possibly experimental bias
- Reducing model error (ER)
  - Identifying/ranking error sources

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Calibrated *A* for Measuring VF (Linear)

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

Considering uncertainty in coefficients

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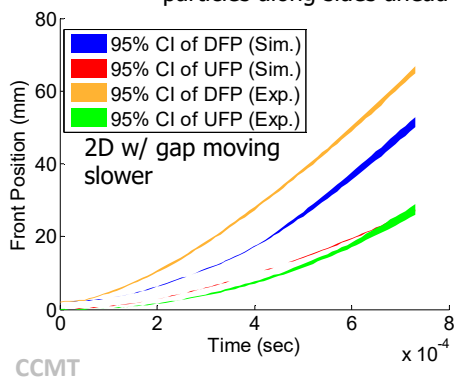
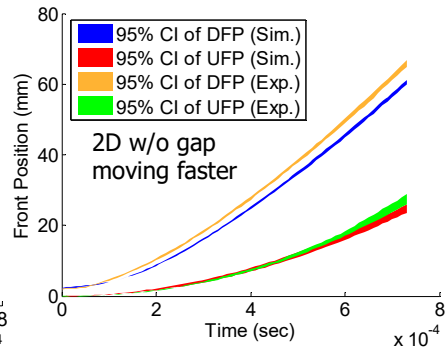
2D Sim. And Exp. W/ and W/O Gaps

- The influence of the gap on experiments and simulations are not consistent
- Experiments are insensitive to the presence of the gaps while 2D sims are not
- Explanation on the unexpected observation is that boundary layer growth over time < 800 μsec mitigated possible movement of particles along sides ahead of the bulk





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CMT-nek: CS Update

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Sanjay Ranka

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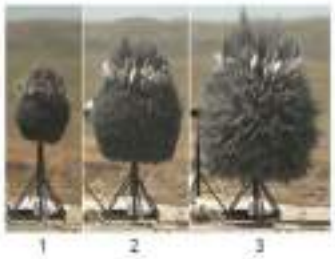
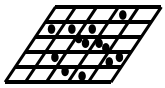
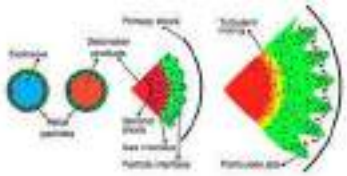
2

Exascale Simulation: CS Challenges

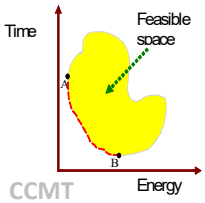


Dynamic Load Balancing





Energy and Performance Tradeoffs



Future Architectures and Hybrid Processors

Parallelization on a million+ processors

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Review Team Questions – 2016

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

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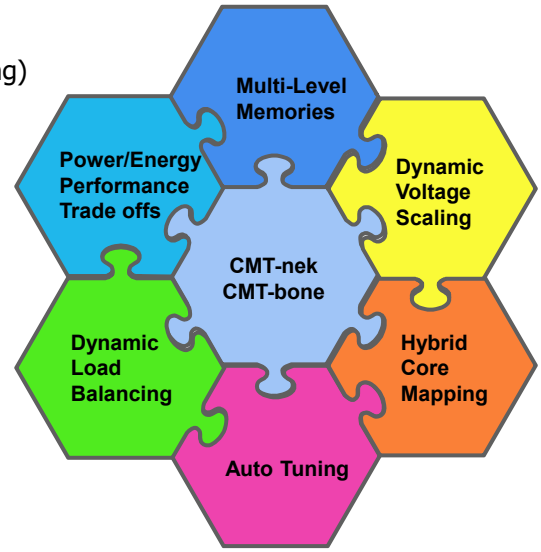
Talk Overview

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



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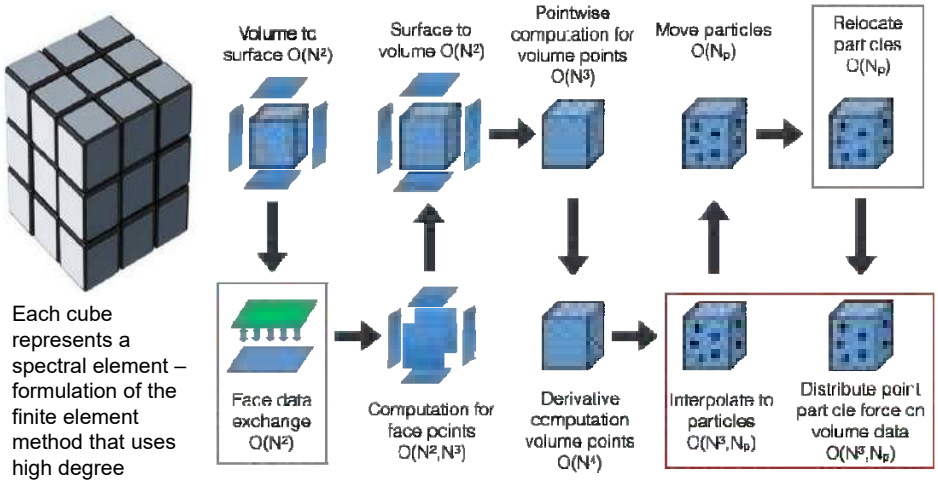
CMT-bone



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, December 2016.

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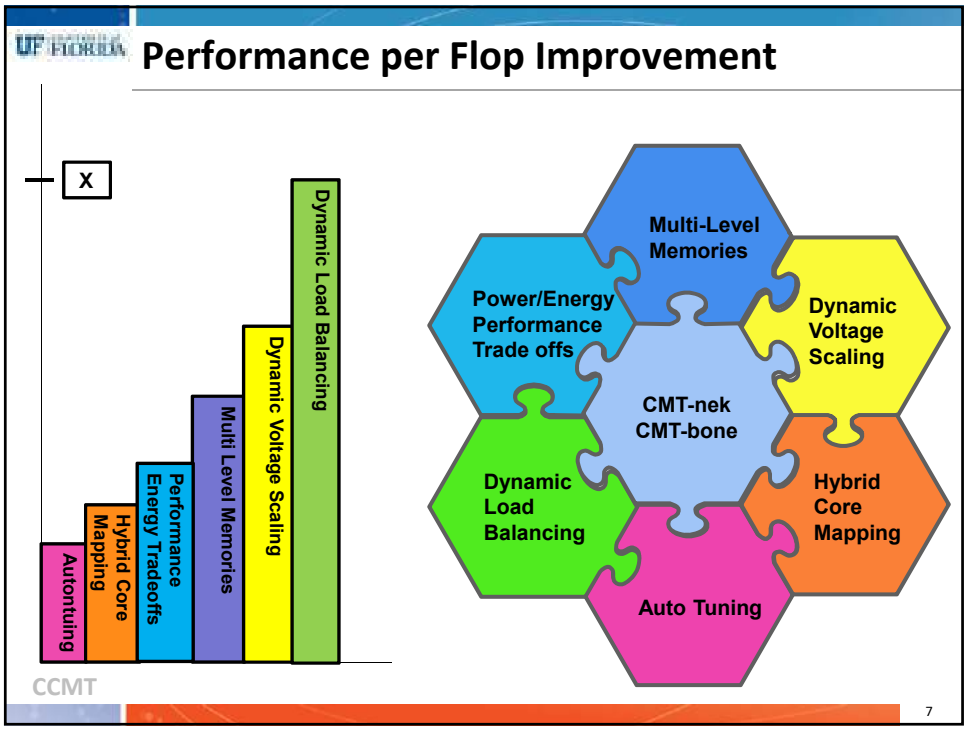
Performance per Flop Improvement
X
Autontuing
Hybrid Core Mapping
Performance Energy Tradeoffs
Multi Level Memories
Dynamic Voltage Scaling
Dynamic Load Balancing
Multi-Level Memories
Power/Energy Performance Trade offs
Dynamic Voltage Scaling
CMT-nek
CMT-bone
Dynamic Load Balancing
Hybrid Core Mapping
Auto Tuning
CCMT
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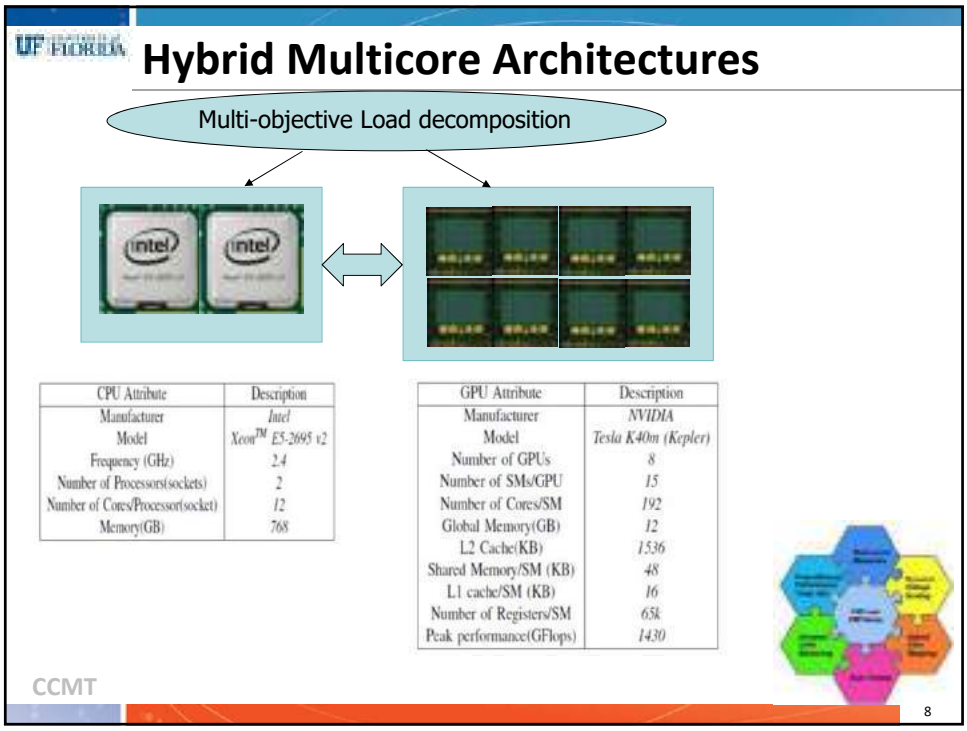
Hybrid Multicore Architectures
Multi-objective Load decomposition
CPU Attribute | Description
Manufacturer | Intel
Model | Xeon™ E5-2695 v2
Frequency (GHz) | 2.4
Number of Processors(sockets) | 2
Number of Cores/Processor(socket) | 12
Memory(GB) | 768
GPU Attribute | Description
Manufacturer | NVIDIA
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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8

Problem formulation

Minimize $E(n, m, f, g, S)$
Subject to $T(n, m, f, g, S) <= T_1 - O(n, m, f, g, S)$

$n <= N \rightarrow 24$
$m <= M \rightarrow 8$
$f \in F \rightarrow 12$
$g \in G \rightarrow 7$

16128 S

X → n CPU cores, freq f

S-X → m GPU cores, freq g

Minimize $E_{CPU}(n, f, X) + E_{GPU}(m, g, S-X)$
Subject to $T_{CPU}(n, f, X) <= T_1 - C_o(m+n, S)$
$T_{GPU}(m, g, S-X) <= T_1 - C_o'(m, S-X)$

$n <= N \rightarrow 24$
$m <= M \rightarrow 8$
$f \in F \rightarrow 12$
$g \in G \rightarrow 7$

E : Energy consumed
n : Number of CPUs
m : Number of GPUs
f : CPU Frequency
g : GPU Frequency
N : Total available CPUs
M : Total available GPUs
F : Set of available CPU frequencies
G : Set of available GPU frequencies

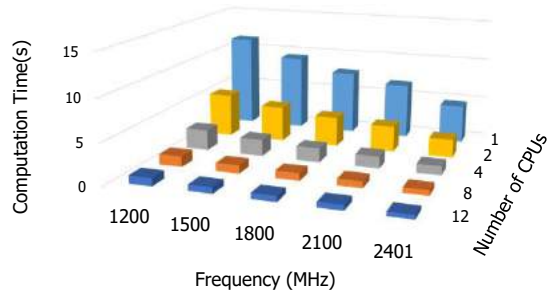
S : Problem size
T : Computation Time
T_1 : Constrained time
O: Communication overhead

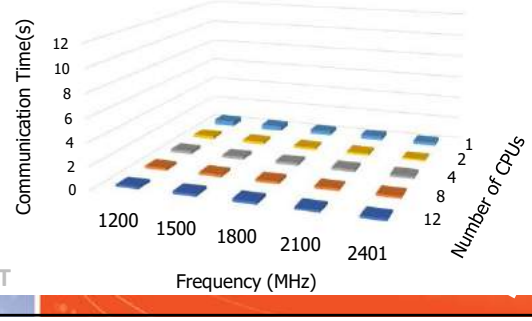
$T_{CPU}(n, f, X) \times P_{CPU}(n, f, X)$ — 344S — $T_{GPU}(m, g, S-X) \times P_{GPU}(m, g, S-X)$

$T_{CPU}(n, X)/f \times P_{CPU}(f) \times n$ — 359+32S — $T_{GPU}(m, S-X)/g \times P_{GPU}(g) \times m$

9

CPU: Computation and Computation Time





Single node

CMT-bone

8192 elements
128000 particles
7x7x7 grid size
Strong scaling

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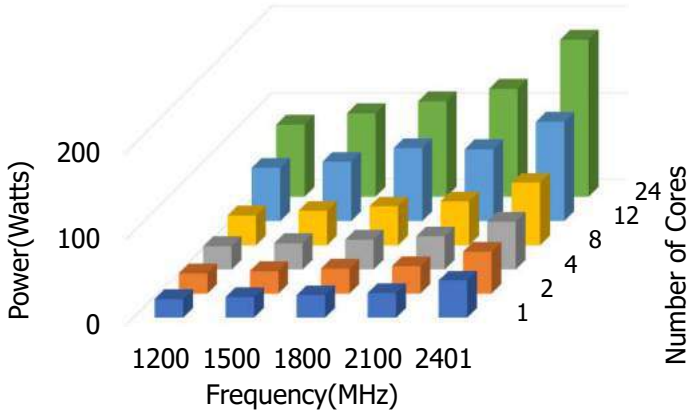
CPU: Power Consumption



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

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

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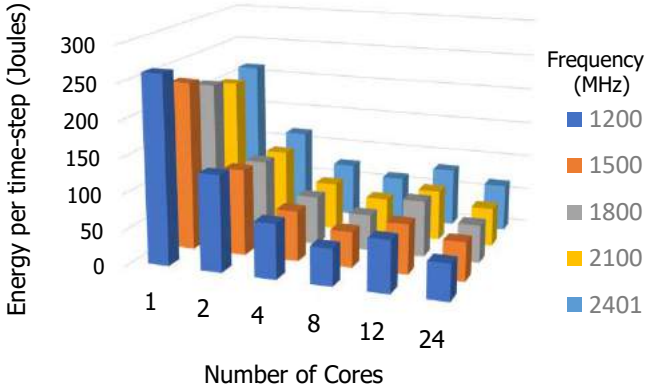
CPU: Energy Consumption



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

- Energy consumption first decreases and then increases with frequency

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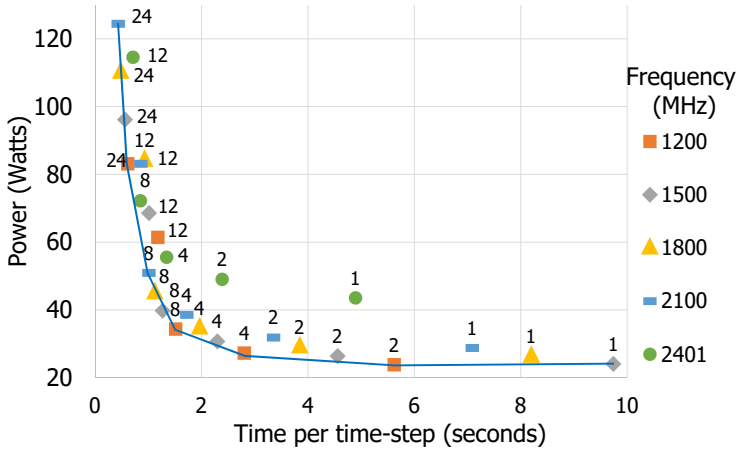
CPU: Power-Performance Tradeoffs



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

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

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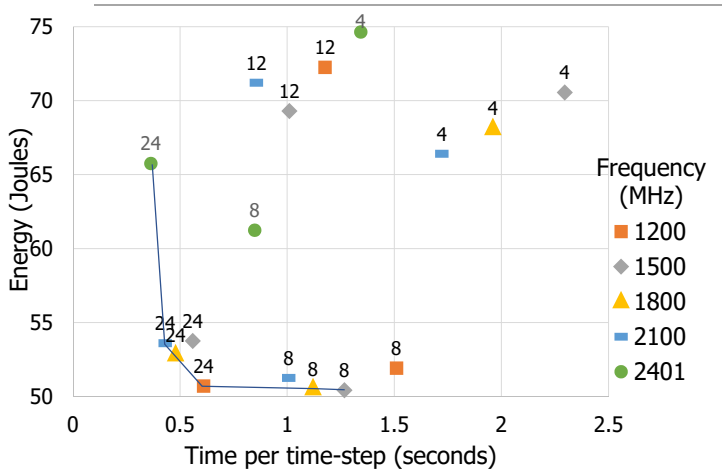
CPU: Energy-Performance Tradeoffs



