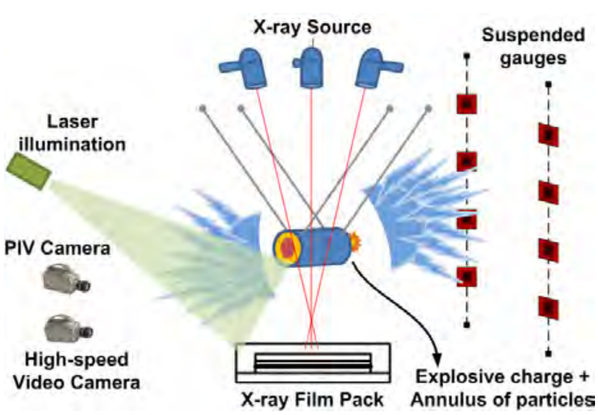
CCMT

CENTER FOR COMPRESSIBLE MULTIPHASE TURBULENCE

AST Meeting

May 7-8, 2015



UF UNIVERSITY of FLORIDA

Center for Compressible Multi-Phase Turbulence

1180 Center Drive
P.O. Box 116135
Gainesville, FL 32611
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Agenda AST Site Visit May 7-8, 2015

<u>Thursday May 7, 2015</u>

7:45	Van pick up at University Hilton
8:00-9:00	Full Breakfast
	(Review Team, AST, other NNSA personnel will meet in small conference room)
9:00-9:10	Introductions and opening remarks (Balachandar, Schofield)
9:10-10:00	CCMT Overview and Background of Center (Jackson)
10:00-10:15	Discussion
10:15-10:30	Coffee break
10:30-11:30	Integration (Balachandar)
11:30-11:45	Discussion
11:45-1:00	Lunch (RT will meet in small conference room)
1:00-1:45	Full-system Simulations (Rollin)
1:45-2:00	Discussion
2:00-3:00	Computer Science (Ranka, Lam, Stitt, George)
3:00-3:15	Discussion
3:00-3:15	Coffee break
3:30-4:00	V&V and UQ (Haftka, Park, Kim)
4:00-4:15	Discussion
4:15-5:15	Poster Session (1st floor lobby; light refreshments served)
5:15-6:30	RT Caucus
6:30-8:00	Dinner (Faculty and Visitors; transportation will be provided for all visitors to the University Hilton)

Friday May 8, 2015

7:45 Van pickup at University Hilton

8:00-9:00 Continental Breakfast (RT will meet in small conference room)

9:00-10:45 Overview of Scientific Goals and Accomplishments

Series of 13-minute talks (8-10 maximum slides for each talk; each speaker must start and end on time)

- Angela Diggs, UF – simulations
- Heather Zunino, ASU – experiments
- Tania Banerjee, UF – CS
- Chanyoung Park, UF – Uncertainty Budget
- Christopher Neal, UF – Microscale simulations
- Nalini Kumar, UF – exascale
- Donald Littrell, Eglin – experiments

10:45-11:00 Discussion

11:00-11:10 Coffee Break

11:10-12:10 Center Response to RT Questions (Balachandar)

12:10-1:10 Lunch (RT will meet in small conference room)

1:10-1:30 Additional Items (Jackson)

1:30-4:00 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 and NNSA (large conf. room)

4:30 Review ends

Center for Compressible Multiphase Turbulence

AST Review May 7-8 Attendee List

Faculty

S. Balachandar "Bala"	University of Florida	bala1s@ufl.edu
Alan George	University of Florida	george@hcs.ufl.edu
Rafi Haftka	University of Florida	haftka@ufl.edu
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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
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Ju Zhang	Florida Institute of Technology	jzhang@fit.edu

Review Team

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Robert Clay (CS)	SNL	rlclay@sandia.gov
Fernando Grinstein (Physics)	LANL	fgrinstein@lanl.gov
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Sriram Swaminarayan (CS)	LANL	sriram@lanl.gov

AST Members

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Nels Hoffman	LANL	nmh@lanl.gov
Dan Nikkel	LLNL	nikkel1@llnl.gov
Bob Voigt	Leidos/NESD	rvoigt@krellinst.org

Research Staff

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Chanyoung Park	University of Florida	cy.park@ufl.edu
Bertrand Rollin	University of Florida	bertrandrollin@gmail.com
Mrugesh Shringarpure	University of Florida	mrugeshs@ufl.edu

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Students

Kasim Alli	University of Florida	kalli@ufl.edu
Saptarshi Biswas	University of Florida	sappy91@ufl.edu
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Brad Durant	University of Florida	neoncrash@ufl.edu
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Christopher Hajas	University of Florida	chrishajas@ufl.edu
Rahul Koneru	University of Florida	rahul.koneru@ufl.edu
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Frederick Ouellet	University of Florida	f.ouellet@ufl.edu
Carlo Pascoe	University of Florida	poppyc@ufl.edu
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Prashanth Sridharan	University of Florida	shan1130@ufl.edu
Cameron Stewart	University of Florida	csstewart10@ufl.edu
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Heather Zunino	Arizona State University	heatherzunino@gmail.com

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Melanie DeProspero	University of Florida	mel7703@ufl.edu

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Overview and Management

T.L. Jackson
Technical Manager

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NNSA

AST Meeting Agenda

Thursday

- Overview and Management (Jackson)
- Integration (Balachandar)
- Full-system Simulations (Rollins)
- Computer Science (Ranka, Lam, Stitt, George)
- V&V and UQ (Haftka, Park, Kim)
- Poster Session (14 Student + 5 Postdoc)
- Dinner

Friday

- Overview of Scientific Goals (7 13-minute talks)
- Center Response to AST Questions (Balachandar)
- Additional Items (Internships, recruitment, etc.) (Jackson)
- RT Deliberations
- RT Summary

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Outline: Overview & Management

- Personnel
- Goals
- Demonstration problem
- Y1 predictions
- Overall V&V and UQ plan
- Simulation roadmap
- Integration
- Y1 accomplishments (Highlights)
- Management/Teams
- Five-year Center-level Gantt Charts for Integration/Simulation Roadmap

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Leadership

Physics and Code Development


S. (Bala) Balachandar


Siddharth Thakur (ST)


Thomas Jackson


Paul Fischer


Ju Zhang

UQ and V&V


Raphael Haftka


Nam-Ho Kim

Experiments


Ronald Adrian


Charles Jenkins


Donald Littrell

CS/Exascale


Alan George


Sanjay Ranka


Herman Lam


Gregory Stitt


Scott Parker

UF members in red

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Research Staff & Senior PhD Students
Bertrand Rollin
Jason Hackl
Chanyoung Park
Mrugesh Shringarpure
Tania Banerjee
Subramanian Annamalai
2Lt. Myles Delcambre
Carlo Pascoe
Nalini Kumar
Dylan Rudolph
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UF UNIVERSITY of FLORIDA
Current Students (Undergraduate & Graduate)
Kasim Alli
Ryan Blanchard
Saptarshi Biswas
Angela Diggs
Brad Durant
Giselle Fernandez
Chris Hajas
Rahul Koneru
Goran Marjanovic
Yash Mehta
Hugh Miles
Christopher Neal
Frederick Ouellet
Prashanth Sridharan
Yiming Zhang
Heather Zunino
David Zwick
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Center Goals

- To radically advance the field of CMT
- To advance predictive simulation science on current and near-future computing platforms with uncertainty budget as backbone
- To advance a co-design strategy that combines exascale emulation, exascale algorithms, exascale CS
- To educate students and postdocs in exascale simulation science and place them at NNSA laboratories

Frost (2012)

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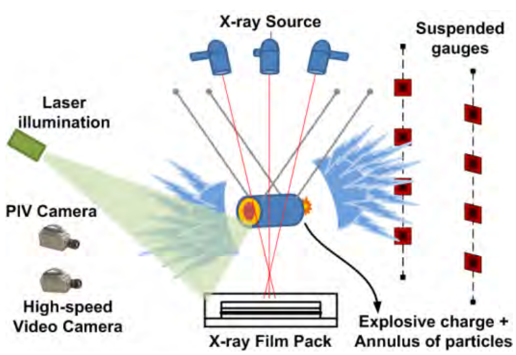
Demonstration Problem

- Explosive-driven cylindrical annulus of particles



- Integrated effort toward predictive simulations
- Experimental measurements for validation

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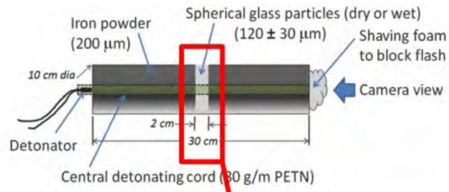
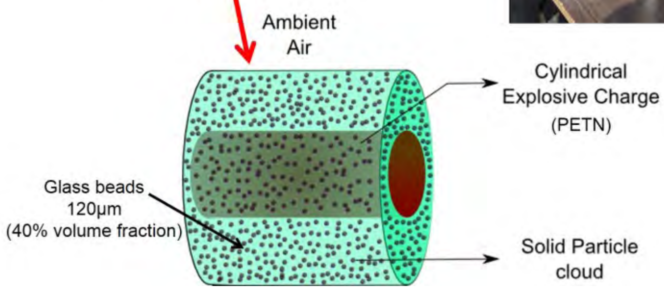
Demonstration problem

Experimental setup of Frost (2012)



Experimental apparatus



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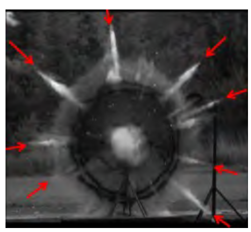
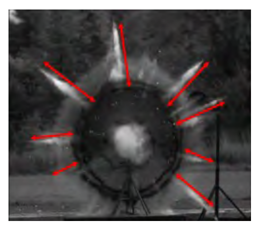
Demonstration Problem – Prediction Metrics

PM-1
Blast wave location

PM-2
Particle front location



PM-3
Number of Instability waves



PM-4
Amplitude of Instability waves

- Y1+ Frost cylindrical charge
- Y3+ Eglin cylindrical charge
- Y2+ Micro- and mesoscale validation quality experiments required for UQ
  - Eglin, ASU, LANL, Sandia

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Demonstration Problem – Simulation Matrix

Case No.	Time Simulated	Outer rad (m)				
2	0-1 ms	0.60	1200	2048	48	
3	0-12 ms	4.00	2400	4096	48	

Y1

	2D	3D	System
Case 1	✓	✓	Mustang (LANL), Vulcan (LLNL)
Case 2	✓		Mustang (LANL), Vulcan (LLNL)
Case 3			Mustang (LANL)

Largest run to date: ➢ **10240 procs, Gas + Particles (5% vol. fraction) (Vulcan)**

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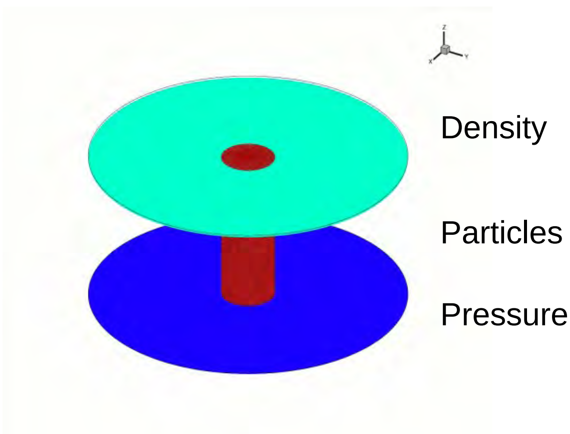
Demonstration Problem – Y1 Predictions

Simulation out to 200 μs
30M cells
5M particles
5% volume fraction
r_{max} = 0.3 cm
512 cores; 6 days



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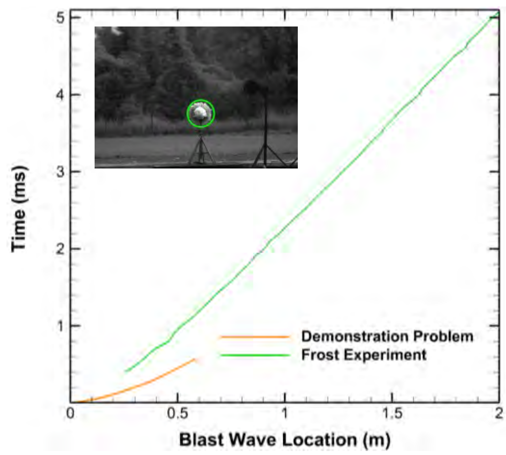
Demonstration Problem – Y1 Predictions

PM1 Comparison



- Data from Frost video starts at 0.4 ms
- Data from simulation ends at 0.575 ms
- Initial packing fraction
  - Frost 40%
  - Simulations 5%
  - As the packing fraction increases, we expect the blast wave to slow down
  - Simple physics

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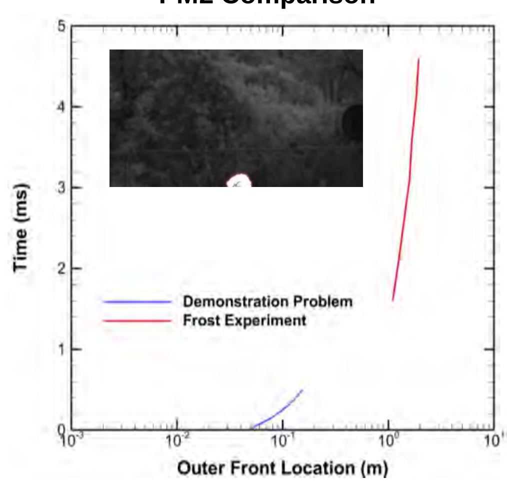
Demonstration Problem – Y1 Predictions

PM2 Comparison



- Data from Frost video starts at 2.6 ms
- Data from simulation ends at 0.575 ms
- Particle front is expanding more slowly in our current simulation
  - Possible sources: EOS, compaction, experimental uncertainties, etc…

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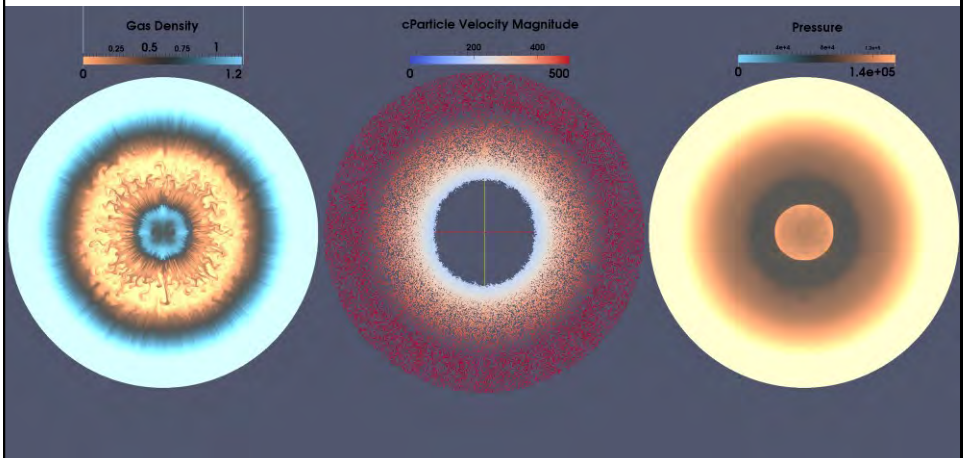
Demonstration Problem – Y1 Predictions

A View Inside Compressible Multiphase Turbulence



Our simulations already provide a detailed look inside the explosive dispersal of particle, up to times when the “jetting” instabilities are likely to originate

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Overall V&V and UQ Plan

- Purpose
  - To outline all errors and uncertainties that contribute to overall predictive capability of Demonstration Problem
  - To outline a sequence of tasks that allow us to quantify different contributions to overall error/uncertainty
  - To outline plan for hierarchical validation
  - Based on multiscale approach

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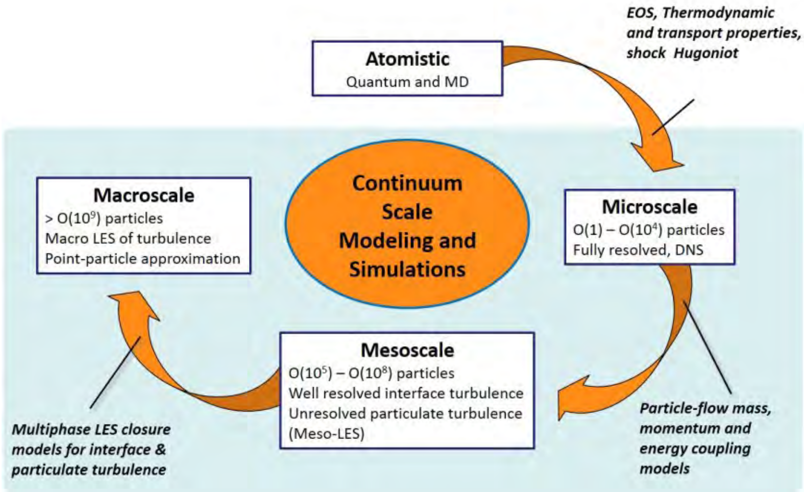
Multiscale Coupling



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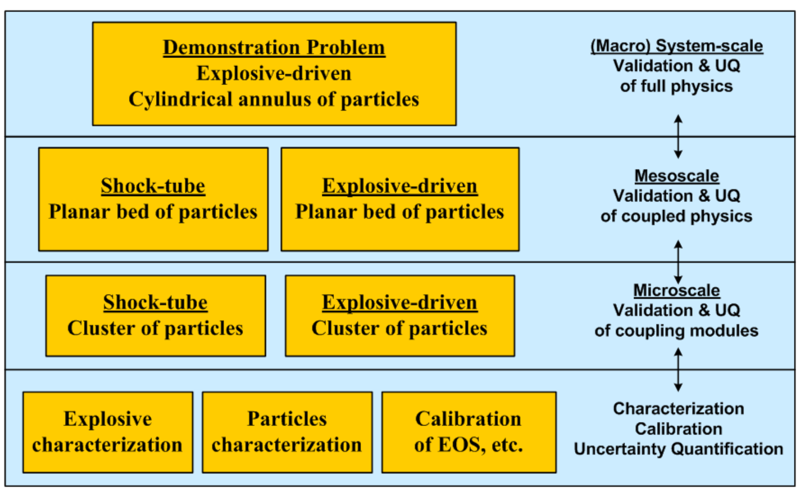
Multiscale Problem Hierarchy



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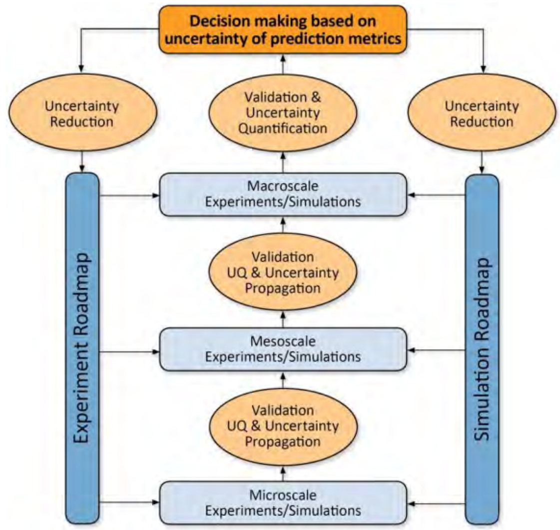
UB Integration - Physics



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Sources of Errors & Uncertainties

- T1: Detonation modeling
- T2: Multiphase turbulence modeling
- T3: Thermodynamics & transport properties
- T4: Particle-particle collision modeling
- T5: Compaction modeling (dense-to-dilute transition)
- T6: Point-particle force modeling
- T7: Point-particle thermal modeling
- T8: Particle deformation and other complex physics
- T9: Discretization and numerical approximation errors
- T10: Experimental and measurement errors & uncertainties

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

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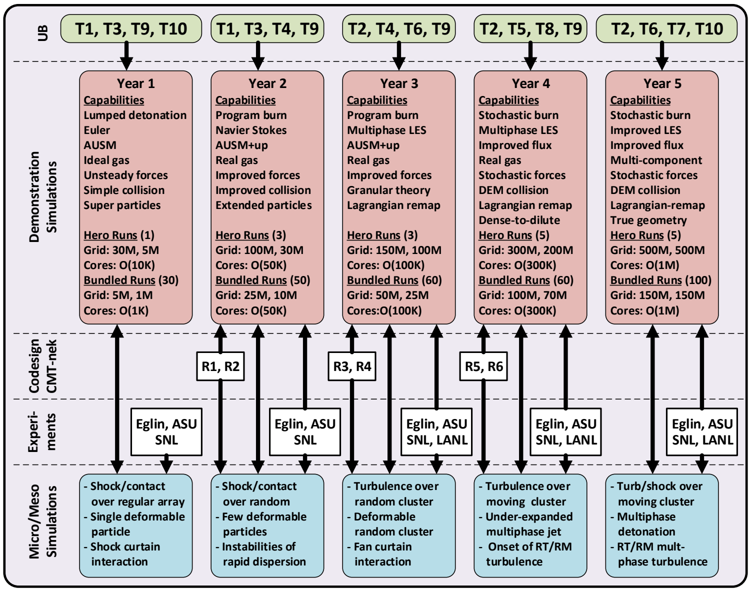
Simulation Roadmap



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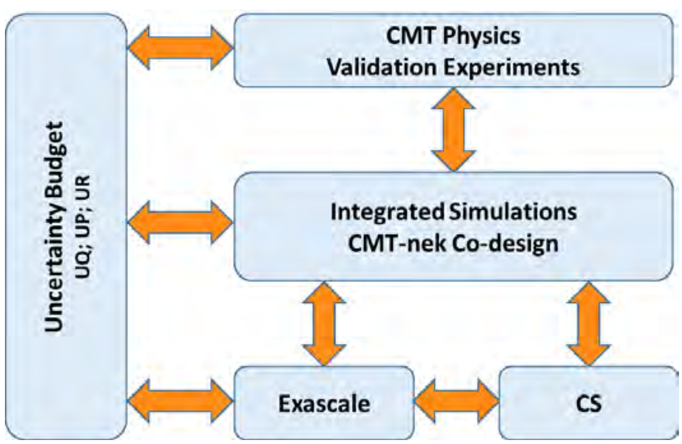
Integration – How Different Pieces Fit



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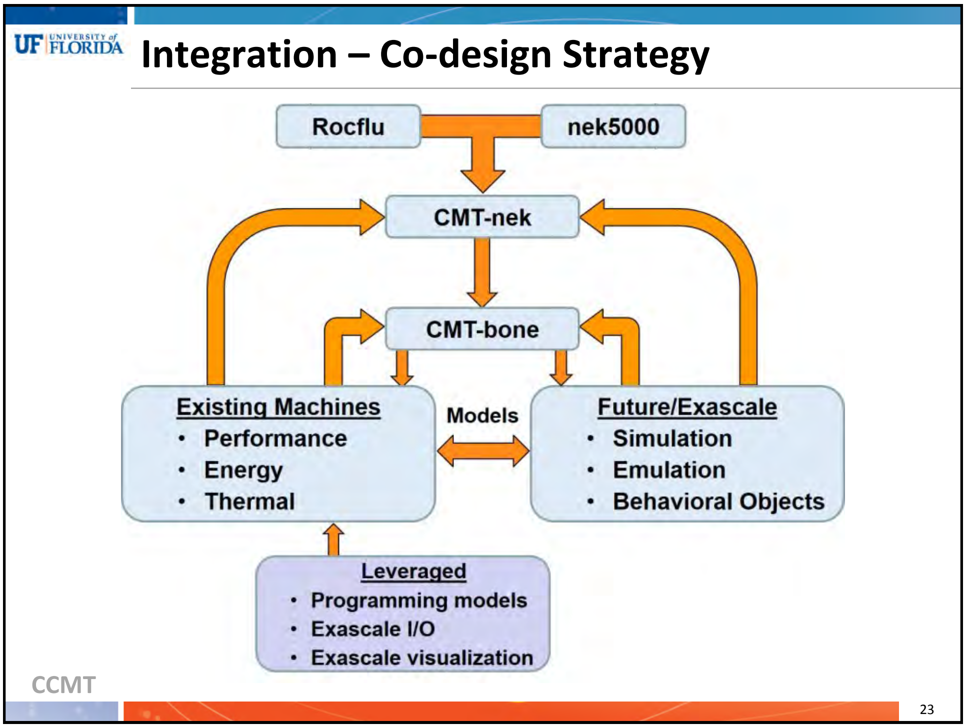
Integration – Co-design Strategy
Rocflu
nek5000
CMT-nek
CMT-bone
Existing Machines
• Performance
• Energy
• Thermal
Models
Future/Exascale
• Simulation
• Emulation
• Behavioral Objects
Leveraged
• Programming models
• Exascale I/O
• Exascale visualization
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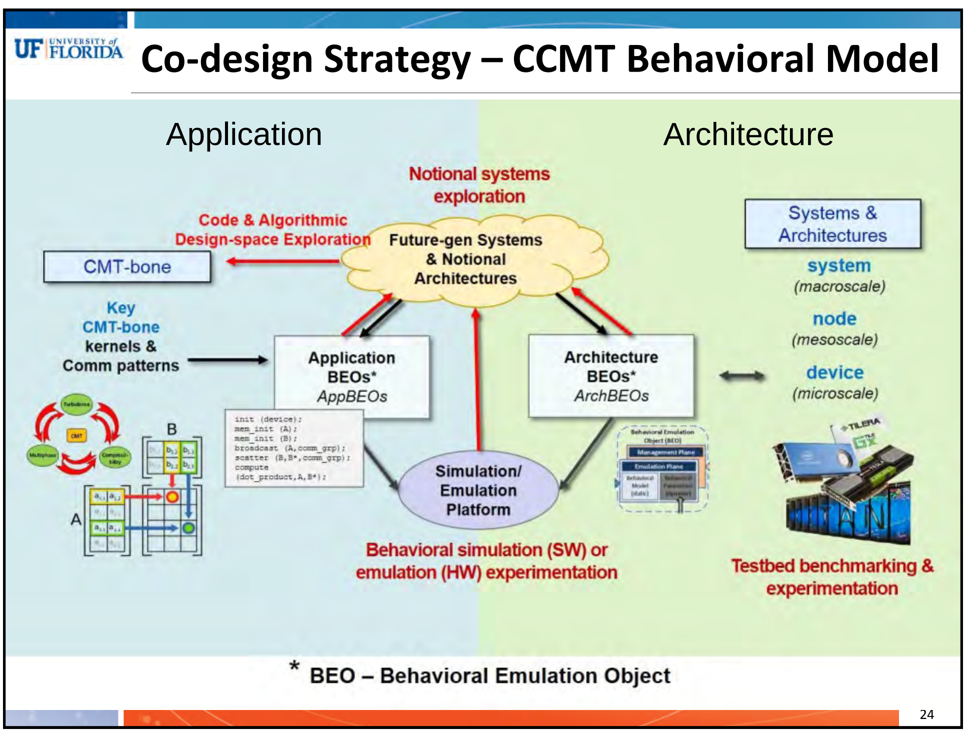
Co-design Strategy – CCMT Behavioral Model
Application
Architecture
Notional systems exploration
Code & Algorithmic Design-space Exploration
Future-gen Systems & Notional Architectures
Systems & Architectures
CMT-bone
system
(macroscale)
node
(mesoscale)
device
(microscale)
Key CMT-bone kernels & Comm patterns
Application BEOs*
AppBEOs
Architecture BEOs*
ArchBEOs
Simulation/ Emulation Platform
Behavioral simulation (SW) or emulation (HW) experimentation
Testbed benchmarking & experimentation
* BEO – Behavioral Emulation Object
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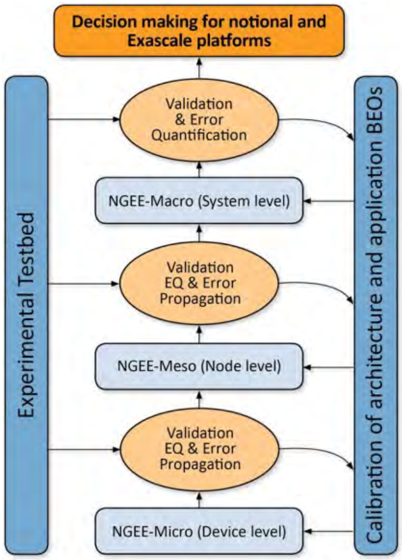
UB Integration – Exascale



Same cycle for notional and exascale platforms but with uncertainty quantification and propagation

Exascale emulation modelling with UQ is one of the unique aspects of the Center, that along with Energy and Thermally aware computing

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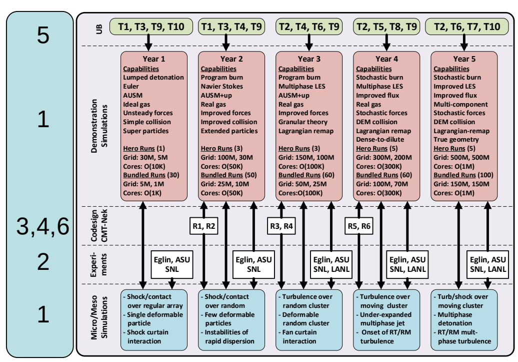
Year 1 Accomplishments (Highlights)

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



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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

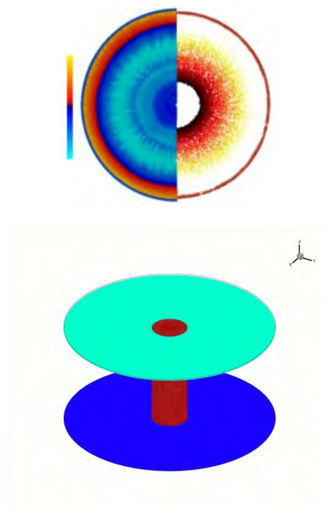
Year 1

- Use existing code to perform petascale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)

Posters

- Dr. Subramanian Annamalai
- Frederick Ouellet; Rahul Koneru; Goran Marjanovic

3-D demonstration Simulations



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1: Mesoscale Simulations

Goal

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

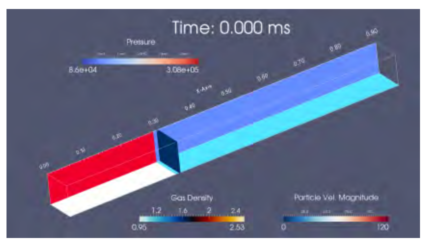
Year 1

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

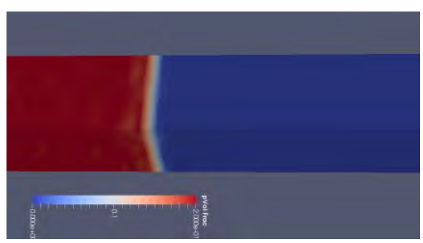
Talks/Posters

- Talks: Angela Diggs
- Posters: Angela Diggs; Saptarshi Biswas

Shock tube



Expansion tube



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1: Microscale Simulations

Goals

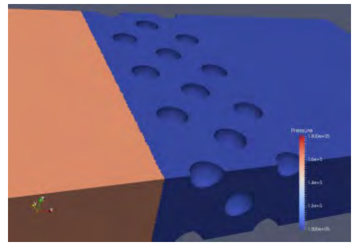
- Compute mean and rms values for drag force modeling (as a function of volume fraction, Mach number, Reynolds number)
- Perform a hierarchy of microscale simulations to allow rigorous validation, uncertainty quantification and propagation to the demonstration problem

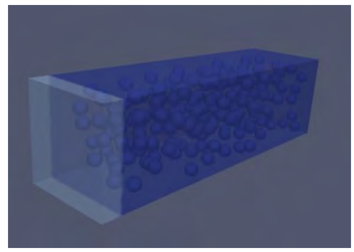
Year 1

- Highly resolved microscale simulations of shock propagation over a random distribution of particles

Talks/Posters

- Talks: Christopher Neal
- Posters: Christopher Neal; Prashanth Sridharan; Yash Mehta





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2: Validation Experiments

Goal

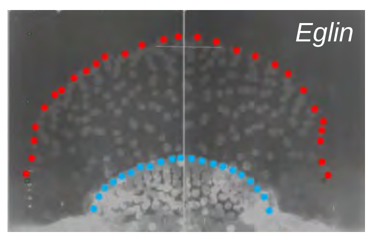
- Obtain validation-quality experimental measurements of the demonstration problem and perform shock-tube and explosive track micro- and mesoscale experiments

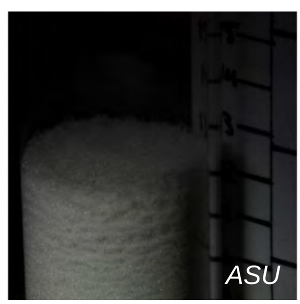
Year 1

- First set of experiments at Eglin AFB on micro- and mesoscale explosive dispersal experiments
- Experimental studies of gas-particle mixtures under sudden expansion at ASU

Talks/Posters

- Talks: Don Littrell (Eglin) and Heather Zunino (ASU)
- Posters: Heather Zunino (ASU)





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3: CMT-nek Development

Goals

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

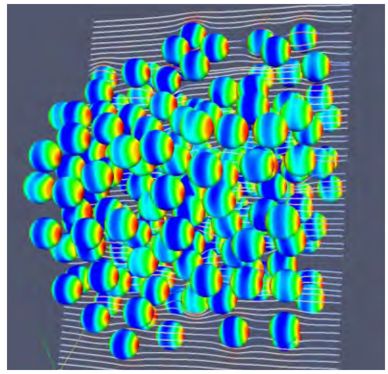
Year 1

- Develop and release first version of CMT-nek

Posters

- Drs. Mrugesh Shringarpure
- Dr. Jason Hackl

CMT-nek simulations



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4: Energy & Thermal Aware Computing

Goal

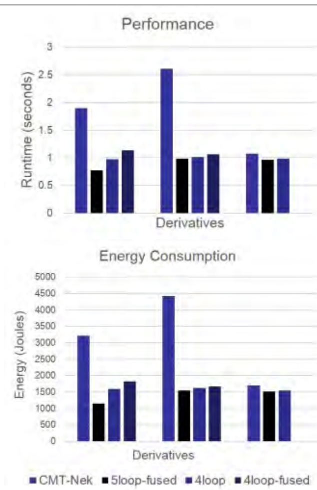
- Derive computationally intensive portions of the CMT-nek code and understand its performance, thermal and energy issues

Year 1

- Carried out extensive investigation of performance and energy issues related to CMT-bone cpu intensive kernels using CHILL and Genetic algorithm

Posters/Talks

- Dr. Tania Banerjee



Performance and energy of CMT-bone normalized wrt original nek5000 kernel

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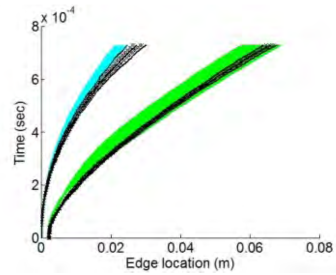
5: Uncertainty Budget

Goals

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

Year 1

- Identify main uncertainty sources and quantify their contributions to the model uncertainty of the shock tube simulation
- Explore parameter space of the shock tube simulation for UQ and found anomalies (possible model errors) in simulation results
- Help introduce UQ and propagation in the context of exascale emulation
- Develop a UQ tool: Multi fidelity surrogate



Propagated uncertainty and measurement uncertainty of the shock tube simulation

Posters/Talks

- Talks: Dr. Chanyoung Park
- Posters: Chanyoung Park; Giselle Fernandez; Yiming Zhang

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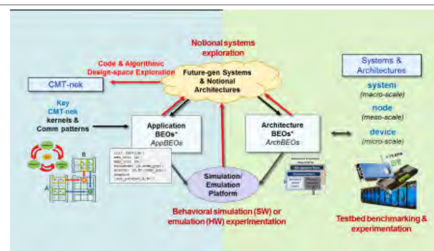
6: Exascale Emulation

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 1

- Demonstrated BE methods for device-level calibration & validation (on existing devices) and prediction (on notional devices) for CMT-bone AppBEOs
- Developed proof-of-concept prototype software PDES simulator for device-level studies & lessons learned; experimentation with single-FPGA hardware-accelerated simulator

Posters/Talks

- Talks: Nalini Kumar
- Posters: Nalini Kumar; Carlo Pascoe; Dylan Rudolph

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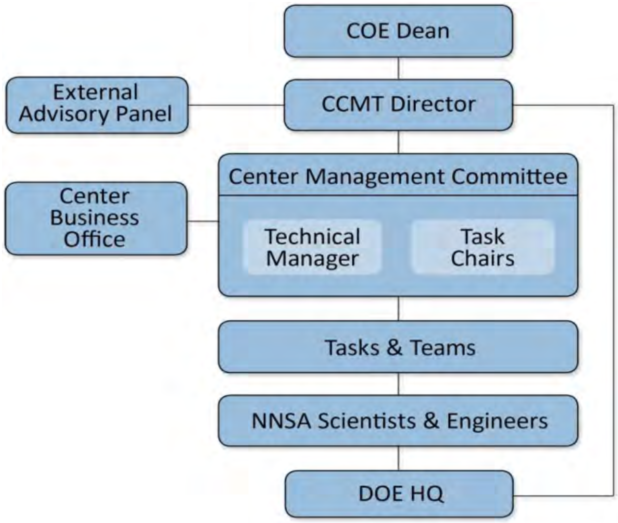
Management: Organizational Chart



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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	UQ	Exp
Exascale	X	X	X			X	
CMT-nek	X	X	X	X	X		
CS	X	X	X				
Micro		X		X	X	X	
Macro		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 PERC
- All meetings held in PERC

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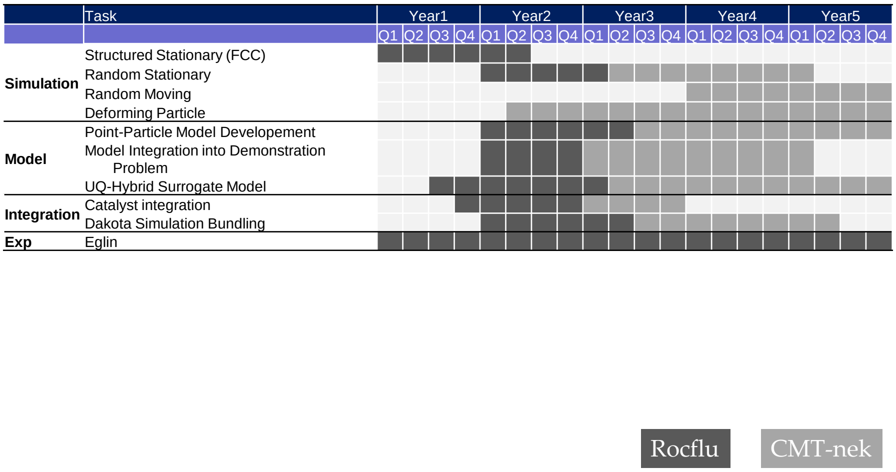
Microscale



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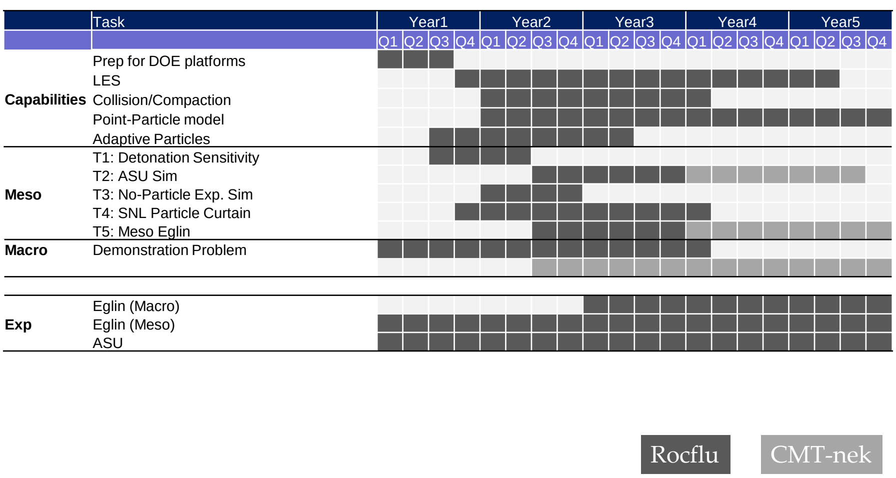
Macro/Mesoscale



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CMT-nek

	Task	Year1				Year2				Year3				Year4				Year5			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
	Euler Solver	■	■	■	■	■	■	■	■	■	■										
	Compressible Navier-Stokes				■	■	■	■	■												
Develop-ment	Lagrangian Point Particles						■	■	■	■	■	■	■								
	Shock Capturing						■	■	■	■	■	■	■								
	Multiphase Turbulence									■	■	■	■	■	■	■	■	■	■	■	■
	Immersed Boundary Method											■	■	■	■	■	■	■			
	Integration with Dakota									■	■	■	■								
Integration	Integration with Catalyst									■	■	■	■								
	Other physics												■	■	■	■	■	■	■	■	■
	CMTMicro						R1				R3				R5						
Release	CMTMacro							R2				R4				R6					
	CMT-bone				B1				B2				B3				B4				

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	Task	Year1				Year2				Year3				Year4				Year5			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
	T1: Detonation Sensitivity Simulation			■	■	■	■														
	T2a: Expansion-Fan ASU Exp	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T2b: Expansion-Fan Simulation							■	■	■	■	■	■	■	■	■	■	■	■	■	
	T3a: No-particle Explosive Exp					■	■	■	■												
	T3b: No-particle Explosive Sim					■	■	■	■												
	T4a: Particle Curtain Sim	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■					
	T4b: Particle Curtain Sim				■	■	■	■	■	■	■	■	■	■							
Physics	T5a: Mesoscale Eglin Exp				■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	
	T5b: Mesoscale Explosive Sim							■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T6a: Microscale Eglin Exp	■	■	■	■	■	■	■	■	■	■	■	■	■	■						
	T6b: Microscale Detonation Sims							■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T7: Microscale Shock Simulations	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T8: Post Detonation Particle Analysis		■	■	■	■	■	■													
	T9: Discretization Error Quantification	■	■	■	■	■	■	■	■	■	■										
	T11: Macroscale Eglin Experiments							■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T10, T11: Macroscale Simulations	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
Exascale /CS	Generating Data for Exascale and UQ		▒	▒	▒	▒	■	■	■	■	■	■	■	■	■	■	■				
	Behavioral Emulation for beyond device level					▒	■	■	■	■	■										
	Behavioral Emulation for CMT									■	■										
	Multi-Fidelity Surrogates (2 levels)	■	■	■	■	■	■														
Tools for UQ	Multi-Fidelity Surrogates (>2 levels)							■	■	■	■	■	■								
	Extrapolation	■	■	■	■	■	■	■	■	■	■	■	■								
	Extreme Events								■	■	■	■	■	■	■	■	■	■	■	■	■

▒ Prep

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CS

	Task	Year1				Year2				Year3				Year4				Year5			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Physics/ CMT-nek	Performance and energy optimization framework applied to CMT-nek	■	■	■	■	■	■	■													
	Integrating performance and energy optimized kernels in CMT-nek					■	■	■													
	Infrastructure for thermal measurements applied on CMT-nek						■	■	■	■											
	Load Balancing algorithms for particulate applications						■	■	■	■	■	■	■								
	Algorithms for thermal optimization applied to CMT-nek								■	■	■	■									
	PET optimization framework applied to CMT-nek									■	■	■	■								
	Extend PET optimization framework to Hybrid Multicore													■	■	■	■				
	Extend load balancing for particulate framework to hybrid multicore													■	■	■	■	■	■		
	PET enabled particulate framework for hybrid multicore													■	■	■	■	■	■		
	Performance evaluation of PET framework on advanced NNSA machines																	■	■	■	■
	Performance evaluation of load balancing framework on advanced NNSA machines																	■	■	■	■
Exascale/ UQ	Generating data for Exascale and UQ experiments		■	■	■	■	■	■	■	■	■	■	■	■	■	■	■				

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Exascale Behavioral Emulation

	Task	Year1				Year2				Year3				Year4				Year5			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Cycle 1	Development of BE methods Platform experimentation	■	■	■	■	■	■														
Cycle 2	Beyond device level comm sync/congestion V1 SW and HW simulators					■	■	■	■	■	■										
Cycle 3	Evolution of methods to support new requirements of CCMT teams V2 SW and HW simulators, tools/services									■	■	■	■	■	■	■	■				
Cycle 4	Explore BE methods to support broader DOE applications V3 SW and HW simulators															■	■	■	■	■	■

Cycle 1:
- **BE concepts and methods:** App BEOs (CMT-bone), Arch BEOs (device level), interpolation techniques for computation
- **Tools:** Prototype SMP software (SW) simulator for device-level studies & lessons learned; experimentation with single-FPGA hardware (HW) simulator

Cycle 2:
- **BE concepts and methods:** Emphasis on beyond device level; communication (synchronization, congestion); focus only on CCMT apps
- **Tools:** V1 SW simulator (leverage other useful simulators) & V1 HW simulator (scalable design); enable early use of simulators for design-space exploration for CCMT researchers

Cycle 3:
- **BE concepts and methods:** Evolution of methods and techniques to support new requirements of CCMT teams
- **Tools:** V2 SW and HW simulators; libraries of arch & app BEOs; more mature services and tools: management, monitoring, reporting, visualization

Cycle 4:
- **BE concepts and methods:** Evolution of methods and techniques to support requirements of new requirements of CCMT teams; Began exploration of using behavioral emulation for other key DOE mini-apps and future architectures
- **Tools:** V3 SW and HW simulators

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Do you have any questions?

