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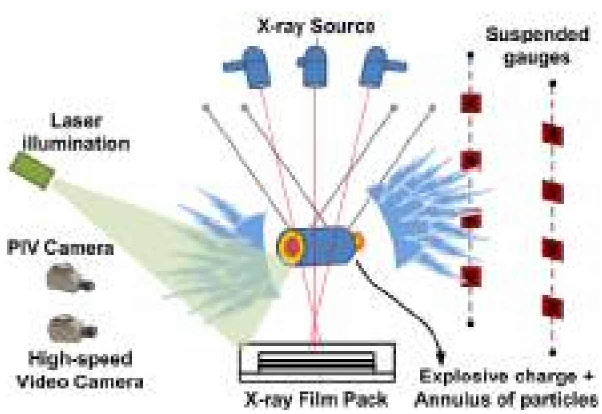
CENTER FOR COMPRESSIBLE MULTIPHASE TURBULENCE

TST Review

October 30-31, 2017



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Center for Compressible Multiphase Turbulence

1180 Center Drive
P.O. Box 116135
Gainesville, FL 32611
Phone: (352)294-2829
Fax: (352) 846-1196

Agenda for TST Site Visit October 30 and 31, 2017

Monday October 30, 2017

7:30	Van arriving University Hilton for pickup
7:45	Van leaving University Hilton
8:00-8:45	Full Breakfast (Review team caucus)
8:50-10:00	T1 - CCMT Overview and Integration (Jackson/Bala)
10:00-10:30	T2 – Full System Simulations (Bertrand Rollin)
10:30-10:45	Coffee break
10:45-11:30	T3 – CMT-nek (Jason Hackl/David Zwick)
11:30-12:00	T4 – ASU Experiments (Blair Johnson)
12:00-1:15	Lunch
1:15-1:45	T5 – Eglin Experiments (Angela Diggs)
1:45-2:30	T6 - UB (Chanyoung Park; Rafi Haftka; Nam-ho Kim)
2:30-3:15	T7 - CS (Sanjay Ranka)
3:15-3:30	Coffee break
3:30-4:15	T8 - Exascale (Herman Lam/Greg Stitt)
4:15-4:30	T9 - Internship presentations by Paul Crittenden, Mohamed Gadou, Trokon Johnson, Yash Mehta
4:30-5:30	Social with Students/Posters (NEB Main Lobby)
5:30	Transportation to University Hilton by CCMT Faculty
6:00-7:30	Dinner at the University Hilton, hosted by CCMT Faculty

Tuesday October 31, 2017

8:00	Van pickup at University Hilton
8:15-9:00	Continental Breakfast
9:00-10:30	Student Presentations
	T10 – EOS Surrogate Modeling (Fred Ouellet)
	T11 – UQ & Instabilities (Giselle Fernandez)
	T12 – PIEP Modeling (Chandler Moore)
	T13 – Microscale Shock-Contact Modeling (Brandon Osborne)
	T14 – BE of CMT-nek (Sai Chenna)
10:30-11:30	Discussions between TST and CCMT PIs
11:30	Box Lunch; Transportation to hotel and/or airport as needed

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TST Review October 30-31, 2017 Attendee List

Faculty

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

Review Team

Abhinav Bhatele	LLNL	bhatele1@llnl.gov
David Daniel	LANL	ddd@lanl.gov
Maya Gokhale	LLNL	gokhale2@llnl.gov
Sam Schofield (Chair)	LLNL	schofield5@llnl.gov
Greg Weirs	Sandia	vgweirs@sandia.gov

Others

Bob Voigt	Leidos/NESD	rvoigt@krellinst.org
Andrew Cook	LLNL	cook33@llnl.gov
Fady Najjar	LLNL	najjar2@llnl.gov
Dan Nikkel	LLNL	nikkel1@llnl.gov
Ryan Houim	University of Florida	rhouim@ufl.edu
Rose McCallen	LLNL	mccallen1@llnl.gov
Kambiz Salari	LLNL	salari1@llnl.gov
Fernando Grinstein	LANL	fgrinstein@lanl.gov