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

- Observations:
  - Using 24 cores with lower frequencies results in an energy and performance efficient configuration

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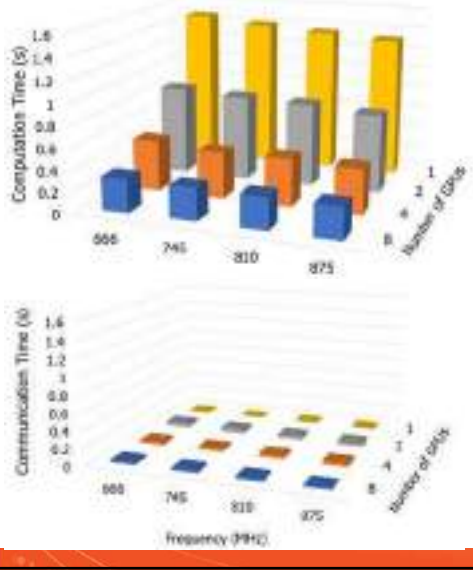
GPU: Computation and Communication Time



Single node

CMT-bone

8192 elements
128000 particles
7x7x7 grid size
Strong scaling

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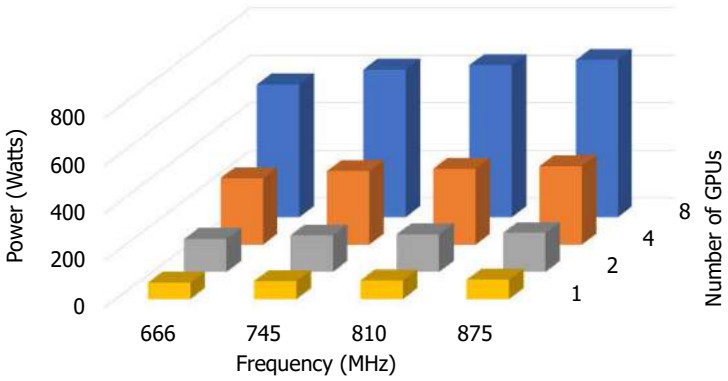
GPU: Power Consumption



Single node

CMT-bone

8192 elements
128000 particles
7x7x7 grid size
Strong scaling

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

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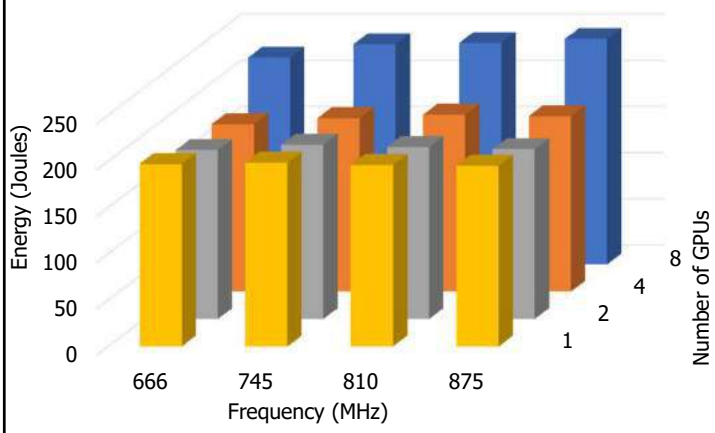
GPU: Energy Consumption



Single node

CMT-bone

8192 elements
128000 particles
7x7x7 grid size
Strong scaling

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

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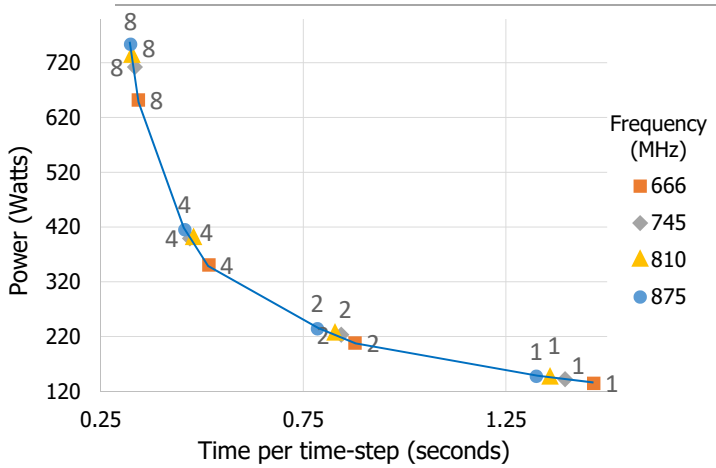
GPU: Power Performance Tradeoff



Single node

CMT-bone

8192 elements
128000 particles
7x7x7 grid size
Strong scaling

- Using 8 GPUs is the most performance efficient setup while using 1 GPU is the most power efficient setup

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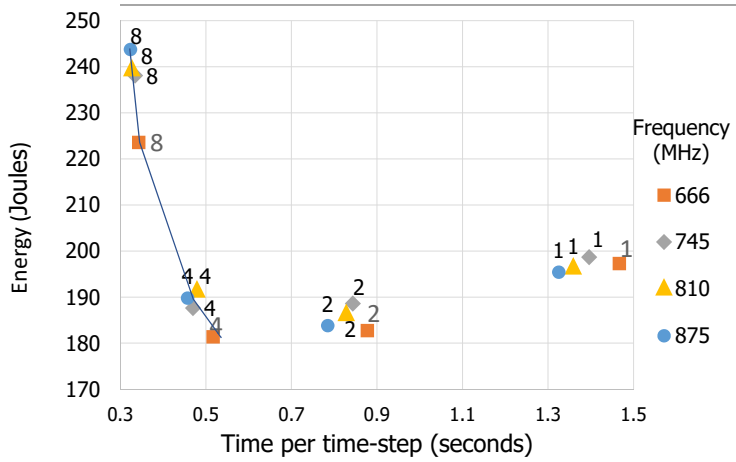
GPU: Energy-Performance Tradeoff



Single node

CMT-bone

8192 elements
128000 particles
7x7x7 grid size
Strong scaling

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

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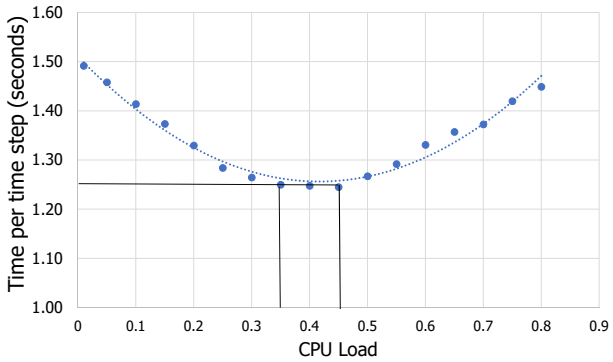
Hybrid: Load Balancing between CPU and GPU



Single node

CMT-bone

8192 elements
128000 particles
7x7x7 grid size
1.8GHz CPU frequency
810MHz GPU frequency
24 CPU cores
2 GPUs

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

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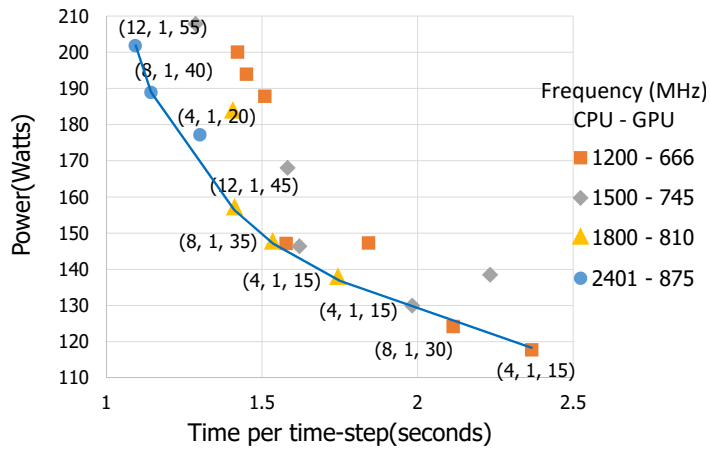
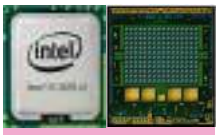
Hybrid: Power-Performance Tradeoff





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

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

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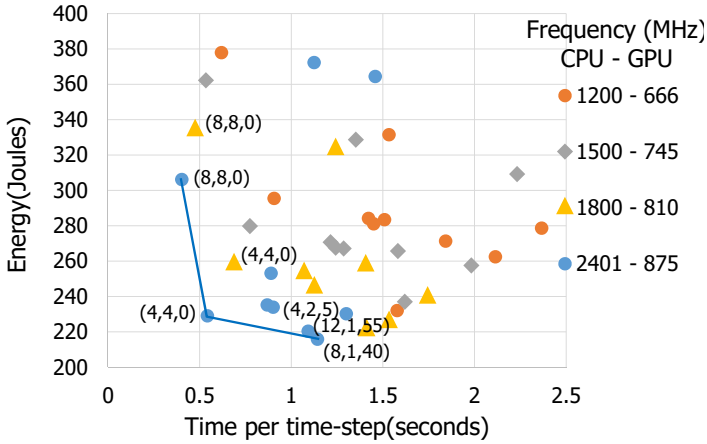
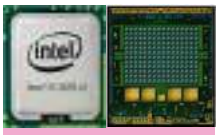
Hybrid: Energy-performance tradeoffs





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

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

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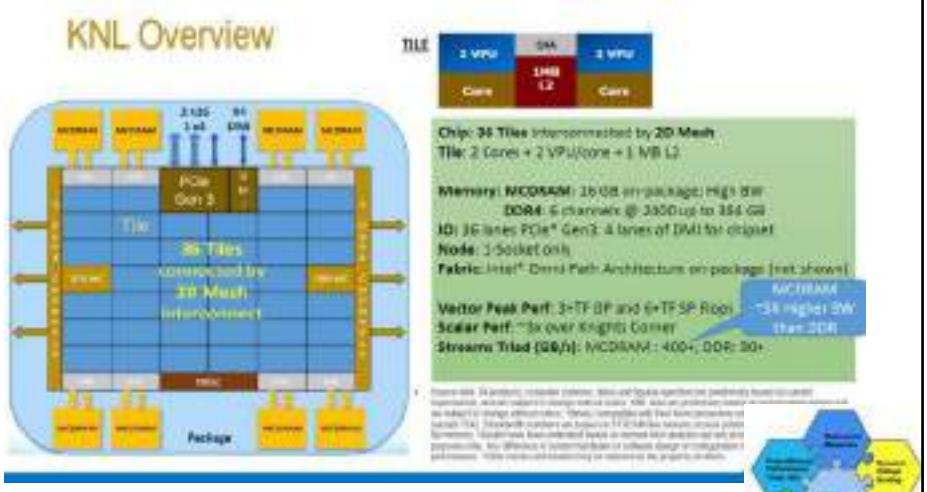
Multi-Level Memories



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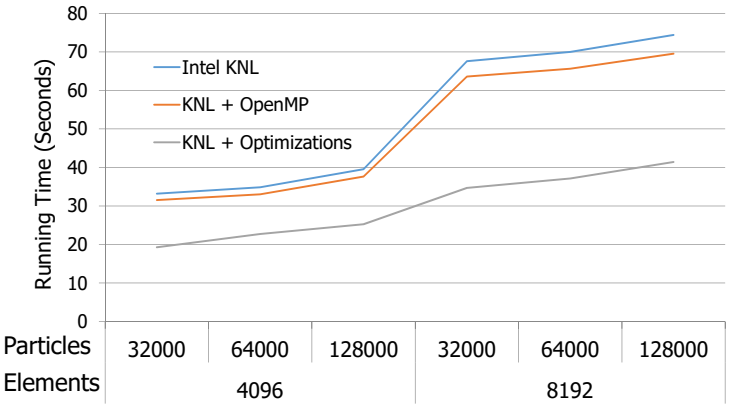
CMT-bone on Intel KNL



Single node

CMT-bone

7x7x7 grid size
1.8GHz frequency
32 MPI ranks
2 OpenMP threads

- Running time is total time taken to complete 100 time steps.
- Optimizations on KNL include autotuning, vectorization AVX-512 instructions, using OpenMP + MPI, using MCDRAM as cache.

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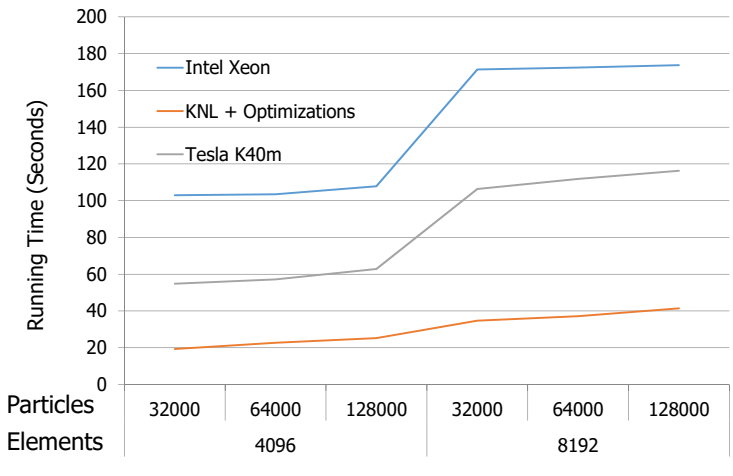
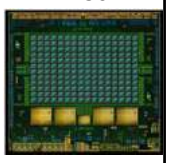
CMT-bone on Different Platforms



TDP: 150W



TDP: 245W

TDP: 215W

- KNL is faster than an Intel IvyBridge by about 4 times
- KNL is faster than Tesla K40m GPU by about 3 times
- KNL is the most energy efficient platform

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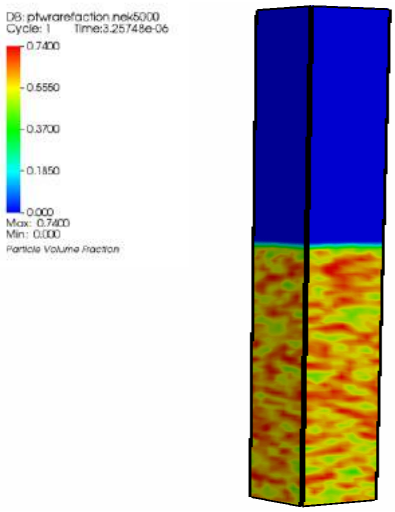
Load Balancing: Expansion Fan



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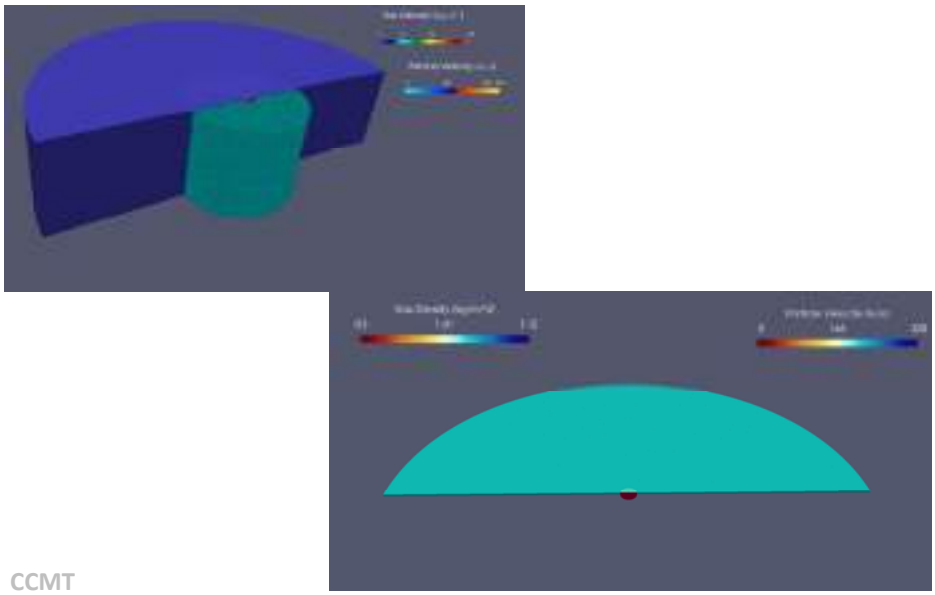
Load Balancing: Cylindrical Scattering



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Dynamic Load Balancing

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

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Load Balancing: Literature Survey

- Liao W, Ou C, Ranka S, Dynamic Alignment and Distribution of Irregularly Coupled Data Arrays for Scalable Parallelization of Particle-in-Cell Problems, ipps, pp.57, 10th International Parallel Processing Symposium (IPPS '96), 1996.
- Joseph RG, Ravunnikutty G, Ranka S, D'Azevedo E, Klasky S, Efficient GPU Implementation for Particle-in-Cell Algorithm, IPDPS, 2011
- Pearce O, Gamblin T, de Supinski BR, Amato N, MPMD Framework for Offloading Load Balance Computation, Olga Pearce, Todd Gamblin, Bronis de Supinski, Nancy Amato, IPDPS, Chicago, IL, USA, May 2016.
- Pearce O, Gamblin T, de Supinski BR, Amato N, Load Balancing N-Body Simulations with Highly Non-Uniform Density, Olga Pearce, Todd Gamblin, Bronis de Supinski, Nancy M. Amato, In Proc. ACM Int. Conf. Supercomputing (ICS), pp. 113-122 , Munchen, Germany, June 2014.
- Gamblin T, de Supinski BR, Schulz M, Fowler R, Reed DA, Scalable Load-Balance Measurement for SPMD Codes SC'08, November2008
- Pearce O, Gamblin T, de Supinski BR, Schulz M, Amato N, Quantifying the Effectiveness of Load Balance Algorithms, International Conference on Supercomputing (ICS), June 2012.
- Pearce O, Gamblin T, de Supinski BR, Schulz M, Amato N, Decoupled load balancing, Proceedings of the 20th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming, 2015
- Adams MF, Ku S, Worley P, et al., Scaling to 150K cores: Recent algorithm and performance engineering developments enabling XGC1 to run at scale, Journal of Physics: Conference Series, 2009.
- Kraeva MA, Malyshkin VE, Algorithms of Parallel Realisation of the PIC Method with Assembly Technology, Lecture Notes in Computer Science, 1999, Volume 1593/1999, 329-338.