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CCMT Integration

S. Balachandar

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Outline of Integration

- Demonstration problem
- Sequence of events and physics models
- Simulation roadmap
- Uncertainty quantification and reduction
- Integration of multiscale physics advancements
  - Mesoscale simulations and experiments
  - Microscale simulations and experiments
- CMT-nek co-design and current capabilities

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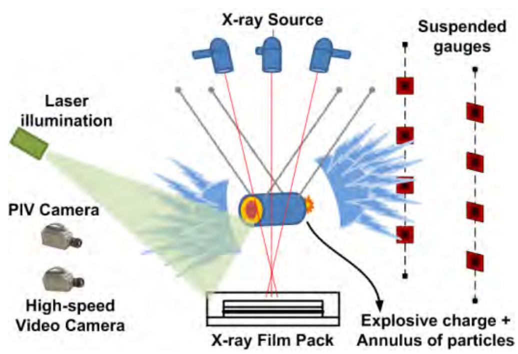
Demonstration Problem

- Explosive-driven cylindrical annulus of particles



- Integrated effort toward predictive simulations
- Experimental measurements for validation

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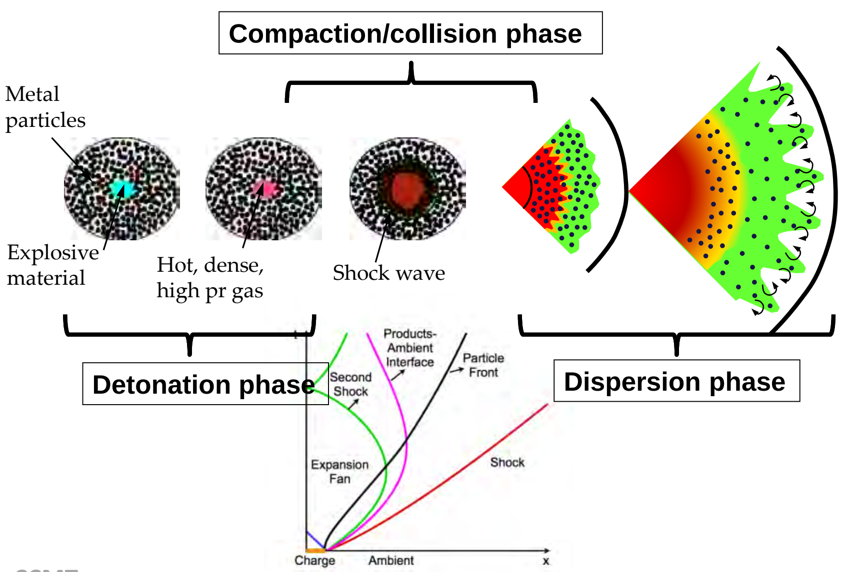
Sequence of Events



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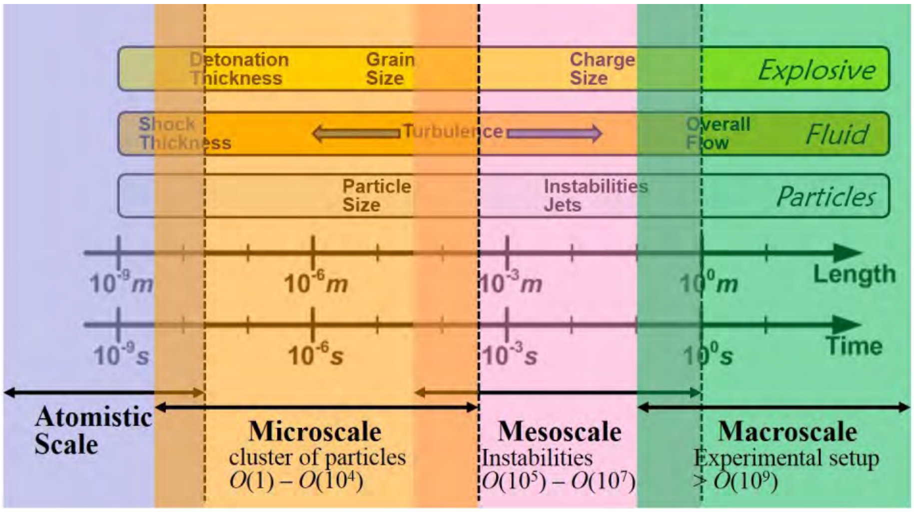
Multiscale Problem



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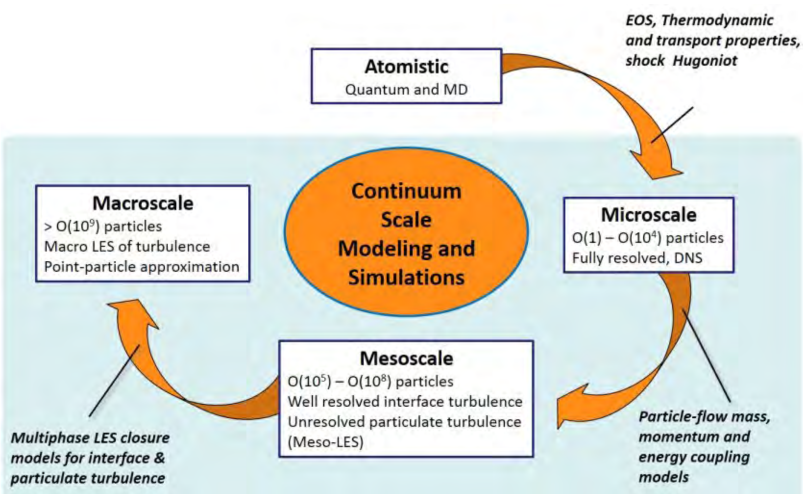
Multiscale Integration Strategy



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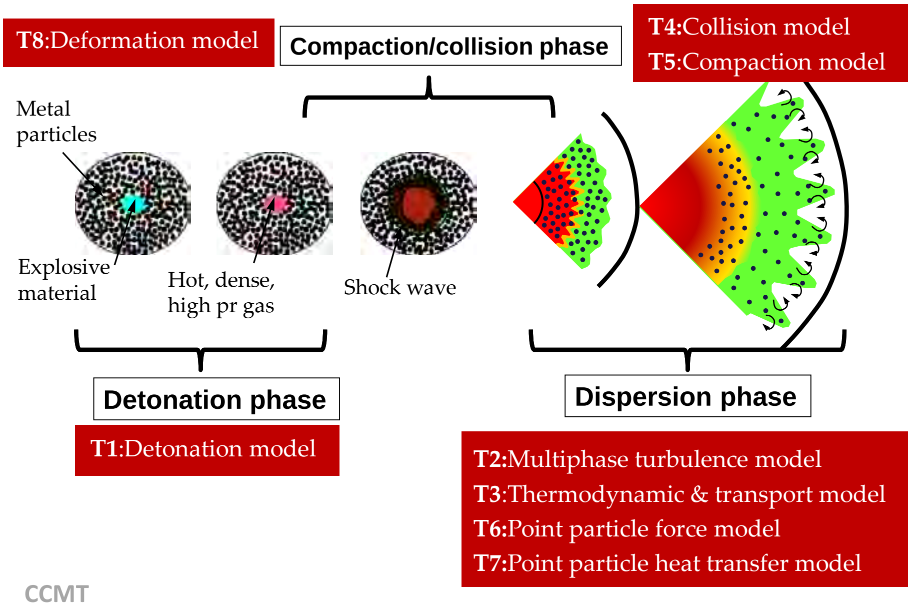
Physical Models – Sources of Error



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Sources of Errors & Uncertainties

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

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

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

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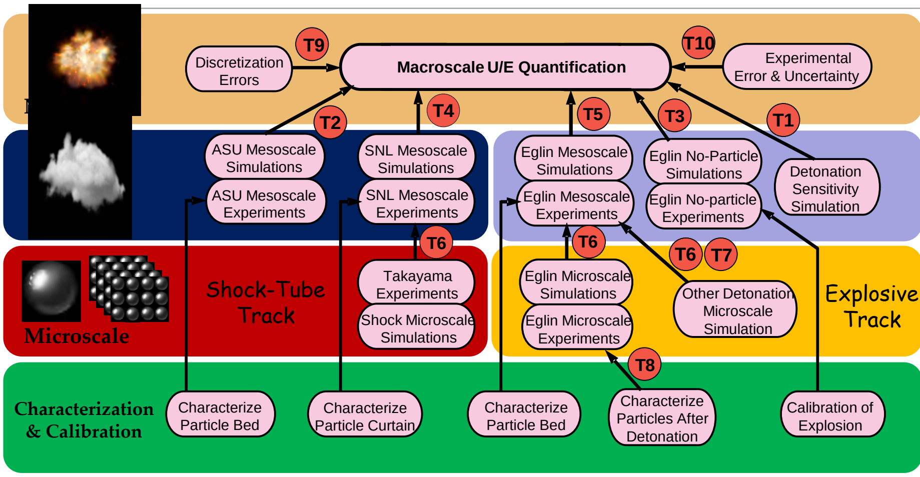
Uncertainty Budget – Overall Plan



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

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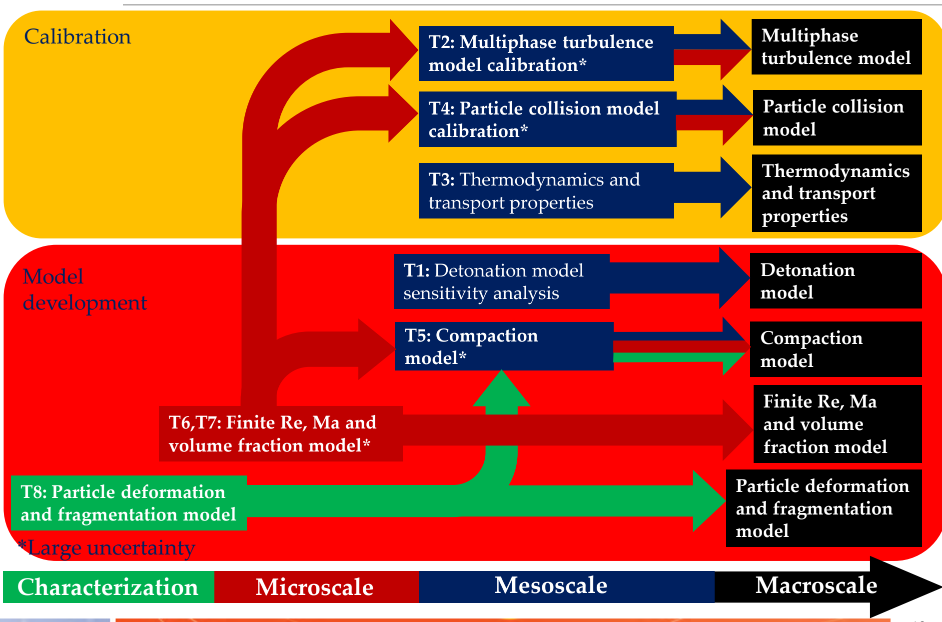
Multiscale Uncertainty Propagarion



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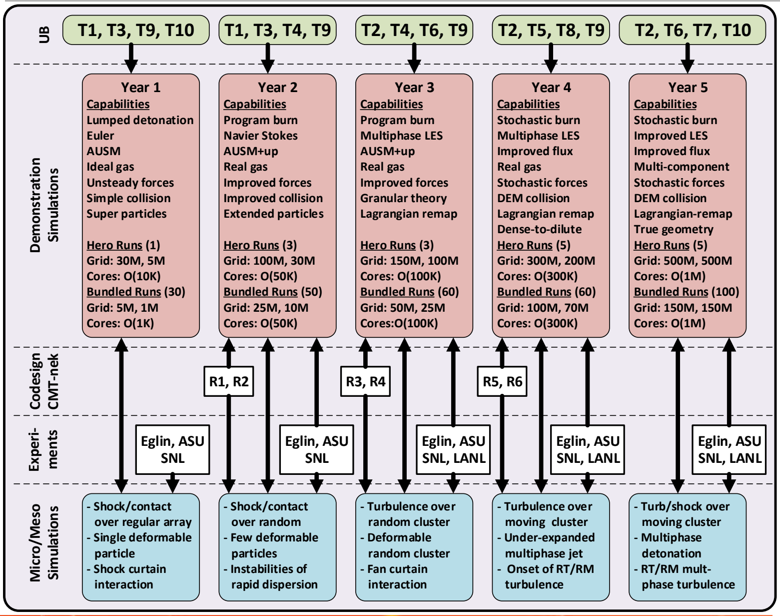
Simulation Roadmap



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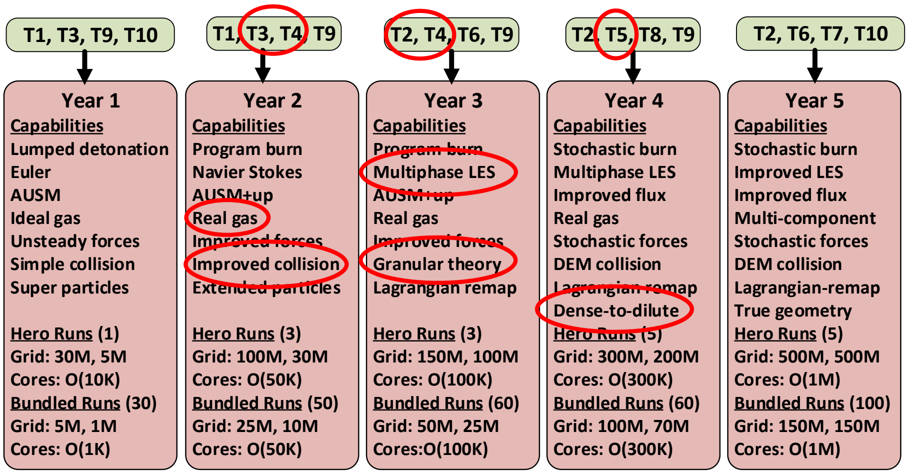
Demonstration Simulations



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

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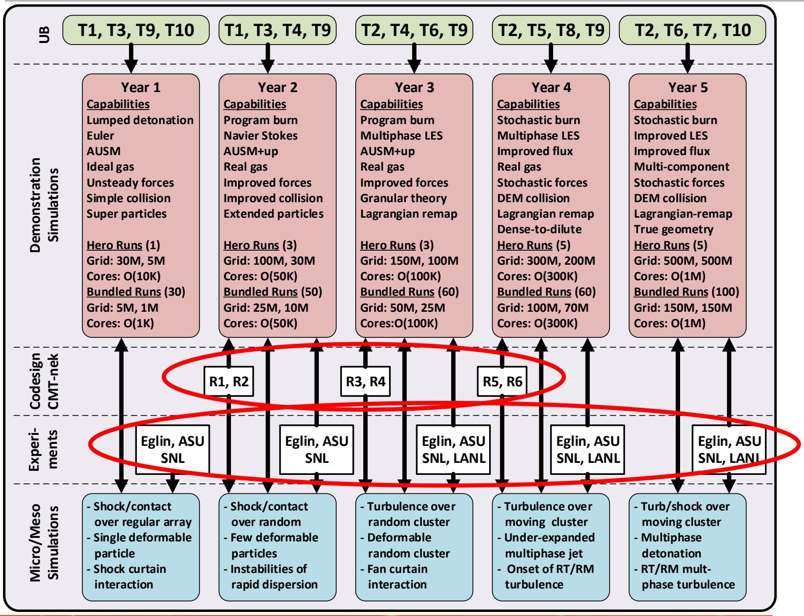
Simulation Roadmap



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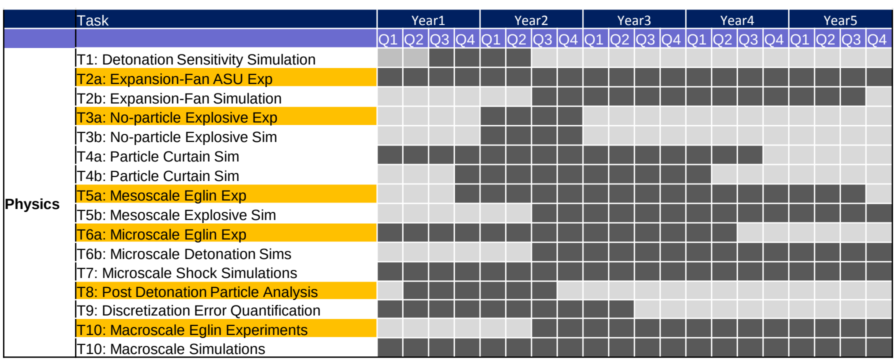
Timeline: T1-T10 Uncertainty Reduction



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T1 to T8: Influence on Macro Simulation

- Gas equations

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

Fluxes (T3) — $\mathbf{G}_{inv} + \boldsymbol{G}_{vis}$

Turbulence LES closure (T2) — $\boldsymbol{G}_{turb}$

Point particle coupling (T6, T7) — $\mathbf{f}_{gp}$

Detonation source (T1) — $\mathbf{f}_{ext}$

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

- Particle equations

$$\frac{d\mathbf{U}_p}{dt} = \mathbf{f}_{pp} + \mathbf{f}_{gp}$$

Collision Model (T4) — $\mathbf{f}_{pp}$

Point particle coupling (T6, T7) — $\mathbf{f}_{gp}$

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

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T6: Point-particle Force Model

$$f = f_{qs} + f_{pg} + f_{am} + f_{vu}$$

- Quasi-steady: $f_{qs} = \frac{\overline{u^g}^s - u^p}{\tau^p} \boxed{} \frac{\mathrm{Re}^p}{24}$
- Pressure-gradient: $f_{pg} = \frac{1}{\rho^p}\overline{\left(\rho^g \frac{Du^g}{Dt}\right)}^v$
- Added-mass:

$$f_{am} = \frac{1}{\rho^p}\int_{-\infty}^{t} \boxed{} \left(\frac{D}{Dt}^v \overline{(\rho^g u^g)}^v - \frac{d}{dt}\overline{(\rho^g u^p)}^v\right) d\chi$$

- Viscous-unsteady: Mei & Adrian (1992)

$$f_{vu} = \frac{1}{\rho^g \tau^p}\int_{-\infty}^{t} \boxed{} \left(\frac{D}{Dt}^s \overline{(\rho^g u^g)}^s - \frac{d}{dt}\overline{(\rho^g u^p)}^s\right) d\chi$$

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T5: Dense-to-Dilute (Compaction) Model

- Compaction equation (Dense limit: Baer-Nunziato model)

$$\frac{\partial \alpha_p}{\partial t} + \boldsymbol{u}_i \cdot \nabla \alpha_p = \frac{1}{\mu}(\tilde{p}_p - p_g)$$

- Compaction equation (Dilute incompressible limit)

$$\frac{\partial \alpha_p}{\partial t} + \nabla \cdot (\boldsymbol{u}_p \alpha_p) = 0$$

- Questions:
  - What is the appropriate interfacial velocity?
  - What is equilibrium pressure between gas and solids?
  - How do we smoothly transition from one limit to the other?
  - How do we numerically implement?

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T5: Dense-to-Dilute (Compaction) Model

- Compaction equation (Dense limit: Baer-Nunziato model)

$$\frac{\partial \alpha_p}{\partial t} + \boldsymbol{u}_i \cdot \nabla \alpha_p = \frac{1}{\mu}(\tilde{p}_p - p_g)$$

- Compaction equation (Dilute incompressible limit)

$$\frac{\partial \alpha_p}{\partial t} + \nabla \cdot (\boldsymbol{u}_p \alpha_p) = 0$$

- Rigorous result (pressure equilibration equation):

$$\frac{d(\tilde{p}_p - p_g)}{dt} + \frac{1}{\tilde{\mu}}(\tilde{p}_p - p_g) = -\varphi_g \nabla \cdot \boldsymbol{u}_g - \varphi_p \nabla \cdot \boldsymbol{u}_p + \cdots$$

$$\boldsymbol{u}_i = \frac{w_g \boldsymbol{u}_g + w_p \boldsymbol{u}_p}{w_g + w_p}$$

- Well suited for numerical implementation

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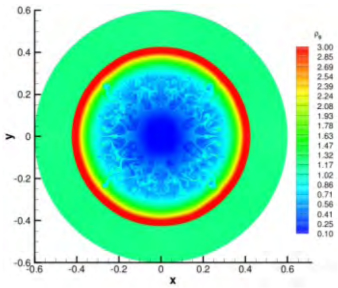
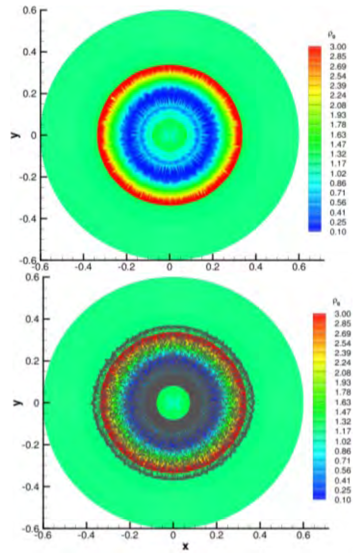
T1: Detonation Modeling Sensitivity

Random Perturbation, no particles



t = 250μs

Random Perturbation, with particles



- Particles annihilate features of initial perturbations in the charge, and imprint a high frequency random perturbation in the underlying gas.

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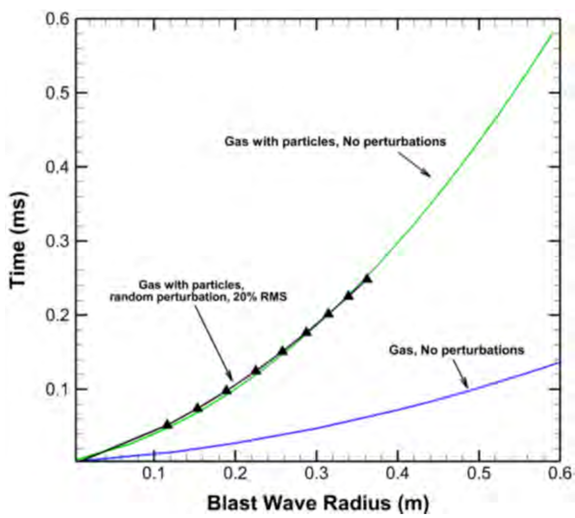
Charge Perturbation Effects on PM-1



- Modest spatial perturbations in the charge density does not affect the blast wave trajectory so long as it is surrounded by a bed a particles

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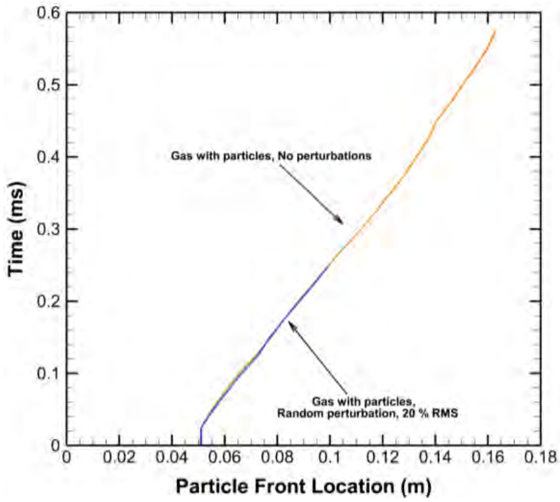
Charge Perturbation Effects on PM-2



- Modest spatial perturbations in the charge density does not affect the particle front trajectory

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Microscale - Goals

- **Conduct microscale simulations and experiments**
  - Various Reynolds and Mach numbers
  - Various volume fractions and particle configurations
  - Particle interaction with shocks, contacts and detonation
- **Develop point-particle models for mesoscale and macroscale**
  - Deterministic aerodynamic forces
  - Deterministic heat transfer
  - Force and heat transfer fluctuation
  - Sub-grid gas-phase Reynolds stress
  - Kinetic models (granular theory)

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Microscale - Tasks

- Develop automated grid generation capability
- Establish grid resolution requirement
- Structured array of particles
  - Shock and contact interaction with an FCC array
- Random array of particles
  - O(10^3) random distribution of particle
  - Sensitivity to volume fraction and force fluctuation
- Freely moving and deforming array of particles
- Hybrid-surrogate model development
- UQ and uncertainty propagation to meso and macroscales
- DAKOTA bundling

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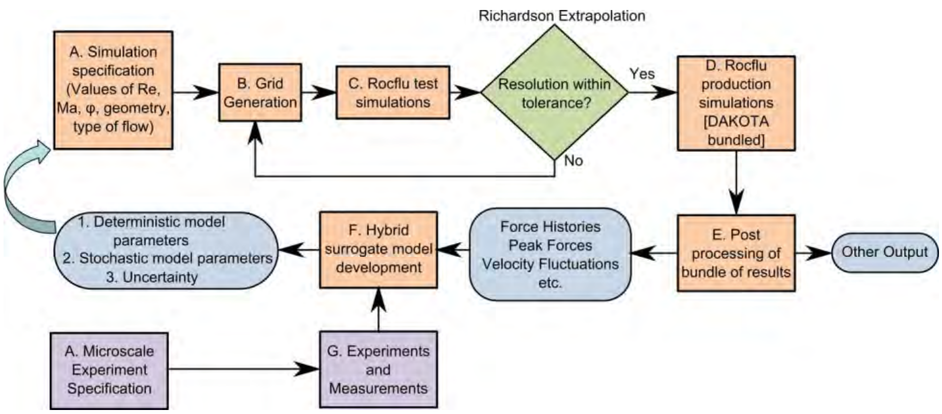
Microscale – Workflow



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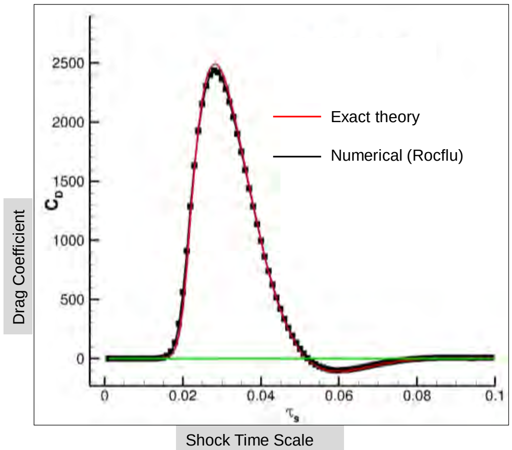
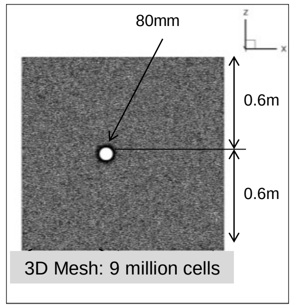
Benchmark Problem: Verification

- Weak shock passing over a particle





Particle Force Model

$$\mathbf{F} = 3\pi\mu d\,\overline{\mathbf{u}}^{S} + \mathrm{V}\rho\,\overline{\frac{D\mathbf{u}}{Dt}}^{V} + \mathrm{V}\int_{-\infty}^{t} K_i(t-\xi)\left(\overline{\frac{D\rho\mathbf{u}}{Dt}}^{V} + \overline{\frac{D\mathbf{r}\nabla.(\rho\mathbf{u})}{Dt}}^{V}\right)d\xi$$

$$C_d = \frac{F_x}{\frac{1}{2}\rho_0 U_0^2 \pi R^2} \qquad \tau_s = \frac{t}{R/U_s}$$

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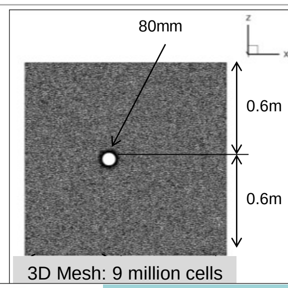
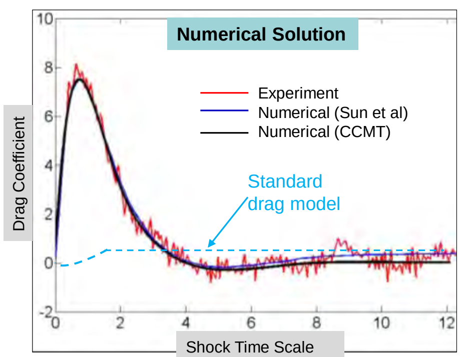
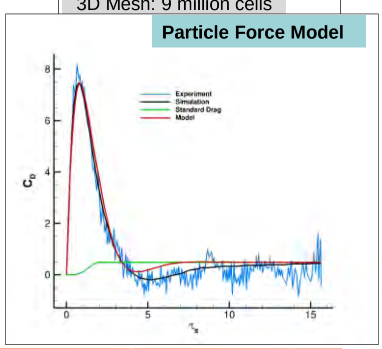
Benchmark Problem: V&V

- Mach 1.22 shock passing over a particle
  - Sun et al., *Shock Waves* (2004).







$$C_d = \frac{F_x}{\frac{1}{2}\rho_0 U_0^2 \pi R^2} \qquad \tau_s = \frac{t}{R/U_s}$$

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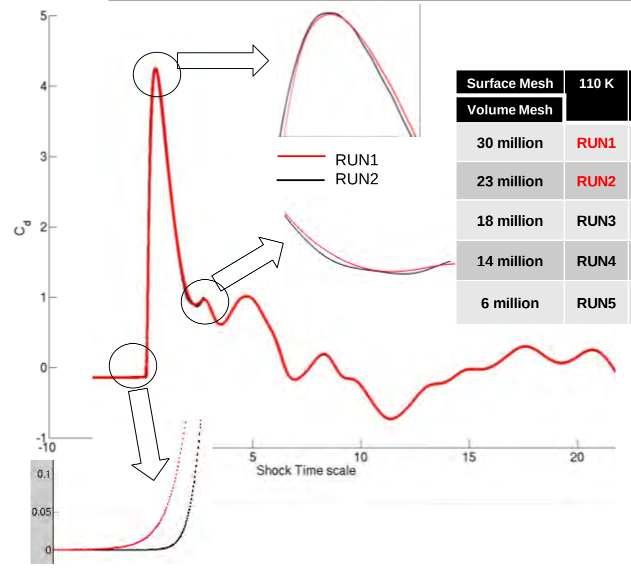
FCC Grid Resolution Studies (Mach 1.5)



Surface Mesh / Volume Mesh	110 K	82 K	70 K	57 K	43 K
30 million	RUN1	RUN6	RUN11	RUN16	RUN21
23 million	RUN2	RUN7	RUN12	RUN17	RUN22
18 million	RUN3	RUN8	RUN13	RUN18	RUN23
14 million	RUN4	RUN9	RUN14	RUN19	RUN24
6 million	RUN5	RUN10	RUN15	RUN20	RUN25

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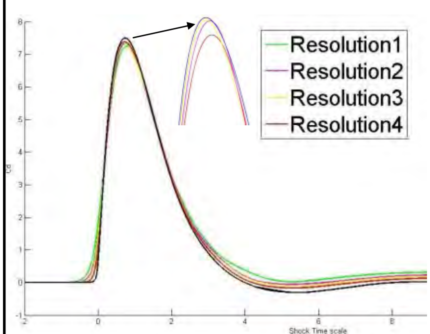
Error Quantification: Richardson Extrapolation



Peak C_d (Percent error compared to extrapolated value)

	Surf_1	Surf_2	Surf_3	Surf_4	
Vol_1	21.94	17.4	13.35	21.22	
Vol_2	10.16	10.85	14.87	18.27	
Vol_3	9.73	4.37	10.24	10.27	
Vol_4	7.51	9.41	5.43	7.26	
					7.4544

Extrapolated value of Peak C_d

Peak C_d on next refined grid (9M volume cells, 250K surface cells): 7.49

- Richardson Extrapolation to get converged estimate of force history for single and multiple particles for different Mach numbers
- Multiple simulations were done to establish optimum grid resolution for the surface mesh of the particle and volume mesh in the domain
- Surface and volume mesh must be refined together to achieve optimum accuracy

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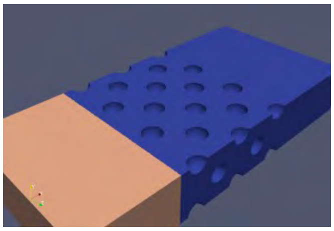
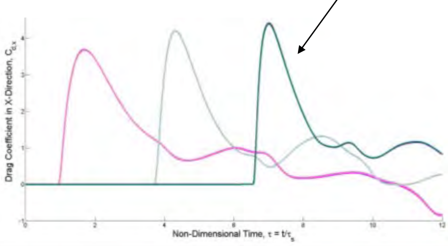
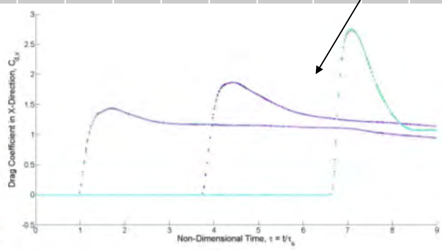
Shock–Particle Interaction Simulation Matrix



Φ=10%, M=1.5, grid=RUN13

Mach → / Volume fraction ↓	1	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	5.5	6.0
					Bundled Runs						
0.1											
0.2											
0.3											
0.4											
0.5											
0.6											





Φ=10%, M=1.5

Φ=10%, M=6.0

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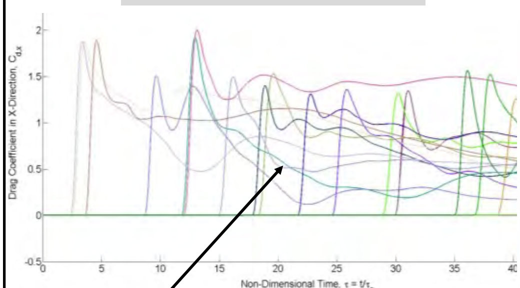
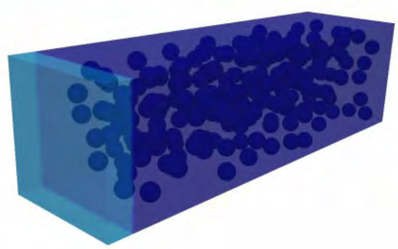
Multi-Particle Simulations

- Simulation of random cluster of particles (10% packing fraction) to extract force history information
- Extracted information is compared with current models to establish areas that need model enhancement.

Force histories of 20 particles

Mach 3 shock over 200 particles





- Current models do not capture this observed effect

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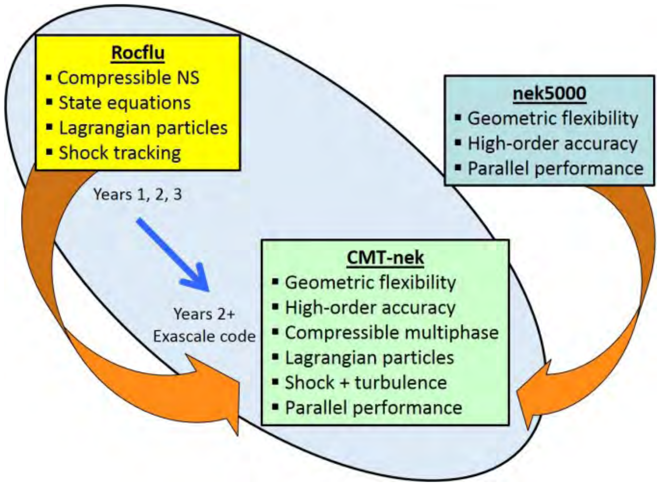
Co-Design of CMT-nek



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nek5000 does... but CMT-nek needs...

nek5000 Wide variety of low-speed flows	CMT-nek Wide variety of rapidly evolving flows
✧ Incompressible Navier-Stokes equations	✧ Compressible Navier-Stokes equations ➢ coupling with dispersed particles
✧ Semi-Implicit time march for elliptic ops	✧ Explicit time marching for acoustics
✧ Smooth solutions	✧ Shock waves, material interfaces
✧ **Global, continuous spectral elements**	✧ **Discontinuous Galerkin (DG)**

From nek5000, take:
map, parallelism
I/O, pre-&post-proc
basis func, quadrature
element geometry

1. New governing equations
2. Mathematical DG formulation
3. Particles
4. Shock capturing

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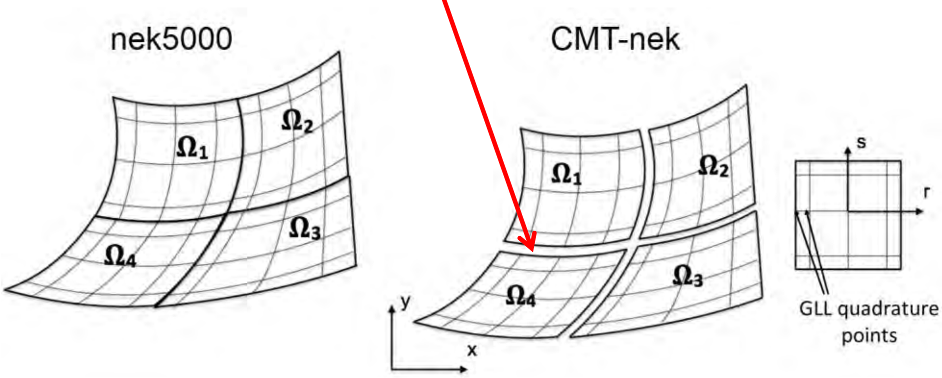
Discontinuous Galerkin Formulation

$$\frac{\partial}{\partial t}\int_V \psi \mathbf{U_i dV} - \int_\Omega (\mathbf{H_{ij}} - \mathbf{H^*_{ij}})\mathbf{n_j d\Omega} + \int_V \psi \frac{\partial \mathbf{H_{ij}}}{\partial \mathbf{x_j}}\mathbf{dV} = \int_V \mathbf{R_i dV}$$



Deville, Fischer and Mund (2002) *Higher-Order Methods for Incomp. Flows* Cambridge
Ronquist and Patera (1987) *Intl. J. Numerical Methods Engrg.* **24**, 2273-2299

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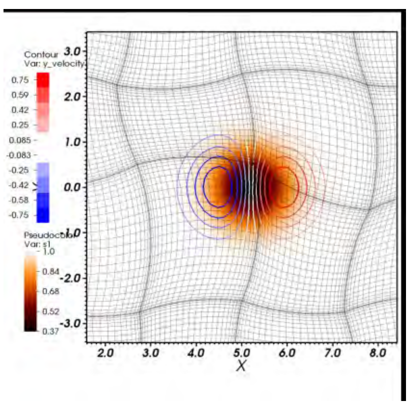
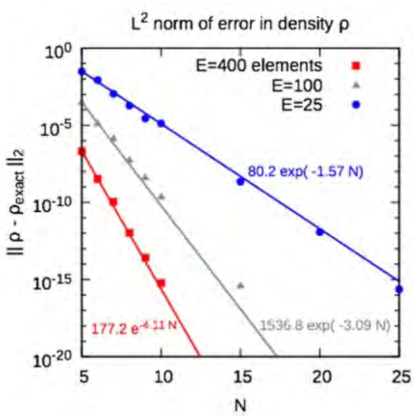
Spectral Convergence - Inviscid Vortex

Spectral convergence in periodic domains, with and without curved elements





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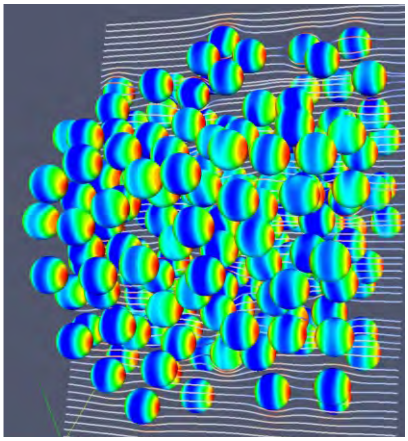
200 Random Sphere in Periodic Box

Free stream Mach number = 0.3
Number of elements ~ 80000; Element resolution = 7*7*7
Simulation performed on Mustang with ~ 4000 MPI ranks



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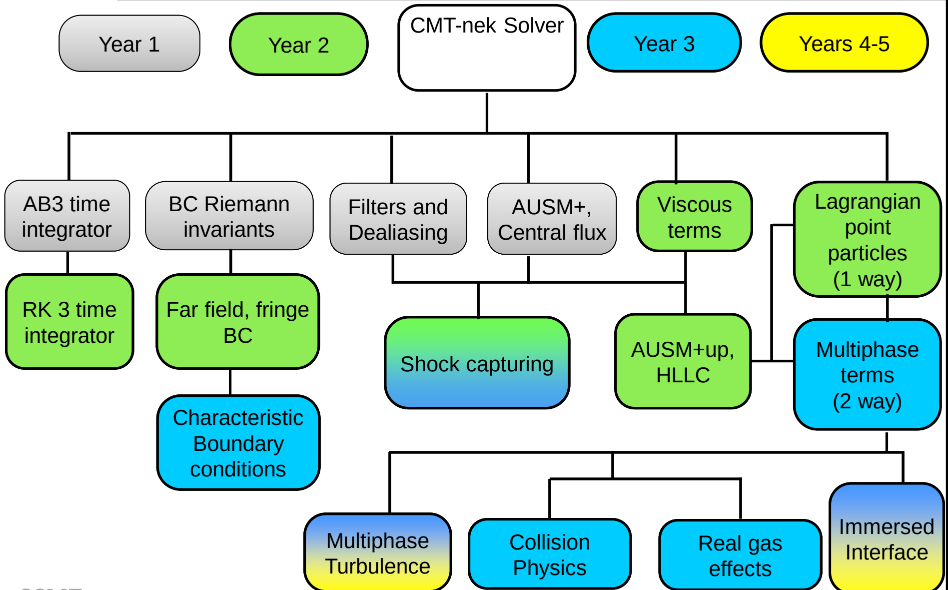
Capabilities and Timeline



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Co-Design With CMT-bone

- **Computation**
  - 3D matrix operations
    - Map element onto itself (derivatives)
  - 3D interpolation
    - Coarse-to-fine, fine-to-coarse (de-aliasing)
  - Surface operations (inviscid & viscous fluxes)
  - Particle tracking (position, velocity, temperature, etc)
  - Lagrangian-Eulerian coupling
  - Shock capturing
- **Communication**
  - Exchange of element interface data
  - Element-to-element particle migration
  - Lagrangian-Eulerian coupling (larger particle foot-print)

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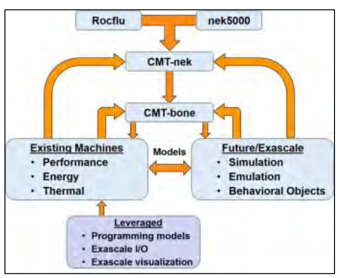
Three-Pronged Co-Design Strategy

- Near term on existing platforms
  - Performance, energy and thermal optimization
  - Dependence on processor/memory architecture
- Future exascale platforms (Architecture & Application BEOs)
  - Address potential show-stoppers and bottlenecks
  - Focus on algorithmic changes
  - Guidelines for multiphase DG-SE parameters
- Leverage (NNSA Labs and PSAAP centers)
  - Programing models
  - Exascale I/O
  - Exascale Visualization



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Co-Design Optimization Questions

- Behavioral emulation on future architectures will guide
  - Cache-optimized order of DG-SE operations
  - Eulerian-to-Lagrangian interpolation and Lagrangian-to-Eulerian projection algorithms and strategies
  - Thermodynamic and transport properties (tabulate vs re-compute)
  - Inter-element communication for IBM
- Optimization on existing platforms (performance, energy, thermal)
  - # of elements (N_e) vs polynomial order (P)
  - Distribution of particles across elements, cores
  - Mapping of elements across nodes and cores
  - Graph selection (nearest neighbor vs crystal router)

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Timeline: CMT-nek and CMT-bone

	Task	Year1				Year2				Year3				Year4				Year5			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Develop-ment	Euler Solver	■	■	■	■	■	■	■	■	■	■										
	Compressible Navier-Stokes				■	■	■	■	■												
	Lagrangian Point Particles						■	■	■	■	■	■	■								
	Shock Capturing						■	■	■	■	■	■	■								
	Multiphase Turbulence									■	■	■	■	■	■	■	■	■	■	■	■
	Immersed Boundary Method											■	■	■	■	■	■	■			
Integration	Integration with Dakota									■	■	■	■								
	Integration with Catalyst									■	■	■	■								
	Other physics												■	■	■	■	■	■	■	■	■
Release	CMTMicro						R1				R3				R5						
	CMTMacro							R2				R4				R6					
	CMT-bone				B1				B2				B3				B4				

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Do you have any questions?