Research Staff

Tania Banerjee	University of Florida	tmishra@cise.ufl.edu
Jason Hackl	University of Florida	jason.hackl@ufl.edu
Blair Johnson	Arizona State University	blairjohnson@asu.edu
Chanyoung Park	University of Florida	cy.park@ufl.edu

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Students

Ryan Blanchard	University of Florida	rlb1116@ufl.edu
Sai Chenna	University of Florida	chenna@hcs.ufl.edu
Paul Crittenden	University of Florida	pcritte@ufl.edu
Brad Durant	University of Florida	neoncrash@ufl.edu
Giselle Fernandez	University of Florida	gisellefernandez@ufl.edu
Mohamed Gadou	University of Florida	mgadou@ufl.edu
Joshua Garno	University of Florida	jgarno@ufl.edu
Trokon Johnson	University of Florida	johnson@hcs.ufl.edu
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Goran Marjanovic	University of Florida	gmarjanovic@ufl.edu
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Yash Mehta	University of Florida	ymehta@ufl.edu
Chandler Moore	University of Florida	wcmoore@ufl.edu
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Raj Rajagoplan	University of Florida	saravana8394@ufl.edu
Ben Reynolds	University of Florida	beynoldsren@gmail.com
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Shirly Spath	University of Florida	spathsy@ufl.edu
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Heather Zunino	Arizona State University	hzunino@asu.edu
David Zwick	University of Florida	dpzwick@ufl.edu

Administration Staff

Hollie Starr	University of Florida	hstarr@ufl.edu

Financial Staff

Melanie DeProspero	University of Florida	mel7703@ufl.edu

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Overview and Integration

T.L. Jackson
S. Balachandar

TST Meeting Agenda

Monday

- T1 - Overview and Integration (Jackson & Balachandar)
- T2 – Full System Simulations (Bertrand Rollin)
- *Coffee Break*
- T3 - CMT-nek (Jason Hackl & David Zwick)
- T4 - ASU Experiments (Blair Johnson)
- *Lunch*
- T5 - Eglin Experiments (Angela Diggs)
- T6 - Uncertainty Budget (Chanyoung Park, Rafi Haftka, Nam-Ho Kim)
- T7 - CS (Sanjay Ranka)
- *Coffee Break*
- T8 - Exascale (Herman Lam & Greg Stitt)
- T9 - Internship presentations
- Social with Students/Posters (NEB Main Lobby)
- *Dinner at University Hilton with CCMT Faculty and Staff*

Tuesday

- Student Talks (5)
- Discussions between TST and CCMT PIs
- *Lunch and transportation to airport*