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Load Balancing: Literature Survey (continued)

- Bhatelé A, Kalé LV, Kumar S, Dynamic Topology Aware Load Balancing Algorithms for MD Applications SC'09 November2009.
- Madduri K, Williams S, Ethier S et al., Memory-efficient optimization of Gyrokinetic particle-to-grid interpolation for multicore processors, SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP10), 2010.
- Stantchev G, Dorland W, Gumerov, Fast parallel Particle-To-Grid interpolation for plasma PIC simulations on the GPU, Journal of Parallel and Distributed Computing, Volume 68, Issue 10, October 2008, Pages 1339-1349.
- Ji Qiang, Robert D. Ryne, Salman Habib and Viktor Decyk, Object-Oriented Parallel Particle-in-Cell Code for Beam Dynamics Simulation in Linear Accelerators, sc, pp.55, Proceedings of the 1999 ACM/IEEE conference on Supercomputing, 1999.
- Viktor K. Decyk, Tajendra V. Singh and Scott A. Friedman, GRAPHICAL PROCESSING UNIT-BASED PARTICLEIN-CELL SIMULATIONS, Proc. Intl. Computational Accelerator Physics Conf. (ICAP2009), San Francisco, CA, Sept, 2009
- V. K. Decyk, UPIC: A framework for massively parallel particle-in-cell codes, Computer Physics Communications, Volume 177, Issues 1-2, July 2007, Pages 95-97 Proceedings of the Conference on Computational Physics 2006 - CCP 2006, Conference on Computational Physics 2006.
- Hariri F, Trana TM, Jockschb A, Lanti E, Progschc J, Messmer P, Brunner S, Gheller C, Villarda L, A portable platform for accelerated PIC codes and its application to GPUs using OpenACC, Computer Physics Communications, October 2016
- Germaschewski K, Fox W, Abbott S, Ahmadi N, Maynard K, Wang L, Ruhl H, Bhattacharjee A, The Plasma Simulation Code: A modern particle-in-cell code with patch-based load-balancing, Journal of Computational Physics, August 2016

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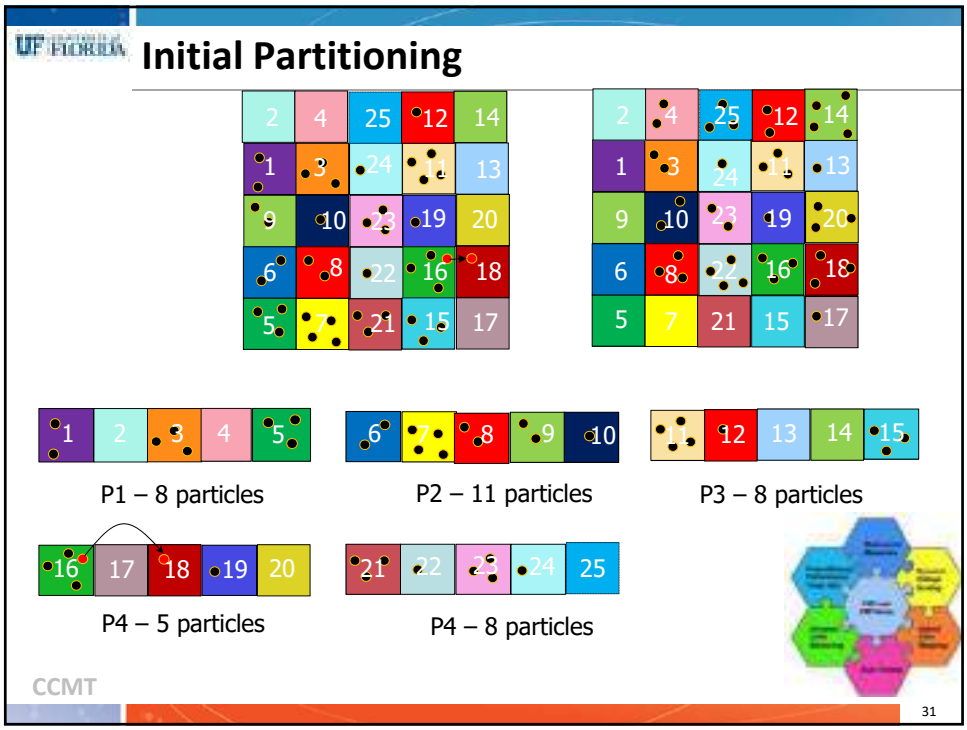
Initial Partitioning
P1 – 8 particles
P2 – 11 particles
P3 – 8 particles
P4 – 5 particles
P4 – 8 particles
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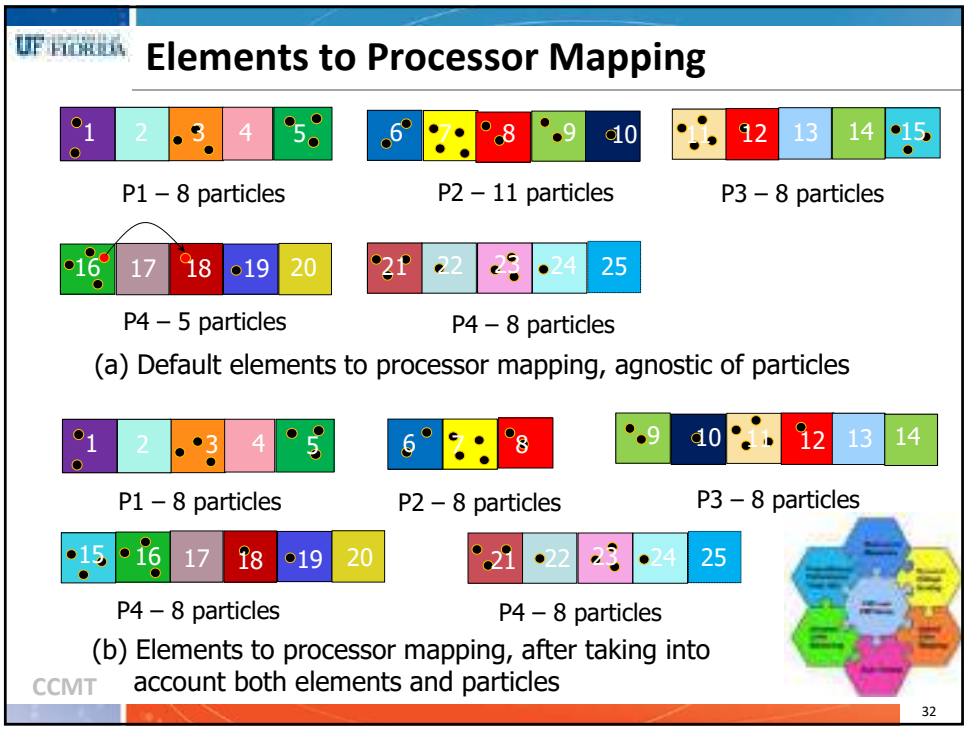
Elements to Processor Mapping
P1 – 8 particles
P2 – 11 particles
P3 – 8 particles
P4 – 5 particles
P4 – 8 particles
(a) Default elements to processor mapping, agnostic of particles
P1 – 8 particles
P2 – 8 particles
P3 – 8 particles
P4 – 8 particles
P4 – 8 particles
(b) Elements to processor mapping, after taking into account both elements and particles
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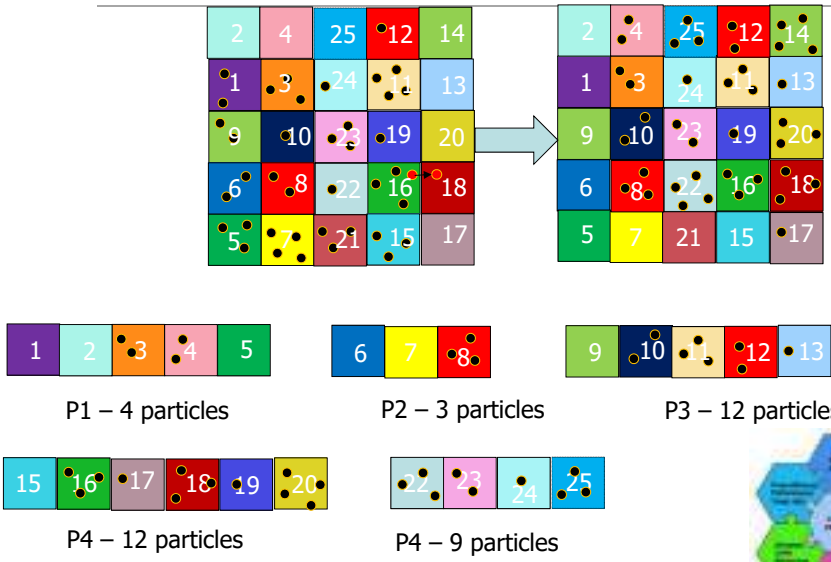
After n time steps



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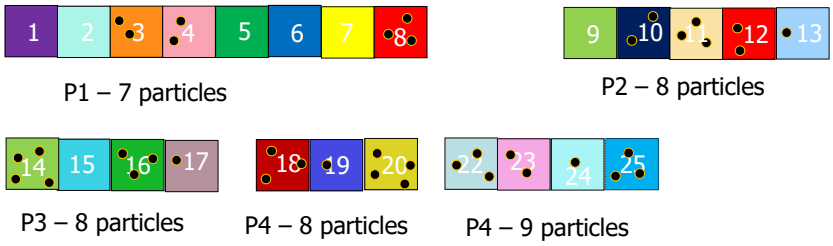
Remapping



- Determine new mapping of elements to processors
- Transfer elements and particles using serialization
- Deserialize newly received elements and particles
- Reinitialize other supporting data structures

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Rebalancing Time

	128p	256p	512p	1024p	2048p
Overhead for remapping, packing, unpacking and transfer(s)	0.099	0.164	0.276	0.540	0.956
Nek5000 reinit time (s)	2.58	6.67	23.13	98.56	389
Time per time step (s)	0.57	0.579	0.575	0.611	0.61
Overhead (in no. of time steps)	0.174	0.283	0.48	0.884	1.567

CMT-nek

16 elements per processor
10,240 particles per processor
Grid size: 5x5x5
Weak scaling

- During rebalancing, some arrays are reinitialized while others are transferred.
- Currently we reuse nek5000 initialization routines, as a result there are some significant additional and redundant operations happening.

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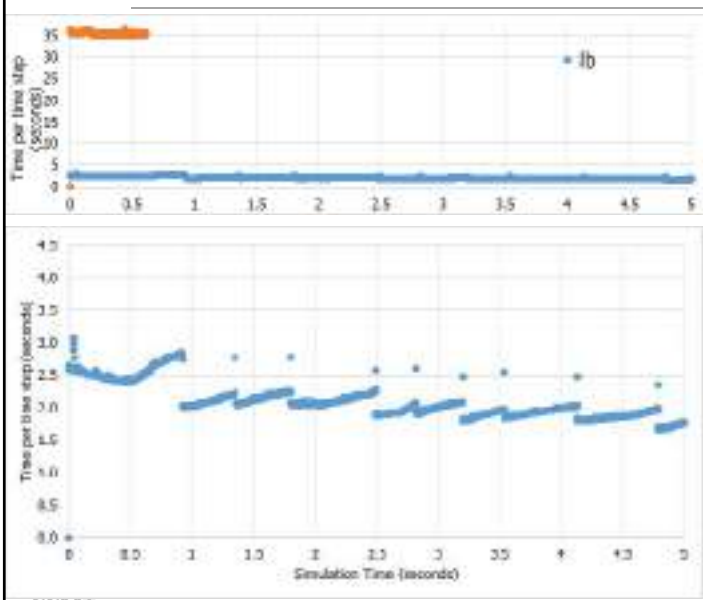
CMT-nek on Vulcan



CMT-nek

256 processors
16384 elements
10,485,760 particles
Grid size: 5x5x5
Cylinder test

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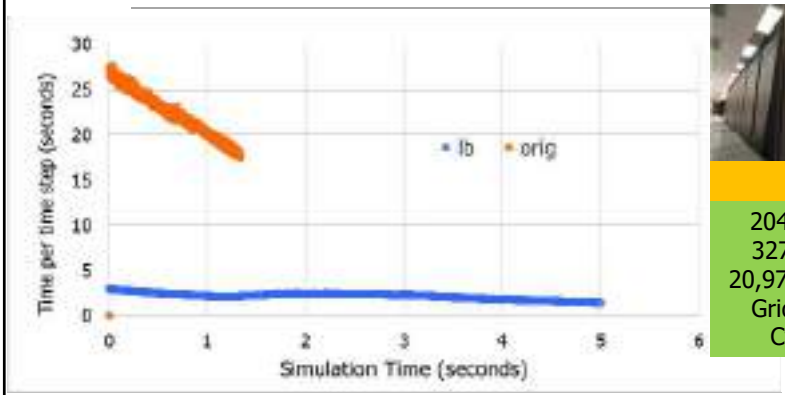
CMT-nek on Vulcan



CMT-nek

2048 processors
32768 elements
20,971,520 particles
Grid size: 5x5x5
Cylinder test

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

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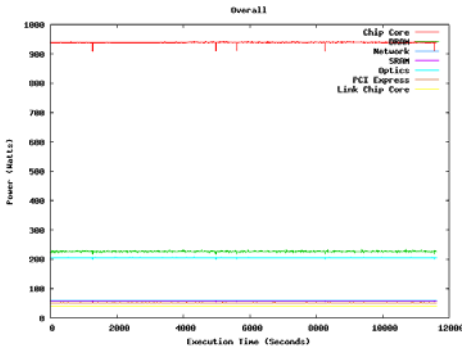
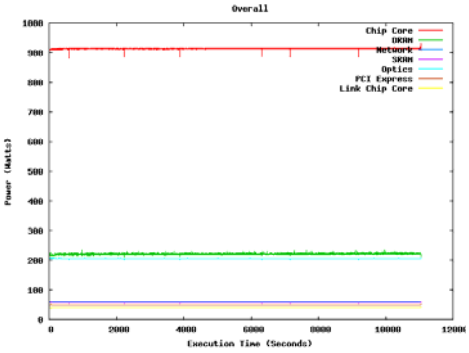
CMT-nek on Mira (setup from previous slide)



Power consumption by original code



Power consumption by load balanced code

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

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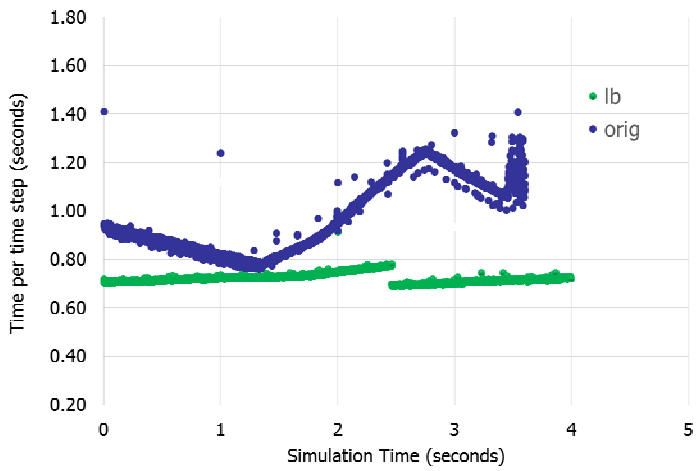
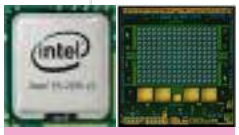
CMT-bone on Titan