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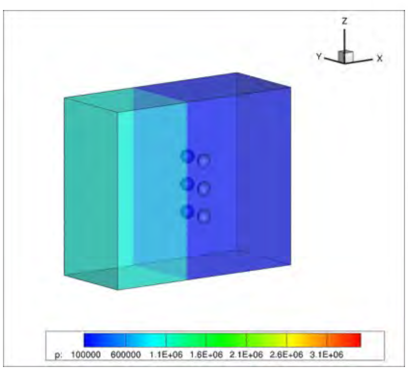
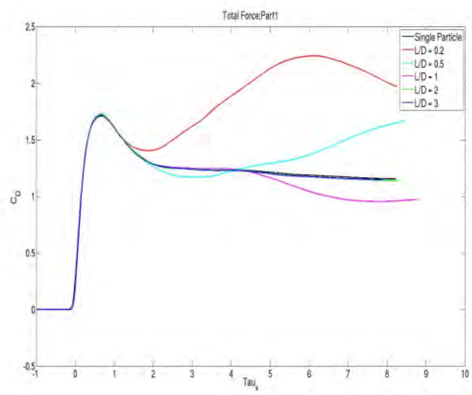
Shock Particle Interaction – Lead particle curtain





- These simulations mimic the effect of shock interaction with lead curtain of particles.
- For different particle-particle spacing total force and fluctuating force are computed.

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Lagrangian-Eulerian Coupling

- Lagrangian description of particles is natural
- Offers subgrid particle resolution
- Consistent interpolation between Eulerian grid and Lagrangian particles
- How many particles per cell?
- How to compute volume fraction?
- Number density fluctuation induced diffusion

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Other Theoretical Advancements

- A rigorous unified mathematical formulation that goes from compaction to contact-dominated to dilute regime
- Accurate microscale models of mass, momentum and energy coupling at extreme conditions of relevance
- Ensure hyperbolicity of governing equations
  - Numerical instabilities without hyperbolicity
  - Pseudo turbulence, Reynolds-stress and added-mass forces play an important role
- Large eddy closure models of particle-wake and interface turbulence

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Microscale Informed Thermal Coupling

$$q = q_{qs} + q_{cu} + q_{du}$$

- Quasi-steady: $q_{qs} = \frac{\overline{T^g}^s - T^p}{\tau_\theta^p} \frac{\mathrm{Nu}(\mathrm{Re}^p, \mathrm{Pr}, \mathrm{M}^p)\mathrm{Re}^p}{24}$
- Compression-unsteady: $q_{cu} =$
- Diffusive-unsteady: Michaelides & Feng (1994)

$$q_{du} = \frac{1}{2\rho^g \tau_\theta^p} \int_{-\infty}^{t} K_{du}(t-\chi, \mathrm{Re}^p, \mathrm{Pr}, \mathrm{M}^p) \left(\overline{\frac{D}{Dt}}^s \overline{(\rho^g T^g)}^s - \frac{d}{dt} \overline{(\rho^g T^g)}^s \right) d\chi$$

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Macroscale and Mesoscale Simulations of Compressible Multiphase Turbulence (CMT)

Bertrand Rollin
Research Scientist

UF UNIVERSITY of FLORIDA — NNSA

CMT in Explosive-Driven Particle-Laden Flows

Sarychev peak (source: wikipedia)

- Why is it interesting?
  - Explosive-driven particles
  - Shock/particle interaction
  - Turbulence/particle interaction
  - Wide range of length and time scale

- Bring predictive capabilities to particle-laden flow simulations

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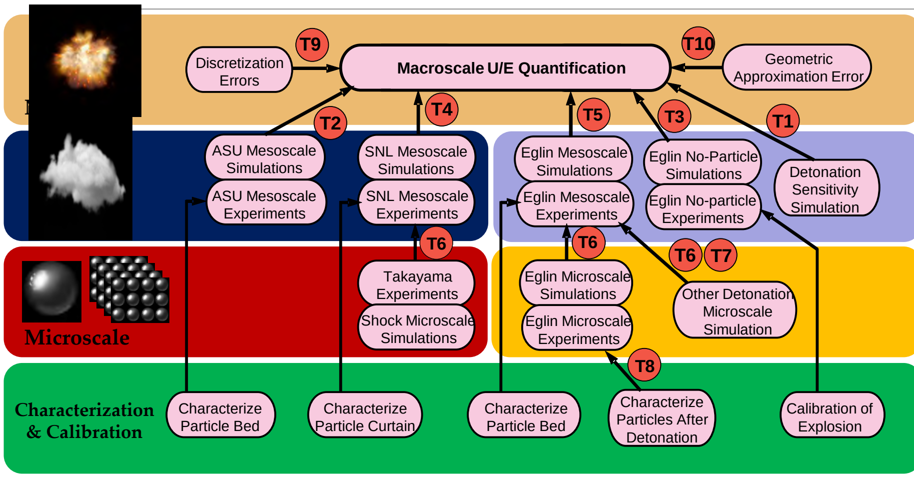
Demonstration Problem



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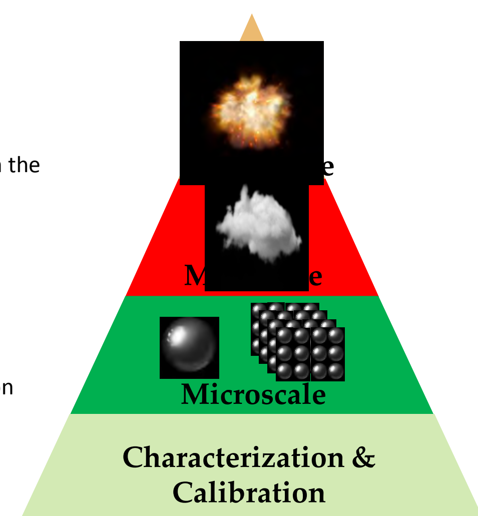
Hierarchical Study of CMT

- Various physics models in the macro simulation
- Validating specific physical models in the meso and micro scales
- Error and variability propagation between scales
- Identify relations between sub-scale validations and macro scale validation



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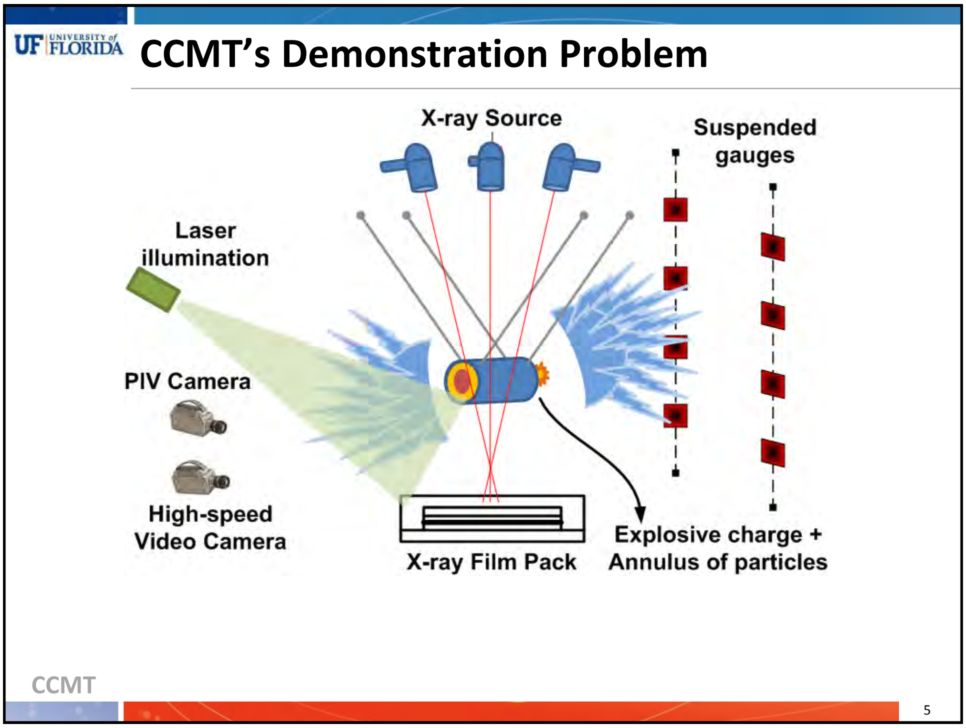
CCMT's Demonstration Problem
X-ray Source
Suspended gauges
Laser illumination
PIV Camera
High-speed Video Camera
X-ray Film Pack
Explosive charge + Annulus of particles
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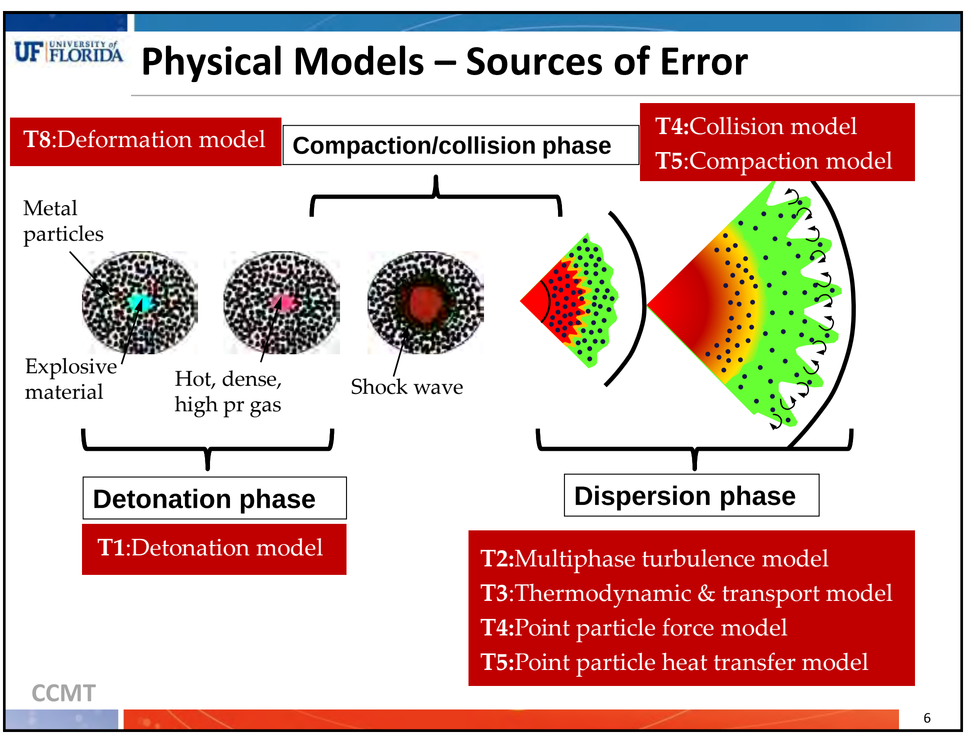
Physical Models – Sources of Error
T8:Deformation model
Compaction/collision phase
T4:Collision model
T5:Compaction model
Metal particles
Explosive material
Hot, dense, high pr gas
Shock wave
Detonation phase
T1:Detonation model
Dispersion phase
T2:Multiphase turbulence model
T3:Thermodynamic & transport model
T4:Point particle force model
T5:Point particle heat transfer model
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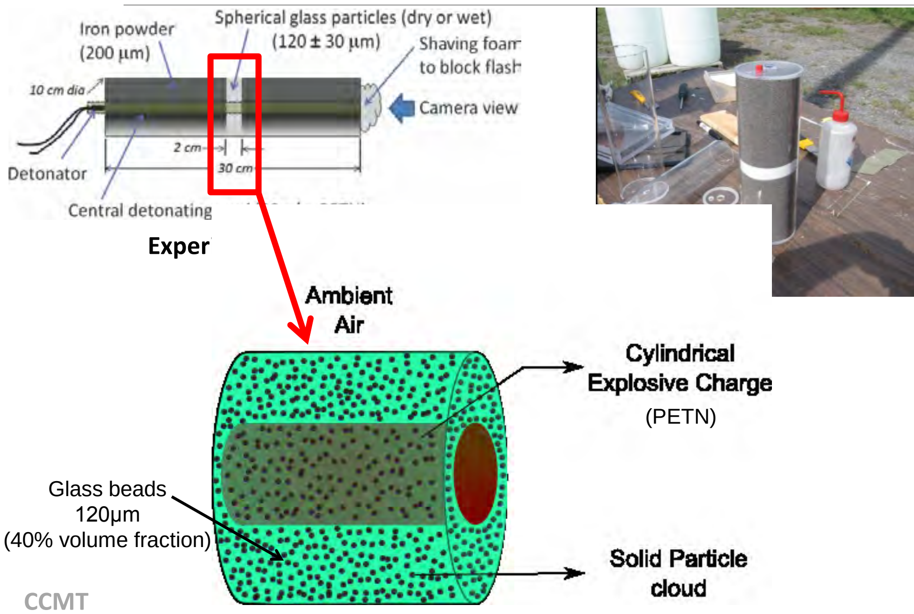
Demonstration problem: Frost et al.'s version



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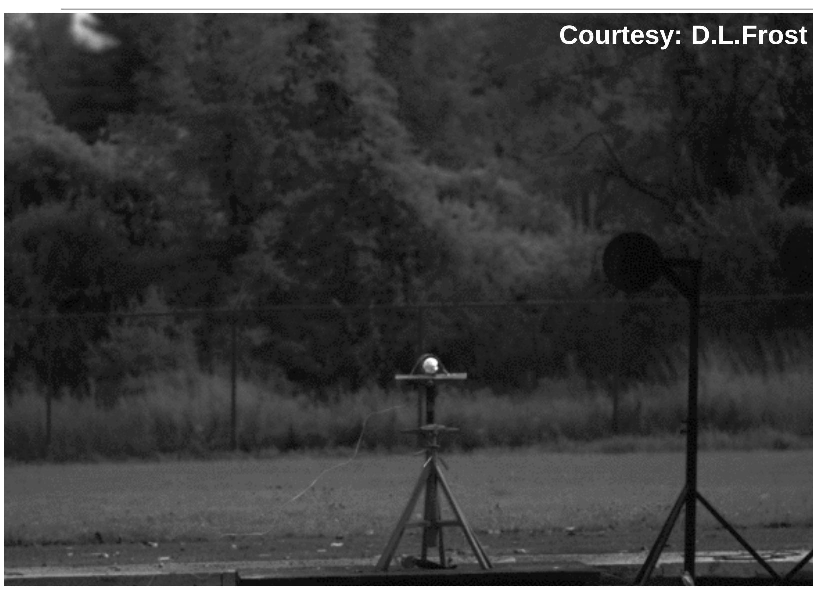
High Speed Video of an Explosive Dispersal of Particles



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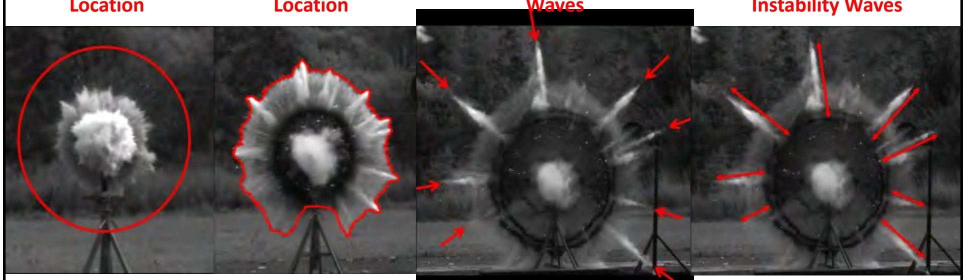
Prediction Metrics

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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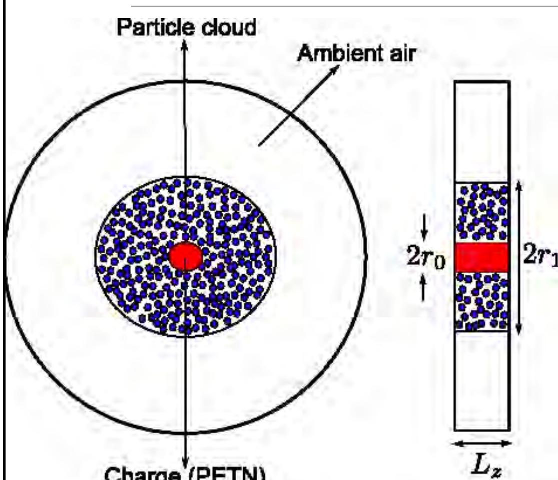
Simulation Description



Parameter	Value
[redacted]	1770 kgm^{-3}
[redacted]	1.203 kgm^{-3}
[redacted]	2500 kgm^{-3}
[redacted]	5 %
[redacted]	3.8 mm
[redacted]	5 cm
[redacted]	2 cm
[redacted]	5 x 10^6

- Boundary conditions:
  - Outflow at the outer radius
  - Slip walls at the back and front when running a 3D case

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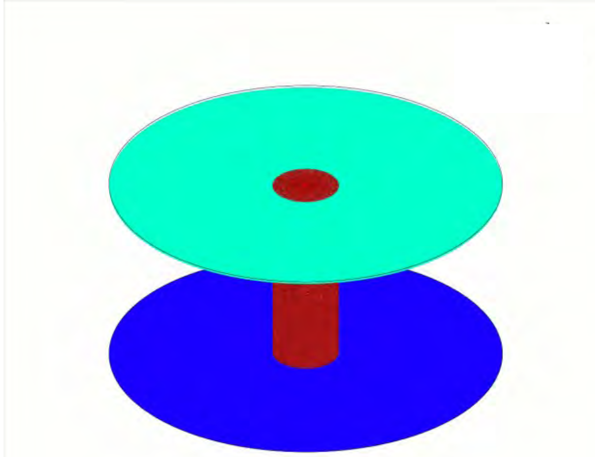
Demonstration Problem: Simulation



- Features:
  - 30 Million computational cells
  - 5 Million computational particles
  - r_{max} = 0.30m

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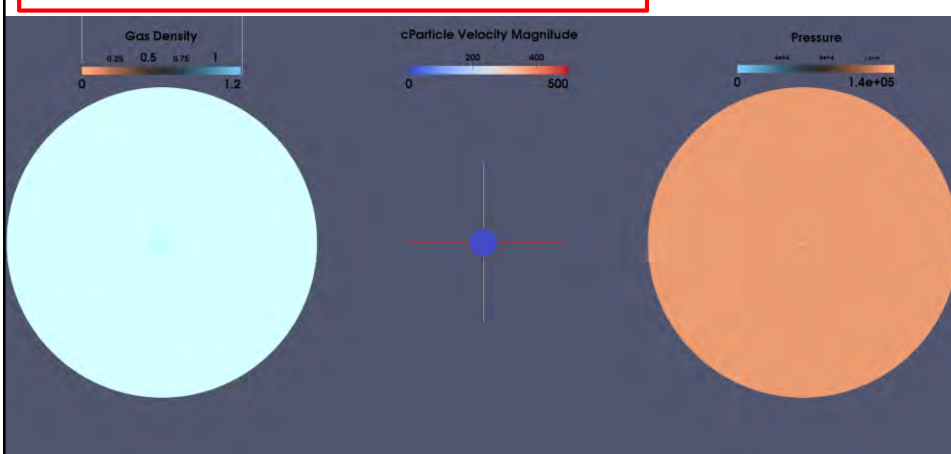
2D Cylindrical Explosive Dispersal of Particles up to 1ms

- Features:
  - 2.5 Million computational cells in a (r,q) plane
  - 1 Million computational particles
  - r_{max} = 0.60m



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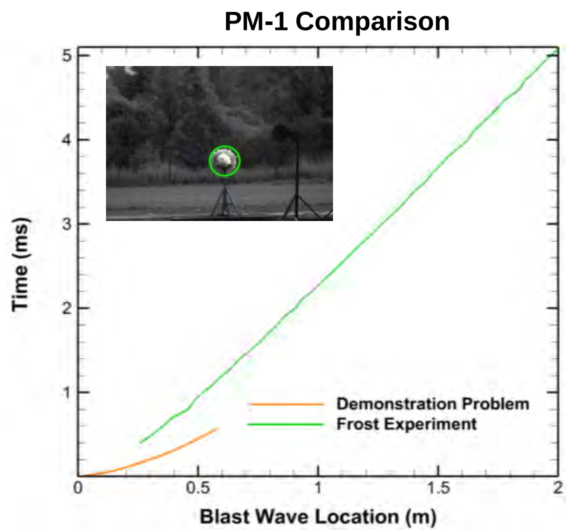
Demonstration Problem: Predictions



- Data from Frost experiment video starts at 0.400 milliseconds
- Data from Demonstration problem ends at 0.575 milliseconds
- Possible sources of discrepancy: EoS, initial particle volume fraction, ...

- The blast wave is slower in the experiment than in our current simulations

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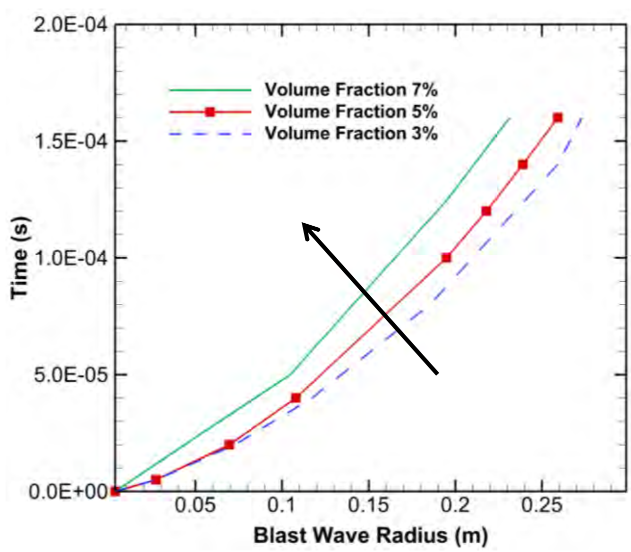
Particle Volume Fraction Effect on Blast Wave



- A Larger Volume Fraction of Particles Slows Down the Blast Wave

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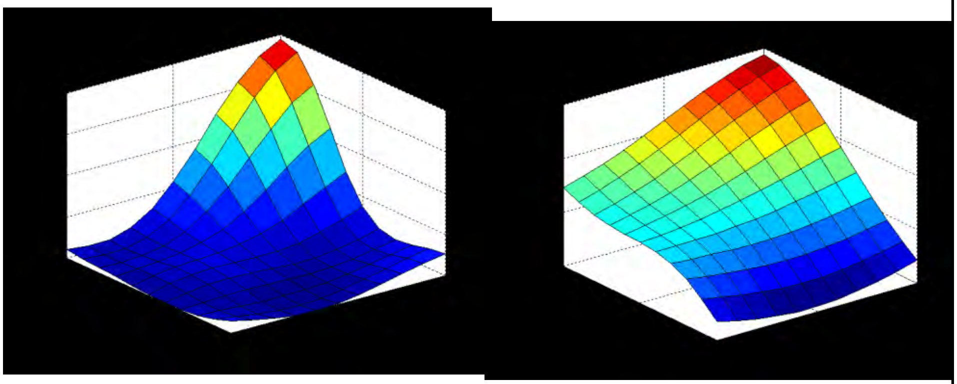
JWL Equation of State Surrogate Model



- The goal is to create a model for mixed explosive/air cells that gives:

$$\rho_{air}, \rho_{dprod}, e_{air}, e_{dprod} = f(\rho_{mixt}, e_{mixt}, Y_{mixt})$$

- This model will remove two iterative root finding methods currently in the code

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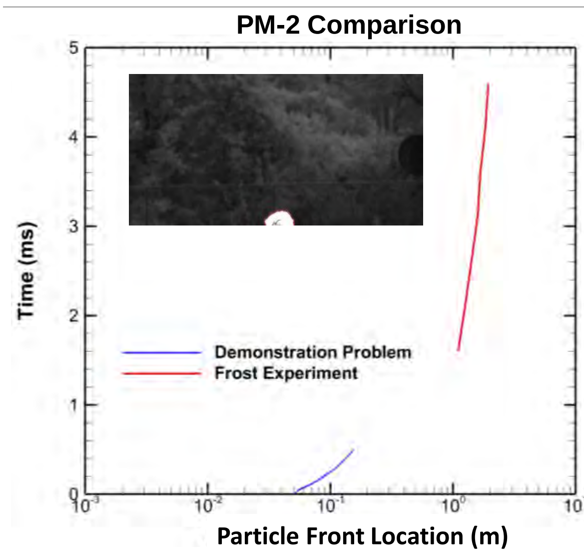
Demonstration Problem: Predictions



- Data from Frost experiment video starts at 2.600 milliseconds
- Data from Demonstration problem ends at 0.575 milliseconds
- Possible sources of discrepancy: EoS, initial particle volume fraction, ...

- The particle front is expanding faster in the experiment than in our current simulation

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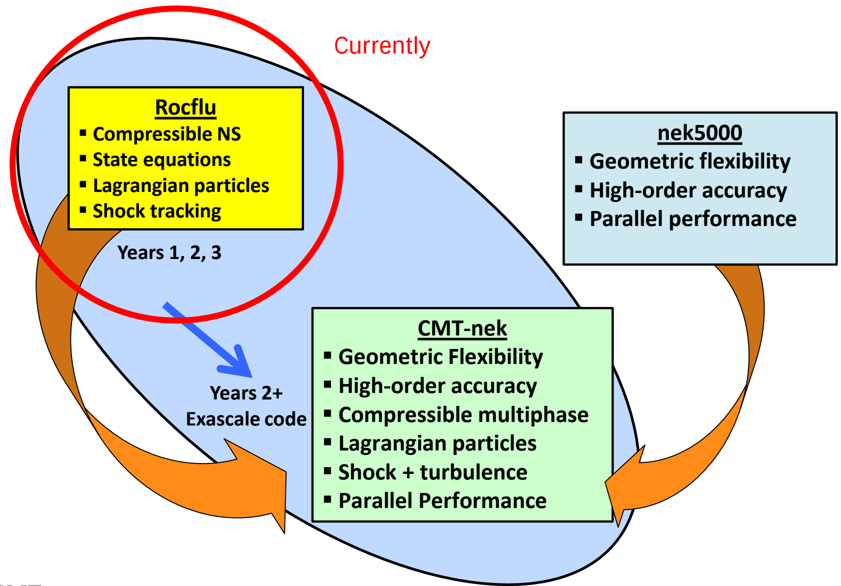
Codes for CMT Simulations



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Governing Equations

Compressible multiphase Euler equations:

$$\frac{\partial(\rho^g \phi^g)}{\partial t} + \nabla \cdot (\rho^g \phi^g \mathbf{u}^g) = 0$$

$$\frac{\partial(\rho^g \phi^g \mathbf{u}^g)}{\partial t} + \nabla \cdot (\rho^g \phi^g \mathbf{u}^g \mathbf{u}^g) + \nabla p^g = -\frac{1}{V_{cell}} \sum_i \chi_{cp} \mathbf{F}_i^{gp}$$

$$\frac{\partial(\rho^g \phi^g E^g)}{\partial t} + \nabla (\rho^g \phi^g \mathbf{u}^g E^g) + \nabla (p^g \mathbf{u}^g) = -\frac{1}{V_{cell}} \sum_i \chi_{cp} (\mathbf{G}_i^{gp} + \mathbf{F}_i^{gp})$$

Particle equations:

$$\frac{\mathrm{d}\mathbf{x}_i^p}{\mathrm{d}t} = \mathbf{u}_i^p$$

$$m_i^p \frac{\mathrm{d}\mathbf{u}_i^p}{\mathrm{d}t} = \mathbf{F}_i^{gp} + \mathbf{F}_i^{pp}$$

$$m_i^p C_i^p \frac{\mathrm{d}T_i^p}{\mathrm{d}t} = \mathbf{Q}_i^{gp}$$

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Micro-informed Inter-Phase Coupling

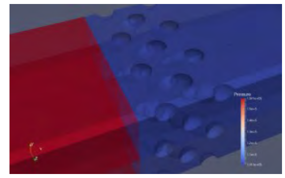
Force due to gas-particle interaction: $\mathbf{F}_i^{gp} = \mathbf{F}_{qs,i} + \mathbf{F}_{pg,i} + \mathbf{F}_{am,i} + \mathbf{F}_{uv,i}$

$$\mathbf{F}_{qs,i} = 3\pi\mu_i^{g} d_i^{p}\left(\mathbf{u}_i^{g} - \mathbf{u}_i^{g}\right)\frac{Re_i^{p}}{24} C_D(Re_i^{p}, M_i^{p}, \phi_i^{p})$$

$$\mathbf{F}_{pg,i} = -V_i^{p}\left(\nabla p^{g}\right)_i$$

$$\mathbf{F}_{am,i} = V_i^{p} C_M(M_i^{p}, \phi_i^{p})\left[-\left(\nabla p^{g}\right)_i - \frac{\mathrm{d}(\rho_i^{g} u_i^{p})}{\mathrm{dt}}\right]$$

$$\mathbf{F}_{am,i} = 3\pi\nu_i^{g} d_i^{p}\theta(\phi_i^{p})\int_{-\infty}^{t} K_{vu}(t-\chi, Re_i^{p}, M_i^{p}, \phi_i^{p})\left[-\left(\nabla p^{g}\right)_i - \frac{\mathrm{d}(\rho_i^{g} u_i^{p})}{\mathrm{dt}}\right]_{t=\chi} \mathrm{d}\chi$$



Force due to inter-particle interaction: $F_i^{pp} = -\frac{V_i^{p}}{\phi_i^{p}}\nabla\tau_{pp,i}$ **where,** $\tau_{pp,i} = \frac{P_s(\phi_i^{p})^{\beta}}{\phi_c^{p} - \phi_i^{p}}$

Heat transfer due to gas-particle interaction: $\mathbf{Q}_i^{gp} = \mathbf{Q}_{qs,i} + \mathbf{Q}_{uu,i} + \mathbf{Q}_{du,i}$

$$\mathbf{Q}_{qs,i} = \pi d^{g}\kappa^{g} Nu(T_i^{g} - T_i^{p})$$

$$\mathbf{Q}_{uu,i} = 0$$

$$\mathbf{Q}_{du,i} = d^{p^2}\sqrt{(\pi\rho^{g} C_p^{g}\kappa^{g})}\int_{-\infty}^{t} K_{vu}(t-\xi)\left[\frac{\mathrm{D}T_i^{g}}{\mathrm{dt}} - \frac{\mathrm{D}T_i^{p}}{\mathrm{dt}}\right]_{t=\xi}\mathrm{d}\xi$$

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Major Challenges Overcome

- "Rigidity" of input for particles
- Rocflu IO incompatible to the size of our cases
- Rocflu memory leak preventing successful run on Vulcan
- Rocflu unadapted post-processing strategy
- rfluinit slowness due to bug and extreme memory requirement
- Inability to have a random distribution of particle

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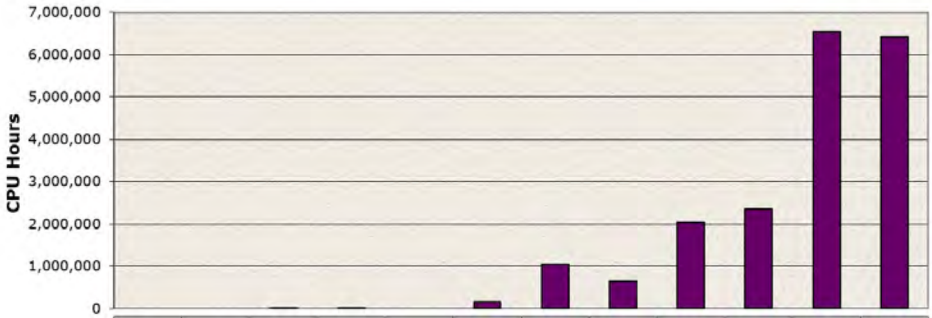
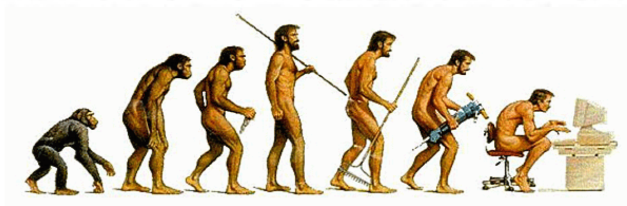
Computer Hour Usage By CCMT

Data courtesy of Rob Cunnigham (HPC-LANL)



	Apr-14	May-14	Jun-14	Jul-14	Aug-14	Sep-14	Oct-14	Nov-14	Dec-14	Jan-15	Feb-15	Mar-15
CMT	0	0	2,111	20,985	0	161,052	1,044,781	651,672	2,039,823	2,343,152	6,537,029	6,420,913



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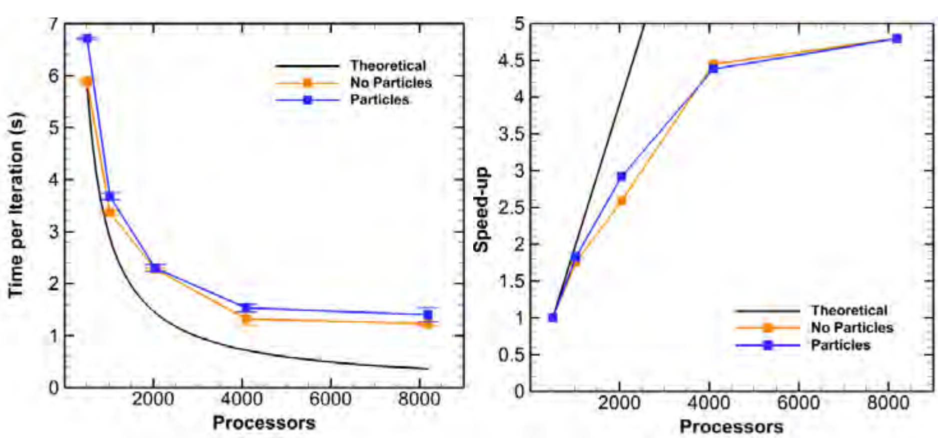
Rocflu's Scaling



- For a demonstration problem simulation counting 30 million cells and 5 million particles, Rocflu is optimum with 4096 cores

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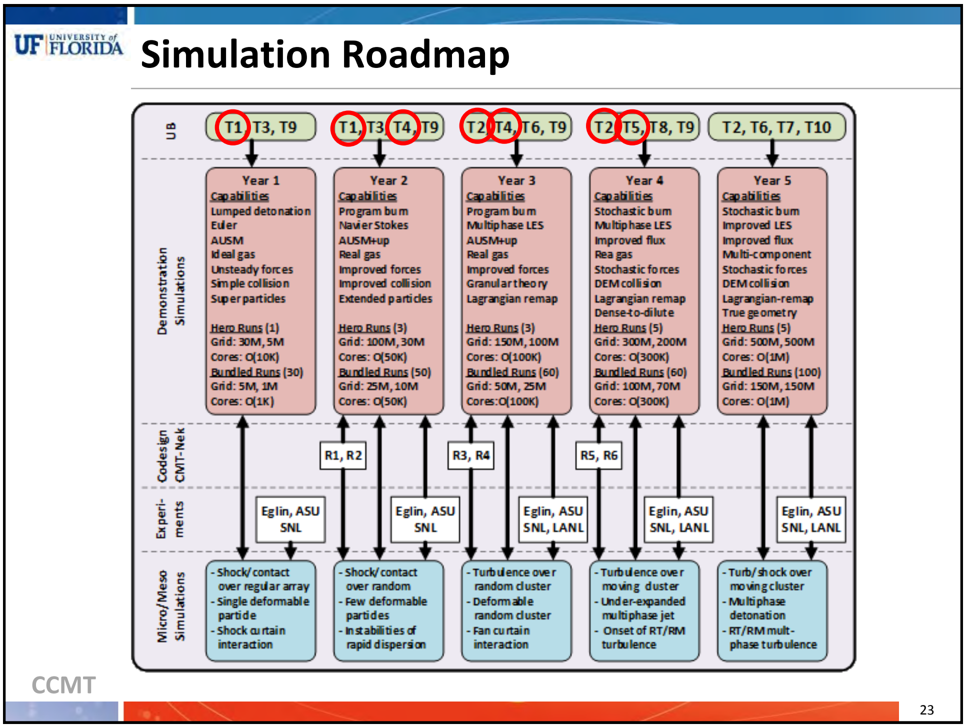
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Simulation Roadmap
UB
T1, T3, T9
T1, T3, T4, T9
T2, T4, T6, T9
T2, T5, T8, T9
T2, T6, T7, T10
Demonstration Simulations
Year 1
Capabilities
Lumped detonation
Euler
AUSM
Ideal gas
Unsteady forces
Simple collision
Super particles
Hero Runs (1)
Grid: 30M, 5M
Cores: O(10K)
Bundled Runs (30)
Grid: 5M, 1M
Cores: O(1K)
Year 2
Capabilities
Program burn
Navier Stokes
AUSM+up
Real gas
Improved forces
Improved collision
Extended particles
Hero Runs (3)
Grid: 100M, 30M
Cores: O(50K)
Bundled Runs (50)
Grid: 25M, 10M
Cores: O(50K)
Year 3
Capabilities
Program burn
Multiphase LES
AUSM+up
Real gas
Improved forces
Granular theory
Lagrangian remap
Hero Runs (3)
Grid: 150M, 100M
Cores: O(100K)
Bundled Runs (60)
Grid: 50M, 25M
Cores:O(100K)
Year 4
Capabilities
Stochastic burn
Multiphase LES
Improved flux
Real gas
Stochastic forces
DEM collision
Lagrangian remap
Dense-to-dilute
Hero Runs (5)
Grid: 300M, 200M
Cores: O(300K)
Bundled Runs (60)
Grid: 100M, 70M
Cores: O(300K)
Year 5
Capabilities
Stochastic burn
Improved LES
Improved flux
Multi-component
Stochastic forces
DEM collision
Lagrangian-remap
True geometry
Hero Runs (5)
Grid: 500M, 500M
Cores: O(1M)
Bundled Runs (100)
Grid: 150M, 150M
Cores: O(1M)
Codesign CMT-Nek
R1, R2
R3, R4
R5, R6
Experi-ments
Eglin, ASU SNL
Eglin, ASU SNL
Eglin, ASU SNL, LANL
Eglin, ASU SNL, LANL
Eglin, ASU SNL, LANL
Micro/Meso Simulations
- Shock/contact over regular array
- Single deformable particle
- Shock curtain interaction
- Shock/contact over random
- Few deformable particles
- Instabilities of rapid dispersion
- Turbulence over random cluster
- Deformable random cluster
- Fan curtain interaction
- Turbulence over moving cluster
- Under-expanded multiphase jet
- Onset of RT/RM turbulence
- Turb/shock over moving cluster
- Multiphase detonation
- RT/RM mult-phase turbulence
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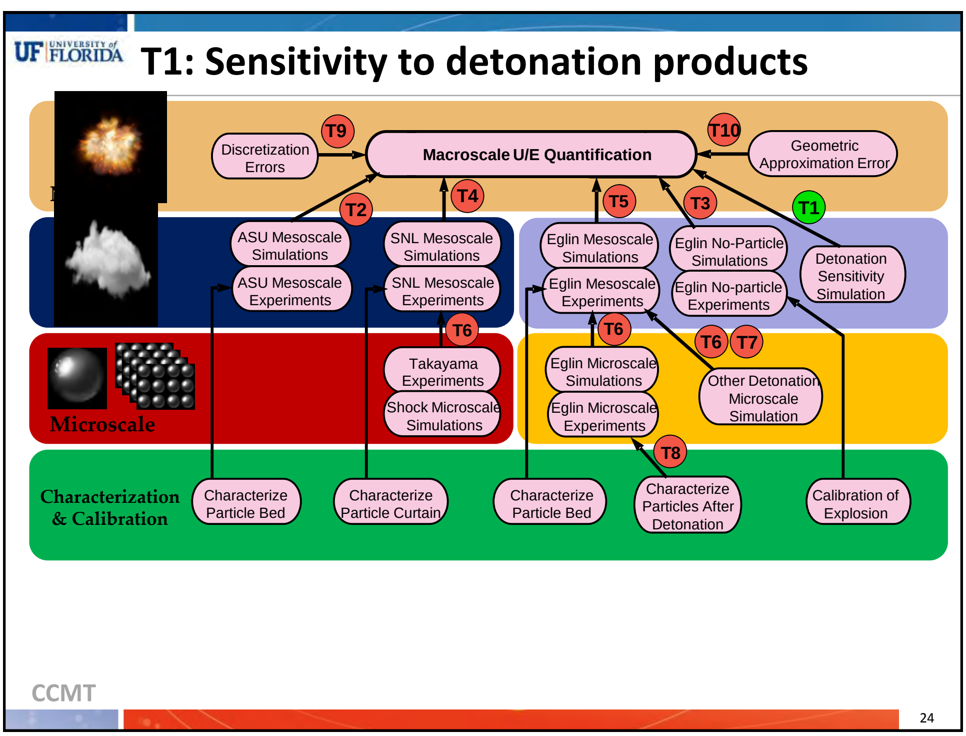
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T1: Sensitivity to detonation products
Discretization Errors
T9
Macroscale U/E Quantification
T10
Geometric Approximation Error
T2
T4
T5
T3
T1
ASU Mesoscale Simulations
ASU Mesoscale Experiments
SNL Mesoscale Simulations
SNL Mesoscale Experiments
Eglin Mesoscale Simulations
Eglin Mesoscale Experiments
Eglin No-Particle Simulations
Eglin No-particle Experiments
Detonation Sensitivity Simulation
T6
T6
T6
T7
Takayama Experiments
Shock Microscale Simulations
Eglin Microscale Simulations
Eglin Microscale Experiments
Other Detonation Microscale Simulation
Microscale
T8
Characterization & Calibration
Characterize Particle Bed
Characterize Particle Curtain
Characterize Particle Bed
Characterize Particles After Detonation
Calibration of Explosion
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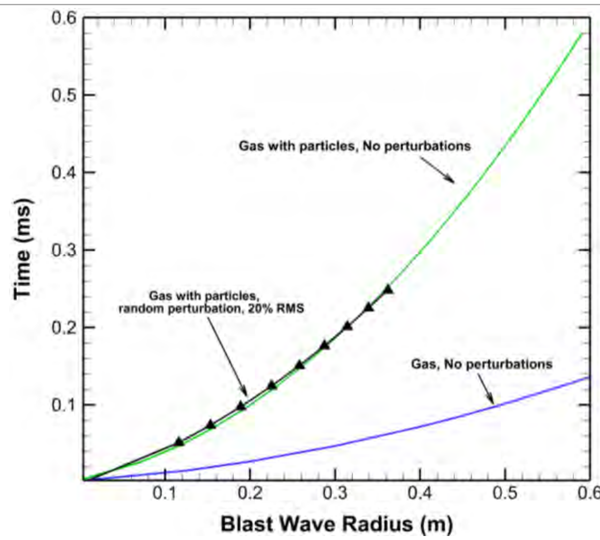
Charge Perturbation Effects on PM-1



- Modest perturbations in the charge density does not affect the blast wave trajectory so long as it is surrounded by a bed a particles

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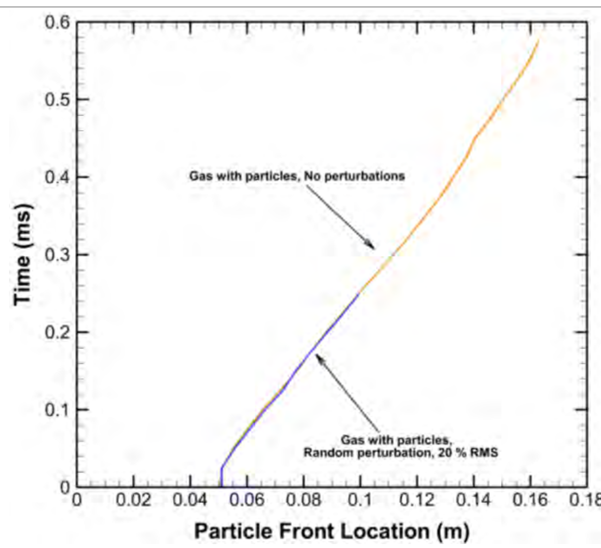
Charge Perturbation Effects on PM-2



- Modest perturbations in the charge density does not affect the particle front trajectory

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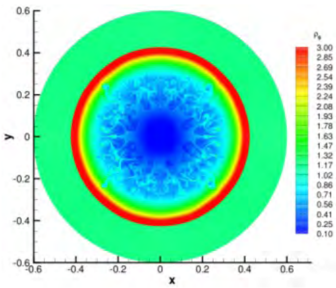
Charge Perturbation Effects

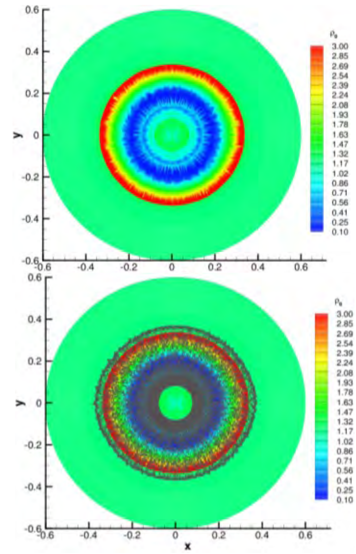
Random Perturbation, no particles



t = 250μs

- Particles annihilate features of initial perturbations in the charge, and imprint a high frequency random perturbation in the underlying gas.