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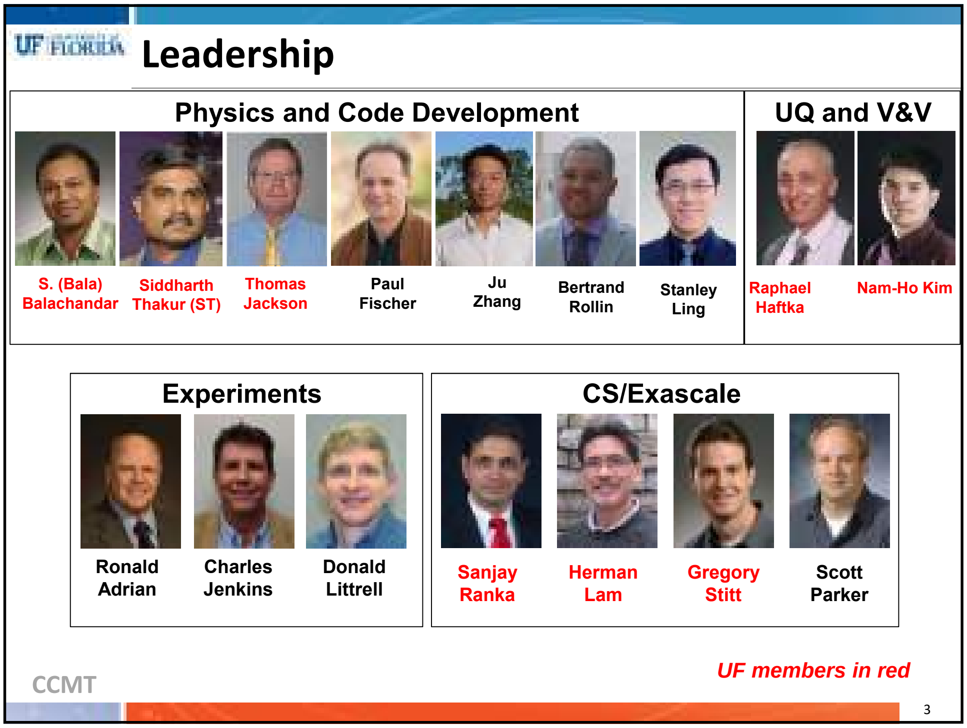
Leadership
Physics and Code Development
S. (Bala) Balachandar
Siddharth Thakur (ST)
Thomas Jackson
Paul Fischer
Ju Zhang
Bertrand Rollin
Stanley Ling
UQ and V&V
Raphael Haftka
Nam-Ho Kim
Experiments
Ronald Adrian
Charles Jenkins
Donald Littrell
CS/Exascale
Sanjay Ranka
Herman Lam
Gregory Stitt
Scott Parker
UF members in red
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Research Staff & Senior PhD Students
Tania Banerjee
Angela Diggs (Eglin AFB)
Jason Hackl
Blair Johnson (ASU)
Chanyoung Park
Carlo Pascoe
Nalini Kumar
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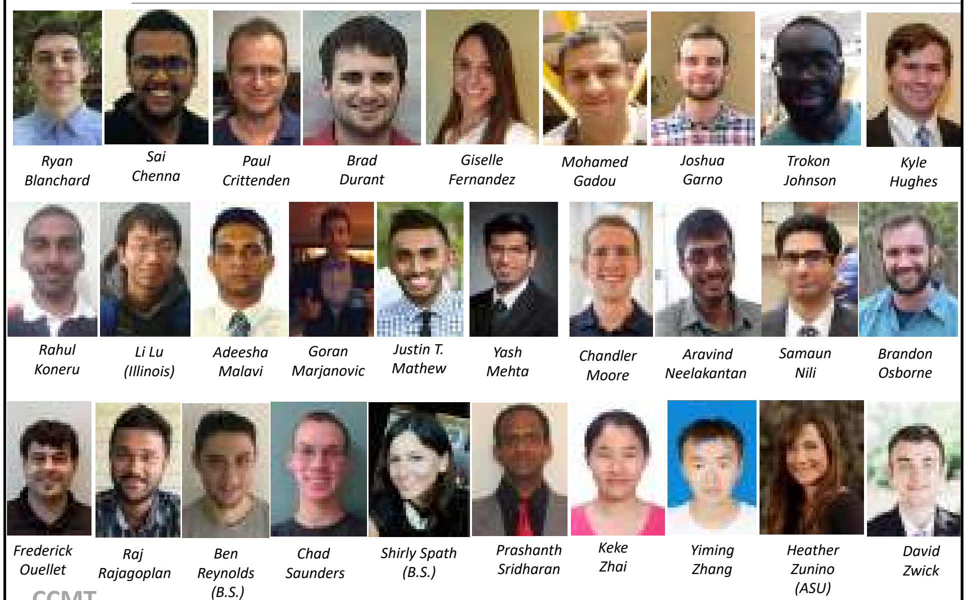
Current Students (Undergraduate & Graduate)



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Internship Program - Completed

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

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Internship Program - Completed

Goran Marjanovic	Sandia	Aug-Nov, 2016	Drs. Paul Crozier & Stefan Domino
Georges Akiki	LANL	May-Aug, 2016	Dr. Marianne Francois
Paul Crittenden	LLNL	Spring, 2017	Drs. Kambiz Salari & Sam Schofield
Mohamed Gadou	LANL	Summer, 2017	Dr. Galen Shipman
Trokon Johnson	LANL	Summer, 2017	Drs. Cristina Garcia- Cardona, Brendt Wohlberg, Erik West
Yash Mehta	LLNL	Summer, 2017	Dr. Kambiz Salari
Kyle Hughes	LANL	Fall, 2017	Dr. Kathy Prestridge

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Internship Program – Not Yet Planned