4 nodes, 16 cores and 1 GPU per node

CMT-bone

16384 elements
1048576 particles
5x5x5 grid size
Expansion fan

- More than 1.3 times improvement in average performance

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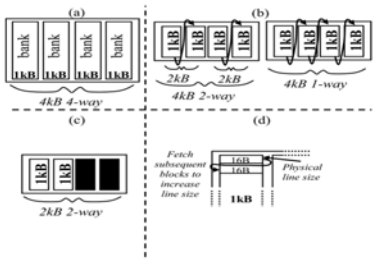
Hardware-Software Autotuning

Algorithm: *dudr-4loop*

```
do k = 1, Nz
 do j = 1, Ny
  do i = 1, Nx
   do l = 1, Nx
    dudr(l, j, k) = dudr(l, j, k) +
                    a(i, l) * u(l, j, k, ie)
   enddo
  enddo
 enddo
enddo
```

Algorithm: *dudr-4loop-fused*

```
do k = 1, Nz* Ny
 do i = 1, Nx
  do l = 1, Nx
    dudr(l, k) = dudr(l, k) +
                 a(i, l) * u(l, k, ie)
  enddo
 enddo
enddo
```



Total number of variants = 20

Algorithm: *dudr-4loop-permuted-and unrolled*

```
do k = 1, Nz
 do i = 1, Nx
  do j = 1, Ny
   do l = 1, Nx,2
    dudr(l, j, k) = dudr(l, j, k) +
                    a(i, l) * u(l, j, k, ie)
    dudr(l+1, j, k) = dudr(l+1, j, k) +
                    a(i, l+1) * u(l+1, j, k, ie)
   enddo
  enddo
 enddo
enddo
```

Number of 4-loop implementations for dudr
$N_x=N_y=N_z=10$
= 4! * 4 ^ 4
= 24 * 256 = 6144 variants
Total number of variants = 98,240 (N=10)
Total number of variants = 217,728 (N=20)
Exhaustive search may not be feasible

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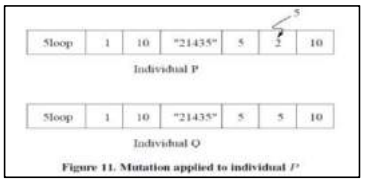
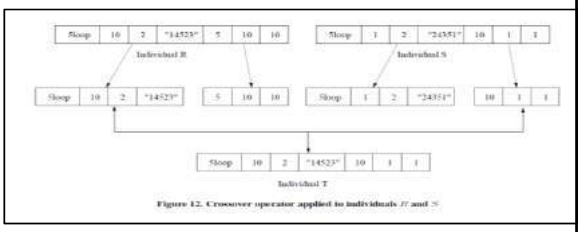
Genetic Algorithm





i=1

- Generate Initial Population
- i=1

- Compile and run each individual
- Set fitness value for each individual based on performance and energy

i < n ?

No

- Population Selection
- Add new individuals using crossover and mutation
- i=i+1

Yes

Report the best individual

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Comparison of GA with Exhaustive Approach

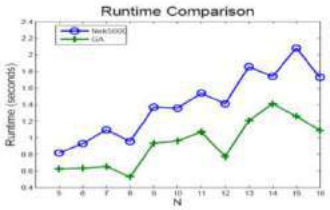
Comparison of performance by platform

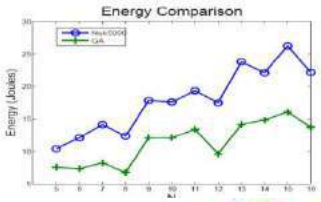
Platforms	CMT-nek time (seconds)	Exhaustive Autotuning			GA based Autotuning			
		Time	Search Space	%Less	Time	Search Space	% Less	%Diff
IBM BG/Q	5.57	2.54	97716	54.3	2.58	1124	53.7	1.1
AMD Opteron	1.81	1.02	97716	43.6	1.06	1283	41.4	3.9
AMD Fusion	1.36	0.95	32652	30	0.95	485	30	0.0

Comparison of energy consumption by platform

Platforms	CMT-nek energy (Joules)	Exhaustive Autotuning			GA based Autotuning			
		Energy	Search Space	%less	Energy	Search Space	%Less	%Diff
IBM BG/Q	292.1	131.7	97716	54.9	135	1124	53.7	2.5
AMD Fusion	17.6	11.98	32652	32	12.11	485	31	1.1

Results (AMD Fusion @ Sandia)





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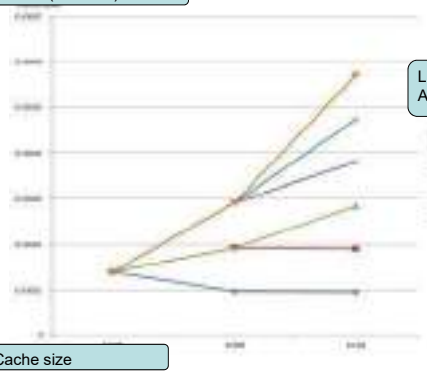
Performance (varying hardware parameters)

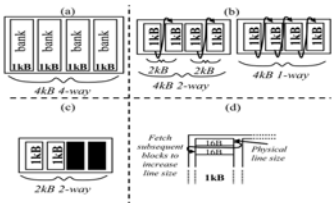
Best Time (seconds)



Cache size

Line Size - Associativity

Associativity Tuning



Capacity Tuning

Line Size Tuning

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

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

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

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Publications

1. Tania Banerjee and Sanjay Ranka, Genetic Algorithm based Autotuning Approach for Performance and Energy Optimization, Proceedings of International Green and Sustainable Computing, 2015
2. Tania Banerjee, Mohammed Gadou, Sanjay Ranka, A Genetic Algorithm based Approach for Multi-objective Hardware/Software Co-optimization, Journal of Sustainable Computing, Vol 10, June 2016, 36 – 47.
3. Tania Banerjee, Jacob Rabb and Sanjay Ranka, Multi-objective Optimization of Spectral Solvers on Hybrid Multicore Platforms, Journal of Sustainable Computing, Vol 12, Dec 2016, 10 - 20.
4. Tania Banerjee, Jason Hackl, Mrugesh Sringarpure, Tanzima Islam, S. Balachandar, Thomas Jackson, Sanjay Ranka, CMT-bone -- A Proxy Application for Compressible Multiphase Turbulent Flows, Proceedings of HiPC, 2016 (and extended version submitted to Journal of Sustainable Computing).
5. Mohammed Gadou, Tania Banerjee, Sanjay Ranka, Multi-objective Optimization of CMT-bone on Hybrid Processors, Proceedings of IGSC 2016, (an extended version submitted to Journal of Sustainable Computing).
6. Keke Zhai, Tania Banerjee, Mohamed Gadou, David Zwick, Jason Hackl and Sanjay Ranka, Dynamic Load Balancing for Compressible Multiphase Turbulence, in preparation.
7. Mohamed Gadou, Meena Arunachalam, Tania Banerjee, Sanjay Ranka, Multiobjective evaluation and optimization of CMT-bone on Intel Knights Landing, in preparation.
8. Sankeerth Mogili, Tania Banerjee, Sanjay Ranka, Multi-objective Optimization on Hybrid Systems using DVFS, in preparation.

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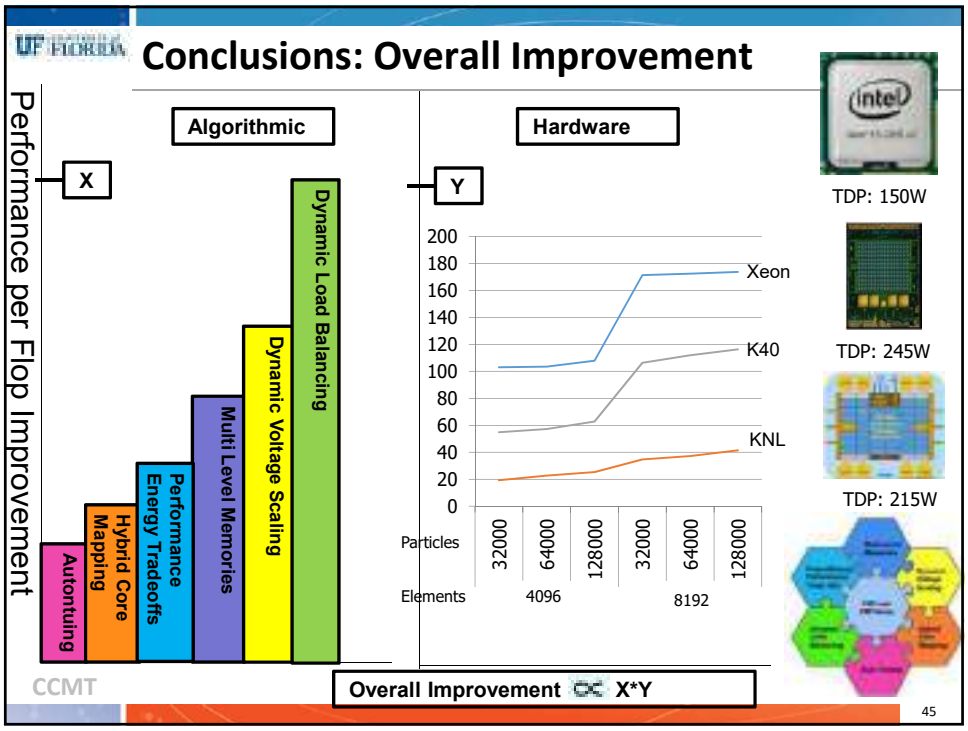
Conclusions: Overall Improvement
Performance per Flop Improvement
X
Algorithmic
Autontuing
Hybrid Core Mapping
Performance Energy Tradeoffs
Multi Level Memories
Dynamic Voltage Scaling
Dynamic Load Balancing
Hardware
Y
200
180
160
140
120
100
80
60
40
20
0
Xeon
K40
KNL
Particles
32000
64000
128000
32000
64000
128000
Elements
4096
8192
TDP: 150W
TDP: 245W
TDP: 215W
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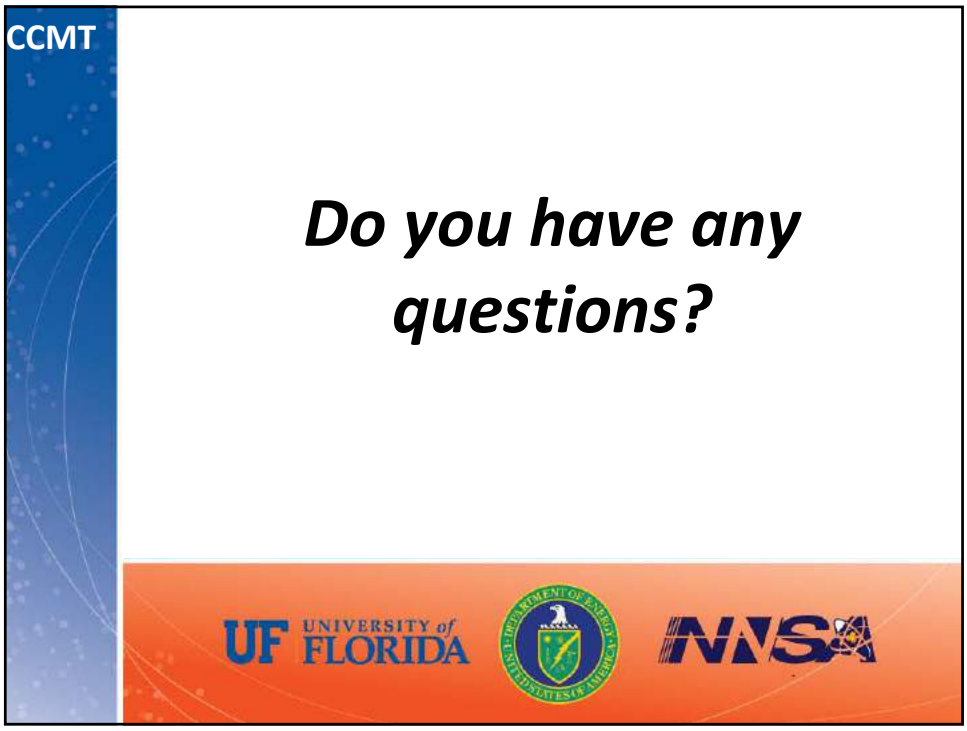
Overall Improvement ∝ X*Y
45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Do you have any questions?
UF UNIVERSITY of FLORIDA
NNSA

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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) Team

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Aravind Neelakantan
(M.S./Ph.D.)

Carlo Pascoe
(Ph.D.)

Ajay Ramaswamy
(M.S.)

Mason Rawson
(B.S./M.S.)

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Review Team Questions & Recommendations - 2016

- RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
  - Feedback loop between physics and CS/BE efforts
  - "Closing the loop": predictive BE simulation of CMT-nek design space
- RQ 5 – Recommendations on Scalability Results
  - Scalability is a major objective in Year 3; will emphasize scalability studies in benchmarking results, predictive BE simulation, and FPGA acceleration
- RQ 6 – Additional Recommendations
  - Scalability of FPGA approach
  - A multi-FPGA scalability projection will be presented

CCMT 3

Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts & Y3 achievements

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

- Summary, conclusions, & future work

CCMT 4

Outline

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- Summary, conclusions, & future work

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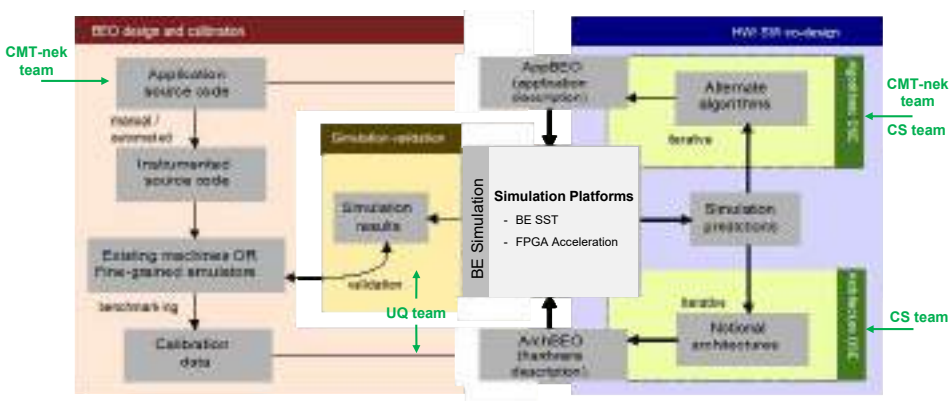
Co-Design Using *Behavioral Emulation*



* BEO – Behavioral Emulation Object

HW/SW co-design

- Algorithmic & architectural design-space exploration (DSE)

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 design space reduction & UQ (Year 2)

Year 3 Accomplishments:

Methods

- BE method enhancement: network models, interpolation schemes, energy & thermal modeling
- Perform large-scale validation (100k+ MPI ranks) on DOE systems (Cab, Vulcan, Titan) and performed *predictive* simulations to million+ MPI ranks
- Closing the loop: Behavioral Emulation & design-space exploration on CMT-nek

Tools

- Completed development of v1.0 of SST-based BE simulator
- Validation of dataflow, pipelined approaches; multi-FPGA scalability prediction

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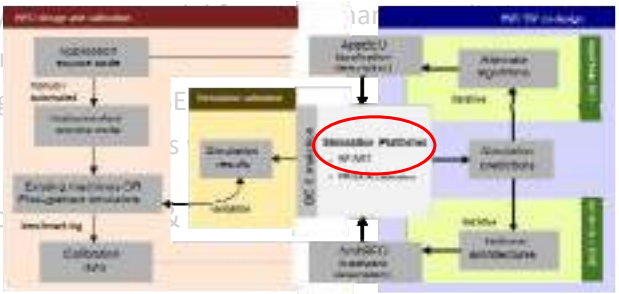
- BE simulatio
- Adding energ
- Accelerating
- Summary, c



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BE-SST Simulator

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

SST Capabilities		BE Influences		BE-SST
• Parallel simulations • Discrete event simulation • Clock and event queues • Network Models • Component Models	+	• Software Definitions • Probabilistic Simulation • Abstract Network Definitions • Abstract Hardware Definitions	=	• Parallel discrete event simulation environment • Distributed component queues • Software Definitions • Probabilistic Simulation • Abstract Network Models • Abstract Component Models

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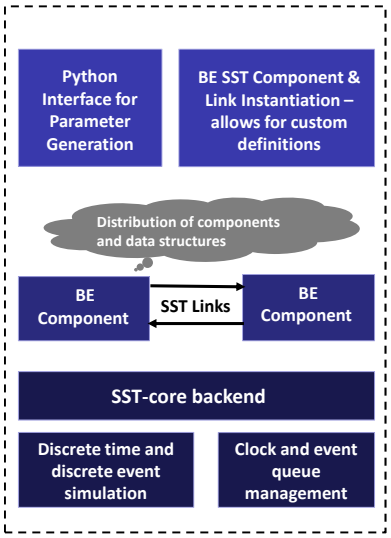
BE-SST model enhancements

- Communication model enhancements:
  - Dynamic generation of network routes provide better performance scaling and parallel performance
  - Overhead modeling at both sender/receiver endpoints
- Interpolation API allows easy switching between different interpolation methods for better accuracy
  - Polynomial Interpolation
  - Lagrange Interpolation
- Improved scalability and robustness of software product
  - Reduced storage by deleting handled events from queues
  - Switched from static routes to runtime routing