Random Perturbation, with particles



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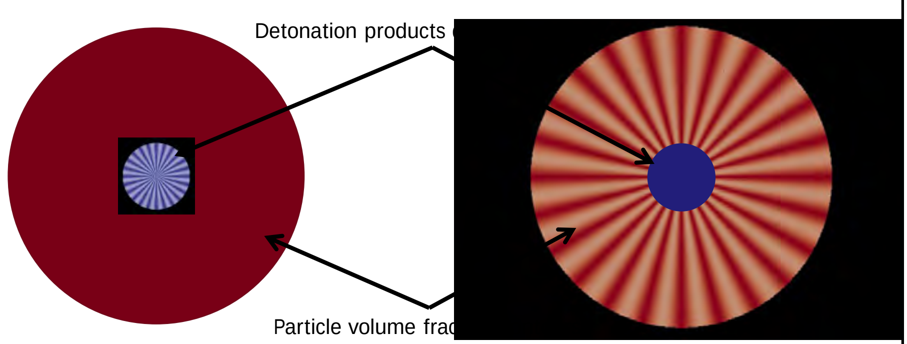
Charge vs. Particle Volume Fraction Perturbation Study

Detonation Products Initially Perturbed

Particle Volume Fraction Initially Perturbed



- The perturbations in the charge and in the particles volume fraction are such that the density rms over the entire cylinder remains the same from one case to the other.

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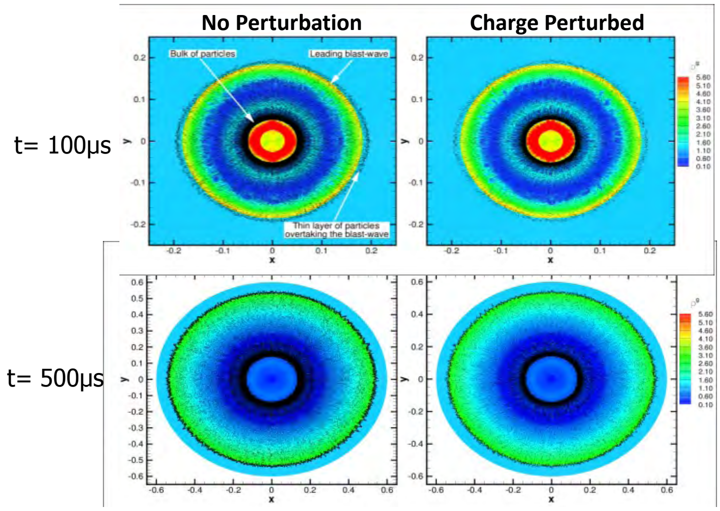
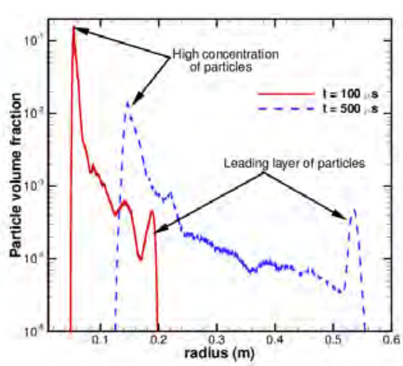
Initial Perturbation in the Explosive Material



- A small perturbation in the charge has no influence on the particle dispersal

Azimuthally Averaged Profile of Particle Volume fraction



- The volume fraction of particles started at 5%, peaked at about 30%, is quickly dropping to 10% by t = 100µs.

- A small concentration of particles that is "riding along" with the blast wave, even over taking it.

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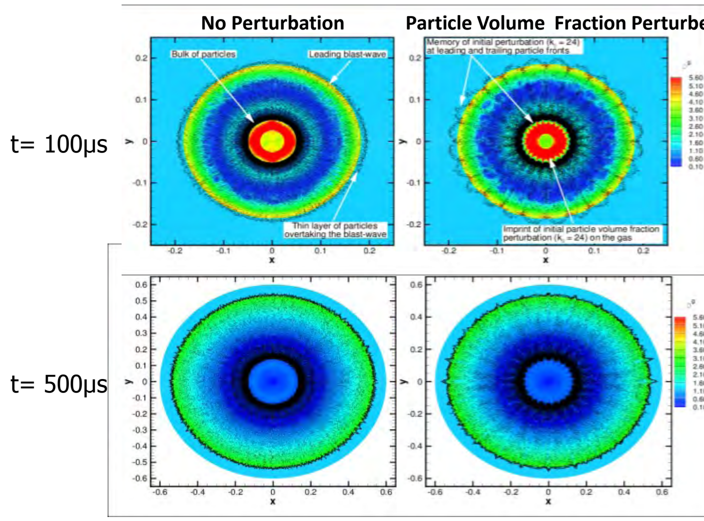
Initial Perturbation in the Bed of Particles



- A small perturbation in the particle volume fraction has a significant effect on the particle dispersal

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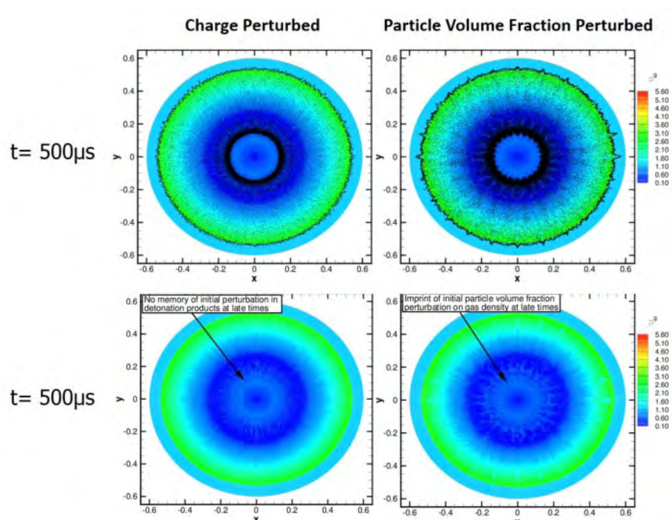
Late Time Behavior Following Initial Perturbation



- Imprint of the initial perturbation in the volume fraction of the underlying gas

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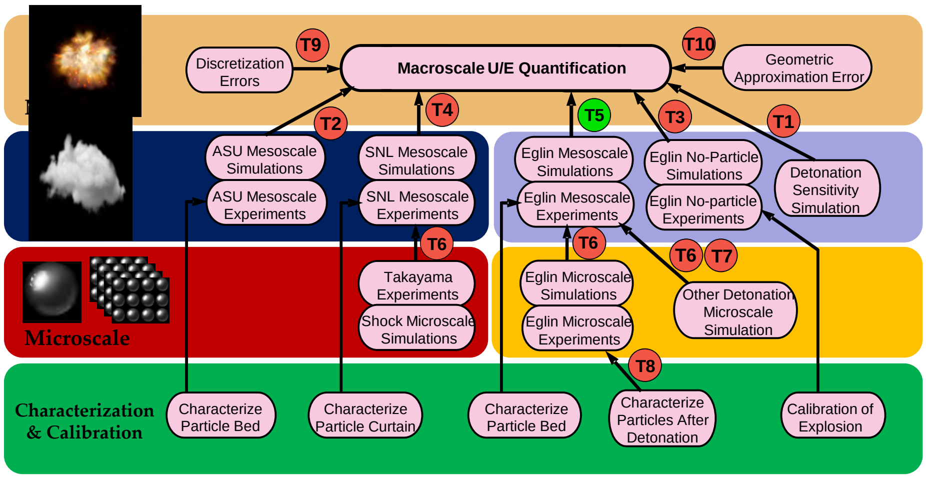
T5: Mesoscale explosive dispersal of particles simulations



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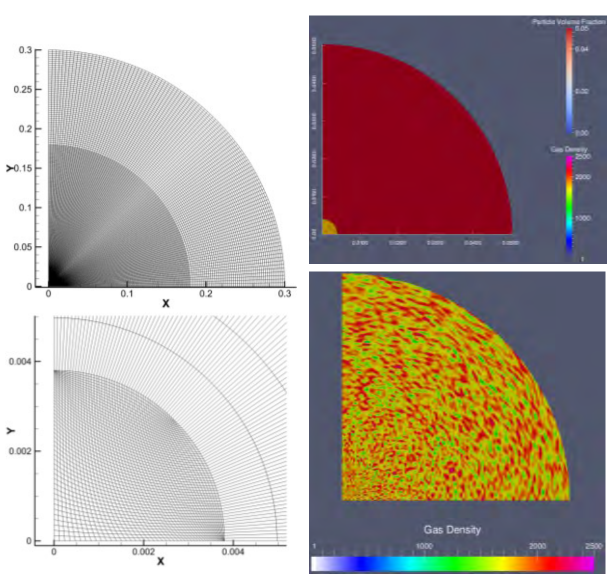
Quarter Cylinder Explosive Problem



- The quarter cylinder problem will be used to test our Compressible Multiphase LES model.
- The quarter cylinder problem allow for extremely fine resolution, necessary to capture the finest scales of turbulence.

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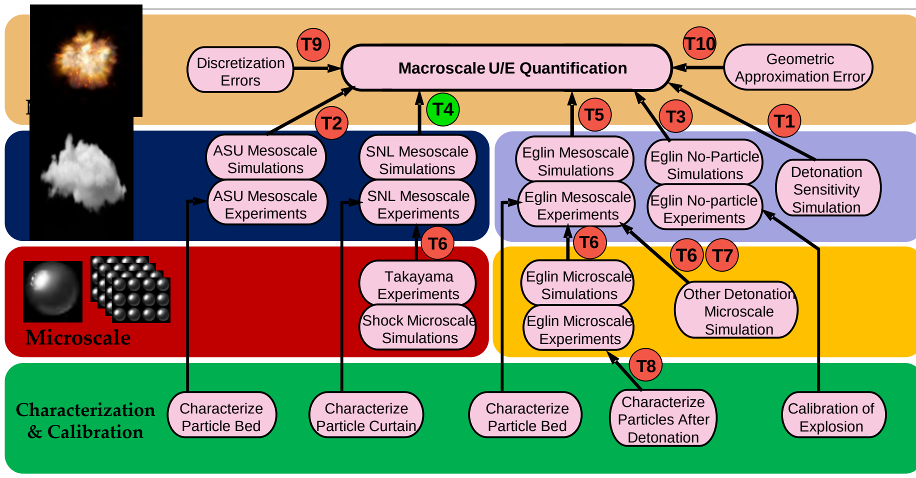
T4: Shock – particle curtain simulations



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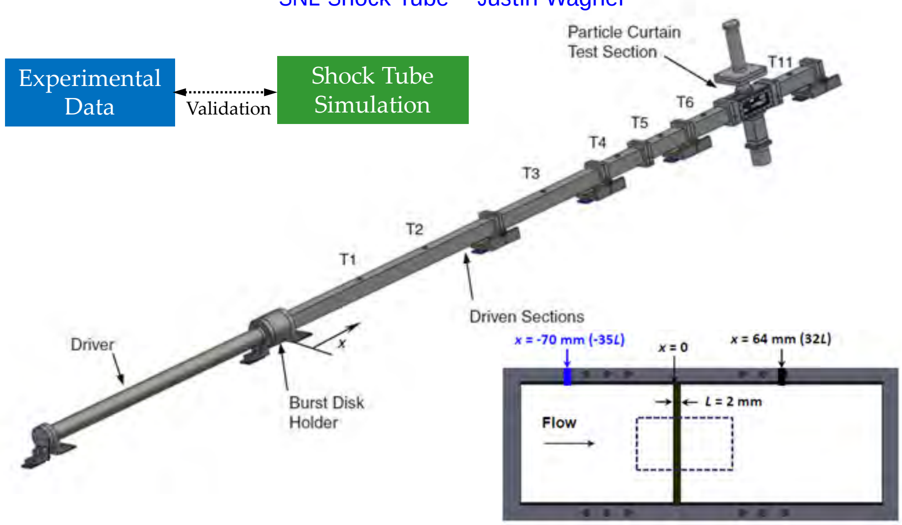
Mesoscale Validation: The Particle Curtain Problem

SNL Shock Tube – Justin Wagner



- Validation of the models for gas and particles interaction

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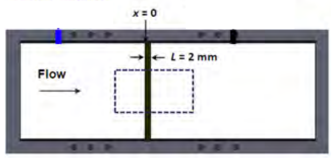
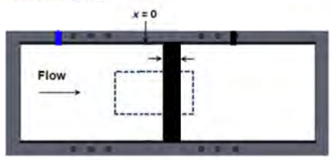
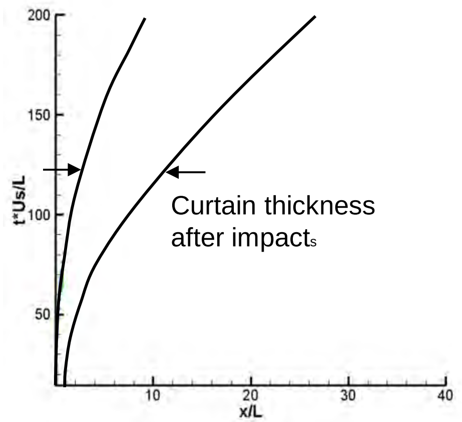
Prediction Metric

Before impact



After impact





- **Prediction Metric:** The locations of the particle curtain edges at upstream and downstream

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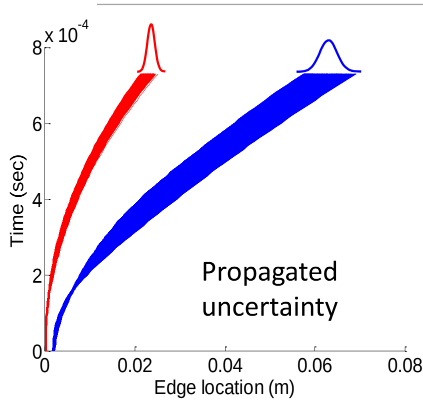
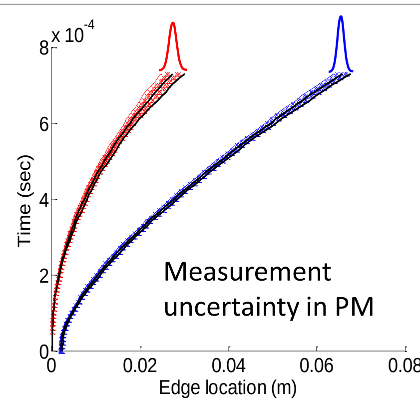
UQ study on 1D Particle Curtain





- **Propagated uncertainty:** reflecting the uncertainties in inputs and the simulation (Rocflu Lite)
- **Measurement uncertainty in PM**: representing the uncertainty in experiments from 4 repeated experiments (SNL)

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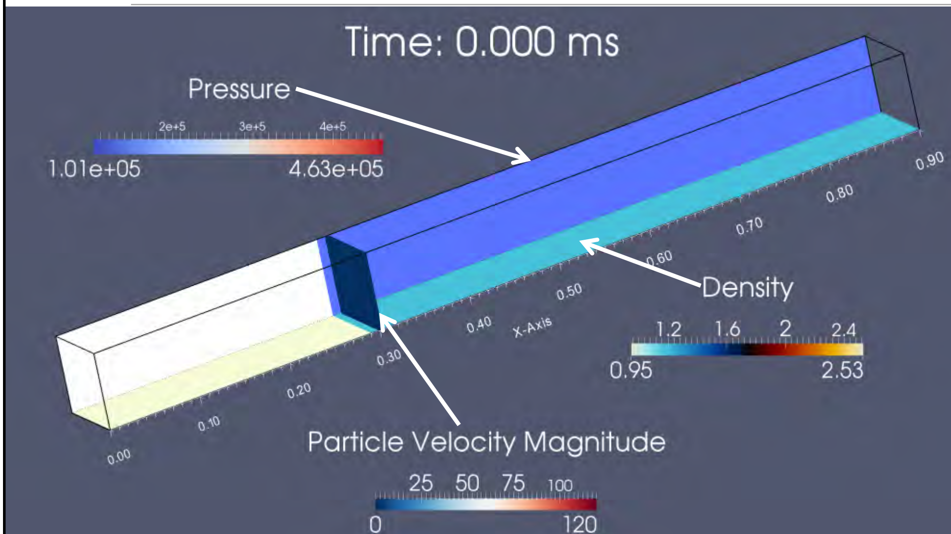
Particle Curtain Simulation (Particle Volume Fraction=23%, Ma=1.66)



- Features:
  - 10 Million computational cells
  - 1 Million computational particles

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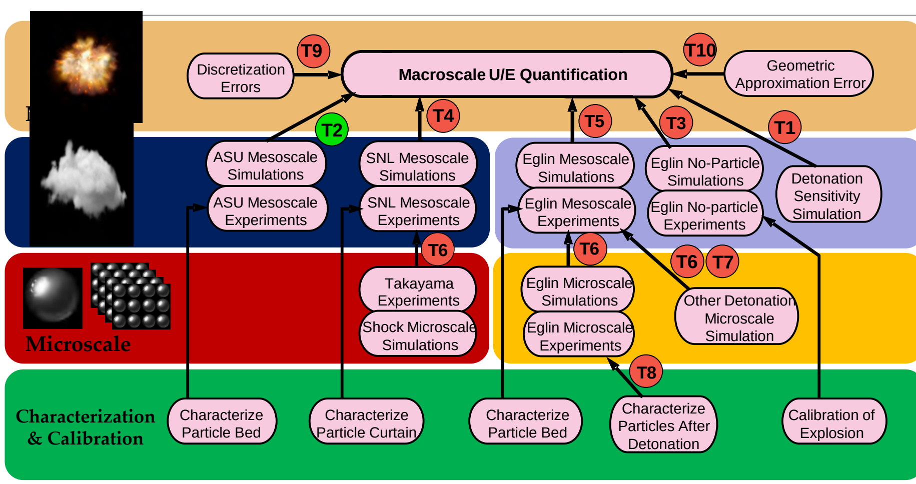
T2: Expansion fan – particles interaction simulations



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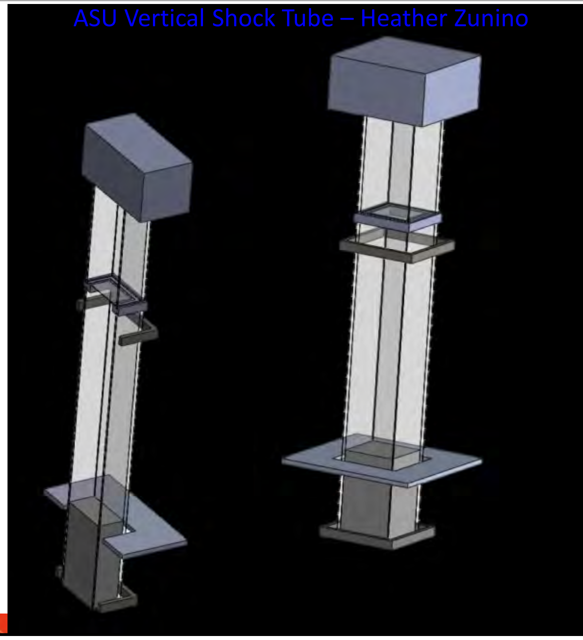
T2: Experimental Setup



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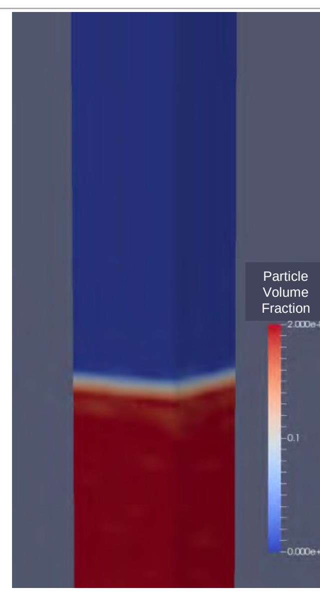
Expansion Fan – Particles Interaction Simulation



- Features: 20% particle volume fraction

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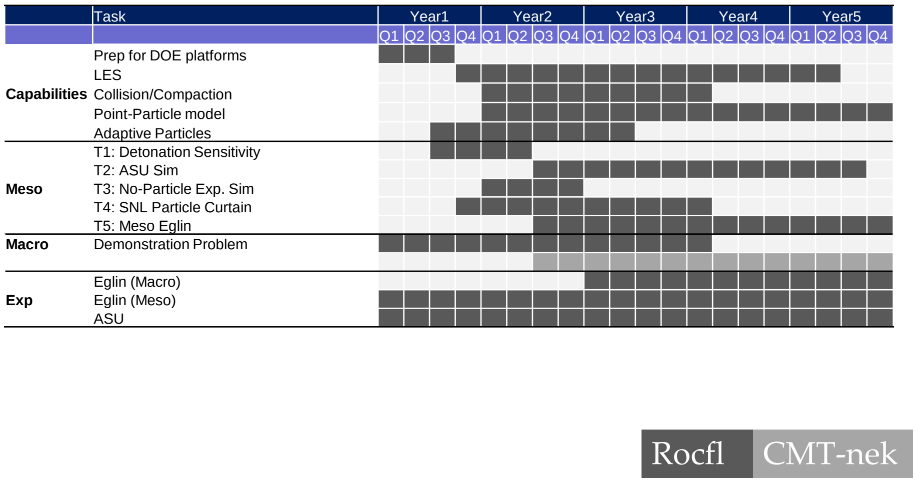
Macro/Mesoscale Gantt Chart



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Do you have any questions?

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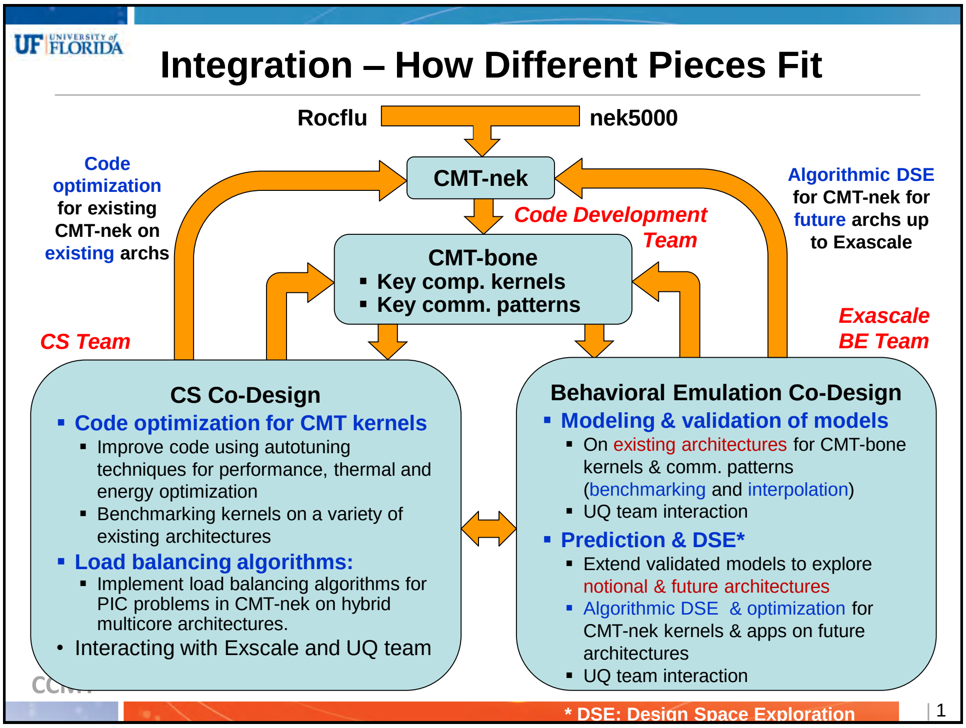
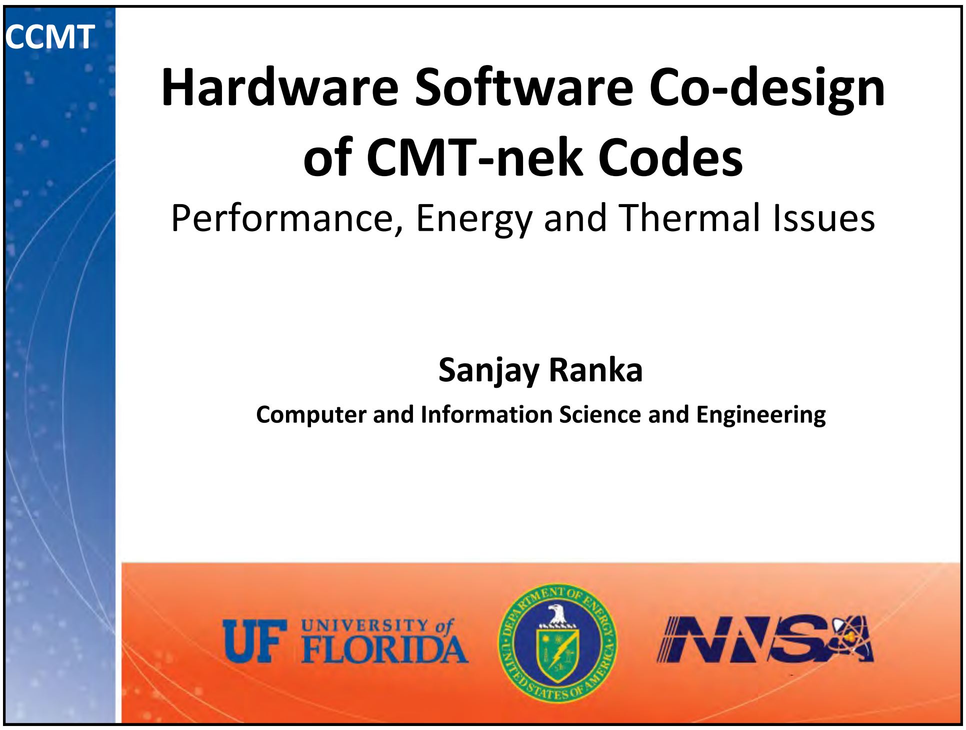
NNSA


Integration – How Different Pieces Fit
Rocflu
nek5000
CMT-nek
Code optimization for existing CMT-nek on existing archs
Algorithmic DSE for CMT-nek for future archs up to Exascale
Code Development Team
CMT-bone
▪ Key comp. kernels
▪ Key comm. patterns
CS Team
Exascale BE Team
CS Co-Design
▪ Code optimization for CMT kernels
▪ Improve code using autotuning techniques for performance, thermal and energy optimization
▪ Benchmarking kernels on a variety of existing architectures
▪ Load balancing algorithms:
▪ Implement load balancing algorithms for PIC problems in CMT-nek on hybrid multicore architectures.
• Interacting with Exscale and UQ team
Behavioral Emulation Co-Design
▪ Modeling & validation of models
▪ On existing architectures for CMT-bone kernels & comm. patterns (benchmarking and interpolation)
▪ UQ team interaction
▪ Prediction & DSE*
▪ Extend validated models to explore notional & future architectures
▪ Algorithmic DSE & optimization for CMT-nek kernels & apps on future architectures
▪ UQ team interaction
* DSE: Design Space Exploration
1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Hardware Software Co-design of CMT-nek Codes
Performance, Energy and Thermal Issues
Sanjay Ranka
Computer and Information Science and Engineering

Long Term Goals

$10^6 \rightarrow 10^7 \rightarrow 10^8 \rightarrow 10^9$ cores

- Parallelization and UQ of Rocflu and CMT-nek beyond a million cores
- Parallel Performance and **Load Balancing**
- **Single Processor (Hybrid) Performance**
- **Energy Management and Thermal Issues**

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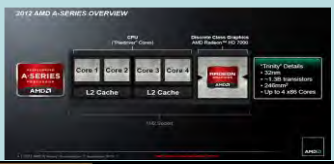
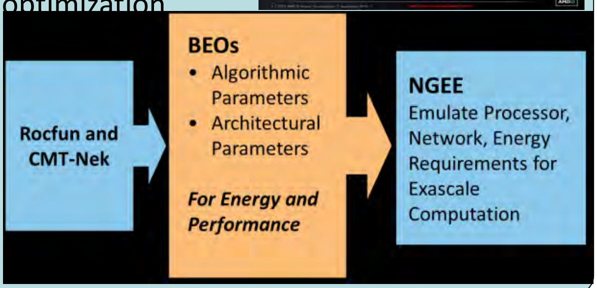
Hybrid Multicores: Performance, Energy and Thermal Management

$10^1 \rightarrow 10^2 \rightarrow 10^3 \rightarrow 10^4$ cores

- Code Generation for hybrid cores
  - Support for multiple types of cores
  - Support for Vectorization
- Multi-objective optimization
  - Energy
  - Performance
- Thermal Constraints





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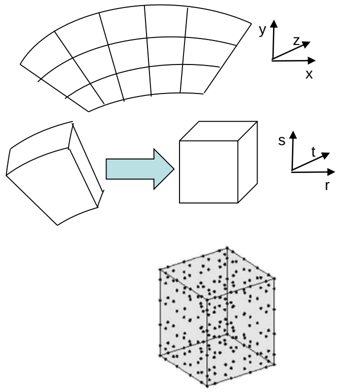
Spectral Element Method



- $\frac{\partial U}{\partial r}$ (i, j, k) = $\sum_{l=1}^{N_x} A_{il} u_{ljk}$
  $\frac{\partial U}{\partial s}$ (i, j, k) = $\sum_{l=1}^{N_y} B_{il} u_{ilk}$
  $\frac{\partial U}{\partial t}$ (i, j, k) = $\sum_{l=1}^{N_z} C_{il} u_{ijl}$
- If $N_x = N_y = N_z = N$
  - Then $B = C = A^T$
- Complexity: $O(N^4)$
- N is typically between 5-25
  - A large number of small matrix multiplications

- Represents a significant fraction of overall time
- More details in Tania's presentation tomorrow

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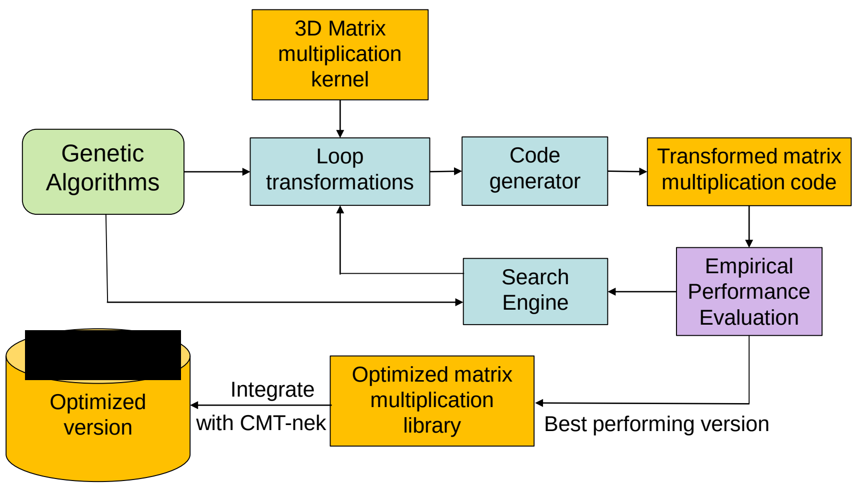
Autotuning Framework



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Performance And Energy

- Software Implementation:
  - CMT-nek
  - 4loop version
  - 4loop-fused version
  - 5loop-version
  - 5loop-fused version
- CPU Platforms:
  - IBM Blue Gene/Q
  - AMD Opteron 6378
  - AMD Fusion
- GPU platform
  - Tesla K20c

Performance and Energy Benchmarking of Spectral Element Solvers, Tania Banerjee, Jacob Rabb, Sanjay Ranka (in preparation)

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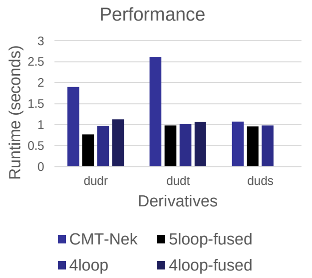
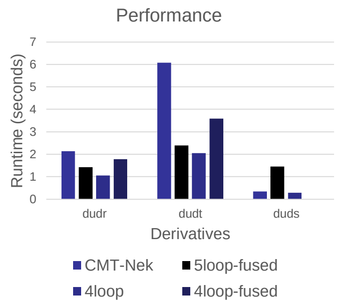
IBM BG/Q (Performance)



- Matrix size 10x10x10, 100 elements
- 51% improvement versus CMT-nek (~ 2 times)
- 34 GFLOPS average



- Matrix size: 16x16x16, 25 elements
- 61% improvement versus CMT-nek (~ 2.53 times)
- 12.7 GFLOPS average

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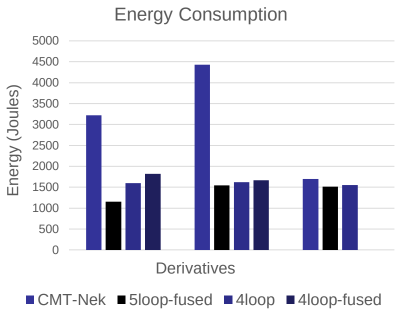
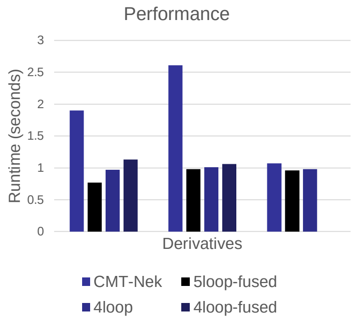
IBM BG/Q (Energy)





- Observations:
  - matrix size 10x10x10, 100 elements
  - 55% reduction in energy versus CMT-nek

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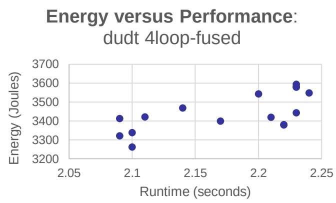
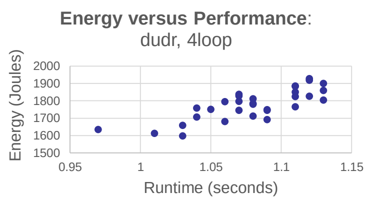
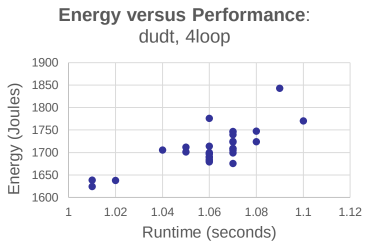
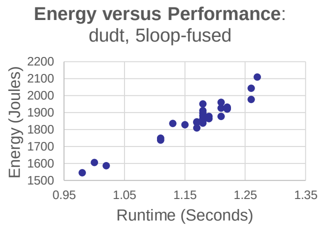
Energy versus Performance Plots









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Results (GA driven autotuning)

Related Work: J.H.Laros, III, P. Pokorny, and D. DeBonis, PowerInsight – A Commodity Power Measurement Capability, The Third International Workshop on Power Measurement and Profiling in conjunction with IEEE IGCC 2013, 2013

- Hipergator (Performance)
- Teller@Sandia (Energy)
  - 104 nodes cluster
  - AMD-Fusion A10-5800K
  - 4 cores operating at 3.8GHz
  - Used PowerInsight to measure power

Derivatives	Min Time (s)	Nek5000 Time (s)	GA Time (s)	#variants
dudr	0.39	0.62	0.41	444
dudt	0.18	0.31	0.2	393
duds	0.45	0.88	0.45	446

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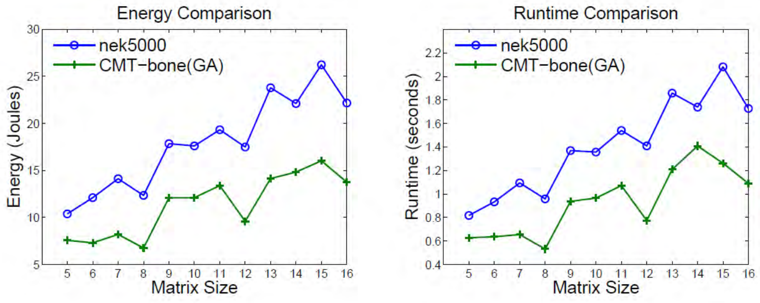
Results (teller@SNL)



- Energy: 27% to 45% improvement average improvement of 37%
- Runtime: 23% to 45% improvement, average improvement of 34%.

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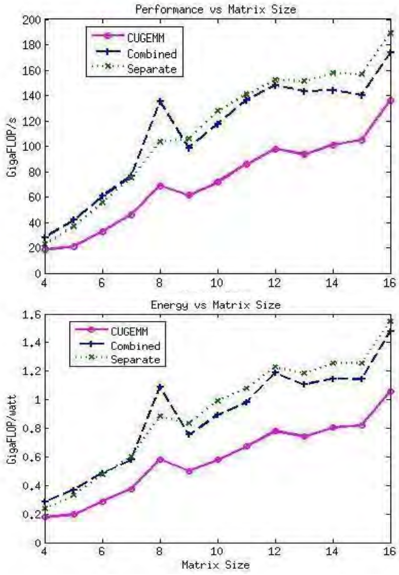
GPU Implementation

- Optimizations:
  - The derivative operator matrices D and D^T matrices are only brought once per block from the device memory to shared memory.
  - The derivative operator matrices D and D^T are stored in registers instead of shared memory.

Related work: A GEMM interface and implementation on NVIDIA GPUs for multiple small matrices, C. Jhurani, P. Mullowney, Journal of Parallel and Distributed Computing September 2014.

GPU (Performance and Energy)



- Performance increases nearly linearly with matrix size
- Over 180 GFLOPS for matrix size 16x16x16
- 39% improvement versus CUGEMM for matrix size 16x16x16
- Power consumed was nearly similar for each kernel
- Hence performance/watt is dominated by performance results

Conclusions

- Benchmarked the derivative computation kernel of CMT-bone for performance and energy
- Our work highlights autotuning as an important strategy for improving both performance and energy, over different architectures
  - Achieved between 23-61% improvement in performance and about 27-55% improvement in energy requirement
- Developed a genetic algorithm based driver which efficiently explores the search space
- Our GPU optimization strategy led to significantly improved performance for small matrix multiplication in spectral elements

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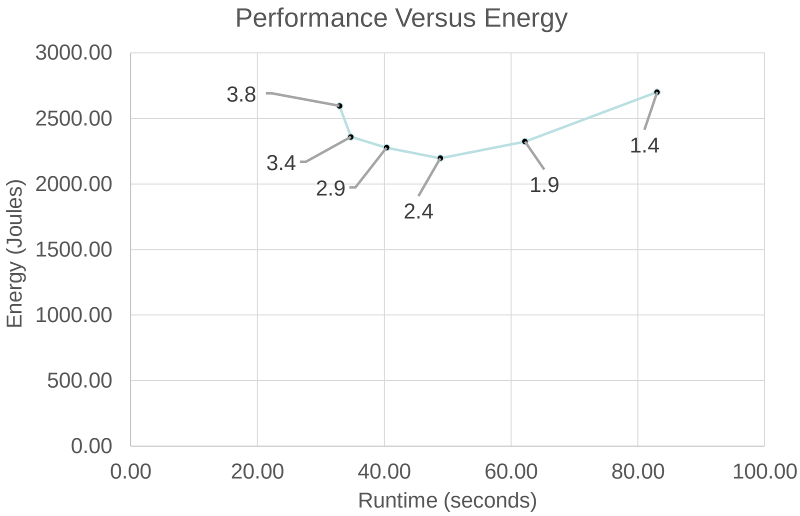
DVFS: Performance Versus Energy



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Integration with CMT-nek

- We achieved about 5% improvement in CMT-nek runtime when the derivative computation kernel is run
- An increased number of cache misses is the primary reason for the differences in performance
- Restructuring CMT-nek code to accumulate accesses to the same array

Working with Applications Code Development Team comprising Mrugesh and Jason

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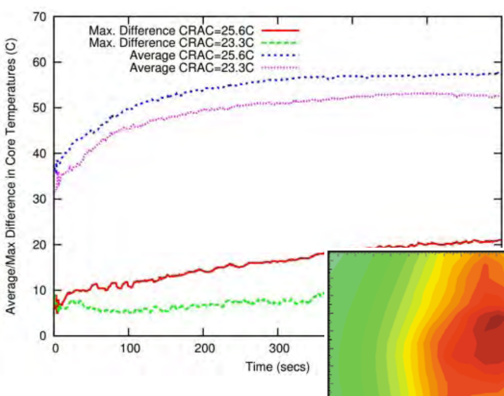
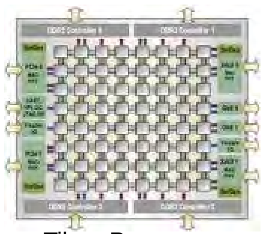
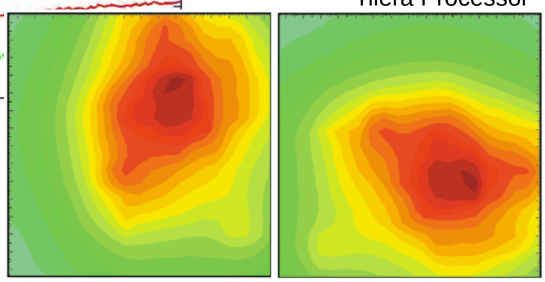
Managing Temperature

Temperature varies on multiple cores





Tilera Processor



[Sarood2011]

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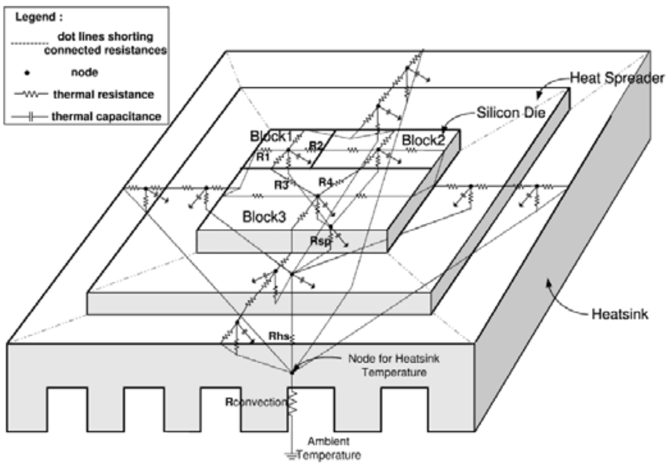
Modeling Thermal Behavior (HotSpot)



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Thermal models

	Core0	Core1	Core2	Core3
Core0	3.66	1.56	1.56	1.31
Core1	1.56	3.66	1.31	1.56
Core2	1.56	1.31	3.66	1.56
Core3	1.31	1.56	1.56	3.66

Steady-state thermal model

- $T(t) = T_A + G^{-1}P$
- Efficient but does not capture transient effects (worst case scenario)

Transient-state thermal model

- If the average power of core is *P* over a time period *t*, then the temperature at the end of this period *T(t)* is given by:
- $T(t) = T_A + e^{-G^{-1}Ct}(T_i - T_A) + G^{-1}(I - e^{-G^{-1}Ct})P$

  G is the thermal conductance matrix
  C is the thermal capacitance matrix
  T_A is the ambient temperature
  T_i is the initial temperature

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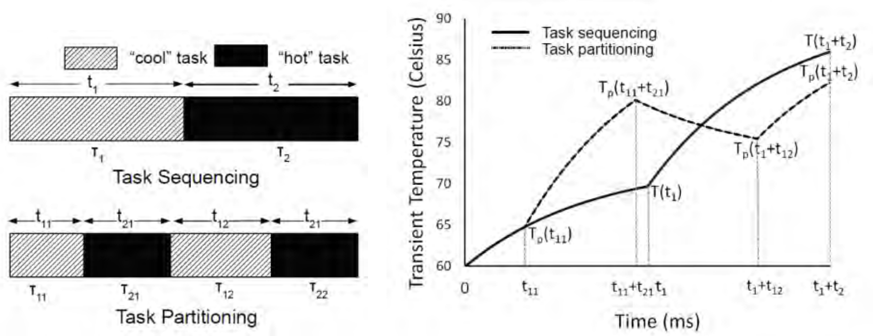
Thermal Optimization for Independent Workloads

Determine data parallel workloads distribution on multicore processor, so that the total throughput across all cores is maximized and the maximum temperature for any core is bounded by a given threshold

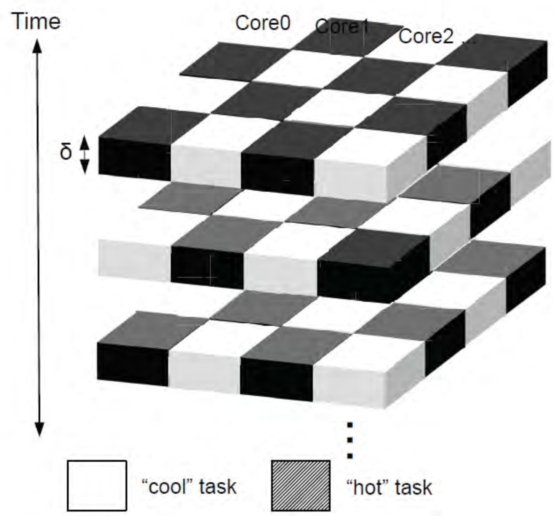
Temperature-aware task partitioning algorithm

Illustrative example



Task Partitioning Algorithm can achieve lower peak temperature than Task Sequencing Algorithm

Multi Core Scheduling



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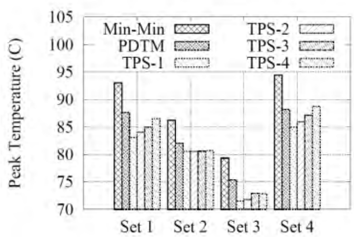
Experiments

- Platform:
  - CPU:
    - Simplescalar, ARM Cortex A9 (multicore)
    - 2-width out-of-order issue, 32KB instruction cache
    - 1.2GHz clock speed.
  - Power simulator:
    - Wattch
  - Temperature evaluation:
    - Temperature simulator: HotSpot
    - Ambient temperature: 45.15ºC
- Tasks:
  - Synthetic tasks and real benchmarks are used
- Algorithms:
  - Min-Min, PDTM [Yeo2008], TPS-1(δ=0.33ms), TPS-2(δ=0.66ms), TPS-3(δ=1.32ms), TPS-3(δ=2.64ms)

THE FOUR SETS OF BENCHMARK TASKS

set1	dijkstra, patricia, adpcm, crc32, fft gsm, ghostscript, cjpeg, blowfish, stringsearch, sha
set2	epic, unepic, rasta, epegwit, ifft dpegwit, ghostscript, dadpcm, ungsm blowfish, susan, basicmath
set3	dijkstra, adpcm, crc32, fft, gsm, rasta ghostscript, jpeg, patricia, rijndael blowfish, stringsearch, sha, epic, pegwit
set4	stringsearch, rasta, unepic, dadpcm, ifft susan, c, ghostscript, dpegwit, blowfish crc32, dijkstra, djpeg, sha



TPS algorithm reduce the peak temperature by up to 9.92oC compared with Min-Min algorithm, 4.52oC compared with PDTM algorithm.