- Brad Durant, PhD (MAE, Physics and UQ)
- Joshua Garno, PhD (MAE, Physics and UQ)
- Brandon Osborne, PhD (MAE, Physics)
- Fred Ouellet, PhD (MAE, Physics and UQ)
- Chandler Moore, PhD (MAE, Physics) (NSF Fellowship)

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Graduated Students & Postdocs

- Kevin Cheng, MS (2014), Dr. Alan George, ECE
- Hugh Miles, BS (2015), Dr. Greg Stitt, ECE
- Chris Hajas, MS (2015), Dr. Herman Lam, ECE
- Angela Diggs, PhD (2015), Dr. S. Balachandar, MAE
  - Currently employed at Eglin AFB and working with center
- Bertrand Rollin, Postdoc in thru August 2014
  - Assistant Professor, Embry Riddle, Daytona Beach FL
- Mrugesh Shringarpure, Postdoc in thru January 2016
  - Research Engineer, ExxonMobil, Houston TX
- Subbu Annamalai, PhD (2015), Dr. S. Balachandar, MAE; Postdoc in thru March 2017
  - Senior Systems Engineer, Optym, Gainesville FL
- Georges Akiki, PhD (2016), Dr. S. Balachandar, MAE; Postdoc thru March 2017
  - Postdoctoral Associate, LANL
- Nalini Kumar, PhD (August, 2017), Dr. H. Lam, ECE
  - Intel, Santa Clara CA

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Additional Information

- Additional Graduate Program Announcements
  - David Zwick – NSF Fellowship Graduate Program (Aug 2016)
  - Georges Akiki - MAE Best Dissertation Award (TSFD; May 2017)
  - Chandler Moore – NSF Fellowship Graduate Program (Aug 2017)
- Other metrics (Y1 – Y3)
  - Publications: 85
  - Presentations: 69
- Deep Dive Workshops
  - Exascale & CS Issues, Feb 3-4, 2015, University of Florida
  - Multiphase Physics, Oct 13-14, 2016, Tampa FL
- APS Special Focus on UQ (July, 2017) – Jackson, Najjar, Najm
- Center Webpage
  - http://www.eng.ufl.edu/ccmt/

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Educational Programs

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

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Management: Tasks and Teams

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

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

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

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3rd Annual CCMT Picnic (March, 2017)

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Outline

- Background
- Scope of the center
- V&V and UQ workflow
- Y4 accomplishments
- Integration and timeline

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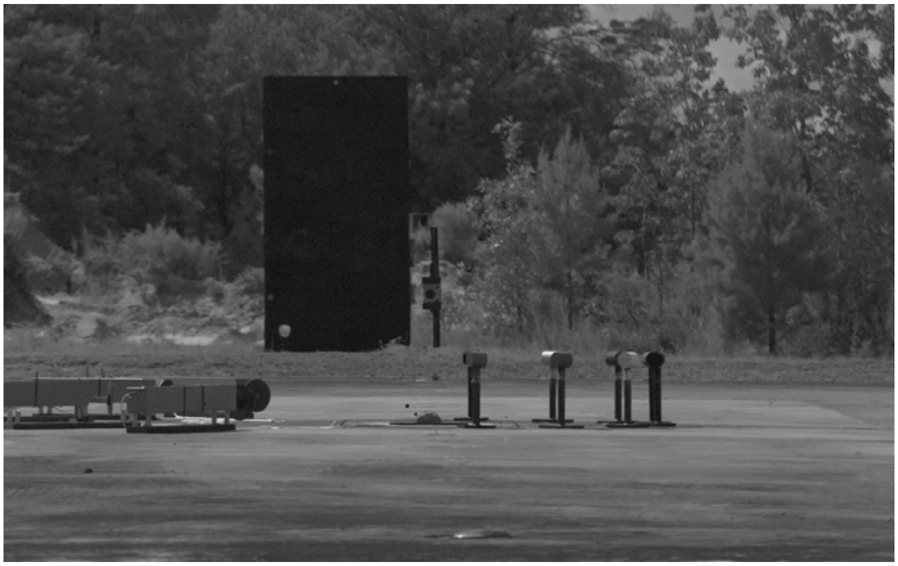
Demonstration Problem