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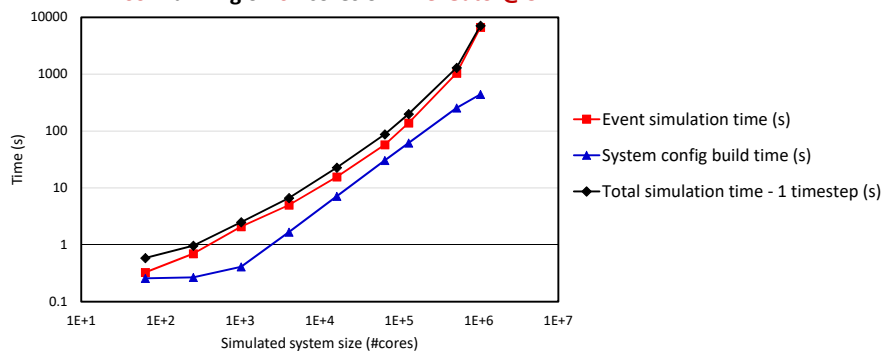
Parallel Performance of BE-SST

- BE simulations of 3d-mesh system running CMT-bone-BE
  - Simulations of machines with up to a million cores
  - With dynamic routing
- System config build time is not a bottleneck for large simulations

BE-SST running on 64 cores of HiPerGator@UF



* See poster from Ajay Ramaswamy

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- Accelerating
- Summary, c

- RQ 5 – Recommendations on Scalability Results

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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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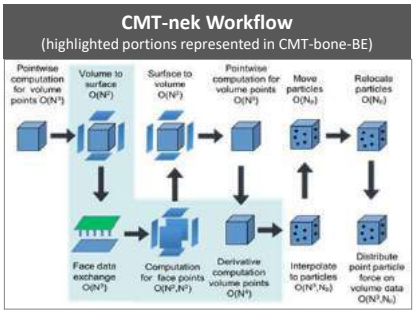
Application Case Study: CMT-bone-BE

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



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

* design-space exploration

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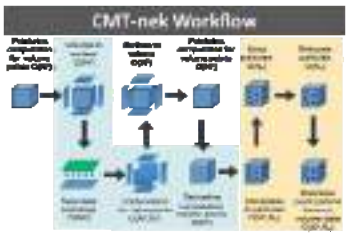
Experiment Setup

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



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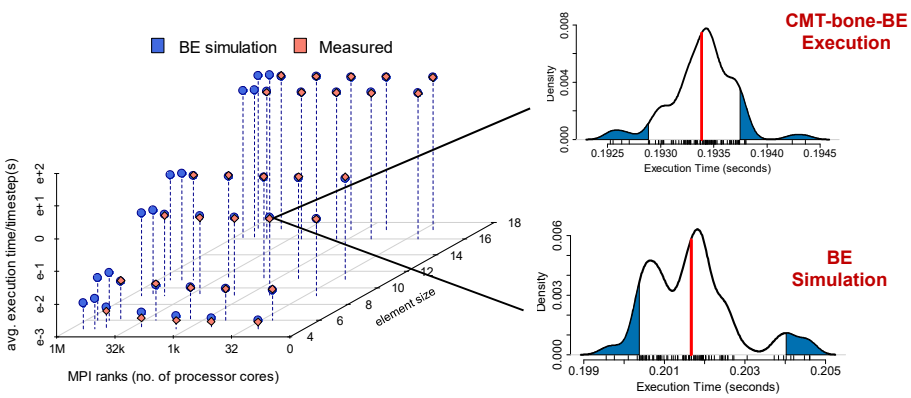
BE Simulations of CMT-bone-BE on Titan



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

$$\%\,error = \frac{\frac{\sum_{i=1}^{N} t_{measured\,i}}{N} - \frac{\sum_{i=1}^{N} t_{simulated\,i}}{N}}{\frac{\sum_{i=1}^{N} t_{measured\,i}}{N}} \times 100$$

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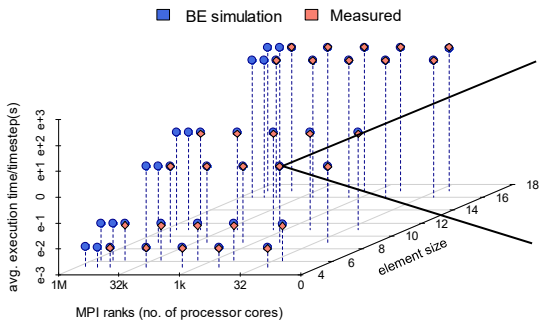
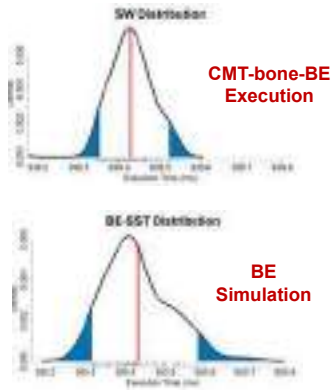
BE Simulations of CMT-bone-BE on Vulcan





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

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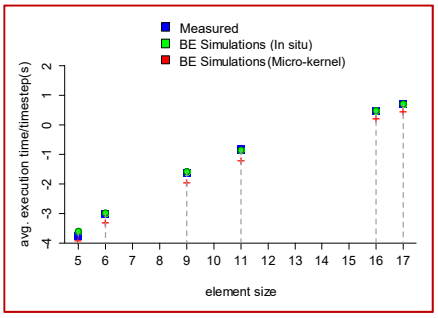
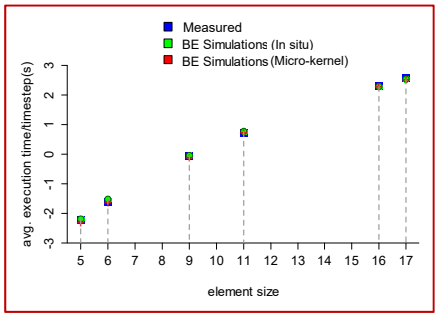
In situ vs. Micro-kernel Benchmarking

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

Titan



Vulcan



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

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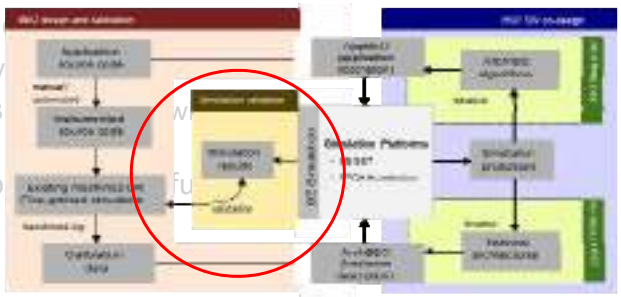
- Adding energy
- Accelerating B

- Summary, co



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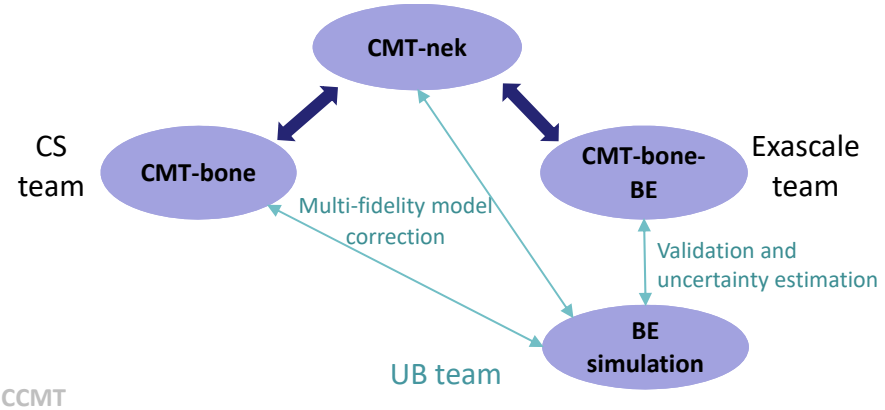
Assessing Behavioral Emulation

w/ UB

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



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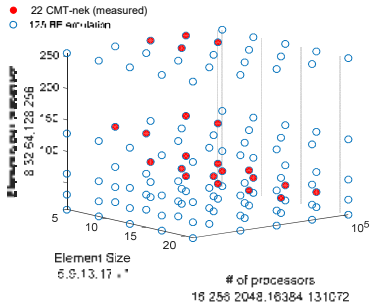
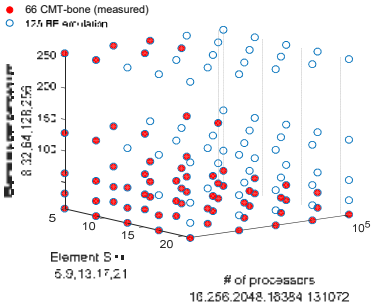
Experimental setup

w/ UB

- Design of experiment (DOE)
  - Element size (ES) = 5,9,13,17,21
  - Elements per processor (EPP) = 8,32,64,128,256
  - Number of processors (NP) = 16,256,2048,16384,131072
- Multi-fidelity surrogate model
  - Fitting CMT-nek and CMT-bone using corrected fitting of BE simulation
  - For large problems, low-fidelity BE simulation is computationally cheaper than high-fidelity CMT-nek or CMT-bone



DOE of CMT-nek



DOE of CMT-bone

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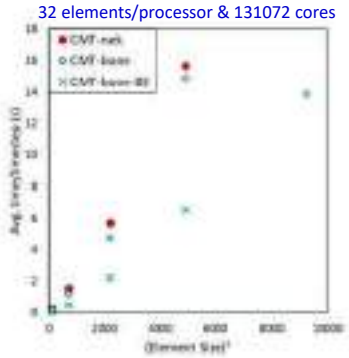
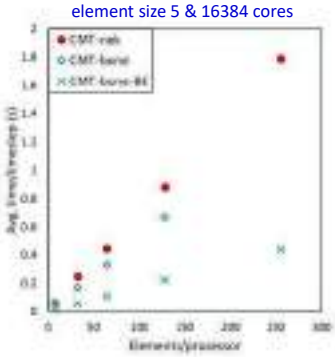
Trends of CMT-nek, -bone, and -bone-BE

w/ UB

Varying **Element Size**
32 elements/processor & 131072 cores



Varying **Elements/processor**
element size 5 & 16384 cores



- Similar trends across three applications:
  - Left: Linear in (element size)^3
  - Right: Linear in elements/processor
- CMT-bone-BE has different slope – captures only spectral element solver kernel of nek/bone

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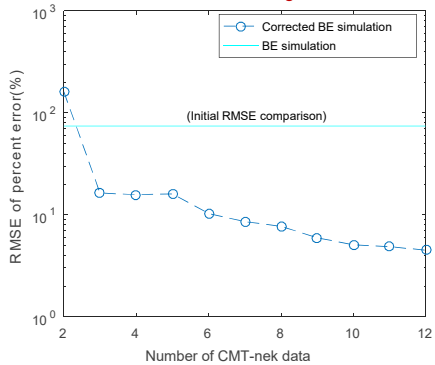
Multi-fidelity Prediction of CMT-nek

w/ UB

Initial RMSE comparison:

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

Corrected BE simulation against CMT-nek



Accuracy of corrected BE sim.

- At 10 left-out CMT-nek test points
- Overall RMSE < 10% with 7 or more CMT-nek data

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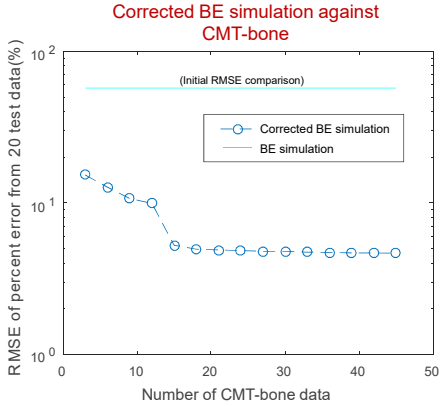
Multi-fidelity Prediction of CMT-bone

w/ UB

Initial RMSE comparison:

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

Corrected BE simulation against CMT-bone



Accuracy of corrected BE sim.

- At 20 left-out CMT-bone test points
- Overall RMSE < 5% with 15 or more CMT-bone data

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* See posters from Aravind Neelakantan and Yiming Zhang

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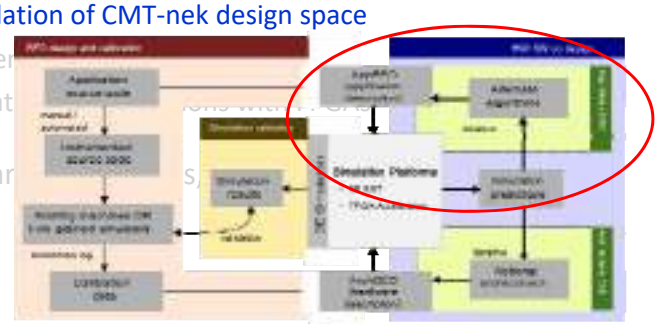
Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts & Y3 achievements

- RQ 4 – Recommendations on Integration of CS/BE & CMT-nek Efforts
  - Feedback loop between physics and CS/BE efforts
- BE simulation of CMT-nek design space
- Adding e
- Accelerat
- Summar



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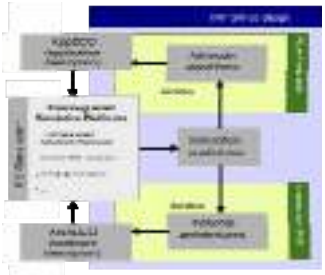
Motivation & Approach

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

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



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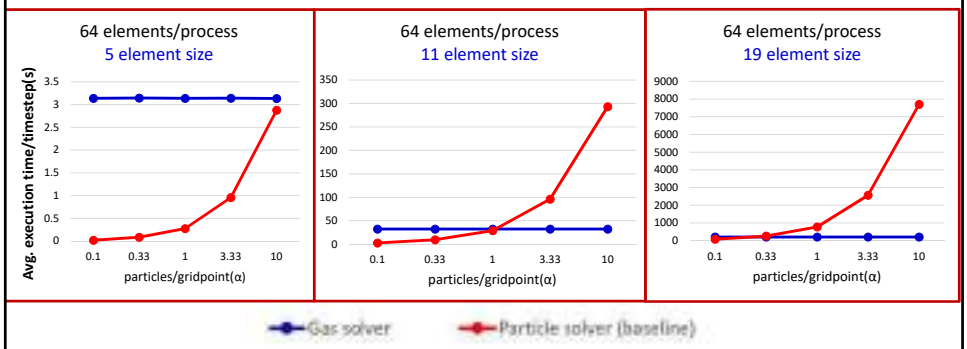
CMT-nek Profiling: Gas vs Particle Solver

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



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

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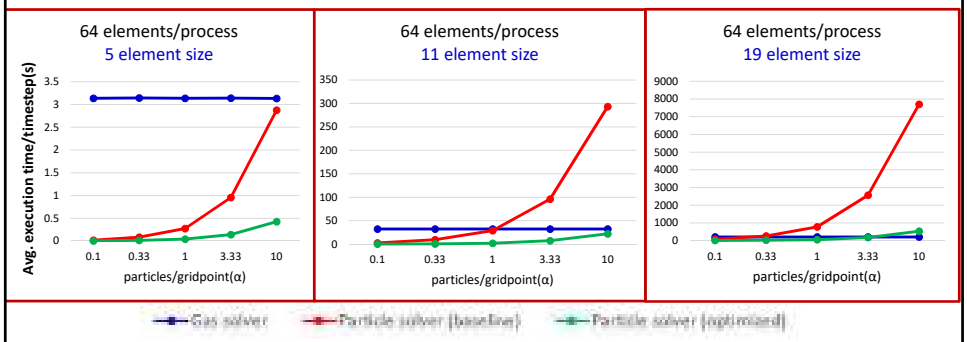
CMT-nek Profiling: Gas vs Particle Solver

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



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

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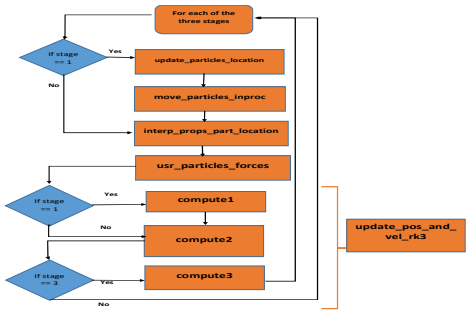
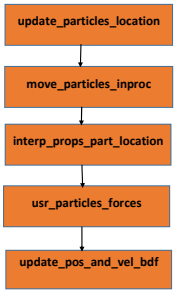
CMT-nek Alternate Algorithms