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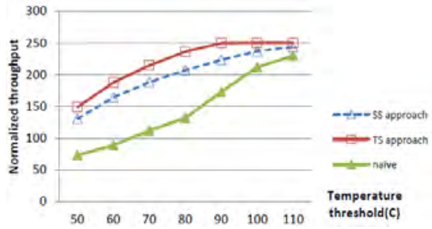
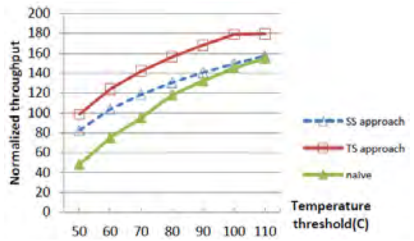
Schemes using Transient Models – Matrix Multiplication

General scheme



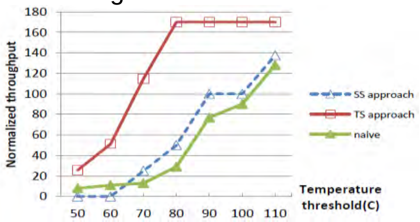
Homogeneous-scaling scheme



- High throughput improvement than w/o HLB
- Around 10% throughput improvement than base solution
- With very large workload, solutions of heuristic and base will converge

N

Non-scaling scheme



Hengxing Tan, and Sanjay Ranka, Thermal-aware Scheduling for Data Parallel Workloads on Multi-Core Processors, ISCC 2014 (Work partially supported by NSF)

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Conclusions

Thermal based approaches can highly improve throughput at a given temperature threshold.

Heuristics with transient thermal models can provide better improvements than methods with steady-state models albeit at a higher computational cost.

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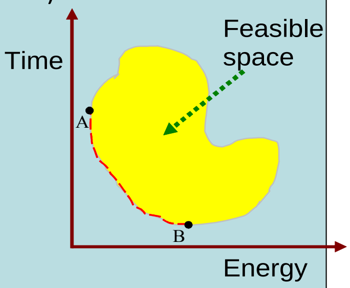
Future Work: Energy and Thermal Management

- Varying Architectural Elements
  - Processor (Dynamic Voltage Scaling)
  - Caches (Dynamic Cache Reconfiguration)
  - Buses
  - Memory
- Developing Optimized Libraries
  - Energy
  - Performance
  - Temperature



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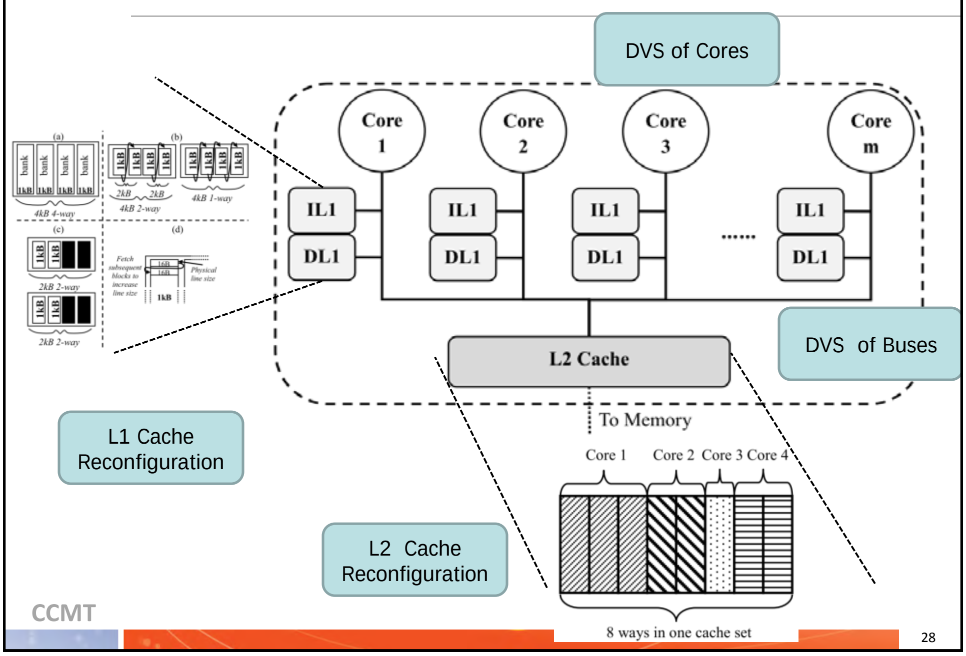
Performance, Energy and Thermal Levers



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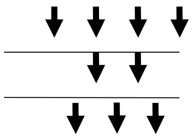
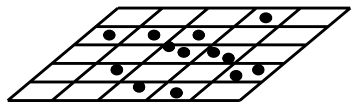
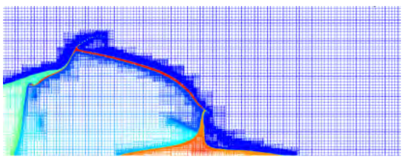
Load Balancing: Types of Adaptivity



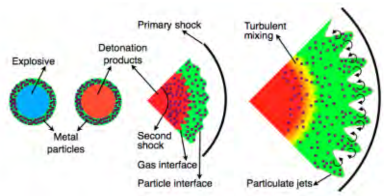
Extreme event UQ-driven
Computational steering



Preferential particle clustering
Lagrangian remap



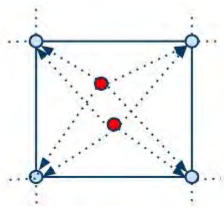
Adaptive mesh refinement



Computational power focusing

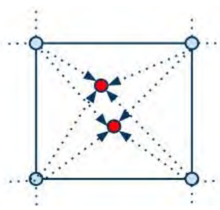
4 Phases of PIC algorithm

1. Charge Deposition Phase

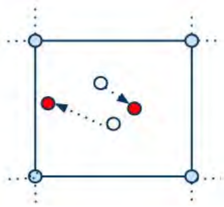


2. Field Solve Phase
- Compute the forces (Poisson equations) needed for particle motion from the accumulated particle charges

3. Force Gathering Phase

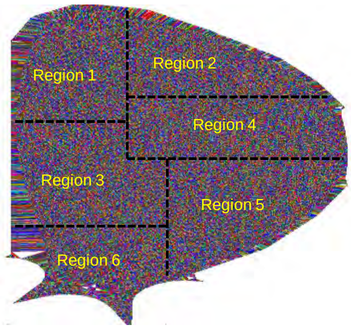


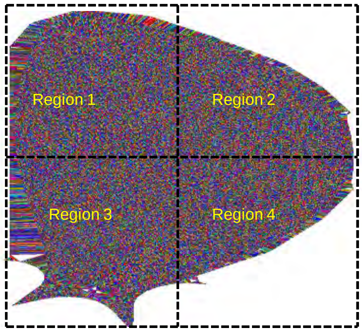
4. Particle push Phase



Triangular Meshes
- Irregular structure makes partitioning complex.
- Each particle requires a search to find the enclosing triangle
  - This step forms an additional **Search Phase** in the PIC algorithm flow
  - Search phase forms one of the time consuming steps in the PIC flow

Different Partitioning Approaches





- Ensures effective load balancing across regions
- Need to use a spatial indexing data structure like KD-tree to partition triangles
- KD-tree is not very well suited for GPU

- The virtual rectangular grid partitions the mesh into regions
- Load imbalance due to difference in triangle density
- The linear search for triangles can be a bottleneck

Fig: Mesh from ORNL used for XGC1 benchmarks

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Experimental Results

- Mesh from ORNL used for XGC1 benchmarks
  - 1.8 Million triangles
  - Randomly distributed 18 Million particles
  - Level 1 partitioning uses 32 X 32 rectangular grid (regions)
  - NVIDIA Tesla T10 GPU with 4GB global memory, 16k shared memory and 240 computing cores

Non-uniform partitioning

GPU blocks	Time (ms)
1024	12561.06
2779	7235.16
22471	989.88
33464	428.51

Uniform partitioning

GPU blocks	Time (ms)
4096	3111.11
9216	1366.21
16384	877.23
25600	609
36864	500.92
50176	427

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Conclusion

- Methodologies to Parallelize PIC on triangular mesh using GPUs
- Shadow entities (replication) provides a simpler and efficient solution
- Algorithms discussed are scalable with the size of mesh, number of particles and can be easily ported to a multi-GPU framework

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Selected Publications

- Hengxing Tan and Sanjay Ranka, Thermal-aware Scheduling for Data Parallel Workloads on Multi-Core Processors, Proceedings of 2014 IEEE ISCC 2014.
- Zhe Wang, Sanjay Ranka and Prabhat Mishra, Efficient Task Partitioning and Scheduling for Thermal Management in Multicore Processors, Proceedings of ISQED 2015.
- Zhe Wang and Sanjay Ranka, A Simple Thermal Model for Multi-core Processors and Its Application to Slack Allocation, Proceedings of International Parallel and Distributed Processing Symposium 2010, pp. 1-11.
- Weixun Wang, Prabhat Mishra and Sanjay Ranka, "*Dynamic Reconfiguration in Real-Time Systems: Energy, Performance, Reliability and Thermal Perspectives*", Springer, 2012
- Performance and Energy Benchmarking of Spectral Element Solvers, Tania Banerjee, Jacob Rabb, Sanjay Ranka (in preparation)
- A simple aggregate power modeling and predicting method on multi-core processors (in preparation)

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Power Modeling and Prediction on Multi-core Processors

Research a power modeling method to integrate power-aware factors including performance counters, architecture scaling factors and application workloads on multi-core processors

- Power consumption is modeled using an accumulated form with multiple input parameters over a set of components.
- Examples of components are CPU, memory, caches (L1, L2, L3)
- The overall power consumption then is formulated as:

  $P = \sum \alpha_i . f_i(X_i) + P_0$
- We determine the coefficients after a training session of sampling data

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Exascale Behavioral Emulation

Principal Investigators:

Dr. Alan George, Dr. Herman Lam, Dr. Greg Stitt

Student Project Leaders:

Nalini Kumar, Carlo Pascoe, Dylan Rudolph

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

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Outline

- Introduction
  - Integration: how different pieces fit
- Goal & approach
  - Behavioral emulation approach
- Overview of behavioral emulation
- Research thrusts & 1st year achievements
  - Behavioral emulation methodology
  - Performance modeling
  - Reconfigurable architectures
- Summary, conclusions, & future work

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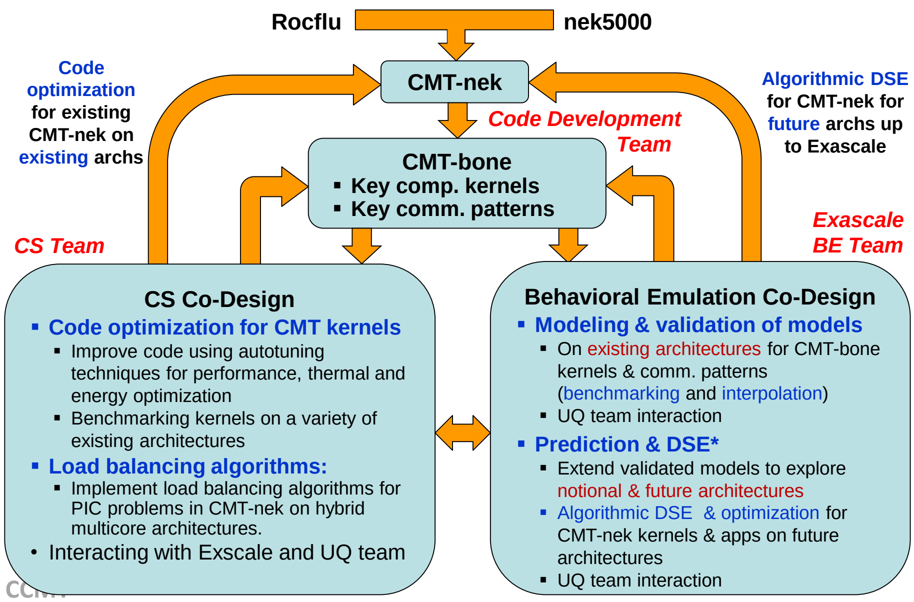
Integration – How Different Pieces Fit



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* DSE: Design Space Exploration | 38

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Goal

Develop ***behavioral emulation*** methods & tools to support:

- Co-design for algorithmic DSE
- Optimization of key CMT-nek kernels & applications

On future architectures, up to Exascale

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Approach: Behavioral Emulation

- How may we study Exascale before the age of Exascale?
  - **Analytical studies** – *systems are too complicated*
  - **Software simulation** – *simulations are too slow at scale*
  - **Behavioral emulation** – *to be defined herein*
  - **Cycle-accurate emulation** – *systems too massive & complex*
  - **Prototype device** – *future technology, does not exist*
  - **Prototype system** – *future technology, does not exist*
- Many pros and cons with various methods
  - We believe **behavioral emulation** is most promising in terms of balance of project goals (accuracy, speed, and scalability, as well as versatility)

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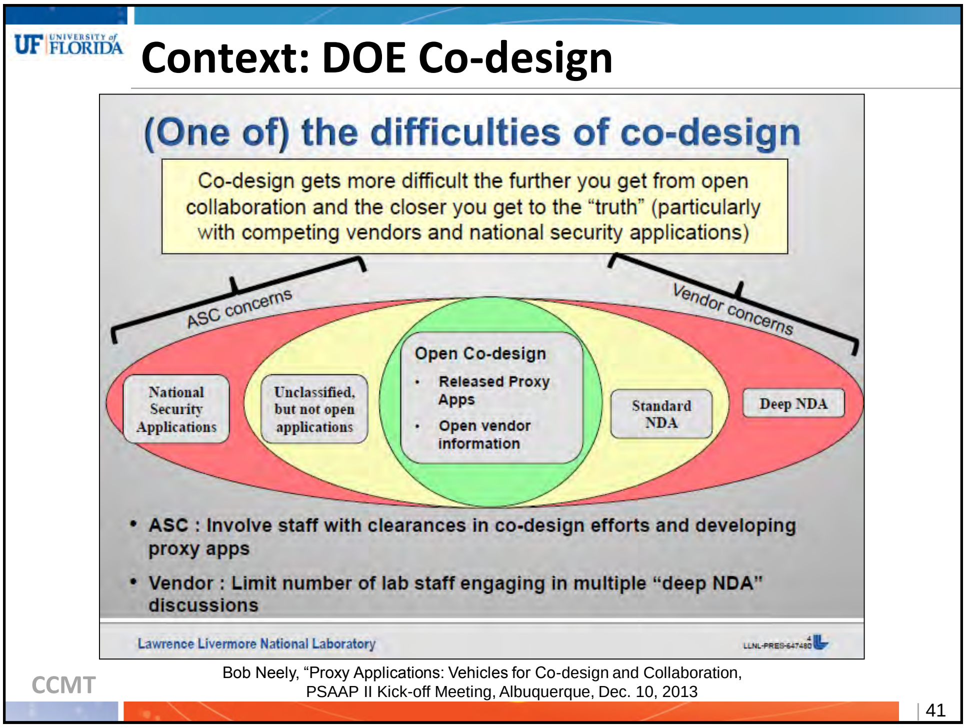
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Context: DOE Co-design
(One of) the difficulties of co-design
Co-design gets more difficult the further you get from open collaboration and the closer you get to the "truth" (particularly with competing vendors and national security applications)
ASC concerns
Vendor concerns
National Security Applications
Unclassified, but not open applications
Open Co-design
Released Proxy Apps
Open vendor information
Standard NDA
Deep NDA
• ASC : Involve staff with clearances in co-design efforts and developing proxy apps
• Vendor : Limit number of lab staff engaging in multiple "deep NDA" discussions
Lawrence Livermore National Laboratory
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Bob Neely, "Proxy Applications: Vehicles for Co-design and Collaboration,
PSAAP II Kick-off Meeting, Albuquerque, Dec. 10, 2013
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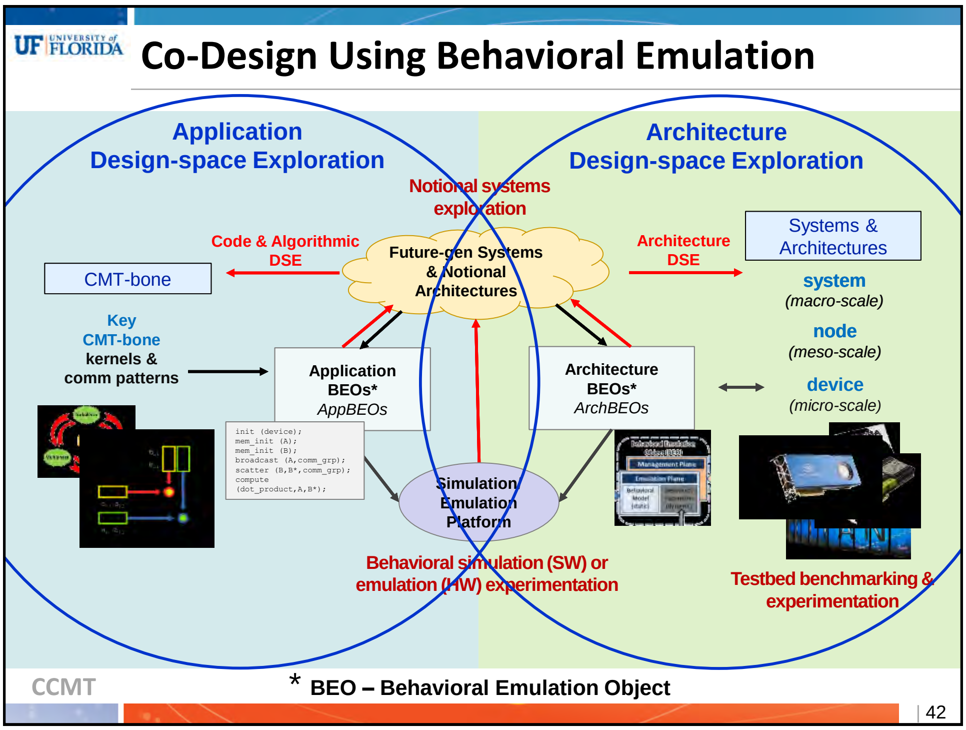
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Co-Design Using Behavioral Emulation
Application
Design-space Exploration
Architecture
Design-space Exploration
Notional systems exploration
Code & Algorithmic DSE
Future-gen Systems & Notional Architectures
Architecture DSE
Systems & Architectures
CMT-bone
system
(macro-scale)
node
(meso-scale)
device
(micro-scale)
Key CMT-bone kernels & comm patterns
Application BEOs*
AppBEOs
Architecture BEOs*
ArchBEOs
init (device);
mem_init (A);
mem_init (B);
broadcast (A,comm_grp);
scatter (B,B*,comm_grp);
compute
(dot_product,A,B*);
Simulation Emulation Platform
Behavioral simulation (SW) or emulation (HW) experimentation
Testbed benchmarking & experimentation
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* BEO – Behavioral Emulation Object
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Behavioral Emulation (BE)

- ***Component-based, coarse-grained*** **simulation**
  - Fundamental constructs called BE Objects (BEOs) act as surrogates
  - BEOs characterize & represent behavior of app, device, node, & system objects as fabrics of interconnected ArchBEOs (with AppBEOs) up to Exascale
- ***Multi-scale*** **simulation**
  - Hierarchical method based upon experimentation, abstraction, exploration
- ***Multi-objective*** **simulation**
  - Performance, power, reliability, and other environmental factors

	Apps	Arch	BEO Models
Macro Level	Skeleton-apps	***System*** BEO fabrics	▪ Models abstracted from Meso-scale ▪ Testbed experimentation in support ▪ Notional ***Exascale system*** exploration
Meso Level	Mini-apps	***Node*** BEO fabrics	▪ Models abstracted from Micro-scale ▪ Testbed experimentation in support ▪ Notional ***Exascale node*** exploration
Micro Level	Kernels	***Device*** BEO fabrics	▪ Architectural studies ▪ Testbed experimentation as foundation ▪ Notional ***Exascale device*** exploration

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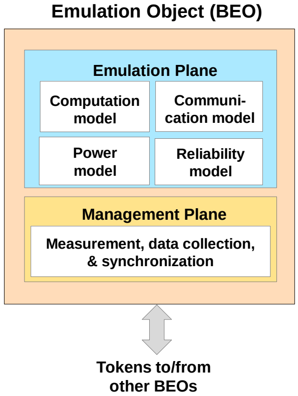
Fundamental Design of an Arch BEO

Arch BEO: *Abstract model (surrogate) of an architecture object*

- Basic primitive in BE approach to studies of Exascale systems

Architecture Behavioral Emulation Object (BEO)



Emulation Plane

- *Mimic* appropriate behavior of modeled object
- *Interact* with other BEOs via tokens to support emulation studies

Management Plane

- Measure, collect, and/or calculate *metrics and statistics*
- Support architectural exploration

Metrics

- *Performance factors* (execution time, speedup, latency, throughput, etc.)
- *Environmental factors* (power, energy, cooling, temperature)
- *Dependability factors* (reliability, availability, redundancy, overhead)

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Behavioral Emulation Tools

- Software PDES* behavioral simulator
  - Initial prototype: In-house developed SMP simulator
  - V2: Leverage existing PDES simulators (e.g., SST, ROSS)
- Hardware-accelerated behavioral simulator
  - FPGA-based reconfigurable computing
  - Leverage emerging reconfigurable supercomputing advances (e.g., UF's Novo-G, Microsoft's Catapult)

*PDES: parallel discrete-event simulator

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Research Thrusts

BE Modeling Research

1. **Behavioral Emulation Methodology**
   - How do we build, calibrate, then validate BEOs?
2. **Performance Modeling**
   - How do we efficiently & effectively model performance?
3. **Synchronization & Congestion**
   - How do we handle sync and congestion at scale?
4. **Resilience & Energy**
   - How do we extend BE methods to other attributes?

Platform Research

5. **Management & Visualization**
   - How do we measure & analyze massive systems & apps?
6. **Reconfigurable Architectures**
   - How do we exploit FPGA hardware for speed & scale?

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Research Thrusts

BE Modeling Research

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Platform Research

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6. **Reconfigurable Architectures**
   – How do we exploit FPGA hardware for speed & scale?

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BE Methodology Thrust

Motivation: Prototyping and validating BE models and simulation framework is essential before developing and optimizing framework for speed and scale

– Develop methods and confidence in BE before investing resources in tool development

Goal: Characterize processors, networks, apps, etc. with Behavioral Emulation Objects (BEOs)

– Explore and evaluate BEO types, structures, and interactions
– Gain insight into abstraction and representation of application behavior

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Application and Architectures BEOs

- AppBEO scripts are abstract representations of the application
  - AppBEO instructions trigger events for procBEOs
  - Whenever possible, event timestamps are generated pre-simulation
- ProcBEOs emulate a processing unit
  - AppBEO instructions are resolved by procBEOs
    - Initialization, computation etc. are internal events
    - Interaction with other BEOs are send/receive events
  - Update clock using performance models of internal events
- CommBEOs emulate network components
  - Send/receive event tokens to other BEOs
  - Update timestamp of each token at each hop

Pseudo-code for ProcBEO

```
if (init) {
   clock=clock+t_init}
if (mem_init){…}
if(compute_dot_product){…}
if(scatter){…}

        ...
```

```
if (input_buffer!=empty) {
   read_event;
   if(output_buffer !=full) {
      forward(x_dir, y_dir);
   }
}
        ...
```

CommBEO model of iMesh switch

```
Topology: 2D mesh
Routing policy: dim-order
Routing policy: cut-through
X-dir latency: testbed data
Y-dir latency: testbad data
Arbitration: round-robin
     ...
```

Network configuration parameters for TILE-Gx36 iMesh

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Overview: Behavioral Emulation Workflow

Calibration

- BEOs: computation & communication
- Performance models
  1. Sample on target platforms for interpolation
  2. Use Kriging method for multi-dim interpolation
  3. Evaluate & recalibrate, if necessary

Validation

- Microbenchmarks
  - Computation
  - Communication
- Kernels
  - 2D matrix multiply
  - Sobel filtering
  - CMT-nek kernel
- Platforms
  - Tile-Gx36

Prediction

- Kernels on
  - Next-gen Tile-Gx72
- Kernels on
  - Notional mesh devices with XeonPhi, 64-bit ARM, Power8 processors

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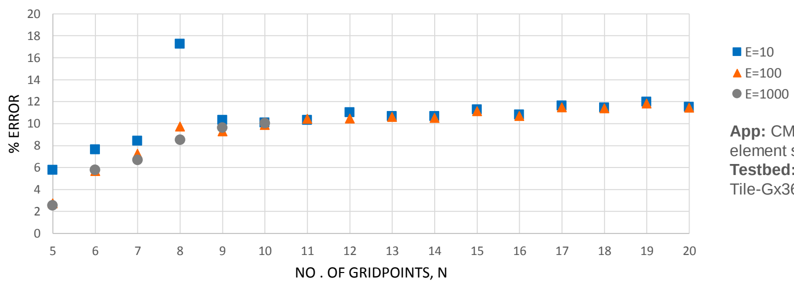
Emulation of Existing Devices

Spectral element solver for partial derivative calculation is the most expensive kernel in CMT-nek

- Large number of small 3D matrix – 2D matrix multiplication (ExN^3xN^2)
- Nearest neighbor updates using pairwise exchanges (ExN^2 words/transfer)
- Calibration data from existing mesh-device was used for developing performance models for ProcBEOs and CommBEOs
  - For E=1000, the device runs out of memory past N=10
- Reasonable error in simulation, in-line with validation results presented earlier (mid-year review and Deep dive)

Validating BE simulations against testbed



App: CMT-nek spectral element solver, **Testbed:** 16 cores on Tile-Gx36

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Emulation of Future/Notional Devices

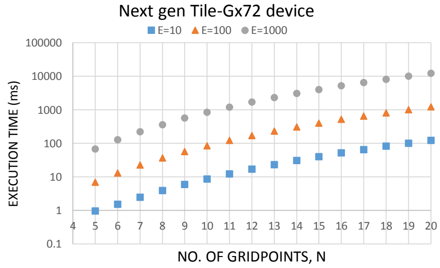
With some confidence in Behavioral Emulation approach we can proceed to study *next-generation devices*

- Ability to evaluate what-if scenarios by changing BEOs parameters

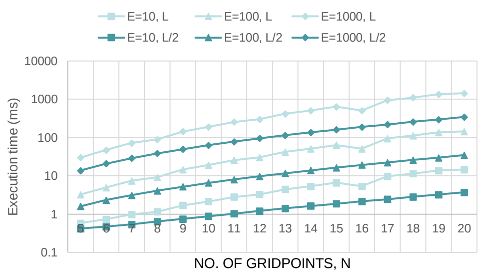
Case studies:

- Tile-Gx72 – largest existing mesh-device from Tilera
- Notional mesh-based processors with Intel Xeon Phi, IBM Power8, and 64-bit ARM cores

Next gen Tile-Gx72 device



Notional Mesh Device with 72 XeonPhi cores



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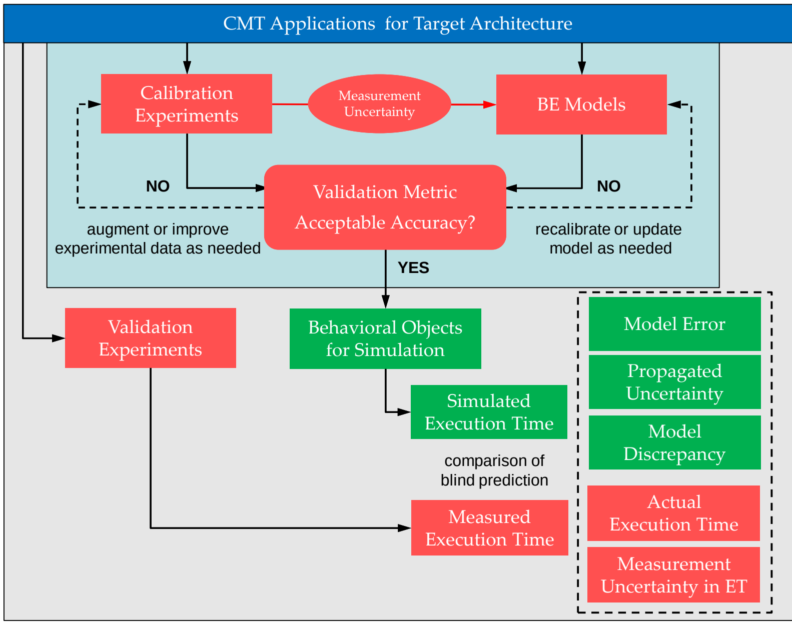
BE Model Validation Framework



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Summary: BE Methodology

- Year 1 achievements
  - Designed, calibrated, and validated architecture BEOs and BE methods
  - Designed application BEOs for key CMT-nek kernels and other kernels (2D matrix multiply, Sobel filtering)
  - Designed Lamport clock based PDES framework and prototyped a multi-threaded simulator prototype
- Interactions with other CCMT teams
  - Code-development team for AppBEO modeling of key CMT-nek kernels
  - CS team for platform data for performance modeling
  - UQ team
- Year 2 plans
  - Extend and modify BE framework for (a) communication modeling and (b) modeling applications and architectures beyond device level

* **Friday Presentation**: *Scalable Network Simulation*, Nalini Kumar

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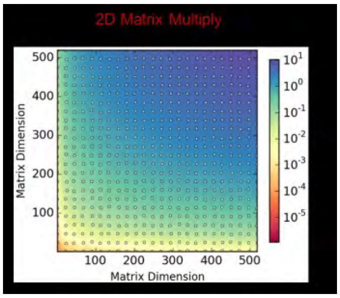
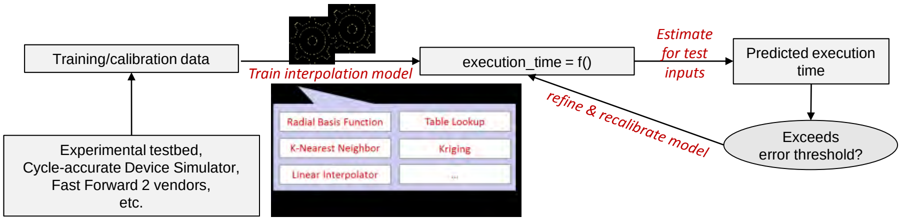
Performance Modeling Thrust

- **Motivation**: BE requires performance estimates for a set of kernels on multiple processing resources
  - Used to update timestamps of simulation events
- **Goal:** Use calibration data to build interpolation models that predict execution time – i.e., *performance models*
  - Sample execution time for small % of input space
  - Use interpolation to predict time for any input
  - Difficult due to multidimensional inputs





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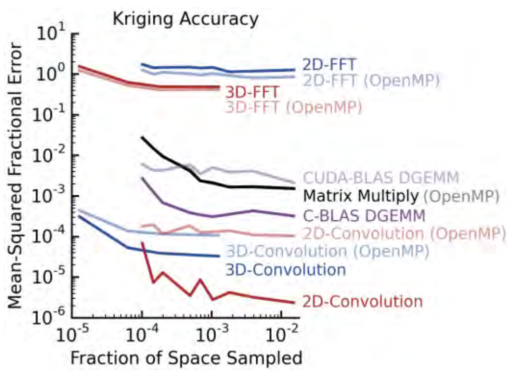
Performance Modeling: Results

- **Approach:** Use Kriging for multi-dimensional interpolation

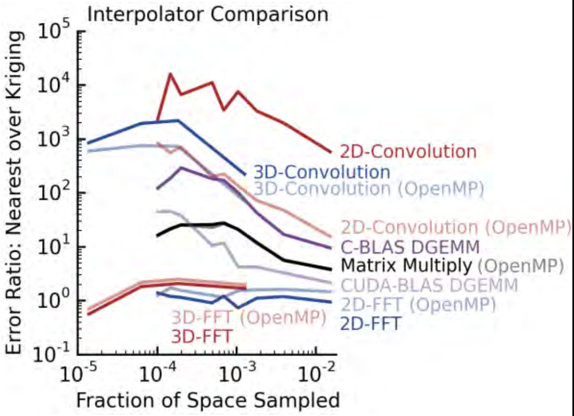
Multi-Dimensional Benchmarks
(Two and Three Input Parameters)



Performance Modeling: Results

Accuracy of Kriging versus Nearest-Neighbor

- Kriging outperforms nearest-neighbor interpolation in (most) all cases (values greater than unity)
- There is little or no improvement for FFT
- For the high-algorithmic-complexity algorithms, Kriging is much better
- Kriging has a better improvement for more sparse sampling



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Summary: Performance Modeling

- Year 1 achievements
  - Determined absolute accuracy of Kriging (as a performance model) for various sample densities
  - Produced an initial set of benchmarks for use in performance modeling research
- Year 2 plans
  - Evaluate Kriging for modeling different system attributes (network parameters, power, etc.)
  - Explore alternative interpolation techniques and determine tradeoffs in speed and accuracy
  - Explore extensions to Kriging which may allow better prediction for difficult cases (e.g., FFT)

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Reconfigurable Architecture Thrust

Motivation: Behavioral emulation (BE) approach attempts to manage exascale complexity via abstraction

- ProcBEOs (micro, meso, macro levels)
- AppBEOs (different kernel granularities)
- Is abstraction enough for exascale?

Goal: Research & develop hardware-accelerated simulator (NGEE) to scale behavioral emulation up to exascale while maintaining required performance

- Explore methods of mapping BEOs onto systems of reconfigurable processors
- Investigate use of large-scale reconfigurable supercomputing, RSC (e.g., Novo-G#, next-gen RSC) in simulation of exa/extreme-scale systems

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NGEEv1 Performance Comparison: 3 Data Points

Tile 6x6	Simulated Time	Prediction Error (Consistent with SMP results)	FPGA Simulation Time†	SMP Simulation Time#
			Speedup	
2D MM 1024x1024 across 36 cores	2.82×10^6 us	-0.35%	3.57×10^1 us	3.41×10^3 us
			~96x	
CMT SES* 20x20x20 100 elements/core across 16 cores	1.23×10^6 us	-11.46%	3.44×10^1 us	2.69×10^3 us
			~78x	

Next-gen

Tile 9x8	Simulated Time	Prediction Error (Consistent with SMP results)	FPGA Simulation Time†	SMP Simulation Time#
			Speedup	
2D MM 1024x1024 across 72 cores	1.66×10^6 us	To be determined	8.11×10^1 us	7.21×10^3 us
			~89x	
CMT SES* 20x20x20 100 elements/core across 72 cores	1.23×10^6 us	To be determined	1.41×10^2 us	1.27×10^4 us
			~90x	

Anticipated

KNL 9x8	Simulated Time	Prediction Error (Consistent with SMP results)	FPGA Simulation Time†	SMP Simulation Time#
			Speedup	
2D MM 1024x1024 across 72 cores	5.87×10^5 us	To be determined	8.11×10^1 us	7.21×10^3 us
			~89x	
CMT SES* 20x20x20 100 elements/core across 72 cores	1.44×10^5 us	To be determined	1.41×10^2 us	1.27×10^4 us
			~90x	

*Spectral Element Solver #Quad Core Intel Xeon E5620 †Quad Core Intel Xeon E5620 + GiDEL ProceV

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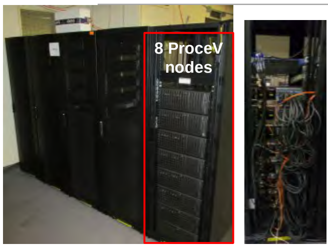
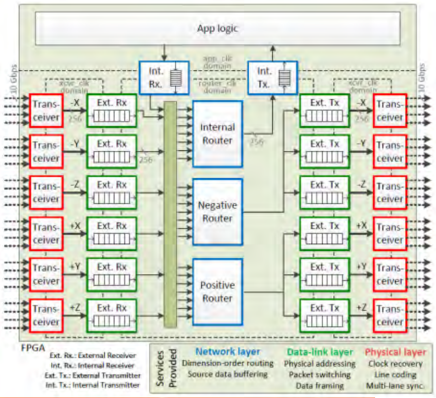
Novo-G#: Reconfigurable, 3D Interconnect for Novo-G



Novo-G# (Novo-*jee*-sharp)

Novel R&D & infrastructure - central and critical to FPGA approach of hardware simulation

- 32 GiDEL ProceV (Stratix V D8), soon to be 64
- 4x4x2 3D torus or 5D hypercube, soon to be 4x4x4
- 6 Rx-Tx links per FPGA, 40 Gbps per link
- Three-layer protocol based on Interlaken
  - CRC32, 64B/67B encoding, multi-lane sync



Acceleration of communication-intensive apps

- Provides support for multi-dimensional FPGA-based apps through three-layer network stack
- Less than 10% memory & logic utilization
- Communication-intensive 3D FFT kernel predicted to show 20x speedup over BG/Q (model validated against Anton and against 2x2x2 Novo-G# hardware)

3D FFT+IFFT kernel execution times (µs)

FFT size	System size						
	2x2x2	2x4x2	2x4x4	4x4x4	4x4x8	4x8x8	8x8x8
16x16x16	3.934	3.669	3.805	4.513	5.203	5.947	-
32x32x32	19.68	14.57	9.897	7.461	6.707	6.935	8.257
64x64x64	147.6	107.6	61.75	39.25	25.52	16.11	12.64
128x128x128	1171	844.4	482.4	298.1	173.9	108.6	65.11

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Scalability Studies & Projections

Definitions:

- Emulation system: Behavioral emulation platform such as *Novo-G#*
- Emulated system: *appBEOs* (e.g., modeling CMT app) stimulating *archBEOs* (e.g., modeling Blue Gene/Q)

Open questions to be answered in the future:

- For a given emulation system architecture (e.g., #FPGAs, BEO core density, core design, interconnect arch, etc.), what are the limits of an emulated system?
  - Including size (e.g., #BEOs) and emulation performance
- For given requirements of an emulated system (e.g., macro-scale emulation with Blue Gene/Q), what emulation system resources are necessary?
  - Including #FPGAs, core density, interconnect arch, etc.

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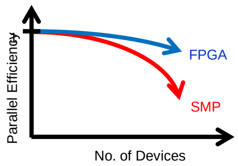
Potential Scalability Measure

Objective:

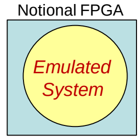
- Compare scalability(HW) vs scalability(SW)
  HW: hardware approach; SW: software SMP approach

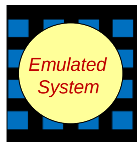


Potential Scalability Measure for HW

- Ideally entire system is on single large FPGA; thus, communication between BEOs is at on-chip rate
  Baseline:
  – Validated BE model for single-FPGA performance **(PfS)** of NGEE (i.e., BE model of FPGA running other BE models)
- Scalability issues arise when BEOs communicate across FPGAs
  – Off-chip communication much more costly
  Approach
  – Validated BE model for multiple-FPGA performance **(PfM)** of NGEE (possible after multi-FPGA experiments)

Notional FPGA





Potential Scalability Measure SM(HW) = PfS/PfM

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Summary: Reconfigurable Architecture

- Year 1 achievements
  – Working single-FPGA prototype (NGEEv1) with max-resource implementation & management plane (no optimization)
  – Beginning stages of performance optimization & scalability evaluation
  – Initial planning for next NGEE design (NGEEv2)
- Year 2 plans
  – Prototype NGEEv1 platform operating on multiple FPGAs
  – Extend SMP simulator performance comparison with NGEEv1 to new set of system architectures e.g.,
    - Anticipated Intel Xeon Phi KNL
    - New CMT-nek centric app case studies
  – Upgraded Novo-G# (4x4x4 torus) supporting BE
  – Updated scalability experiments on Novo-G# incorporating results from multi-FPGA experiments

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Conclusions: BE Modeling Research

- First-year accomplishments:
  - Demonstrated successful device-level calibration, validation, & prediction
  - On existing (Xeon Phi, Tilera) & notional devices
- Going forward
  - Extend methodology beyond device level (node, system)
  - Abstraction, scalable synchronization and congestion issues

❖ **CMT-centric**
  - **CMT kernel, proxy apps (CMT-bone)**
  - **Questions to be answered** for application design-space exploration ("knobs" for tunable design parameters)

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Conclusions: CMT Questions for BE

- BE for notional architectures to guide:
  - Cache-optimized order of DG-SE operations
  - Eulerian-to-Lagrangian interpolation and Lagrangian-to-Eulerian projection algorithms and strategies
  - Thermodynamic state and transport properties (tabulate or re-compute?)
  - Inter-element communication strategy for immersed boundaries
- CMT-bone optimizations on existing platforms:
  - Element count N vs polynomial order P
  - Distribution of particles across elements, cores
  - Mapping of elements across nodes and cores
  - Graph selection (nearest-neighbor vs crystal router)

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Conclusions: Platform Research

- First-year accomplishments:
  - Software PDES simulator
    - Proof of concept prototype: in-house developed SMP simulator
  - Hardware-accelerated simulator
    - Single-FPGA prototype: feasibility study with promising results
- Going forward
  - Software PDES simulator
    - V2: Leverage existing PDES simulators (e.g., SST, ROSS)
  - Hardware-accelerated simulator
    - Extend to multiple FPGAs on Novo-G#
    - Leverage emerging reconfigurable supercomputing advances (e.g., IBM's CAPI coherent accelerator interface, Microsoft's Catapult, Micron's HMC)

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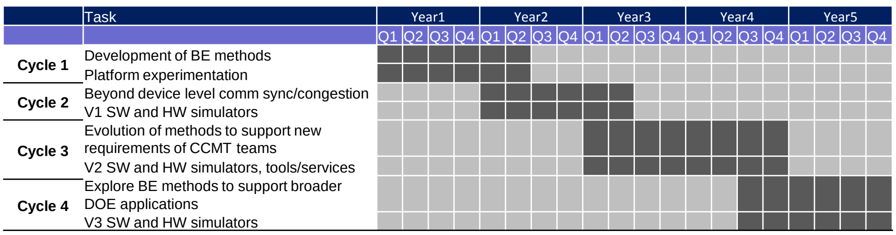
Exascale Behavioral Emulation



Cycle 1:
- **BE concepts and methods:** App BEOs (CMT-bone), Arch BEOs (device level), interpolation techniques for computation
- **Tools:** Prototype SMP software (SW) simulator for device-level studies & lessons learned; experimentation with single-FPGA hardware (HW) simulator

Cycle 2:
- **BE concepts and methods:** Emphasis on beyond device level; communication (synchronization, congestion); focus only on CCMT apps
- **Tools:** V1 SW simulator (leverage other useful simulators) & V1 HW simulator (scalable design); enable early use of simulators for design-space exploration for CCMT researchers

Cycle 3:
- **BE concepts and methods:** Evolution of methods and techniques to support new requirements of CCMT teams
- **Tools:** V2 SW and HW simulators; libraries of arch & app BEOs; more mature services and tools: management, monitoring, reporting, visualization

Cycle 4:
- **BE concepts and methods:** Evolution of methods and techniques to support requirements of new requirements of CCMT teams; Began exploration of using behavioral emulation for other key DOE mini-apps and future architectures
- **Tools:** V3 SW and HW simulators

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Do you have any questions?

Posters:

1. Nalini Kumar, Behavioral Emulation Methodology for Fast Design Space Exploration
2. Carlo Pascoe, NGEE: Novo-G Exascale Emulator
3. Dylan Rudolph, Kriging-Based Performance Modeling

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Uncertainty Budget

Validation and Uncertainty Reduction

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

UF UNIVERSITY of FLORIDA

NNSA

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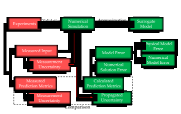
Interaction with Other Teams



Simulation validation and UQ

S. Balachandar
Thomas L. Jackson
Bertrand Rollin
Angela Diggs

Macro/Meso Simulation

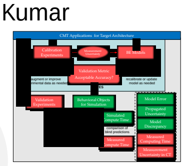
Micro Simulation

Siddharth Thakur

Exascale

BEO validation and UQ

Herman Lam
Dylan Rudolph
Carlo Pascoe
Nalini Kumar



Computer Science

Tania Banerjee

V&V and UQ

Meso Experiment (ASU)

Ronald Adrian
Heather Zunino

Meso Experiment (SNL)

Justin Wagner

Macro/Meso /Micro Exp. (Eglin)

Donald M. Littrell
Charles M. Jenkins

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Outline

- Simulation validation and UQ framework
- Mesoscale validation and UQ (shock tube)
- Simulation verification and modeling support
- BEO validation and UQ framework
- Extrapolation

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Objectives

- In order to validate the prediction capability of the demonstration problem
  - Define measurable quantities of interest including extreme events
  - Validate the prediction capability with metrics
  - Establish appropriate uncertainty quantification and reduction frameworks

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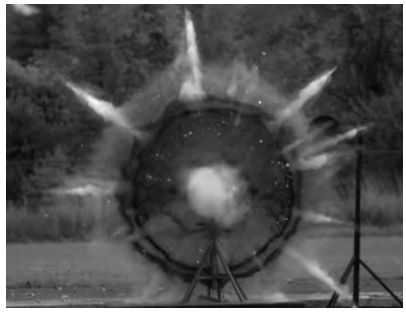
Validation of the CMT Simulation



- Evaluating model errors of the CMT simulation for prediction metrics
  - particle front location
  - shock location
  - number of fingers
  - finger lengths
- Uncertainty quantification and reduction

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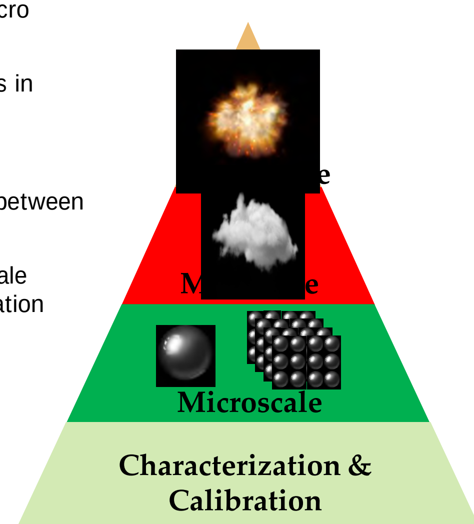
Hierarchical UQ & Validation

- Various physics models in the macro simulation
- Validating specific physical models in meso and micro scales
- UQ as verification aide
- Error and variability propagation between scales
- Identify relations between sub-scale validations and macro scale validation



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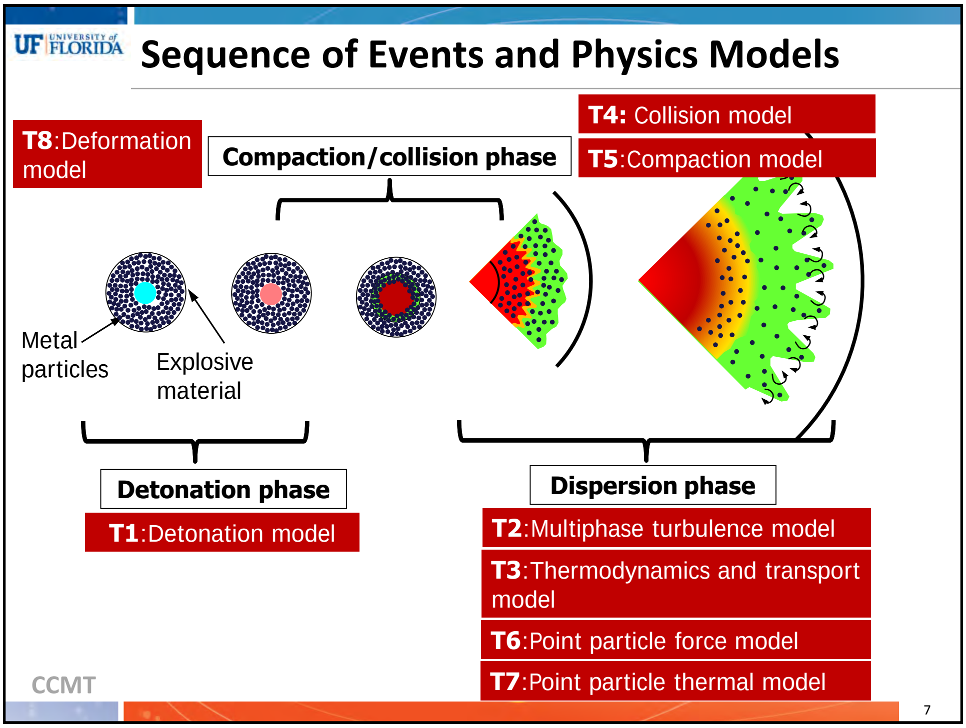
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Sequence of Events and Physics Models
T4: Collision model
T5: Compaction model
T8: Deformation model
Compaction/collision phase
Metal particles
Explosive material
Detonation phase
T1: Detonation model
Dispersion phase
T2: Multiphase turbulence model
T3: Thermodynamics and transport model
T6: Point particle force model
T7: Point particle thermal model
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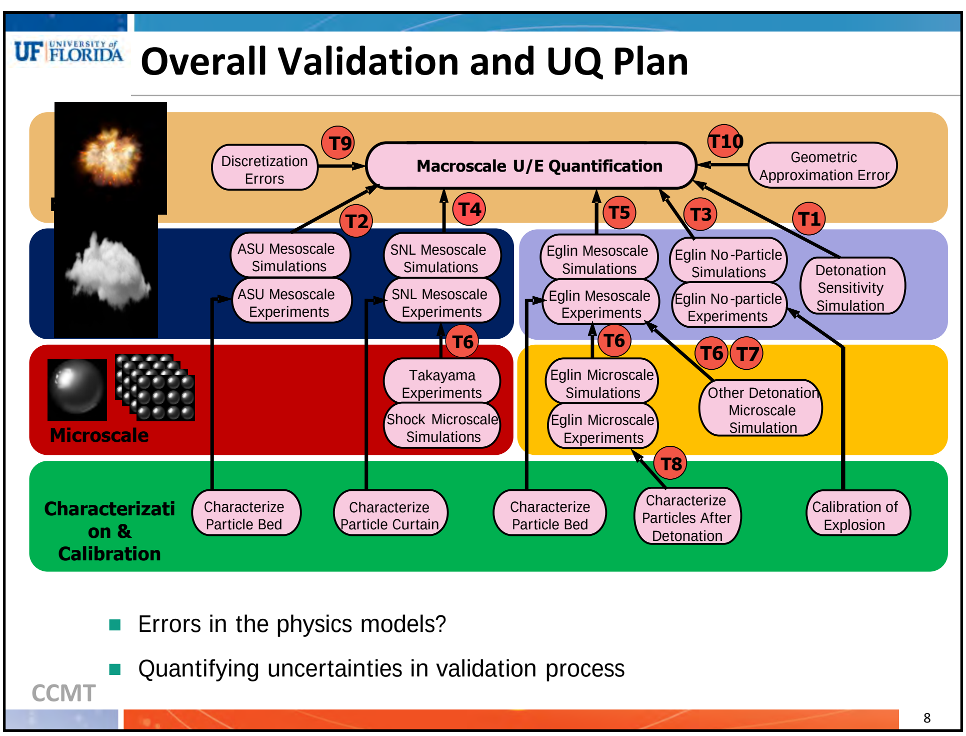
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Overall Validation and UQ Plan
Discretization Errors
T9
Macroscale U/E Quantification
T10
Geometric Approximation Error
T2
T4
T5
T3
T1
ASU Mesoscale Simulations
SNL Mesoscale Simulations
Eglin Mesoscale Simulations
Eglin No-Particle Simulations
Detonation Sensitivity Simulation
ASU Mesoscale Experiments
SNL Mesoscale Experiments
Eglin Mesoscale Experiments
Eglin No-particle Experiments
T6
T6
T6
T7
Takayama Experiments
Shock Microscale Simulations
Eglin Microscale Simulations
Eglin Microscale Experiments
Other Detonation Microscale Simulation
Microscale
T8
Characterization & Calibration
Characterize Particle Bed
Characterize Particle Curtain
Characterize Particle Bed
Characterize Particles After Detonation
Calibration of Explosion
Errors in the physics models?
Quantifying uncertainties in validation process
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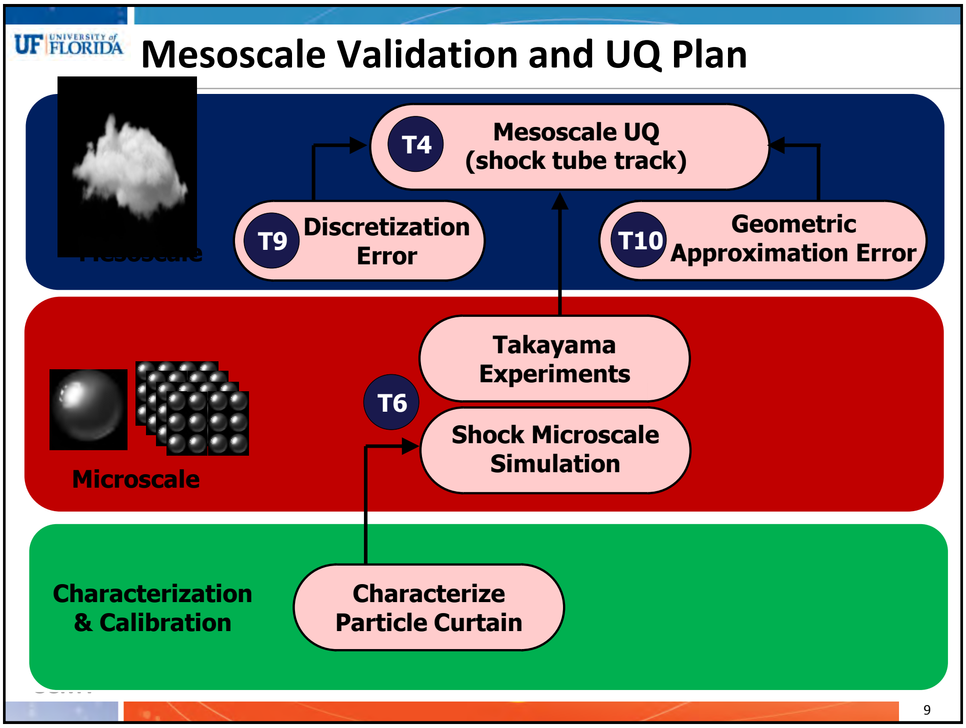

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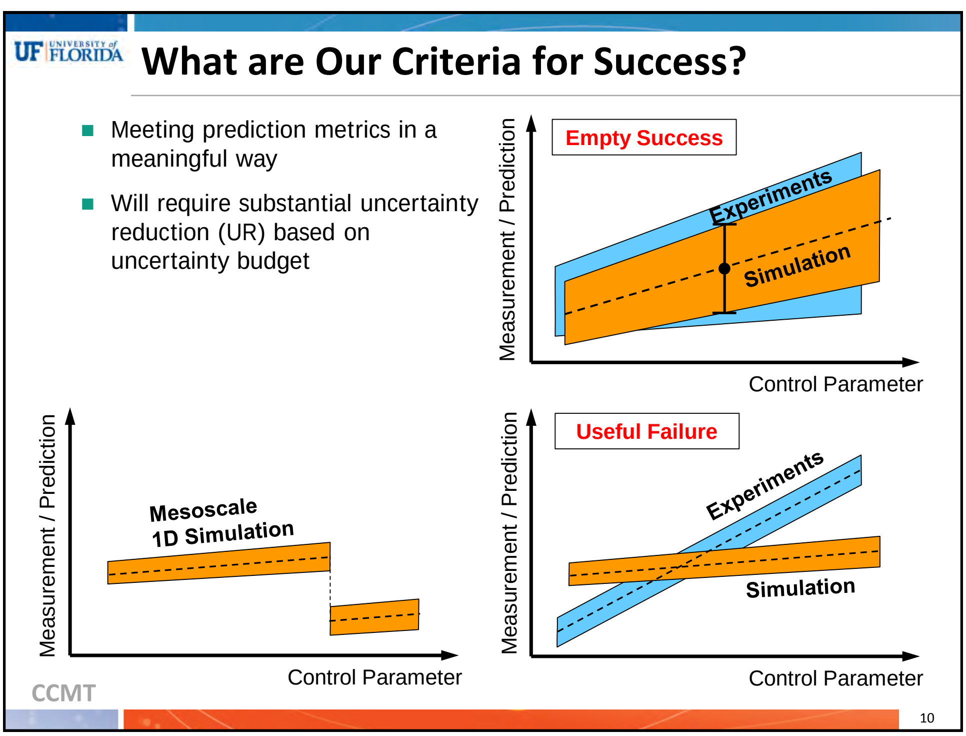
Mesoscale Validation and UQ Plan
T4
Mesoscale UQ
(shock tube track)
T9
Discretization
Error
T10
Geometric
Approximation Error
Takayama
Experiments
T6
Shock Microscale
Simulation
Microscale
Characterization
& Calibration
Characterize
Particle Curtain
9



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What are Our Criteria for Success?
Meeting prediction metrics in a meaningful way
Will require substantial uncertainty reduction (UR) based on uncertainty budget
Empty Success
Experiments
Simulation
Measurement / Prediction
Control Parameter
Mesoscale
1D Simulation
Measurement / Prediction
Control Parameter
Useful Failure
Experiments
Simulation
Measurement / Prediction
Control Parameter
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Uncertainty Budget – Backbone of CCMT

- Periodic experiments and simulations of *"Demonstration Problem"* essential to establish uncertainty deficit
- Determine contributions of various errors to uncertainty
  - Computational challenge of propagating uncertainty within and between levels by extensive use of surrogates
- Prioritize based on potential for reducing uncertainty
  - Improvements in physical models
  - Improvements in numeric
  - Improvements in experimental procedure/measurements
- Essential for achieving accuracy targets here and at NNSA

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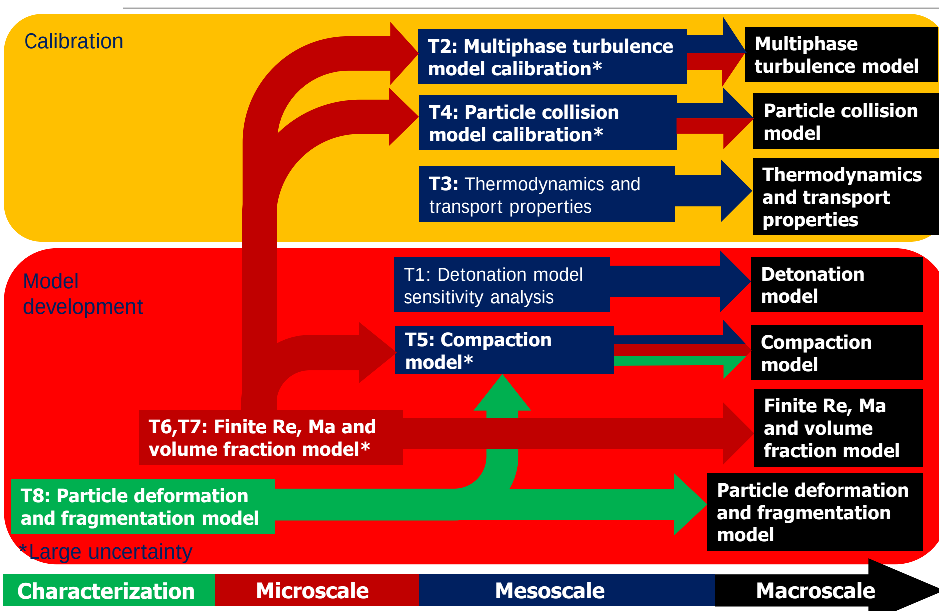
Across-scale Uncertainty Propagation



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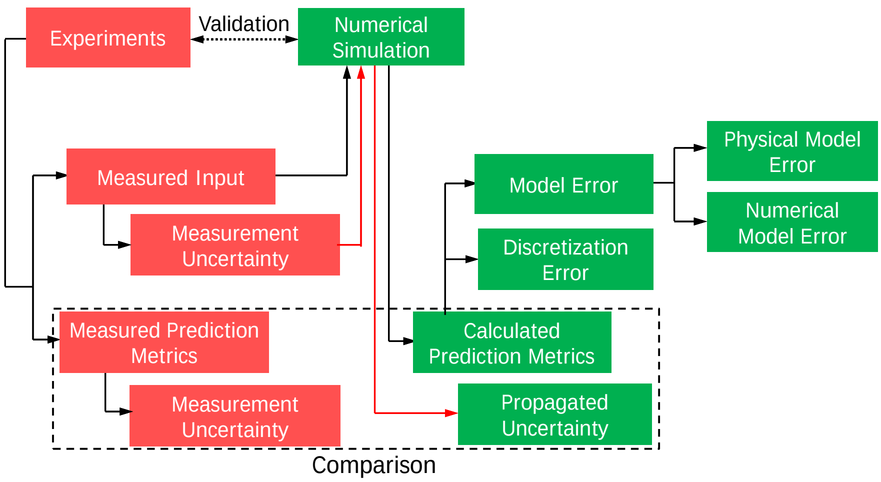
Validation and UQ Framework



- Estimating model errors by comparing measured PMs and calculated PMs based on UQ

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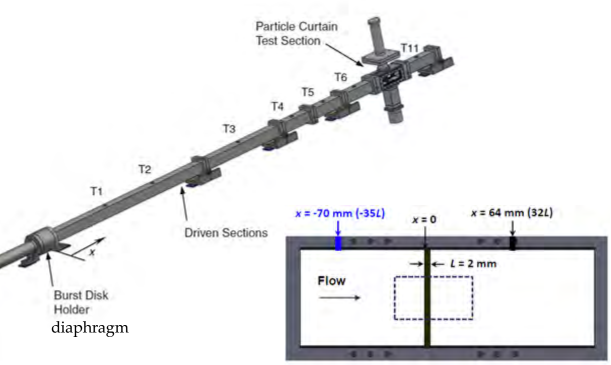
Shock-particle Interaction Model Validation



- Estimating the errors in the collision model (T4) and the particle force model (T6) for simulating gas and particles interaction by quantifying discretization error (T9) and the experiment uncertainty (T10)
- Experiments of Justin Wagner (SNL)
- 1D Simulation (Rocflu Lite)

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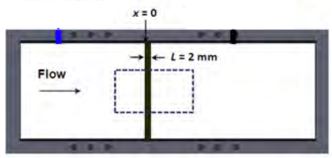
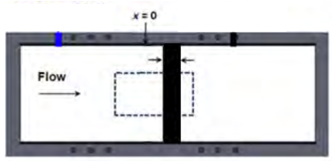
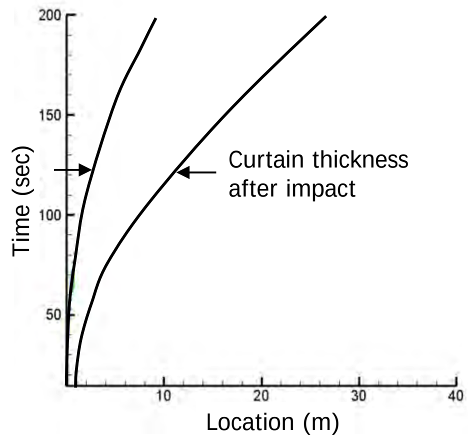
Prediction Metric

- Before impact



- After impact





- **Prediction Metric:** The locations of the particle curtain edges at upstream and downstream
  - Location vs. time

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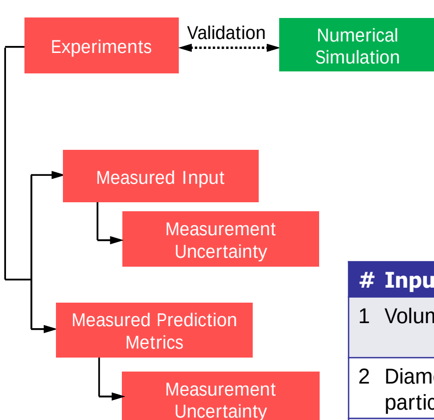
Key Uncertainties and Prediction Metrics



#	Prediction Metrics	Uncertainties in Prediction Metrics
1	Particle curtain location	Large measurement noise
2	Pressure curve	Very small measurement noise
⋮	⋮	⋮

#	Inputs	Uncertainties in Inputs
1	Volume fraction	Measurement error (21%±2%) Local variation in particle curtain
2	Diameter of particle	Errors in distribution type / parameters
3	Particle curtain thickness	Variation in particle curtain thickness
4	Pressure at driver section P	Very small measurement noise
	⋮	⋮

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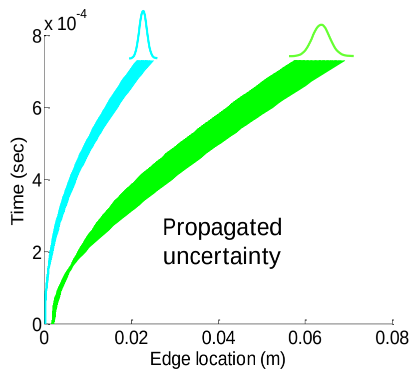
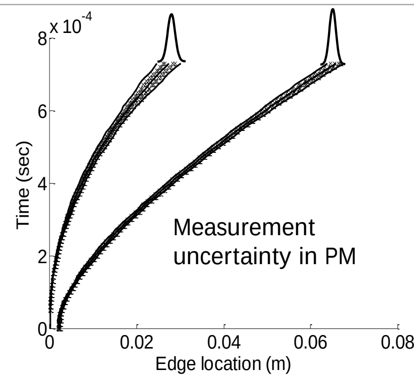
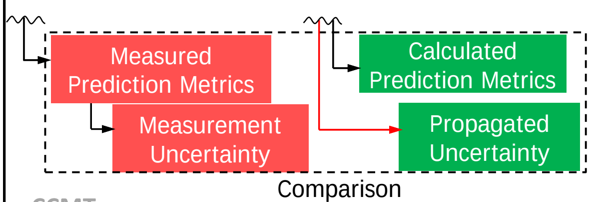
Uncertainty Quantification (1D)







- Measurement uncertainty from 4 repeated experiments (SNL)
- Surrogate model was used for getting propagated uncertainty

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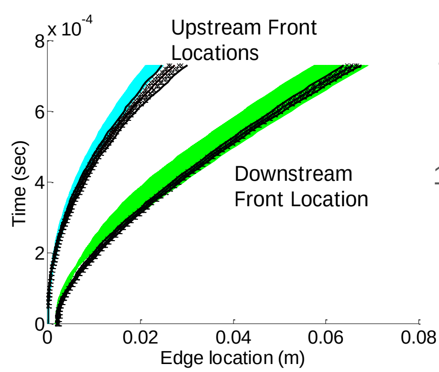
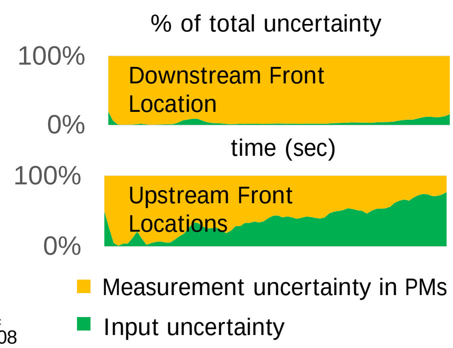
Model Error and UB (1D)





- Propagated uncertainty from the input uncertainty and the measurement uncertainty in PMs (particle curtain edge locations)
- Reducing the input uncertainty is the efficient way to reduce the uncertainty in the discrepancy
- The influence of reducing the measurement uncertainty in PMs is limited for UFL

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Collaborations with the Physics Team

- Modeling support and verification of JWL-EOS in the Macroscale simulation (T3)
- Quantifying and reducing noise in the Mesoscale simulation solution (T4)
- Modeling the drag force kernels from the Microscale simulation (T6)

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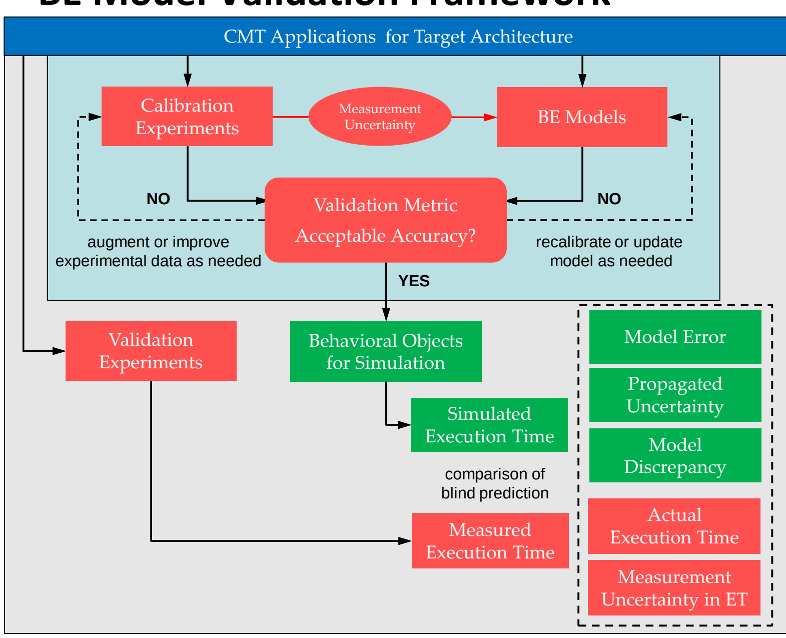
BE Model Validation Framework



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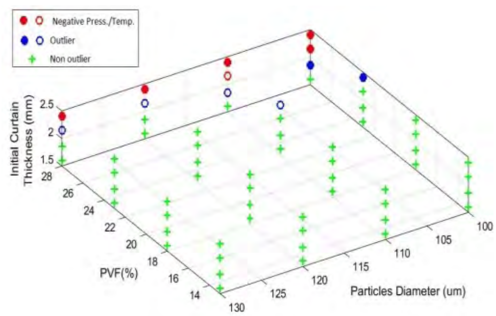
Applicable Region of 1D Simulation



- Sampling reveals the inapplicable region of the mesoscale 1D simulation (validation)
- Negative pressure solutions and outliers were observed
- Extrapolation requires for a prediction at point in the inapplicable region

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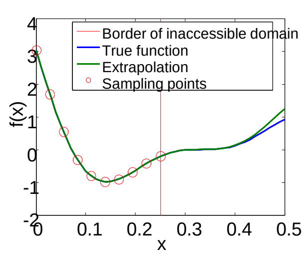
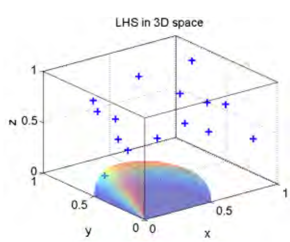
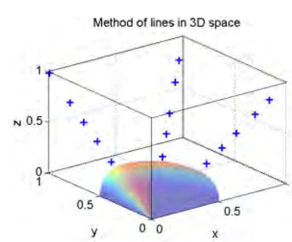
Method of Converging Lines

- Extrapolation at a point using 1D surrogates
  - Transform multi-dimensional extrapolation to 1D extrapolations
  - Consistency check based on multiple 1D extrapolations
  - Develop strategies for making good extrapolations with 1D surrogates and combining multiple extrapolations







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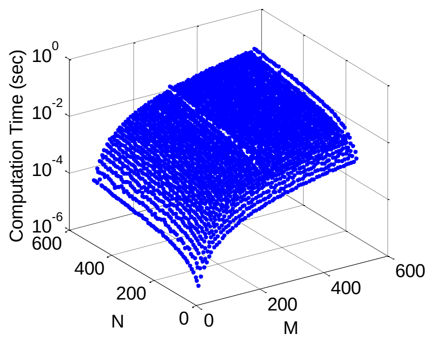
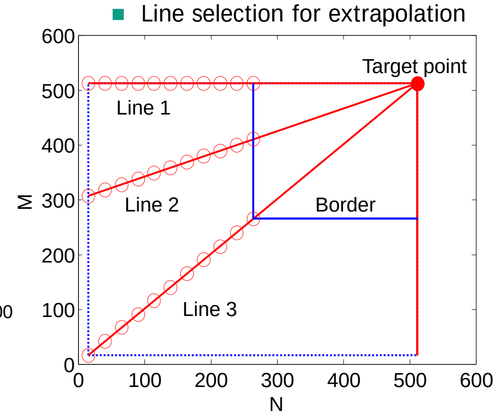
Extrapolation for an Exascale Application

- Matrix multiplication function
  - Basis for predicting computational cost of numerical analysis
  - Extrapolation based on data with strong noise (UQ)

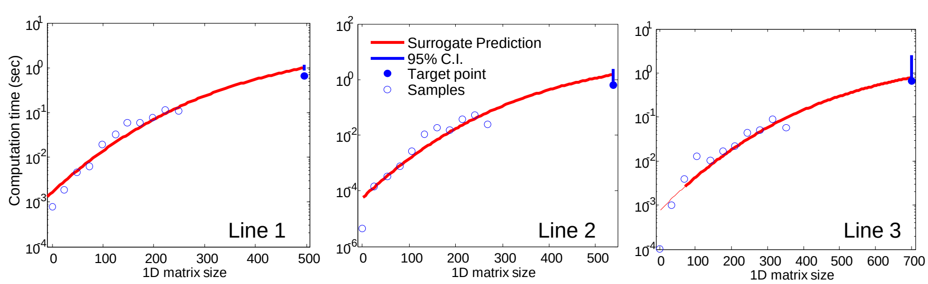
- Function in accessible domain



- Line selection for extrapolation



Extrapolation based on Data with Noise



- 1D extrapolations on the lines using Ridge regressions
- Ridge regression suppresses the effects of high order terms

$$\min_{\boldsymbol{\beta}} \sum_i (y_i - \mathbf{X}_i^T \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

- Extrapolations and the uncertainty predictions were made with λ=5
- Developing a strategy to select λ for better extrapolation

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UB Team

	Task	Year1				Year2				Year3				Year4				Year5			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Physics	T1: Detonation Sensitivity Simulation			■	■	■	■														
	T2a: Expansion-Fan ASU Exp	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	
	T2b: Expansion-Fan Simulation							■	■	■	■	■	■	■	■	■	■	■	■	■	
	T3a: No-particle Explosive Exp					■	■	■	■												
	T3b: No-particle Explosive Sim					■	■	■	■												
	T4a: Particle Curtain Exp	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■					
	T4b: Particle Curtain Sim				■	■	■	■	■	■	■	■	■	■							
	T5a: Mesoscale Eglin Exp				■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	
	T5b: Mesoscale Explosive Sim							■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T6a: Microscale Eglin Exp	■	■	■	■	■	■	■	■	■	■	■	■	■	■						
	T6b: Microscale Detonation Sims							■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T7: Microscale Shock Simulations	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T8: Post Detonation Particle Analysis		■	■	■	■	■	■													
	T9: Discretization Error Quantification	■	■	■	■	■	■	■	■	■	■										
	T11: Macroscale Eglin Experiments							■	■	■	■	■	■	■	■	■	■	■	■	■	■
	T10, T11: Macroscale Simulations	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
Exascale /CS	Generating Data for Exascale and UQ		▒	▒	▒	▒	■	■	■	■	■	■	■	■	■	■	■				
	Behavioral Emulation for beyond device level					▒	■	■	■	■	■										
	Behavioral Emulation for CCMT									■	■										
Tools for UQ	Multi-Fidelity Surrogates (2 levels)	■	■	■	■	■	■														
	Multi-Fidelity Surrogates (>2 levels)							■	■	■	■	■									
	Extrapolation	■	■	■	■	■	■	■	■	■	■	■									
	Extreme Events								■	■	■	■	■	■	■	■	■	■	■	■	■

Prep

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Thank you

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Backup Slides

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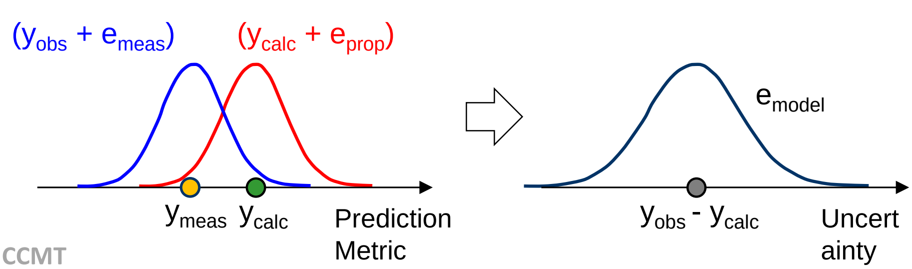
Estimating Model Uncertainty

$$y_{meas} + e_{meas} = y_{calc} + e_{model} + e_{num} + e_{prop}$$

- Only model uncertainty is not quantified
- Assuming the measurement uncertainty is independent
- Little numerical uncertainty in the 1-D simulation

$$e_{model} \approx (y_{meas} + e_{meas}) - (y_{calc} + e_{prop})$$



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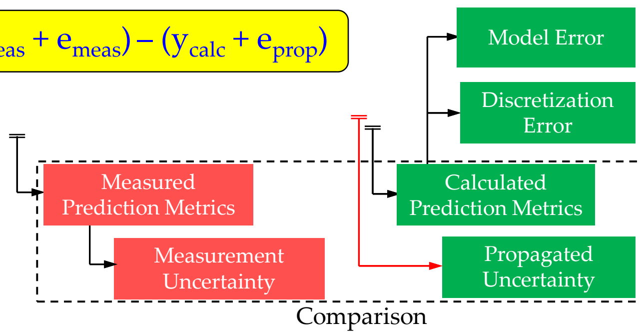
Estimating Model Uncertainty

$$y_{meas} + e_{meas} = y_{calc} + e_{prop} + e_{model} + e_{disc}$$

- Only model uncertainty is not quantified
- Assuming the measurement uncertainty is independent
- Little discretization error in the 1-D simulation

$$e_{model} \approx (y_{meas} + e_{meas}) - (y_{calc} + e_{prop})$$



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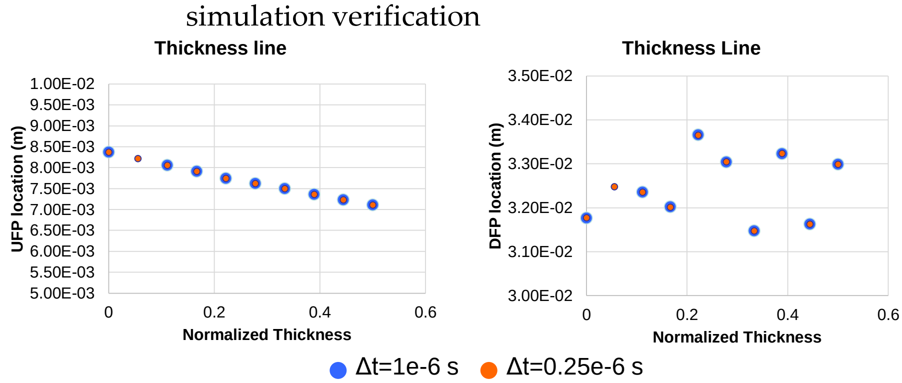
Noise in Solution (T4)

- Noise in Downstream edge location (DFP) prediction
  - Plotting DFP for varying a physical parameter revealed the noise
  - Identification of the noise source is critical for the simulation verification



*DAKOTA was used to execute simulations

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Fitting Force Kernels from Microscale (T6)

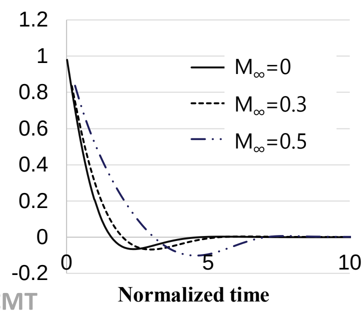
An example: Inter-phase force coupling

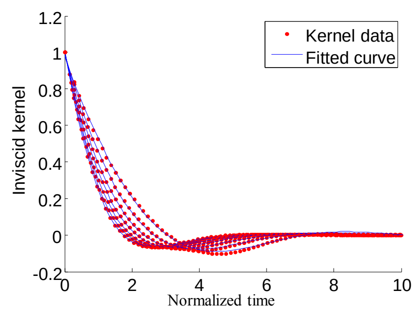
- Hybrid approach using kernels:

$$\mathbf{F} = \text{function of} \{C_D(\mathrm{Re}, \mathrm{M}, \phi), K_{iu}(\mathrm{M}, \phi), K_{vu}(\mathrm{Re}, \mathrm{M}, \phi)\}$$

- Physical-algebraic hybrid surrogates were developed for fitting the inviscid unsteady kernel

$$K_{iu}(\tau) = e \exp\left(-\left(a\tau + b\tau^4\right)\right)\cos\left(c\tau + d\tau^4\right) \quad \text{for } \mathrm{M}_\infty \geq 0$$





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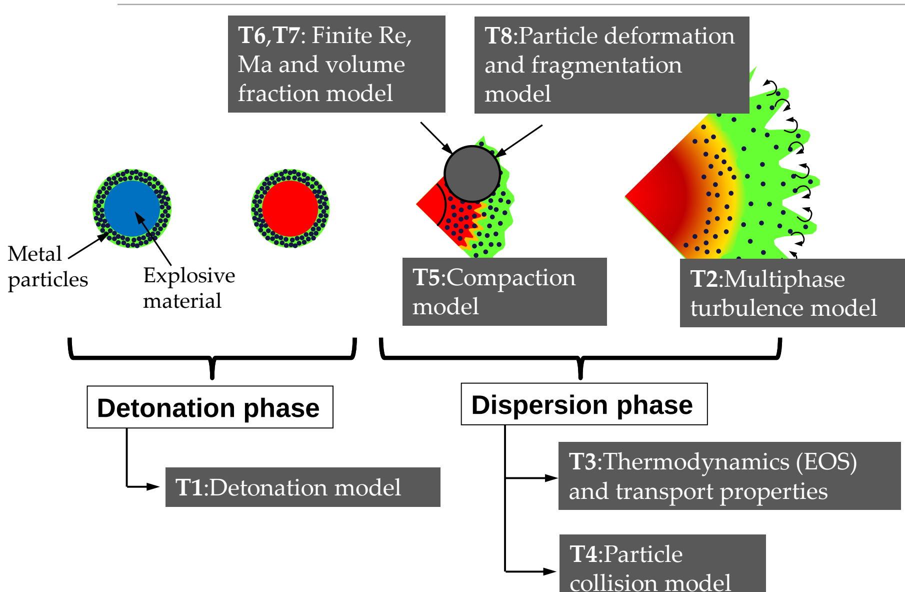
Sequence of Events and Physics Models



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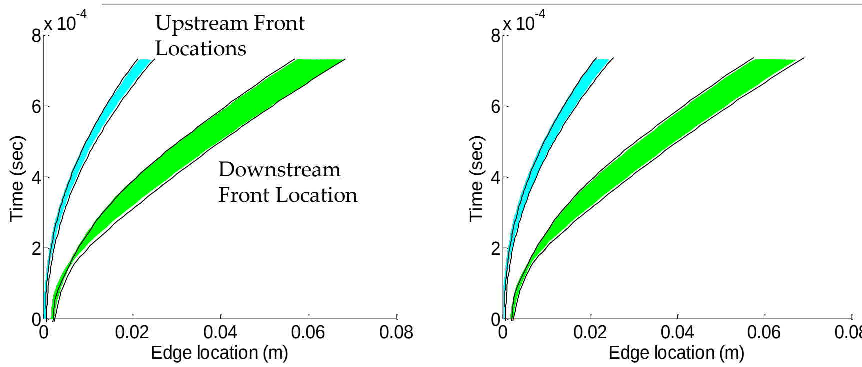
UB (1D)



- Propagated uncertainty from the input uncertainty and the measurement uncertainty in PMs
- Reducing the input uncertainty is the efficient way to reduce the uncertainty in the discrepancy

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CCMT Simulation

Angela Diggs

PhD Student, UF

Air Force Research Lab, Eglin Air Force Base

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Outline

- Fundamental research for simulations
  - Eulerian-Lagrangian coupling
    - High fidelity coupling
    - Rigorous error estimation
  - Flux scheme for multiphase flow
    - Euler-Lagrange AUSM+-up implementation
  - Validation against Sandia multiphase experiments
- Simulation Roadmap
  - Rigorous error estimation of Euler-Lagrange implementation (T9)
  - Critical evaluation of inter-particle collision model (T4) and volume fraction effects (T6)

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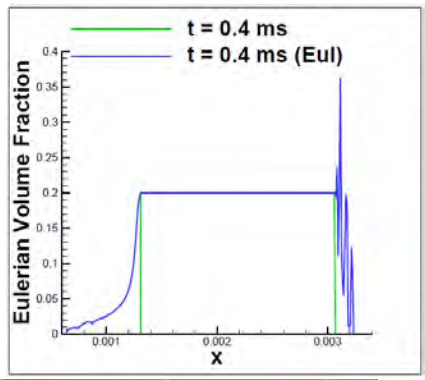
Euler-Lagrange Coupling: Volume Fraction

- Eulerian methods
  - Linear projection (Ling et al, 2012)
  - Sum particles within grid cell (Balakrishnan et al, 2010)
- Particle curtain in uniform flow
  - Expect: lock-step translation downstream
  - Reality:
    - Widening upstream curtain
    - Wild downstream oscillations
- Lagrangian method: sharp edges



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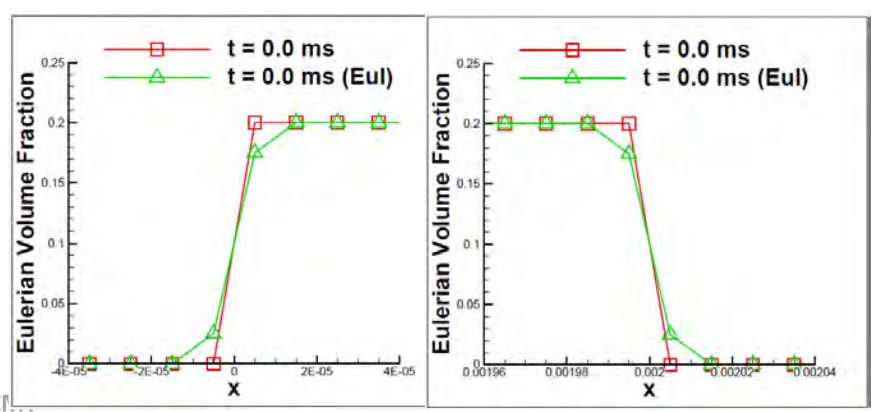
Why?