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



Control-flow graph of rk3 algorithm



Control-flow graph of bdf algorithm

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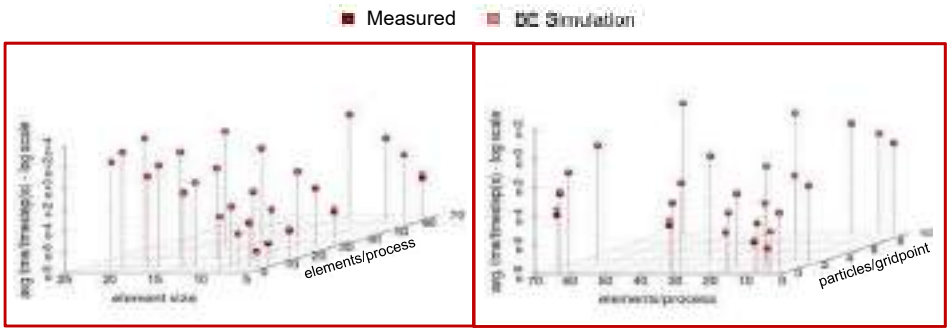
Validation of Particle Solver Models

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



Fixed particles/gridpoint = 0.1
- Element sizes: 5,7,9,13,17,21
- Elements/process: 4,8,16,32,64

Fixed element resolution = 5
- Elements/process: 4,8,16,32,64
- Particles/gridpoint: 0.1,0.33,1,3.33,10

- Observed an average error of 2.57% in simulations
- Reduced Barycentric Interpolation – average error 2%
- Bdf time integration – average error 2.44%

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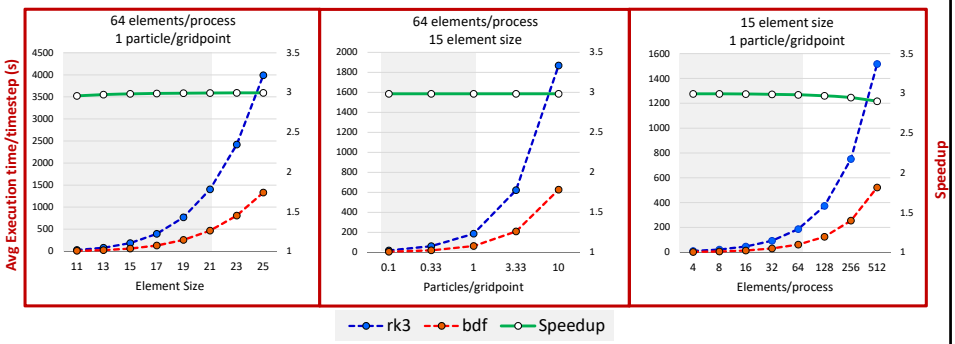
Simulator Predictions: Time Integration

Simulation predictions on Vulcan



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

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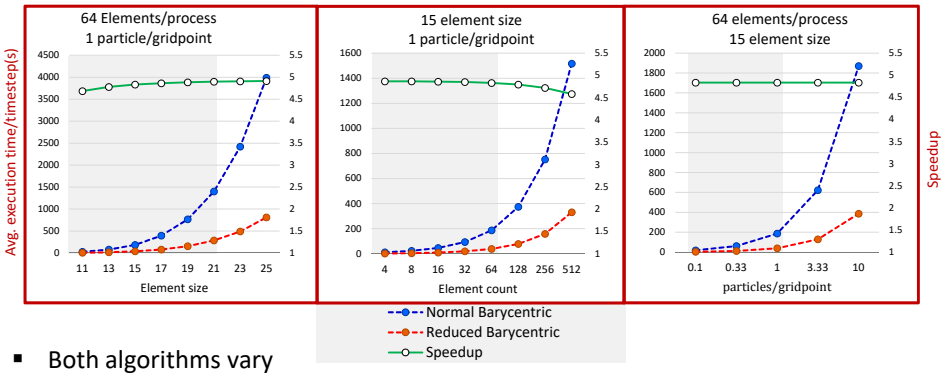
Simulator Predictions: Interpolation

Simulation predictions on Vulcan



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

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* See posters from Sai Chenna and David Zwick

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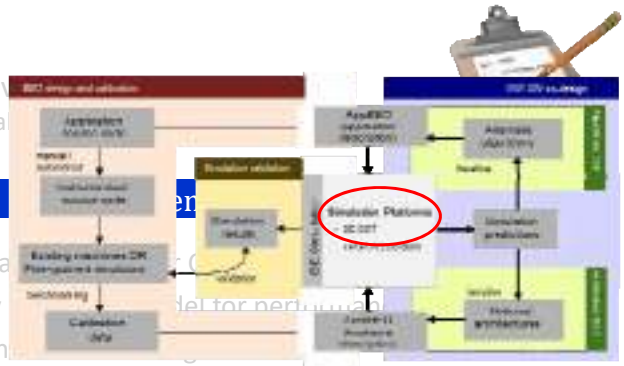
Outline

- Review & Ov
  - Behaviora

Research thrusts



- BE-SST simula
- Multi-fidelity
- BE simulation
- Adding energy models to BE
- Accelerating BE simulations with FPGAs

- Summary, conclusions, & future work

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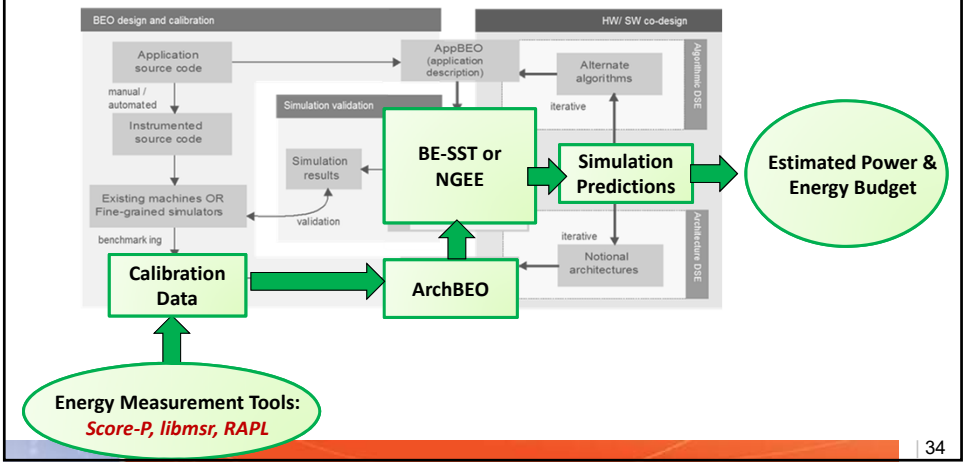
Energy Benchmarking & Modeling

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



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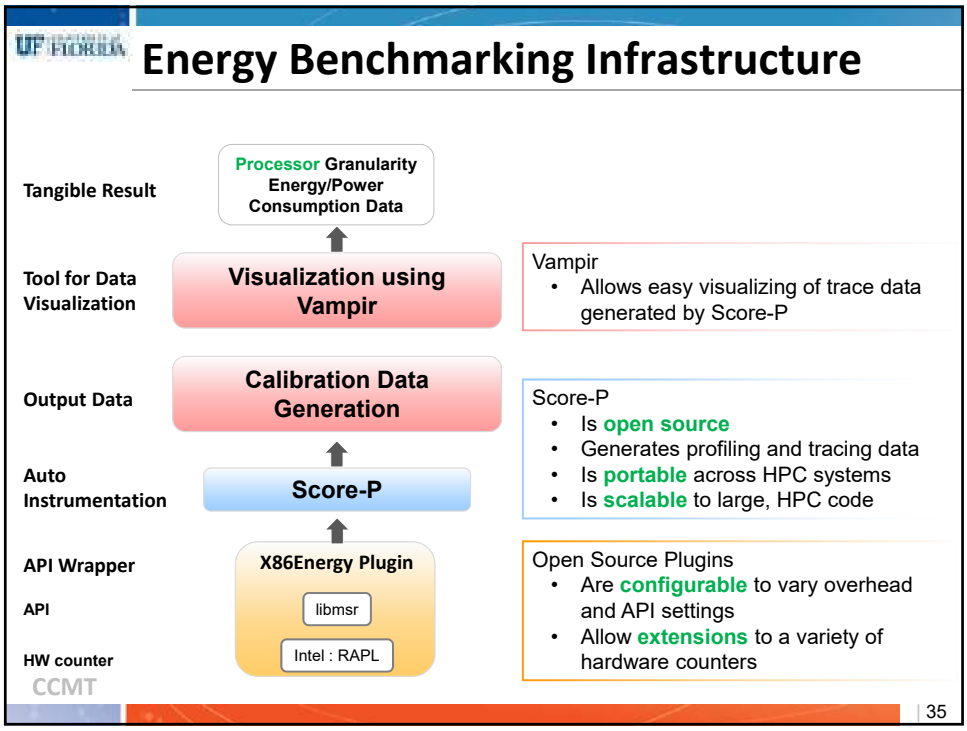
Energy Benchmarking Infrastructure
Tangible Result
Processor Granularity Energy/Power Consumption Data
Tool for Data Visualization
Visualization using Vampir
Vampir
• Allows easy visualizing of trace data generated by Score-P
Output Data
Calibration Data Generation
Score-P
• Is open source
• Generates 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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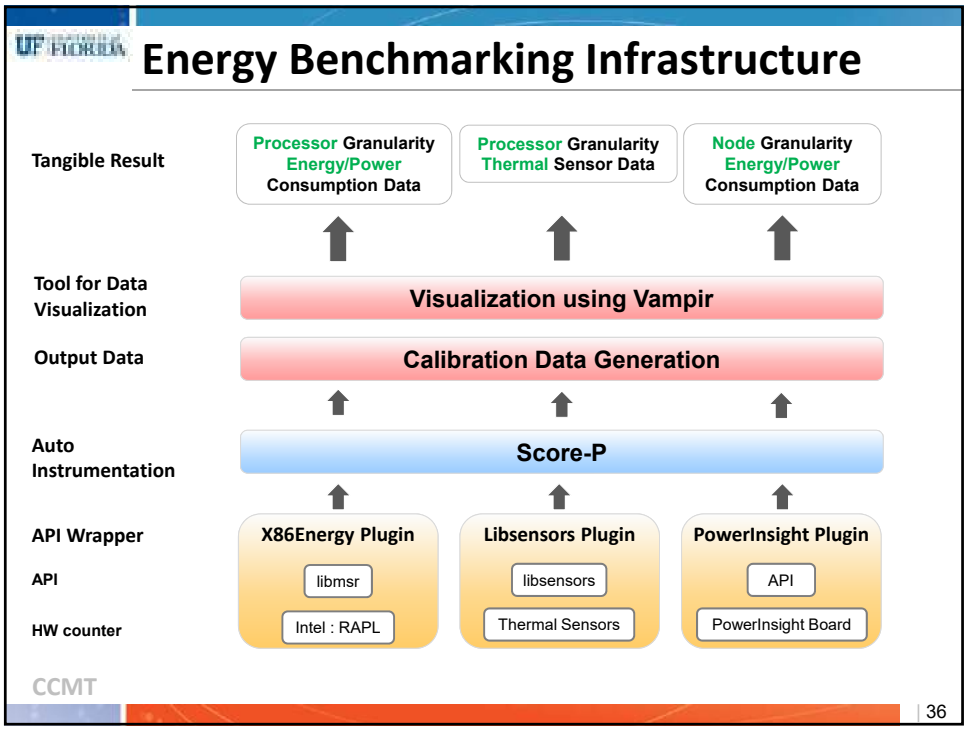
Energy Benchmarking Infrastructure
Tangible Result
Processor Granularity Energy/Power Consumption Data
Processor Granularity Thermal Sensor Data
Node Granularity Energy/Power Consumption Data
Tool for Data Visualization
Visualization using Vampir
Output Data
Calibration Data Generation
Auto Instrumentation
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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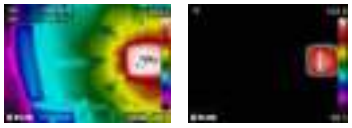
Thermal Aware Computing Lab (TACL)

- Purpose
  - Develop detailed understanding of processor level thermal effects on performance and energy consumption
  - Develop thermal- and energy-aware optimizations for multicores
    - Initial analysis on Intel Knights Landing
  - Working with experimentalist (Kyle Hughes) for IR thermography experience
- Equipment
  - Flir A35c IR Camera
  - Knights Landing (KNL)

Flir A35c IR Camera



Thermal Imaging on Zedboard Zynq Dual Arm-FPGA System-on-Chip

KNL server node

* See posters from Mason Rawson and Tanya Banerjee

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Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts

- BE-SST simula
- Multi-fidelity
- BE simulation
- Adding energ
- Accelerating BE simulations with FPGAs

- RQ 6 – Additional Recommendations
  - Scalability of FPGA approach

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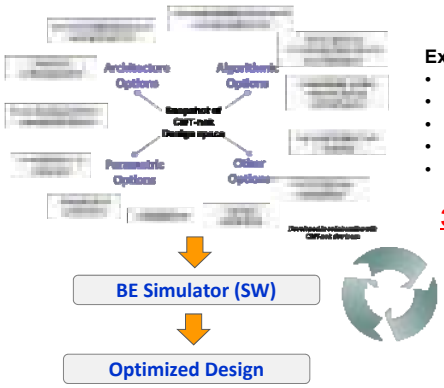
BE Design-Space Exploration



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

~Minutes per simulation

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

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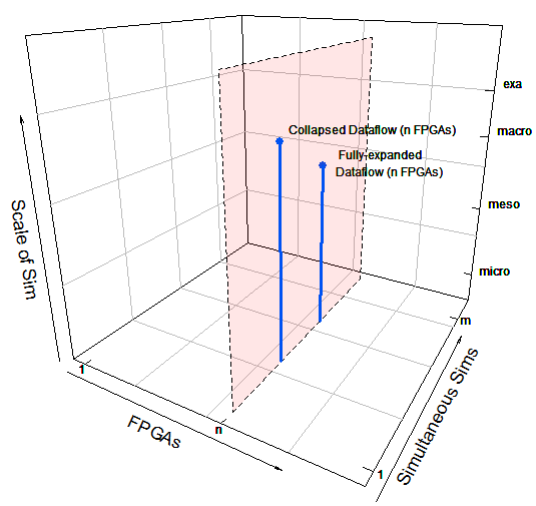
Landscape of FPGA-acceleration Studies



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

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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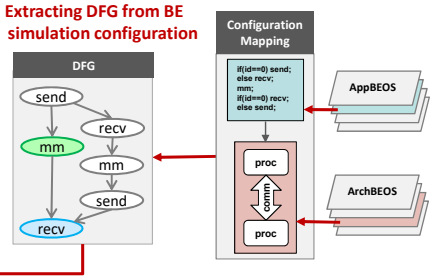
Fully-expanded Pipeline (FEP)

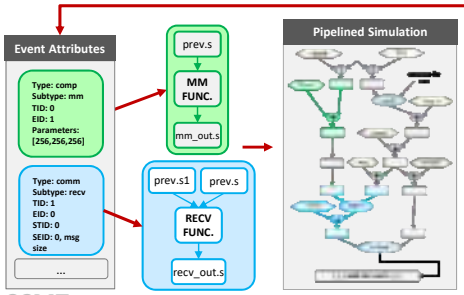
1. Construct Data Flow Graph (DFG) from simulation configuration

- AppBEO+ArchBEO define instructions and operand/output dependencies
- Instructions map to vertices and dependencies map to edges in DFG
- Various opportunities for graph-level optimizations

1. Extracting DFG from BE simulation configuration



2. Mapping DFG to FPGA Pipeline



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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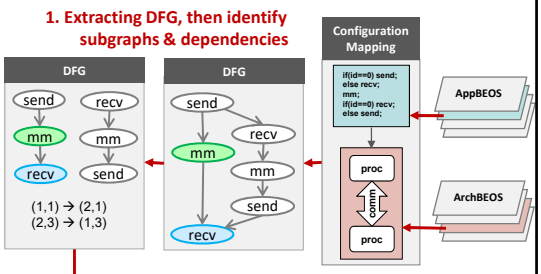
Collapsed Pipeline (CP)

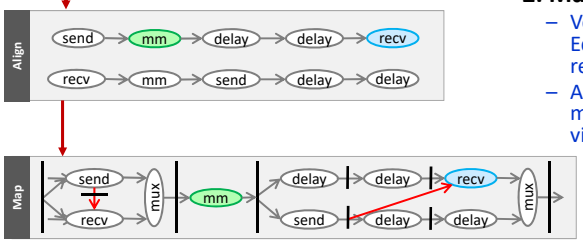
1. Construct Data Flow Graph (DFG) from simulation configuration

- AppBEO+ArchBEO define instructions and operand/output dependencies
- Instructions map to vertices and dependencies map to edges in DFG
- Partition into linear subgraphs and generate dependency lists

1. Extracting DFG, then identify subgraphs & dependencies



2. Mapping DFG to FPGA Pipeline



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*

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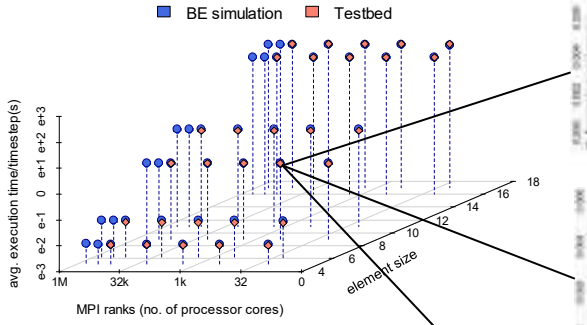
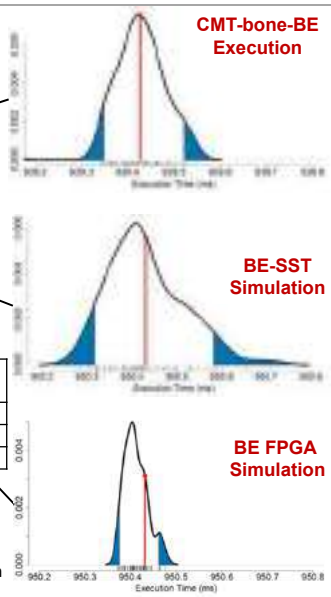
Simulations of CMT-bone-BE on Vulcan