- Volume fraction dependent drag is key
  - Eulerian edges are not sharp
    - Lower volume fraction in rounded edges
    - Edge particles move slower
- Lagrangian calculation, need:
  - Sharp edges
  - Avoid introducing oscillations in curtain middle



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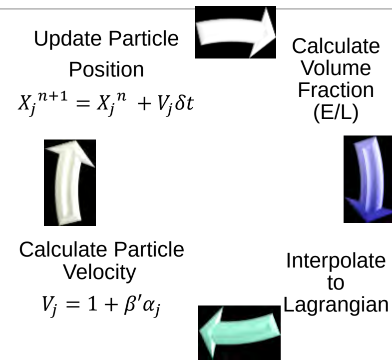
Model Problem

- Compare
  - Eulerian vs. Lagrangian
  - Order of method
  - Initial distribution of particles
  - Handling "edge" particles
  - Projection methods
- Results
  - Eulerian methods
    - Growing peaks at downstream edge
    - Cannot maintain sharp edges
  - Lagrangian methods
    - One-sided at edges
    - Weighted distribution based on particle distance



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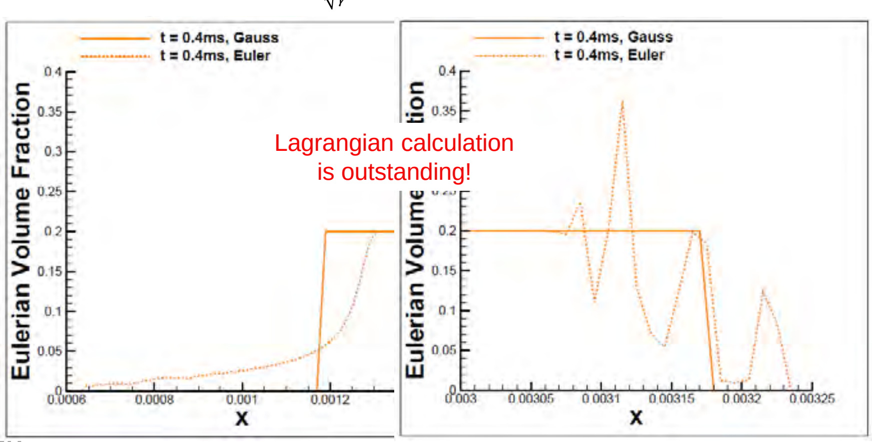
Lagrangian Calculation: Volume Fraction

- Gaussian distribution
  - Interior: $\alpha_j = \frac{1}{S} \sum_{i=1}^{M} \frac{1}{\Delta X \sqrt{\frac{1}{\gamma} * \pi}} exp\left[-\gamma \left(\frac{X_j - X_i}{\Delta X}\right)^2\right]$



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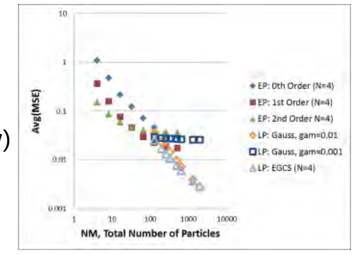
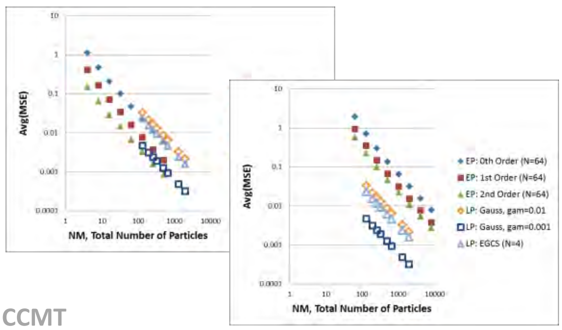
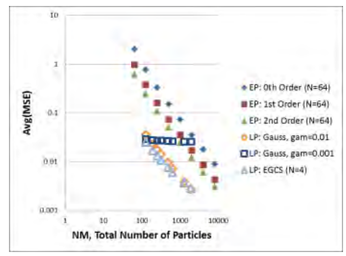
Von Neuman Error Analysis

- Error Analysis for the Average Mean Squared Error
  - Eulerian Projection (EP) methods
  - Lagrangian Projection (LP) methods
  - Estimation of
    - Constant volume fraction (left, below)
    - Sinusoidal volume fraction (right)







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Flux Schemes for Multiphase Flows

- AUSM+-up flux scheme
  - Developed by Liou, et al (2006)
  - Extension of AUSM (1993) and AUSM+ (1996)
  - Eulerian-Eulerian in literature, extended to Eulerian-Lagrangian
  - Rigorous verification using quiescent solid phase to emulate nozzle
    - Subsonic and supersonic flows
    - Match to isentropic solution
  - Investigate effect of shock tube (no analytical solution)
  - Discretization error will be established
- Observations
  - Diffusion parameter (Ku, Kp) only effective after discontinuity
  - Use of non-zero interface pressure coefficient is not recommended

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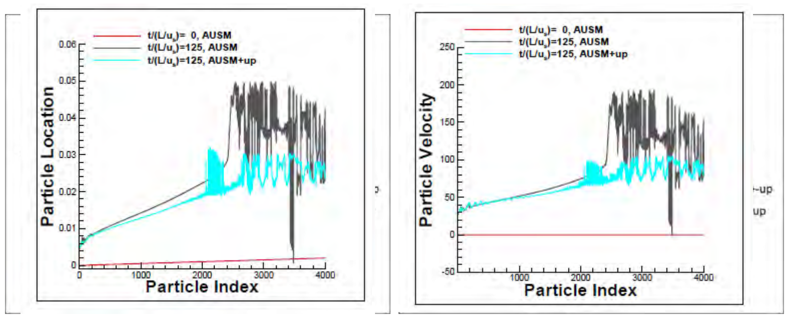
AUSM+up for Planar Shock Tube

- Preliminary Results -- Planar Shock Tube
  - Comparison of AUSM and AUSM+-up
    - Location of upstream and downstream fronts
    - Both give reasonable results for dx=100μm
    - After grid refinement (dx=50μm), AUSM fails



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Key Results and Future Work

- Discovery of new volume fraction instability
- Accurate way to compute volume fraction
- Consistent approaches to interpolation and projection
- Optimal number of computation particles per cell
- Improved fluxes for Euler-Lagrange simulations
- Rigorous error estimation (T9)

- New approaches to Lagrangian remap
- Improved implementation of unsteady force and heat transfer
- Improved implementation of collisional effects
- Validation against Sandia experiments and UQ (T4, T6)

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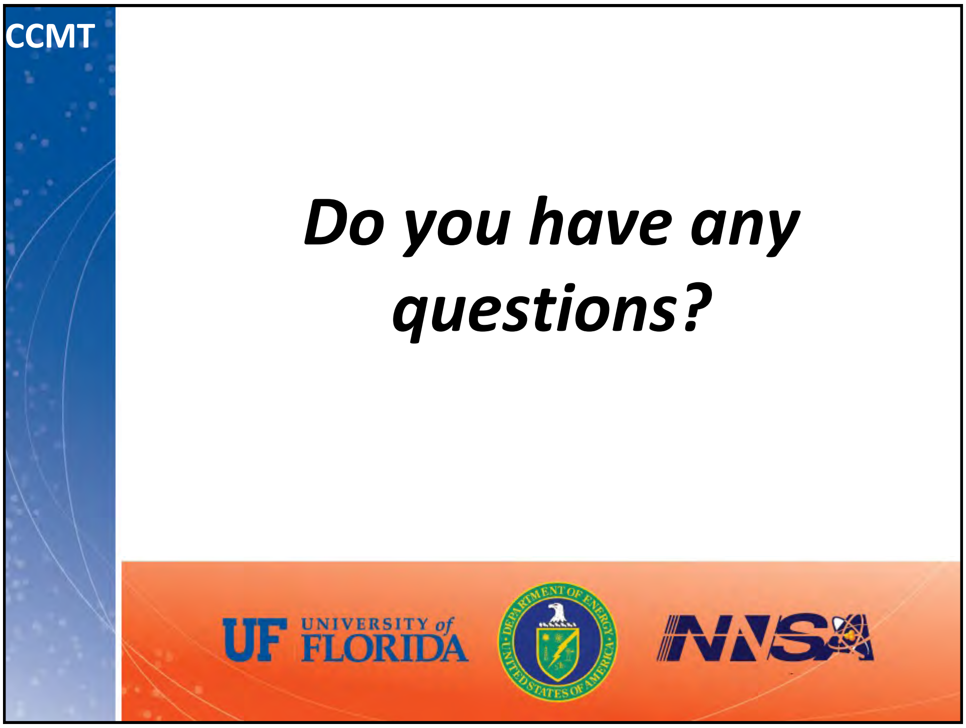
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Experimental Studies of Gas-Particle Mixtures Under Sudden Expansion

Heather Zunino
Ph.D. Student

Ira A. Fulton Schools *of* Engineering
ASU
Arizona State University

Ronald J. Adrian, Ph.D.
Regents' Professor and Ira A. Fulton Professor of Mechanical & Aerospace Engineering

UF University *of* Florida

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Problem Statement and Goals

- Experimental multi-phase studies involving compressible flow are complicated
  - Air and solid particles may move separately
  - Particles generate turbulence
- Need for a simple 1D flow experiment that can be used for early validation of the computational codes developed by the PSAAP center.
  - Simpler physics involved than the PSAAP capstone experiment
  - Reduce the scatter in current data (*Chojnicki, et al.*)
- Perform experiments on existing shock tube setup
  - Determine improvement points and weaknesses
- Design an improved, simple 1D compressible multi-phase flow shock tube experiment
  - Examine expansion fan, flow structures, turbulence, and instabilities
- Provide data for early-stage validation of computational codes developed by the PSAAP Center

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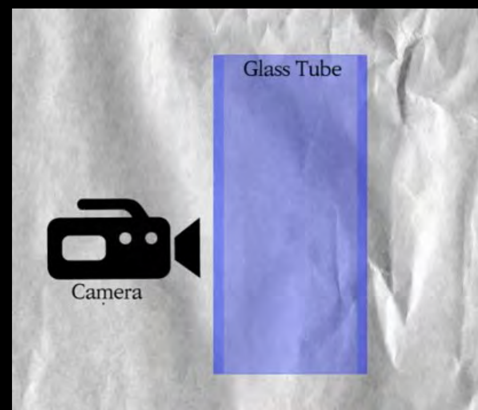
Review Proposed Experiment

- Six foot glass tube
  - Square footprint
    - 6" x 6"
- Particle bed
- Diaphragm
  - Mylar
- High-speed Cameras
  - Schlieren
- Measurements
  - Contact line velocity
  - Gas velocity
  - Particle volume concentration
  - Particle interface
- Parameters: particle size and pressure ratio



Simple Test Bed for Early-Stage Code Nume

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Shock Tube Experimental Structure Setup

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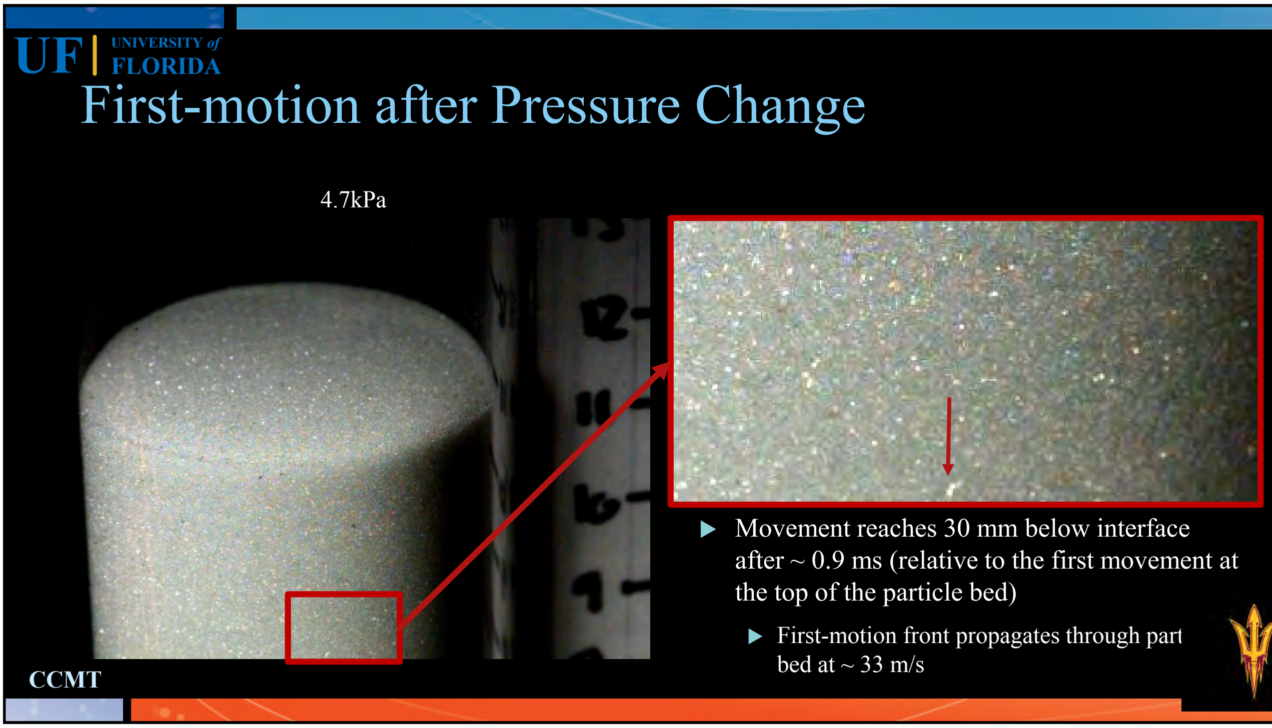
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First-motion after Pressure Change
4.7kPa
Movement reaches 30 mm below interface after ~ 0.9 ms (relative to the first movement at the top of the particle bed)
First-motion front propagates through part
bed at ~ 33 m/s
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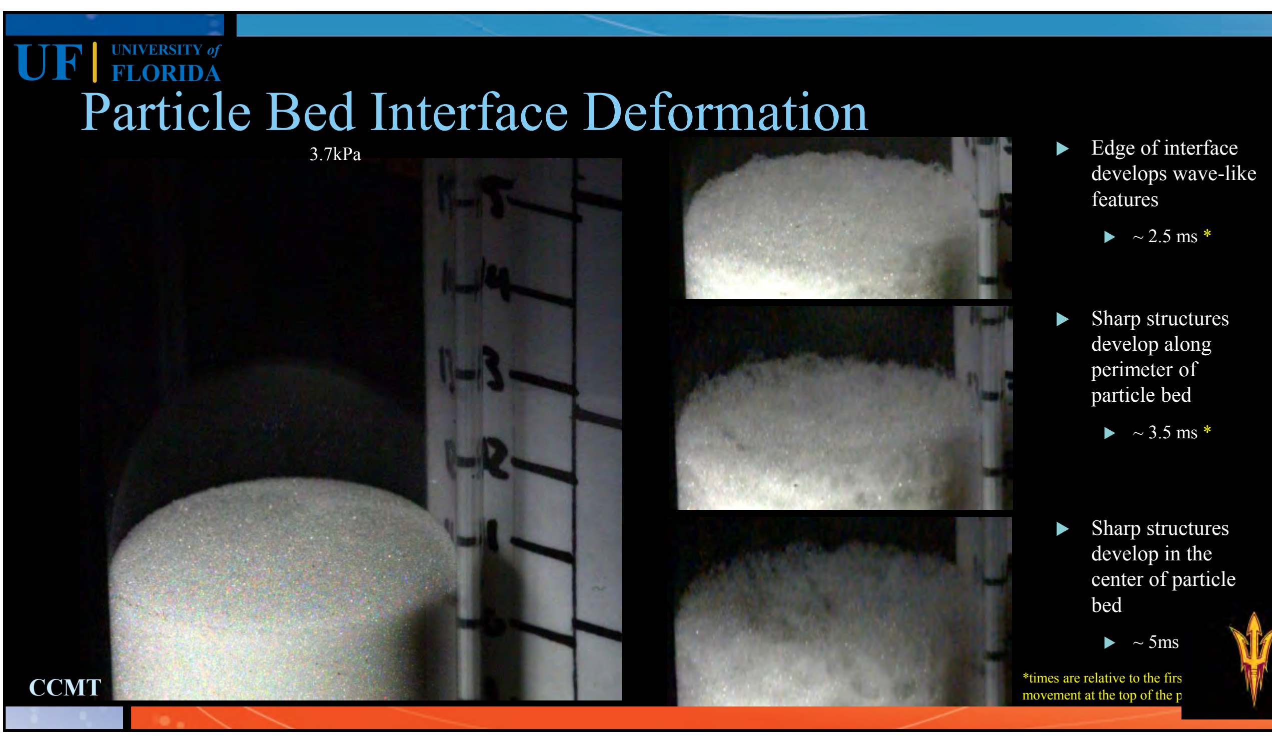
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Particle Bed Interface Deformation
3.7kPa
Edge of interface develops wave-like features
~ 2.5 ms *
Sharp structures develop along perimeter of particle bed
~ 3.5 ms *
Sharp structures develop in the center of particle bed
~ 5ms
*times are relative to the firs
movement at the top of the p
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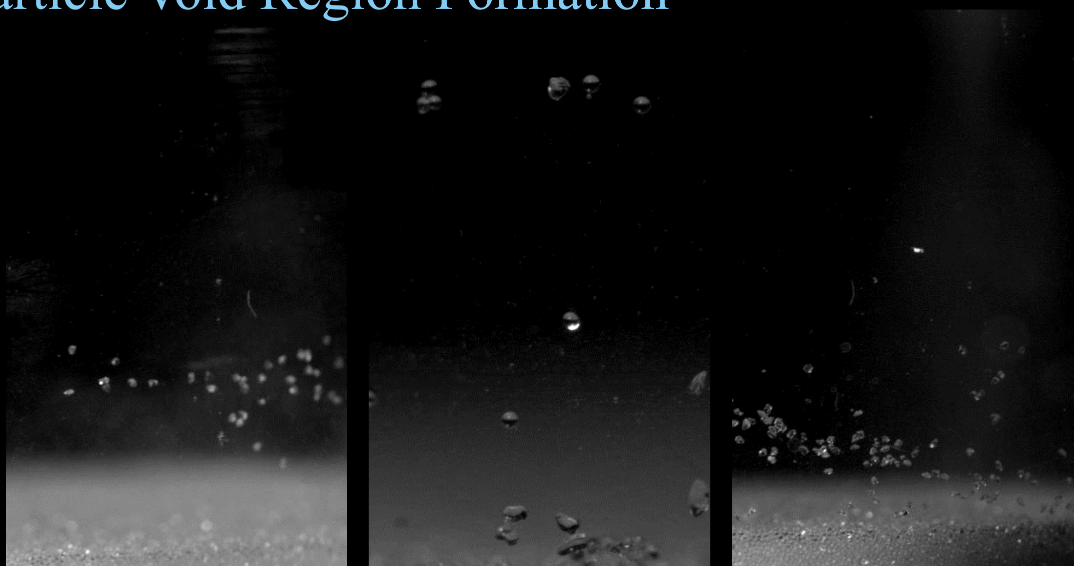
Particle Void Region Formation



8kPa 7kPa Slow Leak 5kPa

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Slow Leak - Slow Decompression

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

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Slow Leak - Rapid Decompression

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

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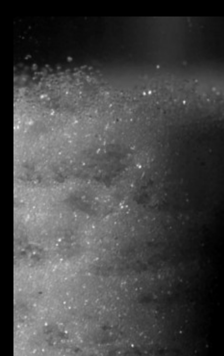
Conclusions



- Experiments performed on existing shock tube at ASU
  - Pressure drop travels approximately 33m/s
  - Particle bed interface deformation
    - Grow in time
    - Edge effects are seen
  - Particle void formation
    - Random inhomogeneities in the particle bed packing at incipient expansion (nucleation sites) may cause random voids that evolve in patterns at later times
- Flow structures resulting from rapid decompression may be directly related to the spikes seen during an explosion
  - Amplification
  - Provide initial perturbations for RM and RT instabilities

PSAAP

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Hardware Software Co-design of CMT-nek Codes

Performance, Energy and Thermal Issues

Tania Banerjee

Computer and Information Science and Engineering

UF UNIVERSITY of FLORIDA

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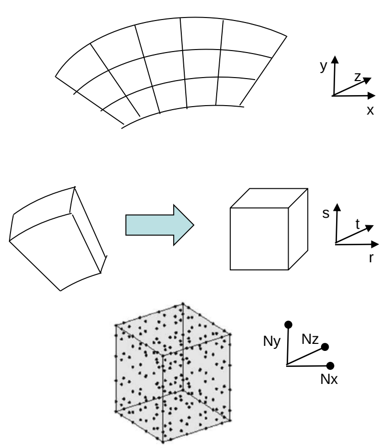
Spectral Element Method



- $\frac{\partial U}{\partial r}$ (i, j, k) = $\sum_{l=1}^{N_x} A_{il} u_{ljk}$

  $\frac{\partial U}{\partial s}$ (i, j, k) = $\sum_{l=1}^{N_y} B_{il} u_{ilk}$

  $\frac{\partial U}{\partial t}$ (i, j, k) = $\sum_{l=1}^{N_z} C_{il} u_{ijl}$
- If $N_x = N_y = N_z = N$
  - Then $B = C = A^T$
- Complexity: $O(N^4)$
- N is typically between 5-25
  - A large number of small matrix multiplications

- Represents a significant fraction of overall time

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Spectral Elements: Derivatives and Codes

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
```

- Similarly, 5loop versions and 5loop-fused versions were considered

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Optimizations

- Autotuning
  - Apply loop transformations
    - Loop permutation
    - Loop unroll
  - CHiLL applies loop transformation automatically on the target code

Related Work: C. Chen, J. Chame, M.W. Hall, CHiLL: A Framework for Composing High-Level Loop Transformations, Technical Report 08-897, University of Southern California, Computer Science Department, 2008.

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Loop permutation

```
do k = 1, nz1
    do j=1,ny1
      do i=1,nx1
        statement
      enddo
    enddo
enddo
```

```
do i = 1, nx1
    do j=1,ny1
      do k=1,nz1
        statement
      enddo
    enddo
enddo
```

```
do i = 1, nx1
    do k=1,nz1
      do j=1,ny1
        statement
      enddo
    enddo
enddo
```

```
do j = 1, ny1
    do k=1,nz1
      do i=1,nx1
        statement
      enddo
    enddo
enddo
```

```
do j = 1, ny1
    do i=1,nx1
      do k=1,nz1
        statement
      enddo
    enddo
enddo
```

```
do k = 1, nz1
    do i=1,nx1
      do j=1,ny1
        statement
      enddo
    enddo
enddo
```

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Loop unroll

```
do k = 1, 10
    do j=1,10
      do i=1,10
        c(i, j, k) = a(j, i) * b(i, k)
      enddo
    enddo
enddo
```