Simulation Method	Num. of MPI Ranks	Num. of Timesteps	Num. of Events	Num. of FPGAs	% Logic Utilization	FPGA Clk Frequency	Latency to First Output	Mega Sims/Sec
BE-SST	128	1	5,952	NA	NA	NA	NA	0.00000152
FEP	128	1	5,952	1	66 %	280 - 320 MHz	66	**280 – 320**
CP	128	1	5,952	1	2 %	315 - 355 MHz	458	**1.68 – 1.99**

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

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Fully-Expanded & Collapsed Pipeline Tradeoffs

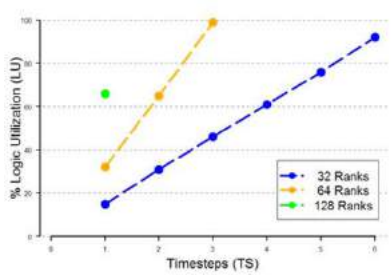
Fully-Expanded Pipeline

Advantages:

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

Limitations:

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



Ranks	TS	% LU	Num. of Events	Lat to First Out (cycles)	Mega Sims /second*	Giga Events /second*
32	1	15	1,344	64	300	403
32	2	31	2,688	118	300	806
32	3	46	4,032	172	300	1,210
32	4	61	5,376	226	300	1,613
32	5	76	6,720	280	300	2,016
32	6	92	8,064	334	300	2,419
64	1	32	2,880	65	300	864
64	2	65	5,760	119	300	1,728
64	3	99	8,640	173	300	2,592
128	1	66	5,952	66	300	1,785

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*Fully-expanded performance of CMT-Bone-BE with varied MPI ranks and simulation timesteps on a single Stratix V S5GSMD8K1F40C2 @ 300MHz

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Fully-Expanded & Collapsed Pipeline Tradeoffs

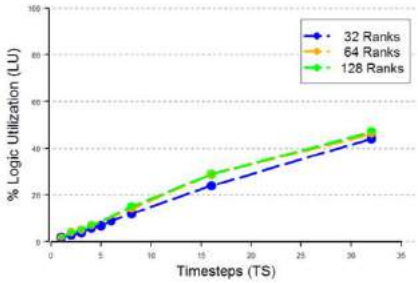
Collapsed Pipeline

Advantages:

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

Limitations:

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



Ranks	TS	% LU	Num. of Events	Lat to First Out (cycles)	Mega Sims /second*	Giga Events /second*
32	1	2	1,344	278	10.5	14.1
32	4	6	5,376	980	10.5	56.3
32	8	12	10,752	1,916	10.5	113
32	16	24	21,504	3,788	10.5	225
32	32	44	43,008	7,532	10.5	450
64	1	2	2,880	394	5.23	15.1
64	4	7	11,520	1,348	5.23	60.3
64	8	14	23,040	2,620	5.23	121
64	16	29	46,080	5,164	5.23	241
64	32	46	92,160	10,252	5.23	482
128	1	2	5,952	458	2.62	15.6
128	4	7	23,808	1,412	2.62	62.3
128	8	15	47,616	2,684	2.62	125
128	16	29	95,232	5,228	2.62	249
128	32	47	190,464	10,316	2.62	498

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

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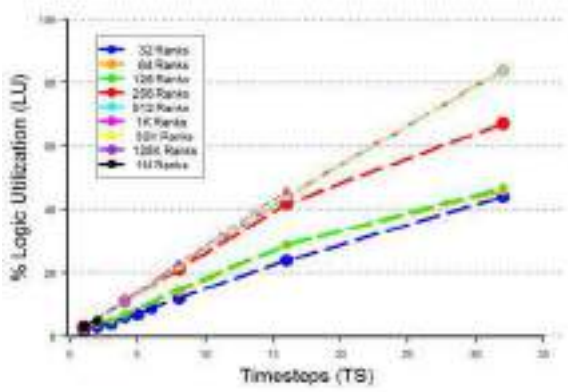
Collapsed Pipeline Single-FPGA Performance/Scalability



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

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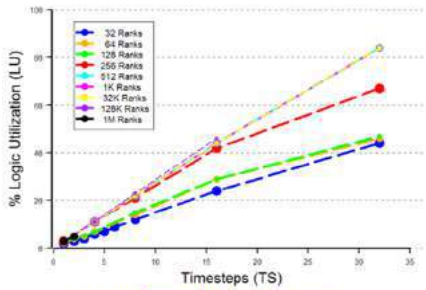
Collapsed Pipeline Single-FPGA Performance/Scalability



Ranks	TS	% LU	Num. of Events	Lat to First Out (cycles)	Mega Sims /second*	Giga Events /second*
32	32	44	43,008	7,532	10.5	450
64	32	46	92,160	10,252	5.23	482
128	32	47	190,464	10,316	2.62	498
256	32	67	393,216	13,516	1.31	515
512	32	84	811,008	20,684	0.65	531
1K	32	84	1,646,592	21,196	0.33	539
32K	32	84	55,443,456	241,868	$1.02E^{-2}$	567
128K	16	46	111,673,344	333,932	$2.56E^{-3}$	285
1M	2	5	112,459,776	1,148,056	$3.19E^{-4}$	36

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

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

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

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

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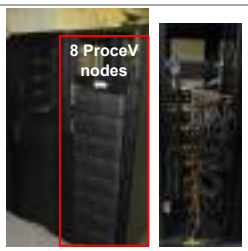
Collapsed Pipeline Multi-FPGA Performance/Scalability

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

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

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

Ranks	TS	FPGAs	Num. of Events	Lat to First Out (cycles)*	Mega Sims /second*	Giga Events /second*
1K	32	1	1,646,592	21,196	0.33	539
1K	64	2	3,293,184	41,439	0.33	1,077
1K	128	4	6,586,368	81,925	0.33	2,155
32K	32	1	55,443,456	241,868	$1.02E^{-2}$	567
32K	64	2	110,886,912	451,039	$1.02E^{-2}$	1,134
32K	128	4	221,773,824	869,381	$1.02E^{-2}$	2,267
128K	32	2	223,346,688	536,863	$2.56E^{-3}$	571
128K	64	4	446,693,376	942,725	$2.56E^{-3}$	1,142
128K	128	8	893,386,752	1,754,449	$2.56E^{-3}$	2,283
1M	**32**	**16**	**1,799,356,416**	**2,641,321**	**$3.19E^{-4}$**	**575**
1M	**64**	**32**	**3,598,712,832**	**4,234,137**	**$3.19E^{-4}$**	**1,150**
1M	**128**	**64**	**7,197,425,664**	**7,414,540**	**$3.19E^{-4}$**	**2,299**



Novo-G#
- 64 GiDEL ProceV (Stratix V)
- 4x4x2 3D torus or 5D hypercube
- 6 Rx-Tx links per FPGA
- Measured 32 Gbps per link
- 150 ns latency across links

- Require 64bits/cycle between FPGAs
- 335MHz, 21.4 Gbps, 51 additional lat
- 450MHz, 28.8 Gbps, 68 additional lat
- 500 MHz before link BW saturation

* See poster from Carlo Pascoe

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

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Summary & Conclusions

- BE methods & tools
  - BE-SST v1.0: parallel BE simulator based on SST
  - Reduction of computational budget using MFS models
  - Began energy & thermal modeling
- Large-scale experiments
  - Validation (100k+ MPI ranks) on Titans, Vulcan, and Cab
  - Predictive simulations to million+ MPI ranks
- CMT-nek DSE using BE simulation
  - Profiling of key CMT-nek particle solver routines
  - Accuracy/performance tradeoffs using BE simulation
- FPGA acceleration of BE simulation
  - Validation of dataflow, pipelined approaches (FEP, CP)
  - Performance/scalability tradeoff analysis for FEP & CP

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Do you have any questions?

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Student Lightning Round

UF UNIVERSITY of FLORIDA

NNSA

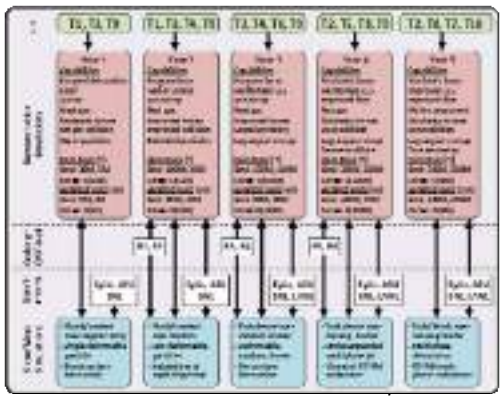
DSE* of CMT-nek using BE**

Sai Prabhakar Rao Chenna

Advisor: Dr. Herman Lam, Dr. Greg Stitt

Department: ECE, UF

- Goals
  - Profile CMT-nek to identify candidates for DSE
  - Perform algorithmic DSE of CMT-nek using BE methods & tools
- Simulation roadmap
  - Early DSE to enhance CMT-nek performance on future exascale systems



Simulation Roadmap

* DSE - Design Space Exploration
**BE – Behavioral Emulation

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2

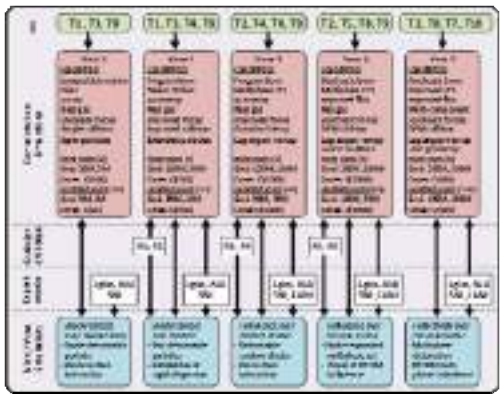
UQ of Sandia Shock Tube Experiments

Brad Durant

Advisor: Prof. S. Balachandar

Department: MAE, UF

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



Simulation Roadmap

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3

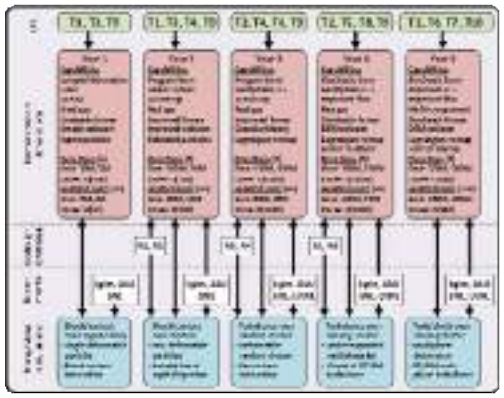
Particles Jet Formation Study

M. Giselle Fernandez

Advisor: Prof. Raphael T. Haftka and S. Balachandar

Department: MAE, UF

- Goals
  - Measurement of PM3 and PM4 in simulations
  - Optimization of initial PVF conditions that grow into jets
- Simulation roadmap
  - Validation of PM4 and PM4



Simulation Roadmap

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4

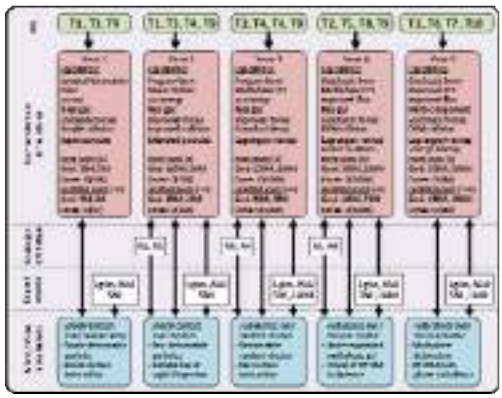
Optimization of CMT-nek on CPUs/GPUs

Mohamed Gadou

Advisor: Prof. Sanjay Ranka

Department: CISE, UF

- Goals
  - Optimization of CMT-bone on hybrid architecture with multiple CPUs/GPUs
  - Performance/Energy modeling of CMT-bone on HMPs
  - Implementation of CMT-bone on Intel KNL
- Simulation roadmap
  - Our research roadmap is closely tied with CMT-nek development



Simulation Roadmap

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5

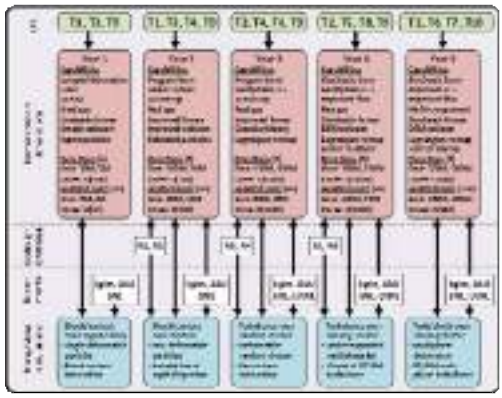
Eglin Explosive Barrel Ejection Simulations

Joshua Garno

Advisor: Dr. S. Balachandar

Department: MAE, UF

- Goals
  - Simulate trajectory of 1, 9 and many particle configurations
  - Simulate dispersal of 0.5 g packet of particles
  - Validate Rocflu models governing particle motion
- Simulation roadmap
  - Real Gas
  - EL-AUSM+UP
  - Improved Forces
  - Program Burn



Simulation Roadmap

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6

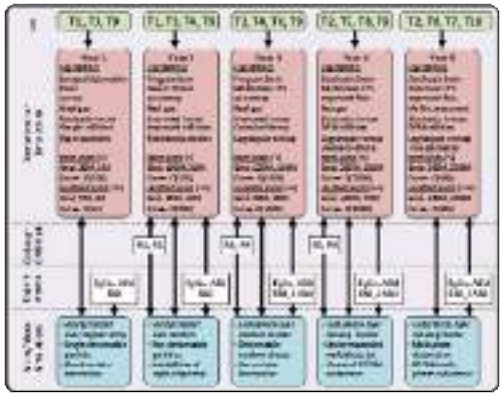
Support for Benchmarking & AppBEO Creation

Trokon Johnson

Advisors: Dr. Herman Lam, Dr. Greg Stitt

Department: ECE, UF

- Goals
  - Benchmarking automation
  - Benchmarking for CMT-nek DSE*
  - Formalize AppBEO creation process
- Simulation roadmap
  - Support for BE* in early DSE of CMT-nek code development
  - Automate & formalize process for BE



Simulation Roadmap

*DSE – Design Space Exploration
*BE – Behavioral Emulation

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7

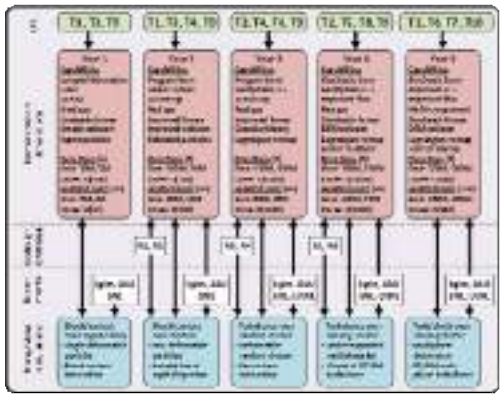
Forensic Uncertainty Quantification

Kyle Hughes

Advisor: Prof. Nam-Ho Kim

Department: MAE, UF

- Goals
  - Quantify uncertainty of past experiments to provide meaningful validation
  - Assist with planning of future experiments to minimize uncertainty
- Simulation roadmap
  - Act as a liaison between simulationalists and experimentalists



Simulation Roadmap

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8

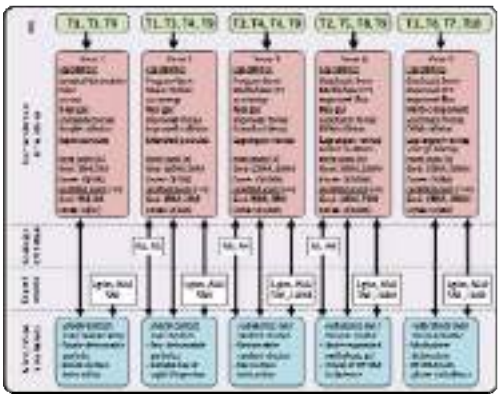
Compressible Multiphase Turbulence Modeling

Rahul Babu Koneru

Advisor: Dr. S. Balachandar

Department: MAE, UF

- Goals
  - Develop multiphase compressible LES model
  - Improved force modeling
  - Validation and integration into Rocflu and CMT-nek
- Simulation roadmap
  - Implement single phase LES and extend it to multiphase flows
  - Validate existing force-models and develop new models in collaboration with microscale team
  - Perform mesoscale simulations