```
do k = 1, 10
    do j=1,10
      do i=1,10,2
        c(i, j, k) = a(j, i) * b(i, k)
        c(i+1, j, k) = a(j, i+1) * b(i+1, k)
      enddo
    enddo
enddo
```

- Unroll factors are preferably divisors of the iteration space
- Advantages
  - Reduces the number of limit checks for iterator
  - Exposes the possibility of vectorization to the back end compiler
    - c (i:i+4, j, k) = a (j, i:i+4) * b (i:i+4, k)
- Disadvantage
  - Code size increases, may result in higher I-cache miss rates

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Possible Combinations

Algorithm: *dudr-4loop*

do k = 1, N_z
 do j = 1, N_y
  do i = 1, N_x
   do l = 1, N_x
    *dudr(l, j, k) = dudr(l, j, k) + a(i, l) * u(l, j, k, ie)*
   enddo
  enddo
 enddo
enddo

Number of implementations for $N_x=N_y=N_z=10$

= 4! * 4 ^ 4

= 24 * 256 = 6144 variants

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

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

Question: Can we use a less expensive search technique?

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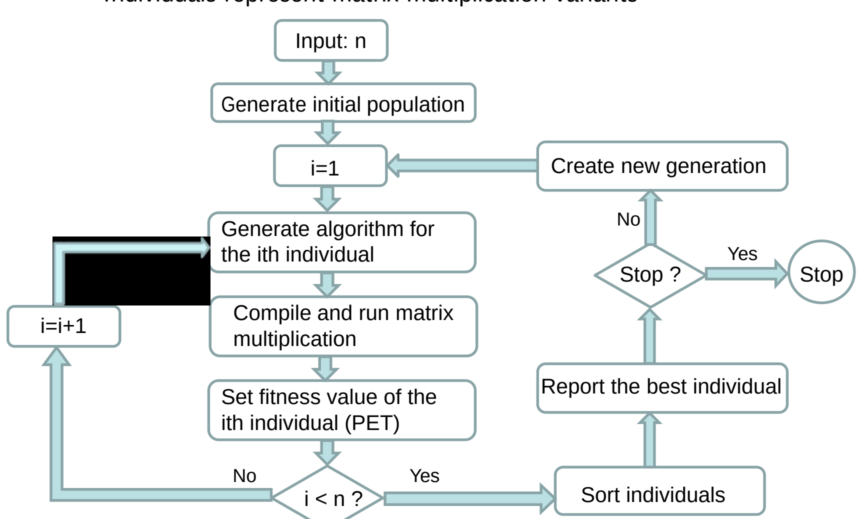
Genetic Algorithm

- We use genetic algorithms to search the exploration space efficiently.
- Individuals represent matrix multiplication variants



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Results (HiPerGator)

- Matrix size: 10x10x10

Derivatives	Min Time (s)	nek5000 Time (s)	GA Time (s)	#variants
dudr	0.39	0.62	0.41	444
dudt	0.18	0.31	0.2	393
duds	0.45	0.88	0.45	446

- Best variant found by GA is
  - Near optimal
  - Better than nek5000 variant
- Total number of variants analyzed is about 1%

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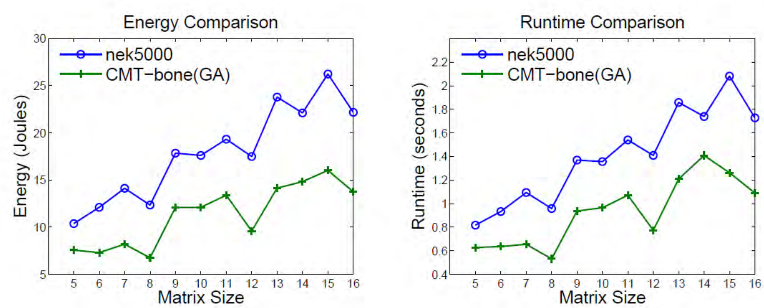
Results (teller@SNL)



- Energy: 27% to 45% improvement average improvement of 37%
- Runtime: 23% to 45% improvement, average improvement of 34%.

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Conclusions

- We benchmarked the derivative computation kernel of CMT-bone for performance and energy.
- Our work highlights autotuning as an important strategy for improving both performance and energy, over different architectures
  - We got between 23-61% improvement in performance and about 27-55% improvement in energy requirement
- We developed a genetic algorithm based driver which efficiently explores the search space.
- We are getting about 5% improvement in CMT-Nek runtime when the derivative computation kernel is run.
- An increased number of cache misses is the primary reason for the differences in performance.
- Working with Applications Code Development Team comprising Mrugesh and Jason, to restructure CMT-nek code to accumulate accesses to the same array

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Do you have any questions?

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Surrogate Models

For CCMT

Chanyoung Park

Department of Mechanical & Aerospace Engineering

UF UNIVERSITY of FLORIDA · NNSA

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Outline

- Surrogate for mesoscale UQ
- CCMT Applications using surrogates
- Multi-fidelity surrogate (MFS) for UQ based on multiple simulations

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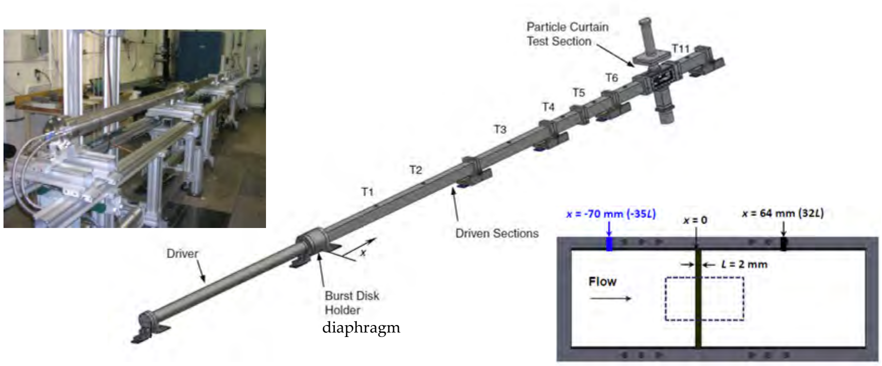
Shock-particle Interaction Model Validation



- T4, T6, T9, T10
- Estimating the error in the drag model for simulating gas and particles interaction
- Experiments of Justin Wagner (SNL)
- 1D Simulation (Rocflu Lite)

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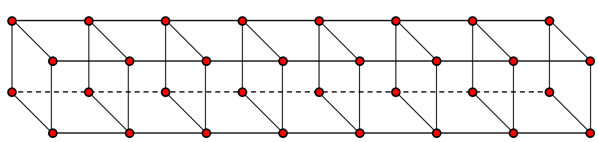
3D and 1D Shock Tube Simulations

- 3D and 1D simulations for the shock tube experiment
- 3D/1D simulations
  - 3D simulation: high fidelity physics models and low fidelity resolution



32 grid points and 7 cells

  - 1D simulation: low fidelity physics models and high fidelity resolution

32 grid points and 31 cells

- Multi-fidelity surrogate (MFS) makes predictions by combining data from 3D and 1D simulations

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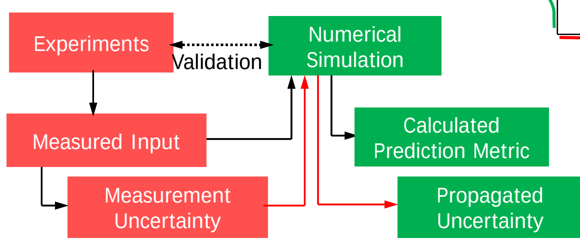
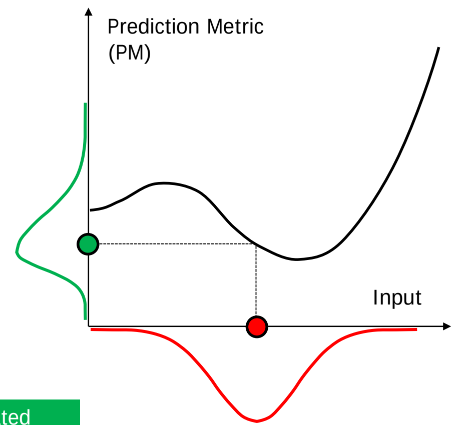
Computational Challenge of UQ

- UQ requires to propagate uncertainty in input to uncertainty in prediction metric
- General uncertainty propagation approach Monte Carlo method often requires thousands of simulations
- How to address the computational challenge of UQ?





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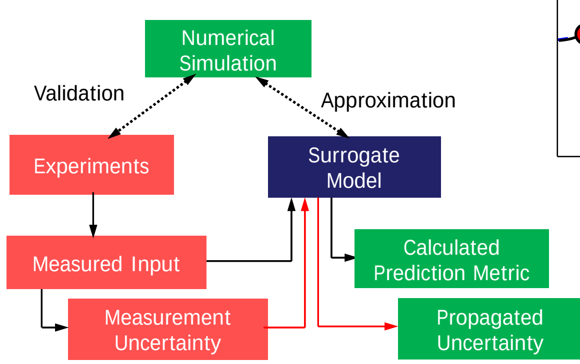
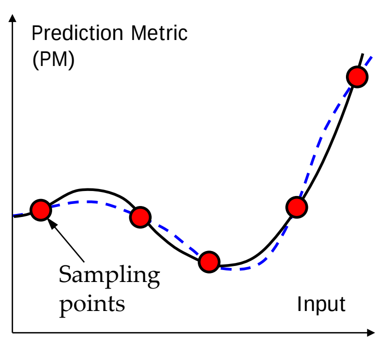
Surrogates for UQ

- Surrogates are fits to a set of data points called design of experiments
- Surrogate models are approximation of the prediction metric for inputs using cheap algebraic functions





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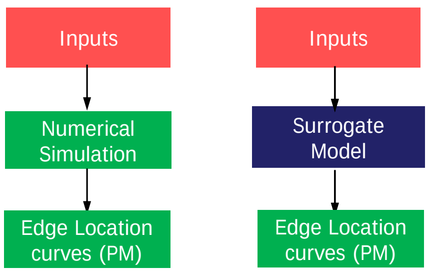
Surrogate of the Mesoscale Simulation

- Key uncertainties

#	Inputs	Uncertainties in Inputs
1	Volume fraction	Measurement error (21%±2%)
2	Diameter of particle	Errors in distribution type / parameters
3	Particle curtain thickness	Variation in particle curtain thickness



- Surrogate model is a cheap representative model of the numerical simulation
- Surrogate model of the mesoscale simulation gives edge location curves for given inputs as the simulation does

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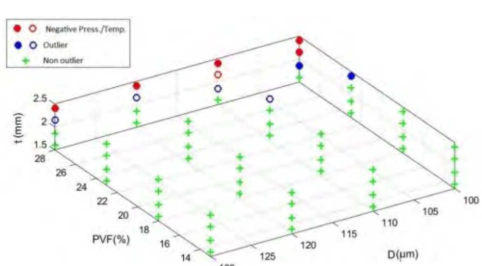
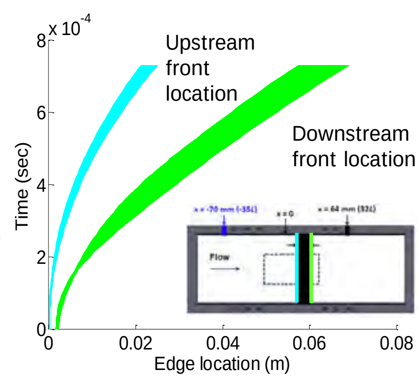
Propagated Uncertainty of Mesoscale Sim.





- Propagated uncertainty was calculated based on 10,000 curves
- 64 simulation runs for fitting a surrogate for the curves
  - Kriging surrogate was used
  - DAKOTA was used to evaluate samples by managing simulation runs
  - Sampling also revealed the valid parameter domain of the simulation

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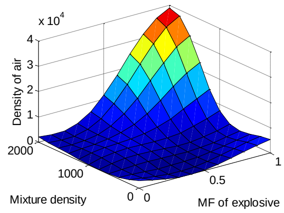
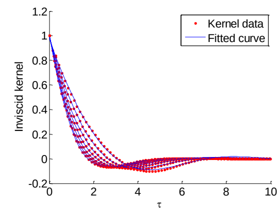
Applications using Surrogate Models

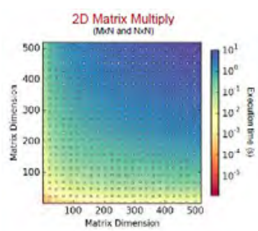
- JWL-EOS (Meso/macroscale team)



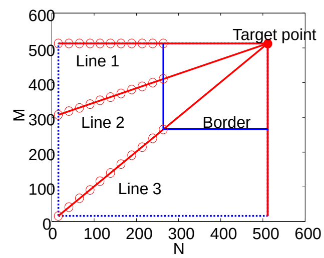
- Inviscid force kernels (Microscale team)



- Behavioral Emulation (Exascale team)



- Extrapolation (UB team)



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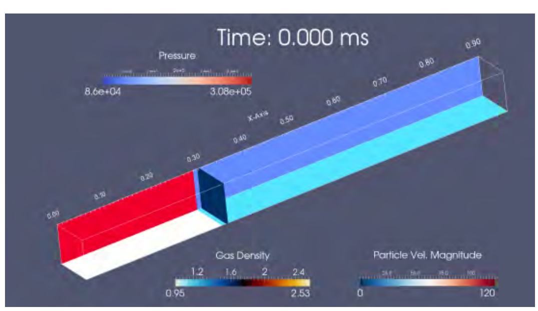
Validation and UQ of 3D Mesoscale Sim.



Mesoscale 3D simulation (Preliminary)

- Building a surrogate by combining samples from multi-fidelity simulations (MFS) based on 1D/2D/3D simulations
- MFS will be used for the UQ of the macroscale 3D simulation
- 9 data points from the 3D simulations and 64 data points from the 1D simulation

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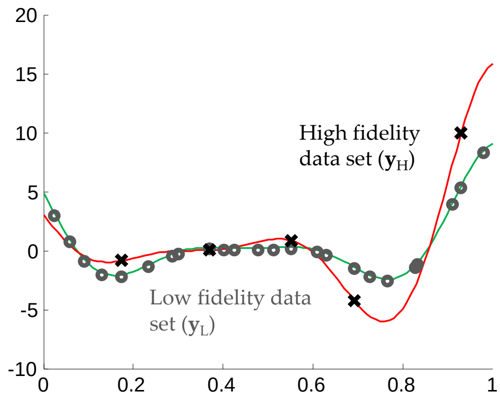
MFS for UQ of High Fidelity Simulations



- Compensate a small number of expensive high fidelity samples with a large number of cheap low fidelity samples
- Building a surrogate by combining samples from multi-fidelity simulations (MFS) based on 1D/2D/3D simulations

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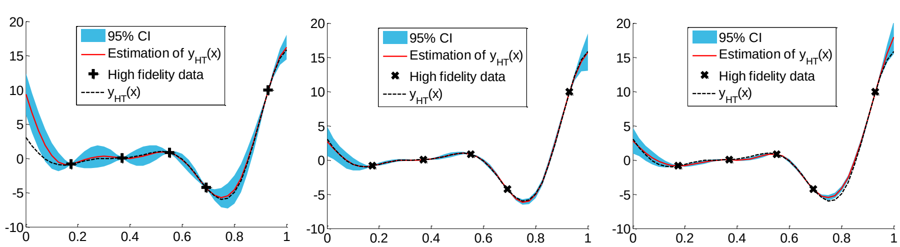
Frameworks for Fitting MFS

- There are various frameworks are available for modeling discrepancy between low and high fidelity simulations



$$\hat{y}_H(x) = \rho \hat{y}_L(x) + \hat{\delta}(x)$$

Discrepancy function based framework

$$\hat{y}_H(x) = \rho \hat{y}_L(x, \theta)$$

Calibration based framework

$$\hat{y}_H(x) = \rho \hat{y}_L(x, \theta) + \hat{\delta}(x)$$

Comprehensive framework

- Predicting a best framework for a specific problem
- Carrying out case studies for minimizing the approximation error for given computational budget

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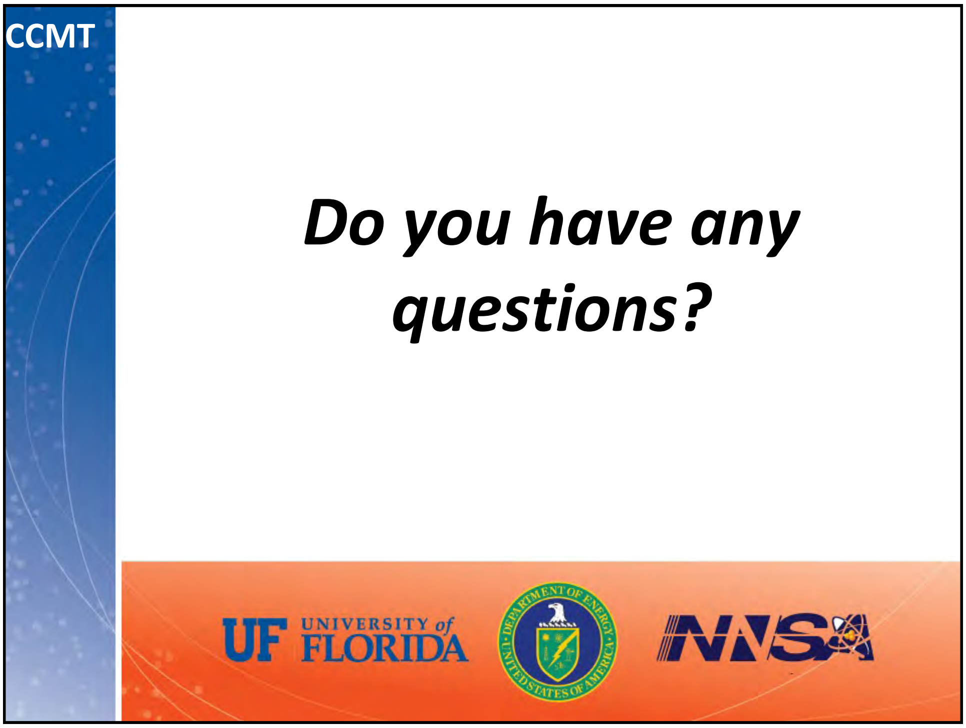
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Microscale Simulations

Chris Neal
CCMT MicroscaleTeam

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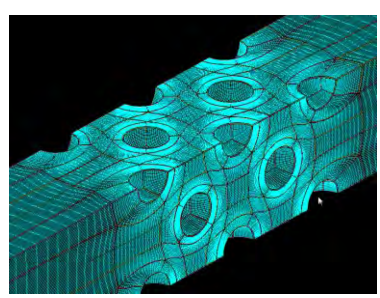
Microscale Simulations Goals

Goals

- Perform hero & bundled runs for varying Re, Ma and particle arrangement
  - Under conditions of relevance
  - Establish numerical errors
- Validate against microscale experiments
- Develop point particle models
  - Force and heat transfer
- Explore new microscale physics



FCC Mesh

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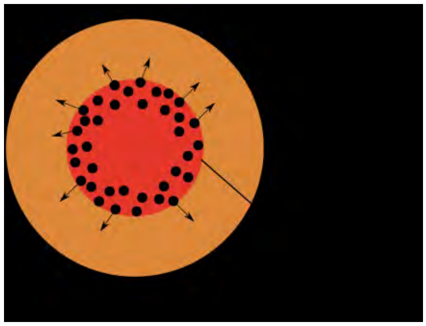
Flow Conditions of Relevance

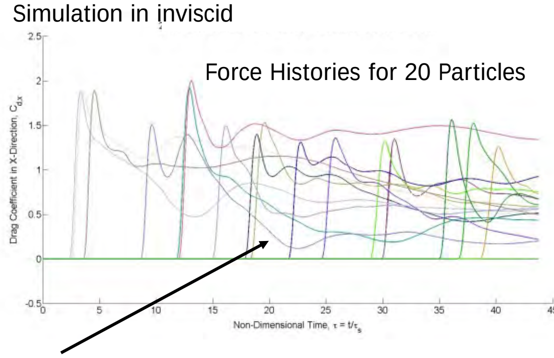


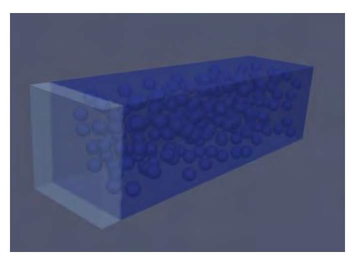
Multiphase Detonation

- What is the strength of the force arising from a shock and contact interface interaction with a particle in a compressible flow?

Shock Propagation Over a Particle Bed

- Shock Mach number is 3.0
- Post shock flow is supersonic
- 200 Particles at 10% volume fraction
- Particle diameter is 80mm
- Simulation in inviscid





200 Particles

- Current models do not capture these effects

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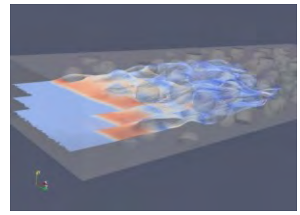
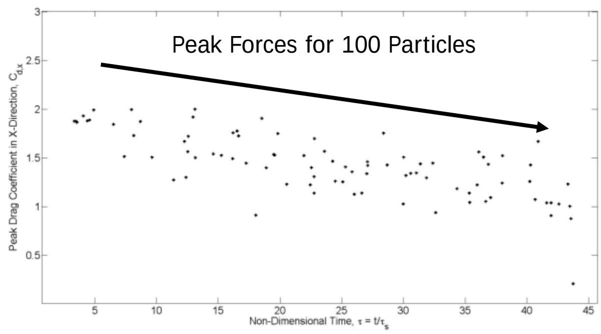
Multiparticle Simulations

- Data processing is ongoing because 200 particle simulation data is preliminary
- The force data will be compared with current model to identify areas that need enhancement





- Shock strength decreases as shock pushes through the particle pack

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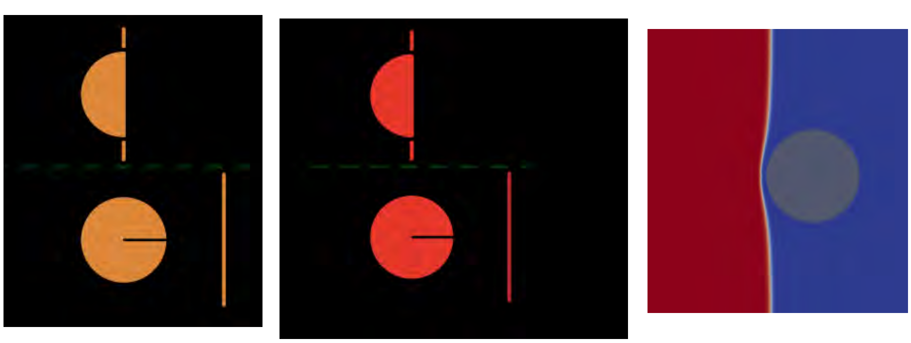
Contact Interface Force Models

- The point-particle model worked well for shock-particle interaction
- How good is it for shock-contact interaction?



- Contact-interface travels subsonically, so the flow will react to the impinging interface

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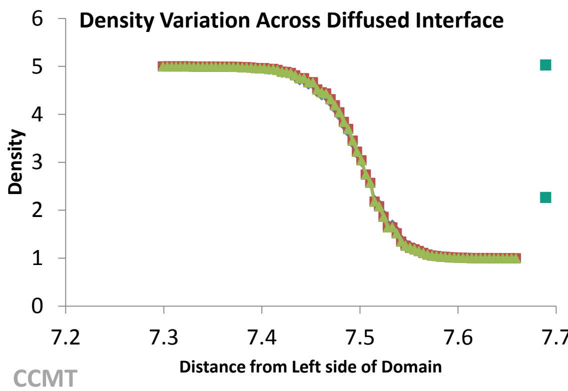
Contact Interface Simulation Challenges

- Different flux schemes are available in Rocflu. Is there is a scheme for running simulations involving contact interfaces?



- The contact interface simulations, showed negligible differences in the interface diffusion
- The contact interface diffusion is not a strong function of the flux scheme used

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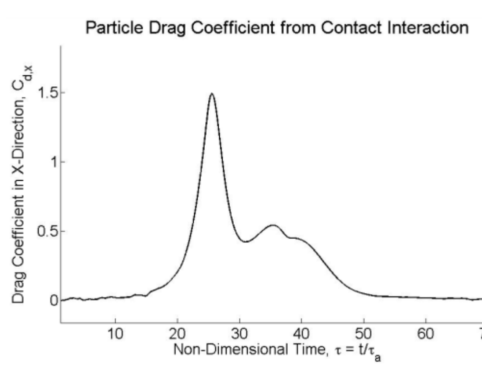
Simulation Results

- For a density ratio of 5 with subsonic flow of Mach 0.1. Results are still being generated for these cases

- Numerical Schlieren to enhance the position and shape of the interface



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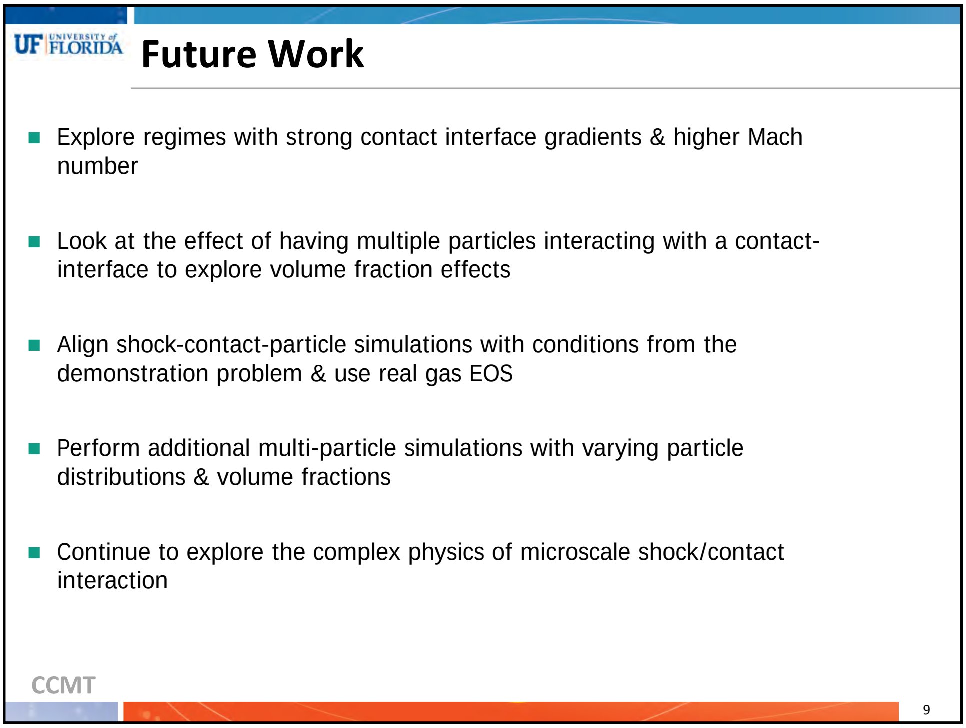
Future Work
Explore regimes with strong contact interface gradients & higher Mach number
Look at the effect of having multiple particles interacting with a contact-interface to explore volume fraction effects
Align shock-contact-particle simulations with conditions from the demonstration problem & use real gas EOS
Perform additional multi-particle simulations with varying particle distributions & volume fractions
Continue to explore the complex physics of microscale shock/contact interaction
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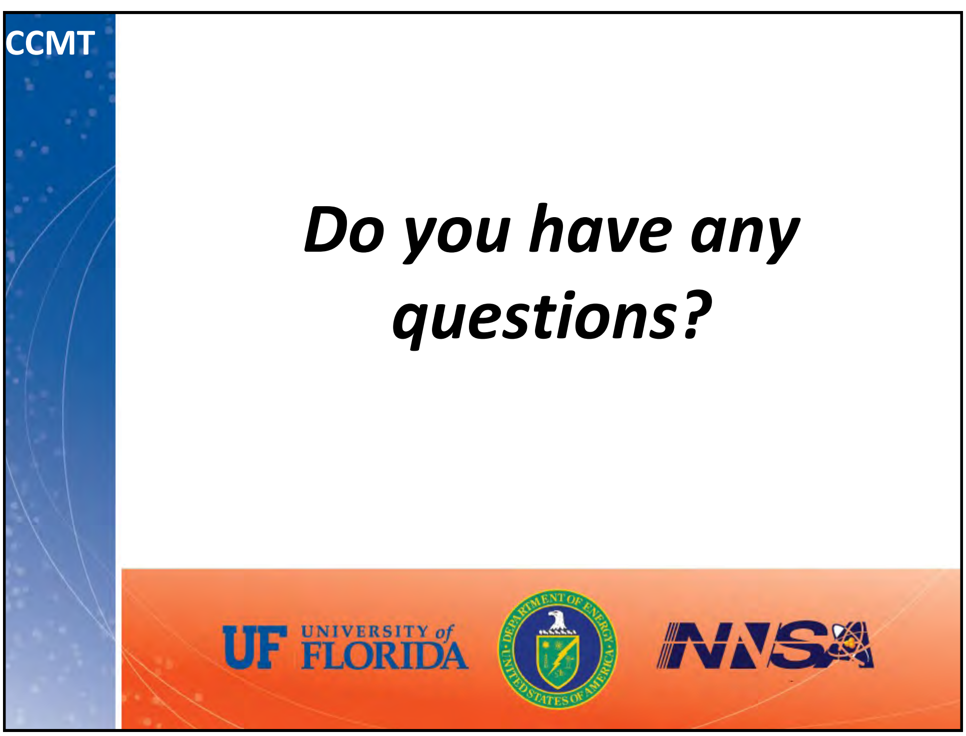
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Scalable Network Simulations

Nalini Kumar

PhD Student, ECE, University of Florida

Sandia National Laboratories

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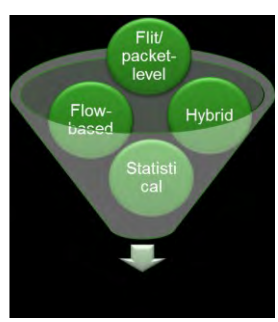
NNSA

Scalable Network Simulation

- Explore existing congestion models for use in Behavioral Emulation
  - Most recent simulators use low-level network models
  - SST* (Micro) uses high-fidelity component models for system simulations
  - SST (Macro) uses very coarse-grained models for system networks
  - FSIM allows functional network simulation and BigSim allows high-level latency models and detailed model of communication fabric
- Developing highly-scalable parallel simulator is a big-task
  - We are looking at leveraging existing simulator cores/frameworks to support network modeling using our Behavioral Emulation approach
  - Reduce development and support effort, and possibly leverage existing models developed by other users of the tool



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* Structural Simulation Toolkit

2

Characterizing Communication in CMT-nek

- First we need to understand communication behavior of target CMT-nek app
  - Since full application is too complex and cumbersome to do targeted study, we are using **'CMT-bone'** miniapp

- Polynomial degree of Nx=Ny=Nz=N
- Total no. of elements, E
- No. of MPI ranks, P
- Physical quantities, Q = 5
- No. of bytes, B

- Nearest-neighbor update using pairwise exchange:
  - No. of transfers per MPI rank = 6
  - Best-case, all exchanges across all MPI ranks occur in parallel
  - Worst-case, all transfers are serialized = $6P$
  - Average transfer size = $6N^2\left(\frac{E}{P}\right)^{\frac{2}{3}}$; total data transferred = $30N^2\left(\frac{E}{P}\right)^{\frac{2}{3}}$
- Nearest-neighbor update using crystal router:
  - No. of transfers per MPI rank = Optimal no. of transfer steps = log_2P
  - Transfers at each comm stage = P ; Total no. of transfers = $P\,log_2P$
  - At each transfer stage, largest transfer size = $6N^2\left(\frac{E}{P}\right)^{\frac{2}{3}}$; total data transferred > $30N^2\left(\frac{E}{P}\right)^{\frac{2}{3}}$

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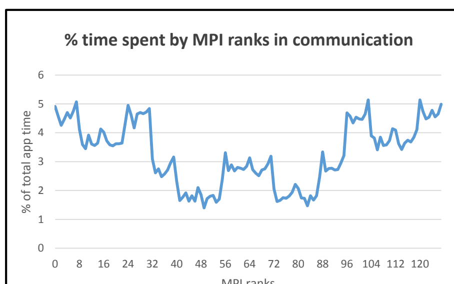
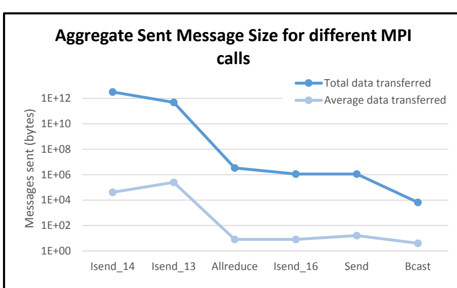
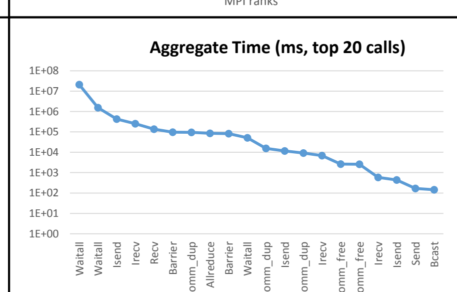
CMT-bone MPI Profiling Data

- Experimental setup:
  - 128 MPI ranks, 1 rank/node
  - mpiP profiling data
  - Best-case, all exchanges across all MPI ranks occur in parallel

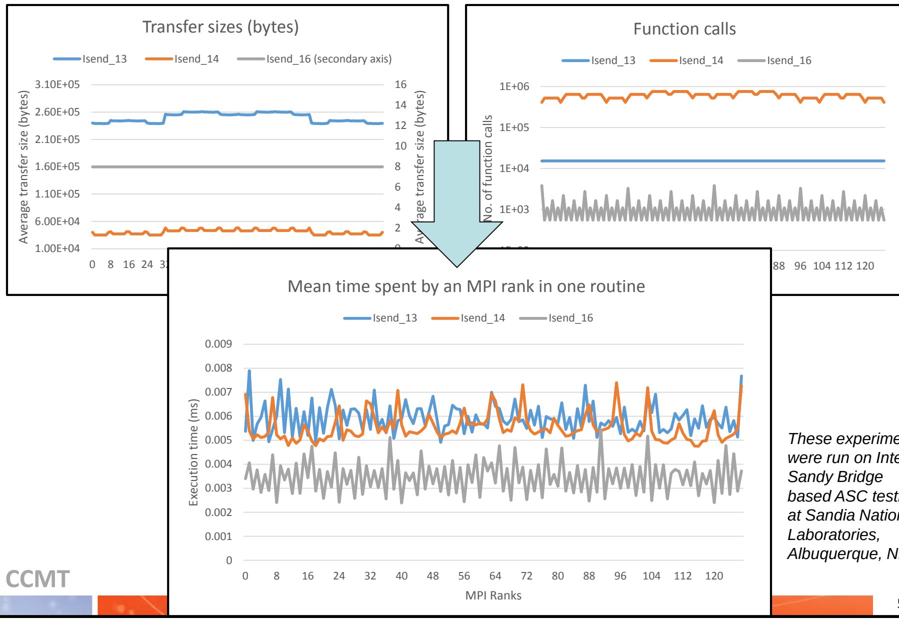
These experiments were run on Intel Sandy Bridge based ASC testbed at Sandia National Laboratories, Albuquerque, NM.







Data for Estimation of Transfer Times



These experiments were run on Intel Sandy Bridge based ASC testbed at Sandia National Laboratories, Albuquerque, NM.

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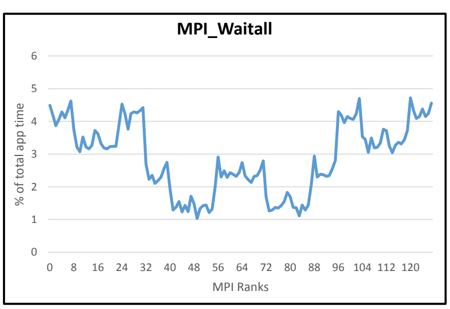
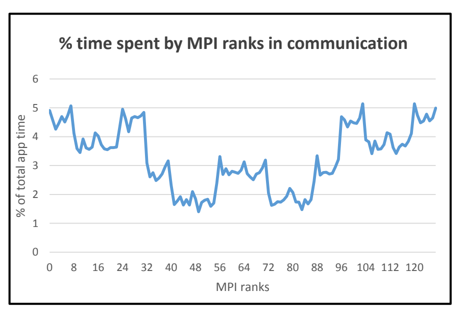
Overall Communication Time Estimation





These experiments were run on Intel Sandy Bridge based ASC testbed at Sandia National Laboratories, Albuquerque, NM.

- Most of the time is spent in MPI_Waitall
  - Need timed simulations to look at these effects
  - It may still be possible to use coarse models for actual transfer time estimations

Sandia National Laboratories

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Scalable Network Simulation using SST

- Develop abstract end-point models '**motifs**' for various communication routines used in CMT-nek
  - Identified routines: Nearest-neighbor communication using pairwise exchange, all-to-all using crystal routing, allreduce, bcast etc.
- Ember is an end-point model for network communications
  - Motifs are condensed, efficient models of communication which are able to correctly represent the target, size and data type of messages in larger applications, libraries and mini-apps
  - Events generated by motifs are interpreted by the Ember engine and then handed off to the Hermes middleware emulation layer
  - Hermes provides timing for basic middleware operations such as MPI message matching
  - Currently supports SHMEM/MPI-3 one-sided communications

Ember → Hermes → Firefly → Merlin

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Scaling & Speeding up SST Simulations

- Currently working on evaluating the sensitivity of simulations to different model parameters
  - Run simulations across a sweep of different parameters such as MPI match latency, packet size, buffer sizes etc.
  - Quantify the effect of these parameters on simulated time
- Final goal is to speedup the simulations by reducing
  - Number of components being simulated,
  - Number of parameters that are needed to describe a system, and
  - Number of events being generated by each component
- It has to be good enough to provide a first-order approximation of performance which can enable application developers to do some early design space exploration

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Microscale Experiments: Explosive Testing Update

Principal Investigator:
Don Littrell
Air Force Research Laboratory
Munitions Directorate
Eglin Air Force Base, Florida

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Experimental Timeline

- Year 1+: Focus on microscale experiments
  - Millimeter-sized particles; single/few particles; planar geometry
  - Controlled experiments where
    - a few well-characterized finite-sized metal particles are placed outside a well-characterized explosive in a precise manner
    - particles embedded inside the explosive interact with the detonation wave and the post-detonation flow
    - complex particle arrays (*e.g.*, stacked particles or spaced particles) are embedded in a frangible, inert matrix material that is impedance-matched to the explosive
- Year 2+: Focus on macroscale experiments
  - 10-100 µm particles; >10^3 particles; planar geometry
- Year 2+: Focus on mesoscale experiments
  - 10-100 µm particles; >10^3 particles; cylindrical geometry

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Objectives for Microscale Experiments

Objectives	Parameters/Diagnostics
Accurate extraction of particle position, velocity and acceleration in the near/intermediate field	• Position vs time / X-ray images & high speed video – Velocity – derivative – Acceleration – double derivative
Extraction of the flow field in the region of the particles in the near field	• Light transmission / high speed video with strong back-lighting • Fireball temperature / Fourier Transform Infrared (FTIR) video • Blast pressure / piezoelectric pressure transducers
Quantify the deformation of the particle	• Soft catch • 3-D scan of deformed particles
Uncertainty quantification	• Repeat selected experiments

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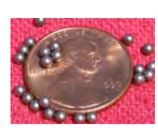
Experiment Design Goals & Approaches

- Well characterized explosive (precision explosive charges)
  - Composition N-5 explosive
    - Pressed 0.5” OD x 0.5” L pellets for good density control
    - L/D=~3 charge (stacked pellets with interface control)
      - Sufficient length for steady-state detonation (> DDT length)
      - Minimal explosive charge for better near-field diagnostics
  - 2” OD mild steel case. Heavy radial confinement ensures:
    - Fixed boundary conditions
    - Planar detonation waves
  - RP-83 Exploding Bridge Wire Detonator (EBW) or equivalent
- Well-characterized finite-sized metal particles (spheres & hexes)
  - Tungsten alloy (ρ=17)

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Experimental Diagnostics

- Hewlett Packard 150 keV pulsed X-ray system
  - Multiple heads, multiple timings
  - Orthogonal views
- Phantom 5/9/11 high speed video cameras
  - Up to 1632x1200 resolution
  - Up to 100,000 fps
- Simacon high speed framing camera
  - 16 frames
  - 1,000,000 fps
- Kistler piezoelectric pressure transducers (calibrated)
- Witness panels (ray tracing from origin to frag impacts)

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Test Set-up

- Feedback from UF-CCMT researchers concerning prior experiments included:
  - a desire to quantify the reproducibility of the pressure measurements;
  - positive feedback on x-ray imaging of particles in the fireball;
  - a desire to track the trajectories of individual particles; and
  - a desire for improved visualization of the fireball and flow fields.
- Based on this feedback, RWMW made the following upgrades to the diagnostics:
  - increasing the number of pressure probes from two to eight – covering a wider array of azimuths and elevations, and redundant measurements to assess accuracy and repeatability;
  - calibrating the scale of the x-ray images by taking x-rays of static objects of known size;
  - increasing the number of x-ray images from three to four;
  - adding a Simacon camera with a 825±25 nm band pass filter matched to a Xenon light source;
  - adding matched linear polarizers attached to a flash bulb and a second high speed camera; and
  - adding an alternate non-explosive particle driver – a gas from a high speed valve and compressed helium reservoir combination – as an alternative to the explosive particle driver.

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Test Series Description

Test #	Date	Driver	Particle(s)
1	2/25/2015	Compressed helium at 400 psi	Large tungsten spheres
2	2/25/2015	Compressed helium at 400 psi	Salt
3	2/25/2015	Compressed helium at 500 psi	Salt
4	2/25/2015	Compressed helium at 500 psi	Salt
5	2/25/2015	Compressed helium at 500 psi	Salt
6	2/25/2015	Compressed helium at 1000 psi	Salt
7	2/26/2015	RP83 + 3 N5	Single small tungsten sphere
8	2/26/2015	RP83 + 3 N5	Single small tungsten sphere
9	2/26/2015	RP83 + 3 N5	3 tungsten hexes
10	2/26/2015	RP83 + 3 N5	Salt
11	2/26/2015	RP83 + 3 N5	Salt
12	2/26/2015	RP83 + 3 N5	4 small tungsten spheres (diamond pattern)

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Wide-view Photograph of the Test Set-up

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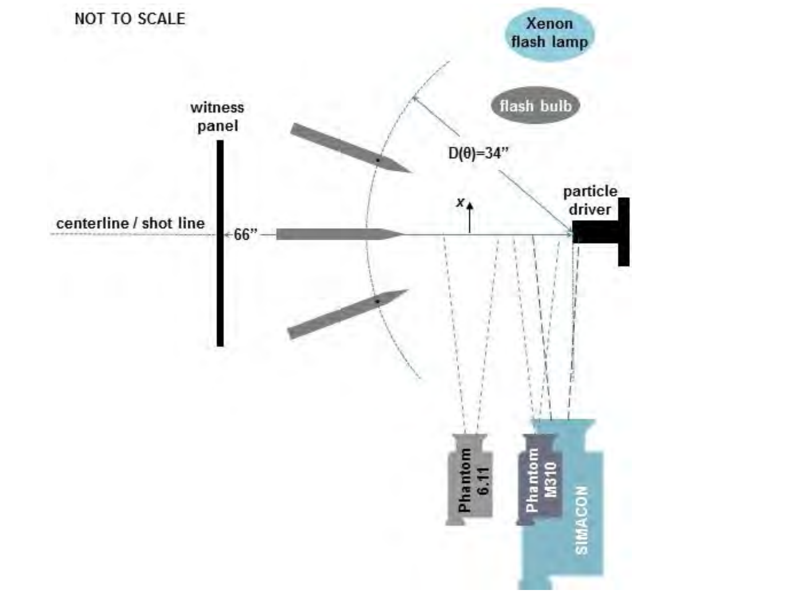
Overhead Schematic of the Test Set-up



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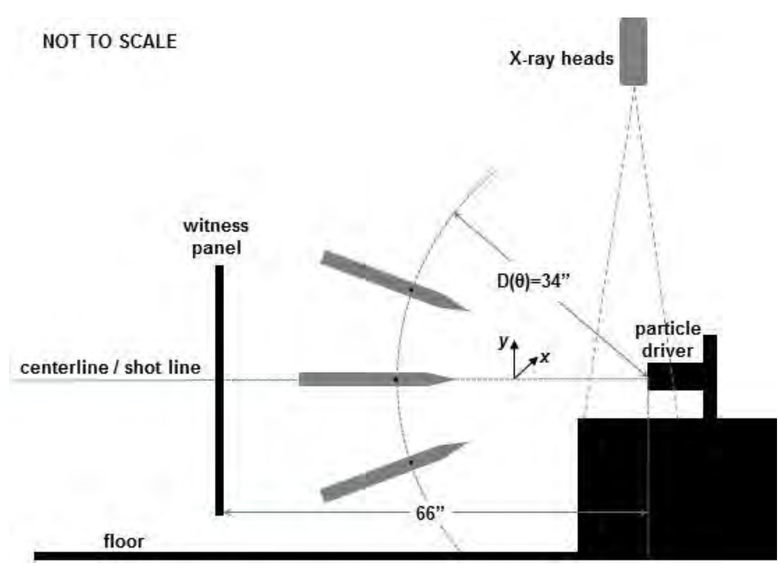
Side-view Schematic of the Test Set-up



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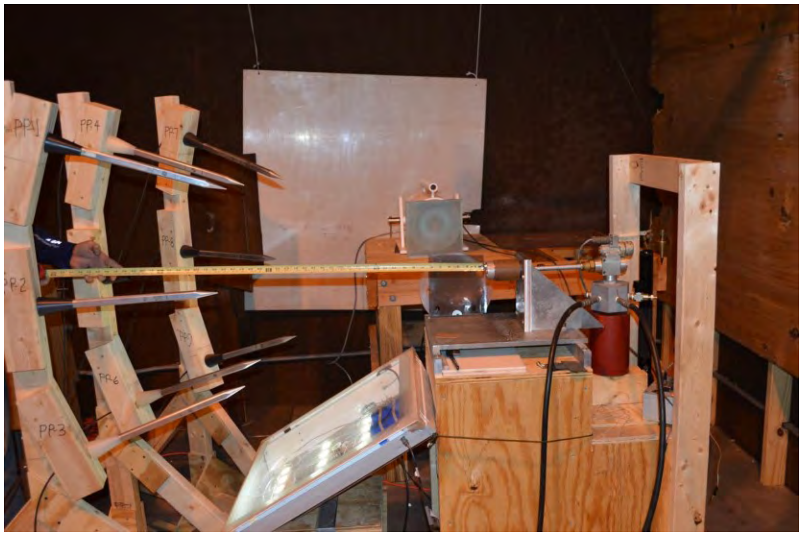
Photograph of Concave Pressure Probe Array



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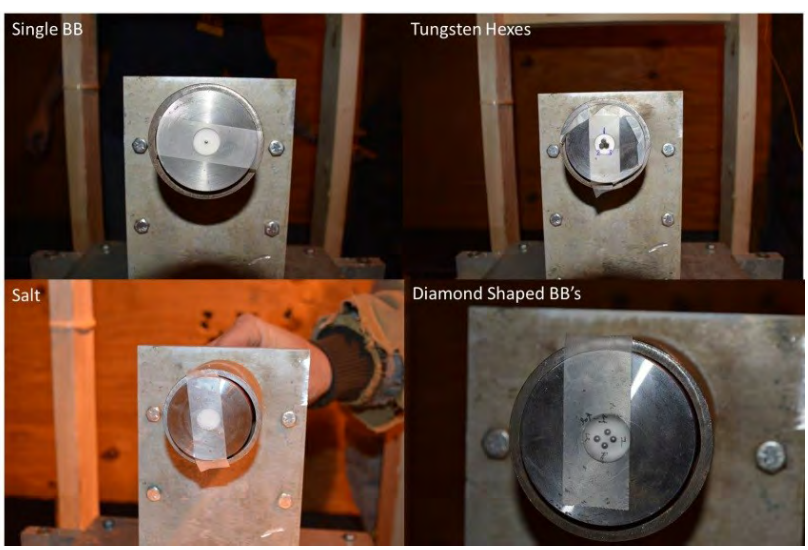
Test Items



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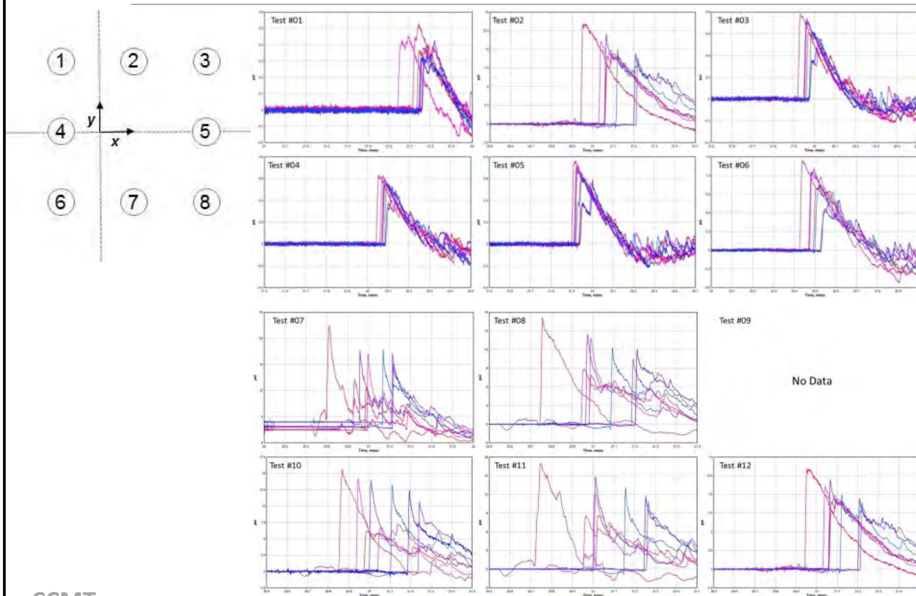
Pressure Traces



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Shock Arrival Times (in milliseconds)

Test	#1	#2	#3	#4	#5	#6	#7	#8
Test #01	21.733	21.713	21.750	21.641	21.760	21.757	21.745	21.742
Test #02	22.150	22.120	22.168	22.053	22.174	22.172	22.155	22.156
Test #03	21.959	21.919	21.950	21.947	21.977	21.950	21.975	21.974
Test #04	22.072	22.039	22.068	22.058	22.087	22.067	22.086	22.081
Test #05	21.034	21.898	21.916	21.910	21.935	21.912	21.939	21.918
Test #06	22.491	22.424	22.468	22.471	22.524	22.469	22.529	22.498
Test #07	20.960	20.440	20.716	20.981	21.217	20.775	21.225	20.919
Test #08	20.978	20.552	20.757	20.978	21.183	20.962	21.201	20.869
Test #09	---	---	---	---	---	---	---	---
Test #10	20.972	20.654	21.038	20.935	21.235	20.999	21.185	20.894
Test #11	21.010	20.531	20.756	20.995	21.255	21.000	21.242	20.934
Test #12	21.054	20.941	21.058	21.024	21.208	21.056	21.199	21.112

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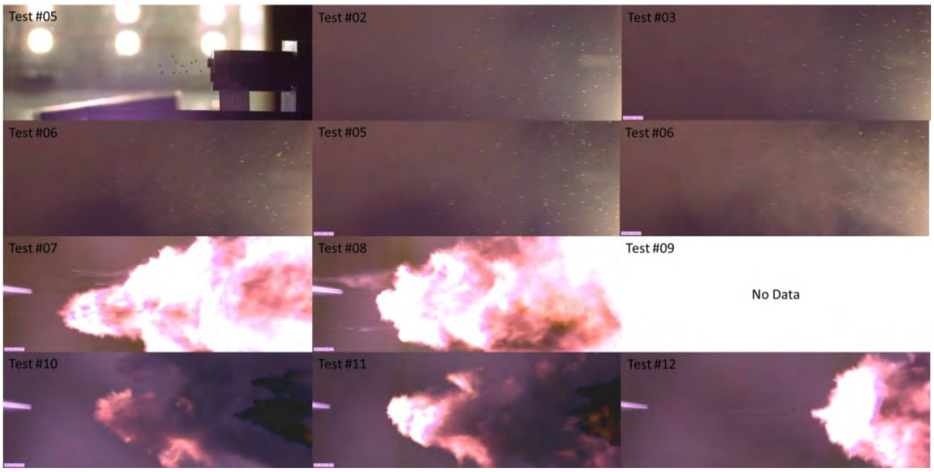
Representative Images from the Phantom 6.11



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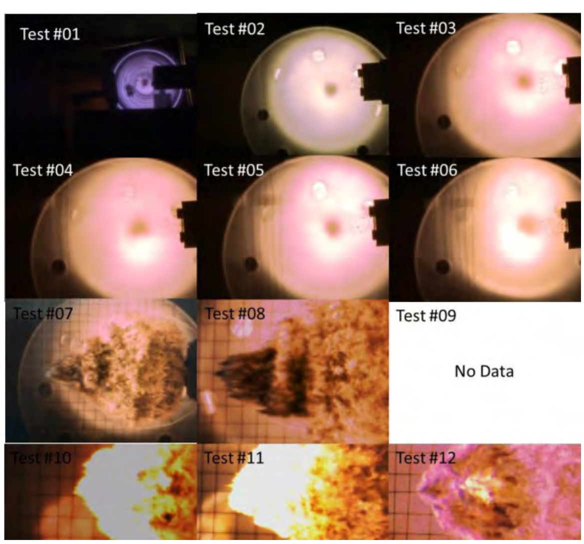
Representative images from the Phantom Miro M310



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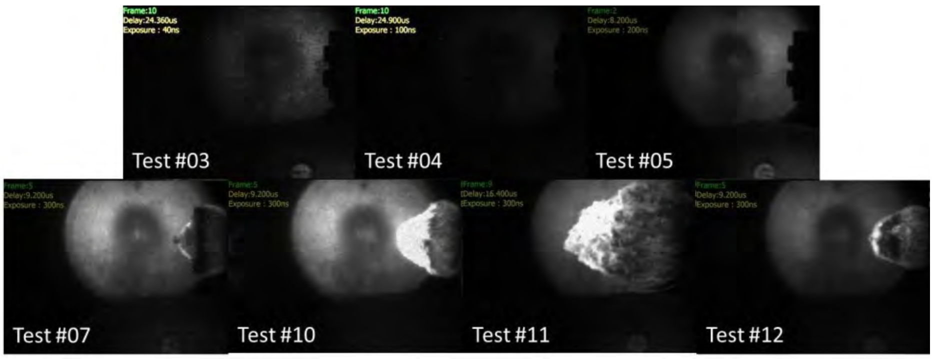
Representative images from the SIMACON



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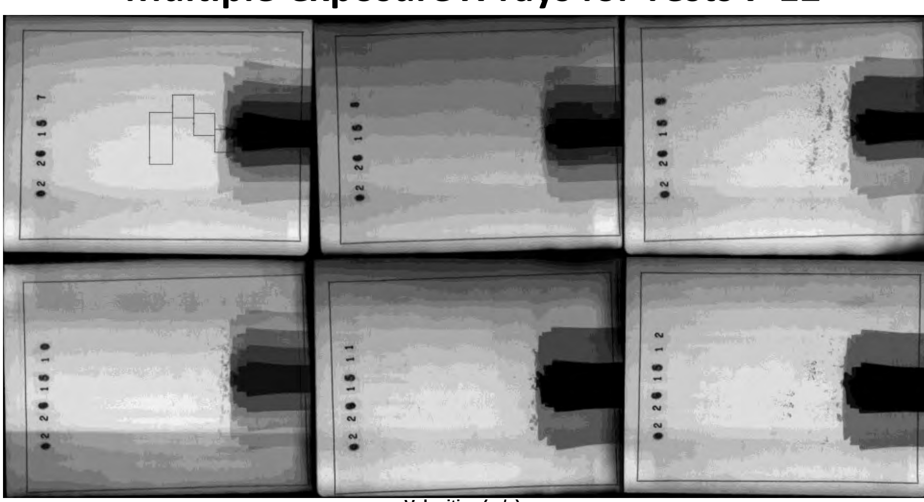
Multiple-exposure X-rays for Tests 7-12



Velocities (m/s)

	Test #07	Test #08	Test #09	Test #10	Test #11	Test #12
Head 1	550	550	759	---	---	---
Head 2	651	560	751	---	---	---
Head 3	723	644	707	---	---	631
Head 4	776	576	---	---	---	806

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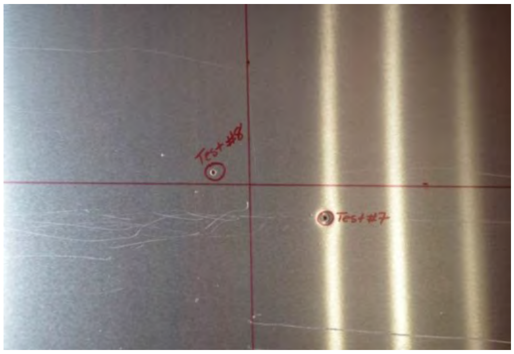
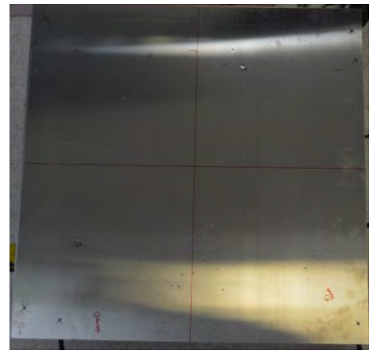
Witness Panels





X,Y coordinates (in millimeters) for witness panel impacts

	Test #07	Test #08	Test #09	Test #10	Test #11	Test #12
Particle1	-19, -46	7, 21	---	---	---	84, 182
Particle2	---	---	---	---	---	-192, -148

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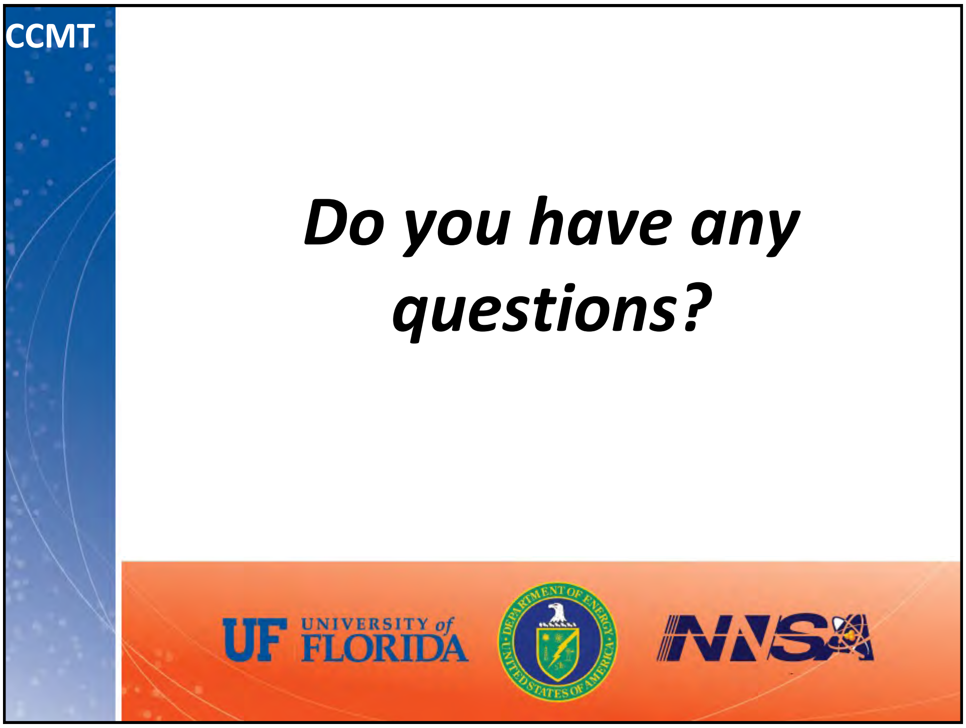
Summary

- Year 1+: Focus on microscale experiments
  - Millimeter-sized particles; single/few particles; planar geometry
  - Controlled experiments where a few well-characterized finite-sized metal particles are placed outside a well-characterized explosive in a precise manner
  - Diagnostics to:
    - Quantify the reproducibility of the pressure measurements
    - Accurately determine particle position and velocity in the fireball via X-ray imaging
    - Track the trajectories of individual particles via witness panels
    - Take high quality imagery of the fireball and flow fields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Additional Items

T.L. Jackson

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Recruiting

- Outstanding PhD students on campus at start of program
- Personal contacts by Faculty to outstanding students
  - Dr. Haftka's optimization class
  - Introduction from colleagues from other Universities
- ECE recruits outstanding BS and MS students for Ph.D. program
- MAE - gave talks to incoming PhD students (recruited David Zwick, ASU, and Frederick Ouellet, UF)

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Educational Programs

- Verification, Validation and Uncertainty Quantification: a new course started in 2014 in anticipation of CCMT with the help of visiting faculty from Korea, was offered the second time in 2015 by Drs. Haftka and Kim with revamped experimental project
- Computational Science – Dr. Sanjay Ranka taught a specialized course for HPC for computational scientists (as part of the Computational Engineering Certificate); five students in the course

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Internship Program

- Staff
  - Dr. Chanyoung Park – Sandia, March 2014
  - Dr. Jason Hackl – LLNL, February 2015
  - Dr. Bertrand Rollin – LANL, March 2015
  - Dr. Tania Banerjee – LLNL, May 25-29, 2015 (Martin Schulz and Barry Rountree)
  - Dr. Mrugesh Shringarpure – not required; cost share
  - Dr. Subramanian Annamalai – not required; cost share

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Internship Program

- Student Internships Planned or Completed

Heather Zunino	LANL	May-August, 2014	Dr. Kathy Prestridge
Kevin Cheng	LLNL	May-August, 2014	Dr. Maya Gokhale
Nalini Kumar *	LLNL	March-May, 2015	Dr. James Ang
Christopher Hajas	LLNL	May-August, 2015	Dr. Maya Gokhale
Christopher Neal	LLNL	June-August, 2015	Dr. Kambiz Salari
Carlo Pascoe	LLNL	June-August, 2015	Dr. Maya Gokhale
Giselle Fernandez	Sandia	Fall, 2015	

**cost share*

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Internship Program

- Student Internships Not Yet Planned
  - Kasim Alli
  - Angela Diggs (other funding; not required)
  - Goran Marjanovic
  - Yash Metha (cost share; not required)
  - Fred Ouellet
  - Dylan Rudolph
  - Prashanth Sridharan
  - Yiming Zhang (cost share; not required)
  - David Zwick (will be starting PhD program in June 2015)

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Additional Information

- CRT Site Visit – August 19, 2014
- Deep Dive Workshop. Held at the University of Florida on Feb 3-4, 2015.
- "Good Software Engineering Practices and Beyond" Workshop - Internal workshop - organized by Bertrand Rollin, held Feb 19, 2015.
- Center Webpage
  - http://www.eng.ufl.edu/ccmt/

1. Carlo Pascoe
2. Frederick Ouellet
3. Mrugesh Shringarpure
4. Nalini Kumar
5. Yash Mehta
6. Christopher Neal
7. Bertrand Rollin
8. Siddharth Thakur (ST)
9. Subramanian Annamalai
10. S. Balachandar (Bala)
11. Dylan Rudolph
12. Prashanth Sridharan
13. Tom Jackson
14. Tania Banerjee
15. Jason Hackl
16. Chanyoung Park
17. Jacob Rabb

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