Simulation Roadmap

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9

Improving Accuracy and Scalability of Behavioral Emulation (BE) Methodology

Nalini Kumar

Advisors: Dr. Herman Lam, Dr. Greg Stitt

Department: ECE, UF

- Goals
  - Apply BE methodology, demonstrated for device and system simulations, to simulation of large-scale systems
  - Design & validate simulation models of existing machine architectures
  - Improve communication modeling in BE
- Simulation roadmap
  - Design and evaluate BE simulation framework which will enable early design-space exploration to aid and assist CMT-nek code developers

Simulation Roadmap

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10

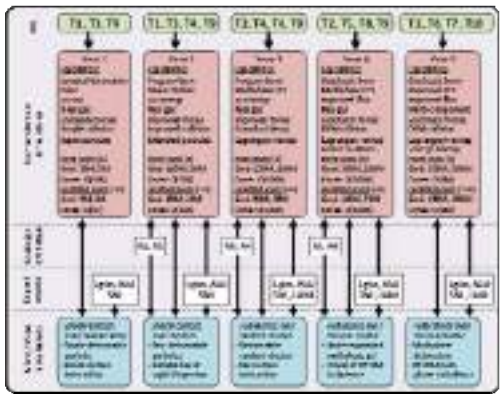
CMT-nek Microscale Simulation

Goran Marjanovic

Advisor: Prof. S. Balachandar

Department: MAE, UF

- Goals
  - Demonstrate CMT-nek capabilities
  - Verification
  - Validation
- Simulation roadmap
  - Microscale simulation
  - Expansion over curtains of particles



Simulation Roadmap

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11

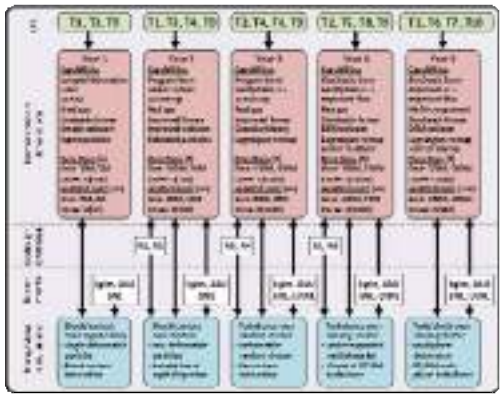
Uncertainty Quantification of Shock Tubes

Justin Mathew

Advisor: Prof. Kim and Prof. Haftka

Department: MAE, UF

- Goals
  - Reproduce measurement processing from Sandia and ASU shock tubes to identify sources of uncertainty
  - Propagate identified sources of uncertainty from experiments into simulations
- Simulation roadmap
  - T2: Multiphase turbulence modeling and uncertainty
  - T4: Validation, UQ and UR of the shock tube simulation



Simulation Roadmap

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12

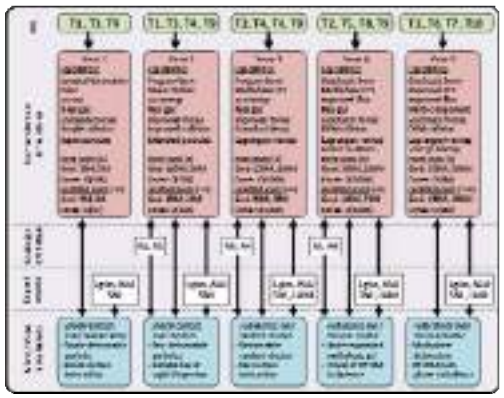
Microscale – Shock Particle Interaction

Yash Mehta

Advisor: Prof. S. Balachandar

Department: MAE, UF

- Goals
  - Fully resolved DNS of shock interaction with particles
  - Developing models for predicting particle motion and force history
- Simulation roadmap
  - Simulating shock interaction with random bed of particles (Inviscid and Viscous)
  - Integration of force models in Meso-Macro scale simulations



Simulation Roadmap

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13

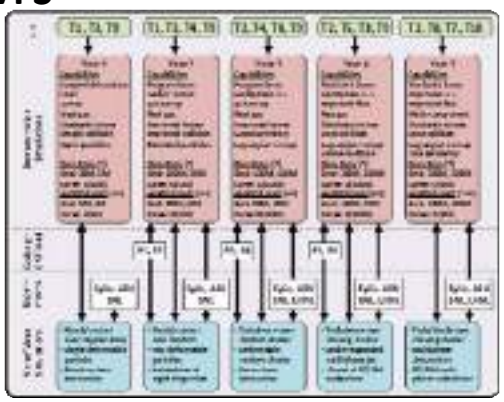
Multi-objective optimization on Hybrid Systems using DVFS

Sankeerth Reddy Mogili

Advisor: Prof. Sanjay Ranka

Department: CISE, UF

- Goals
  - Power Minimization
  - Energy Optimization
  - Time per time-step minimization
- Simulation roadmap
  - Our research roadmap is closely tied with CMT-nek development



Simulation Roadmap

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14

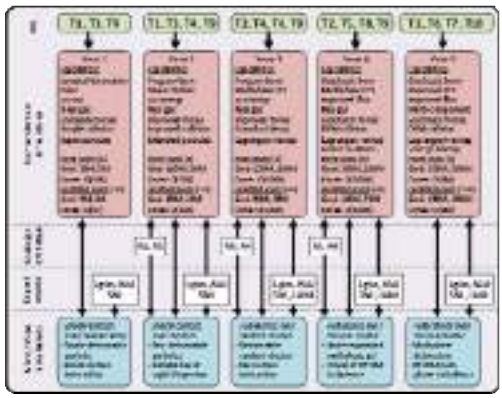
Behavioral Emulation (BE) Models

Aravind Neelakantan

Advisor: Dr. Lam, Dr. Stitt

Department: ECE, UF

- Goals
  - Validation and uncertainty estimation of BE
  - Reduce computation budget of CMT-nek (with UB team)
  - Verify trend among CMT-nek, CMT-bone, and CMT-bone-BE
- Simulation roadmap
  - BE helps in simulating CMT-nek on exascale systems (notional architectures)



Simulation Roadmap

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15

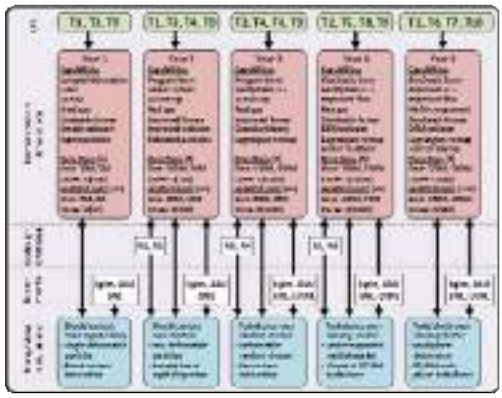
Eulerian-Lagrangian Interphase Coupling UQ and UR

Sam Nili

Advisor: Prof. Kim, Haftka & Balachandar

Department: MAE, UF

- Goals
  - Identify and quantify potential errors for numerical force models of Eulerian-Lagrangian multi-phase dispersed
  - Reduce the errors by model improvement
- Simulation roadmap
  - T4: Verification and validation of the shock tube simulation
  - Uncertainty reduction via model improvement



Simulation Roadmap

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16

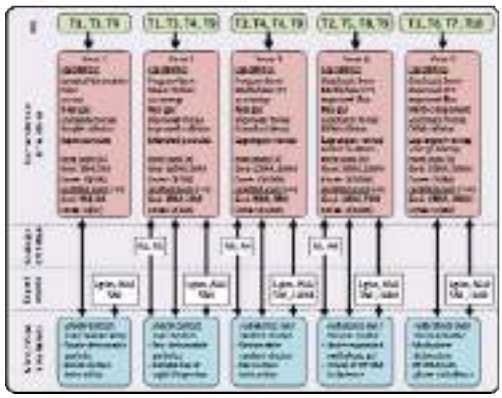
Shock and Contact Interaction with Particles

Brandon Osborne

Advisor: Prof. S. Balachandar

Department: MAE, UF

- Goals
  - DNS of shock and contact interaction with structured and random arrangements of particles
  - Development of models for predicting particle motion
- Simulation roadmap
  - Microscale simulations for shock-contact-particle interaction



Simulation Roadmap

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17

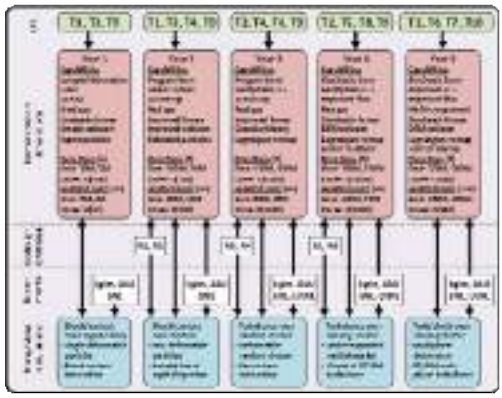
Surrogate Modeling of the Equation of State

Frederick Ouellet

Advisor: Dr. S. Balachandar

Department: MAE, UF

- Goals
  - Develop a surrogate model for use in evaluating the equation of state in mixed air/product cells
  - Perform and analyze simulations of the Eglin blastpad experiments
- Simulation roadmap
  - Real gas equation of state capabilities in code
  - Analysis of instabilities of rapid dispersion



Simulation Roadmap

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18

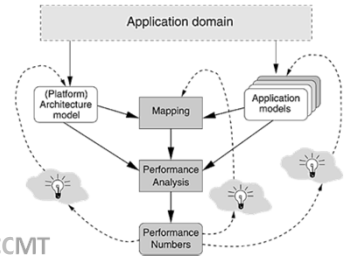
FPGA Pipelined Simulations for CMT-nek

Carlo Pascoe

Advisors: Dr. Herman Lam, Dr. Greg Stitt

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

Simulation Roadmap



- Goal: Pipeline simulations to explore a different design option every cycle
  - After some initial latency, quickly explore large number of different configurations – fast DSE
- Ideal for an FPGA
  - Pipeline is bounded by resources rather than I/O
  - Multiple FPGAs can be used to explore a vast input space – almost embarrassingly parallel
  - **Up to eight orders-of-magnitude faster DSE**

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19

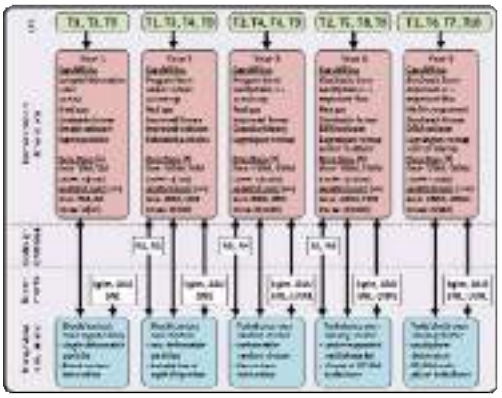
BE-SST* Simulator

Ajay Ramaswamy

Advisor: Dr. Lam, Dr. Stitt

Department: ECE, UF

- Goals
  - Use SST framework to develop BE methods and run parallel, scalable simulations
  - Run simulations of large HPC systems
  - Improve communication models and interpolation API
- Simulation roadmap
  - BE-SST simulator enables scalable design space exploration on exascale systems



Simulation Roadmap

*SST: Structural Simulation Toolkit from Sandia National Laboratory

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20

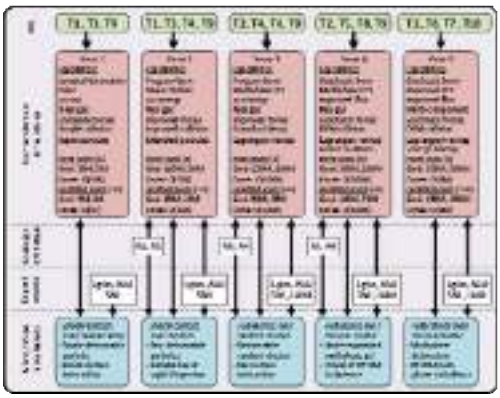
Energy and Thermal Modeling

Mason Rawson

Advisor: Dr. Lam, Dr. Stitt

Department: ECE, UF

- Goals
  - Design and implement a framework for assessing performance and energy consumption tradeoffs across entire HPC systems
  - Understand processor level thermal effects on performance and energy consumption
- Simulation roadmap
  - Explore design space of future HPC systems to incorporate power and energy



Simulation Roadmap

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21

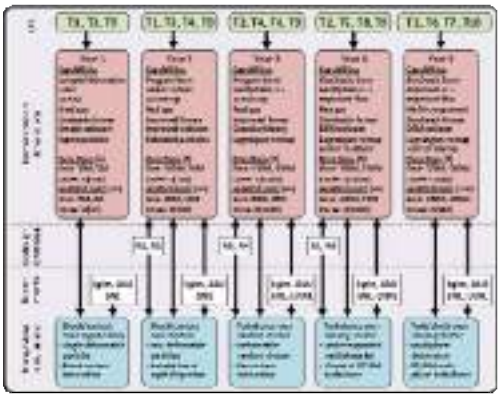
RocSDT: Shock-Particle Interaction

Prashanth Sridharan

Advisor: Dr. Thomas L. Jackson

Department: MAE, UF

- Goals
  - Investigate aluminum spherical particles under various shock loading conditions
  - Implement modelling technology to create robust level-set algorithms that handle mixture of deforming and rigid particles
- Simulation roadmap
  - Preliminary research conducted to produce transient force/drag histories



Simulation Roadmap

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22

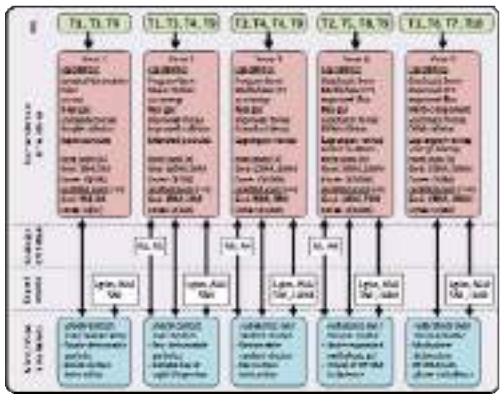
Dynamic Load Balancing for CMT-nek

Keke Zhai

Advisor: Prof. Sanjay Ranka

Department: CISE, UF

- Goals
  - To reduce simulation time and decrease power consumption on CMT-bone and CMT-nek by utilizing dynamic load balancing
- Simulation roadmap
  - This simulation includes moving particles and gas to simulate the actual particle movement within a fixed box



Simulation Roadmap

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23

Correction of Performance Emulation

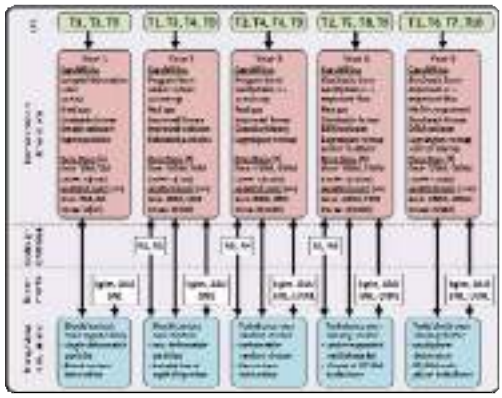
Yiming Zhang

Advisor: Prof. Raphael T. Haftka

& Prof. Nam H. Kim

Department: MAE, UF

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



Simulation Roadmap

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24

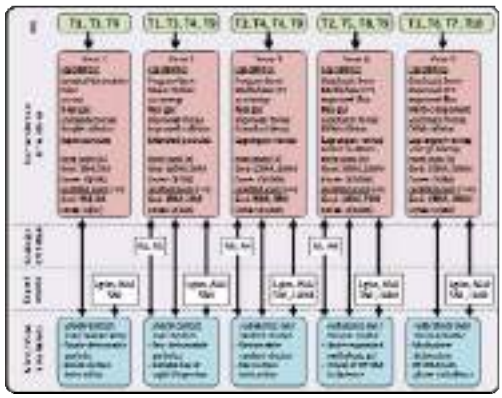
Gas-Particle Mixtures Under Sudden Expansion

Heather Zunino

Advisor: Prof. Ronald Adrian

Department: SEMTE, ASU

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



Simulation Roadmap

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25

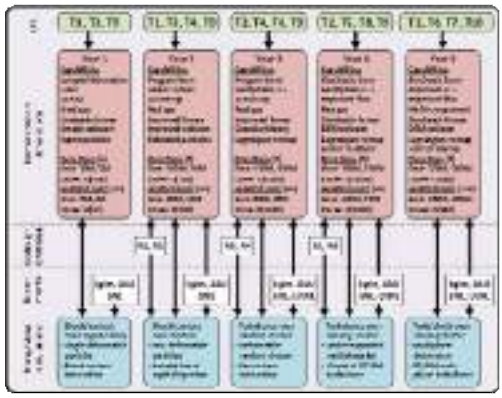
Two-way Coupling in CMT-nek

David Zwick

Advisor: Dr. S. Balachandar

Department: MAE, UF

- Goals
  - Understanding of physics in ASU experiment through simulation
  - Development of state-of-the-art Eulerian-Lagrangian capabilities in CMT-nek
- Simulation roadmap
  - Detailed modeling of particle simulations of ASU experiment in CMT-nek
  - Two-way coupling



Simulation Roadmap

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