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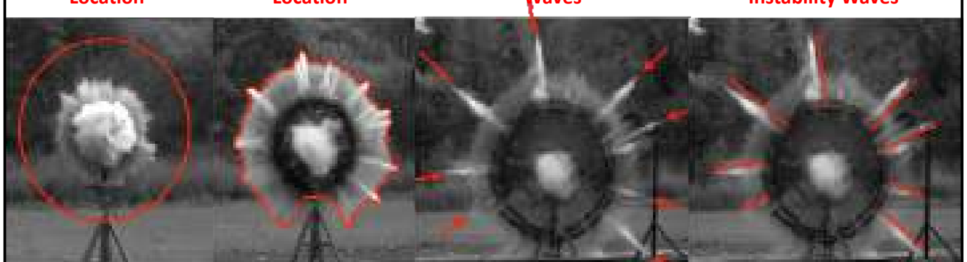
Prediction Metrics

PM-1: Blast Wave Location

PM-2: Particle Front Location

PM-3: Number of Instability Waves

PM-4: Amplitude of Instability Waves



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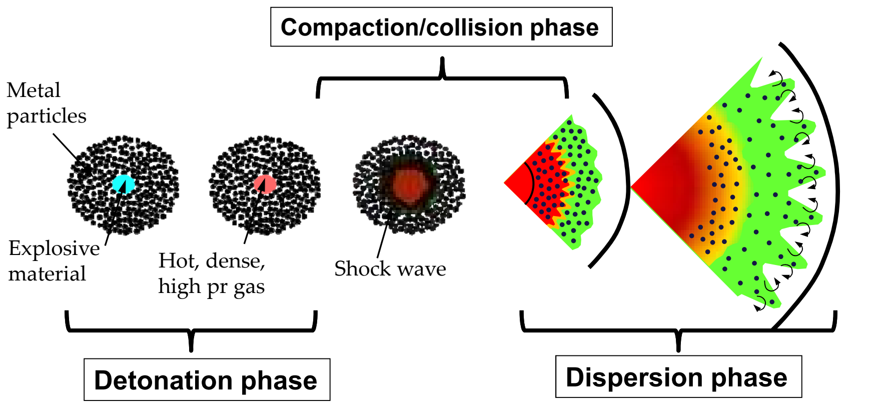
Sequence of Events



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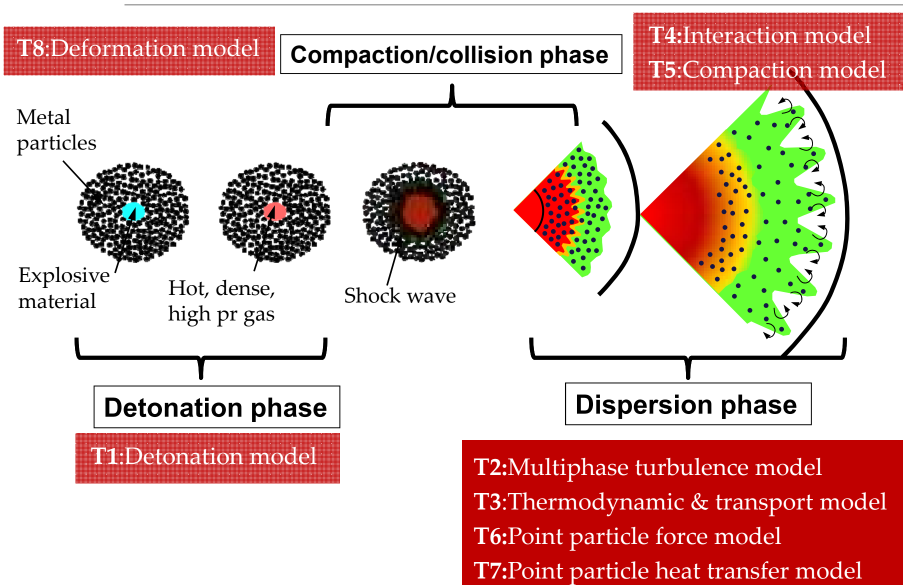
Physical Models – Sources of Error



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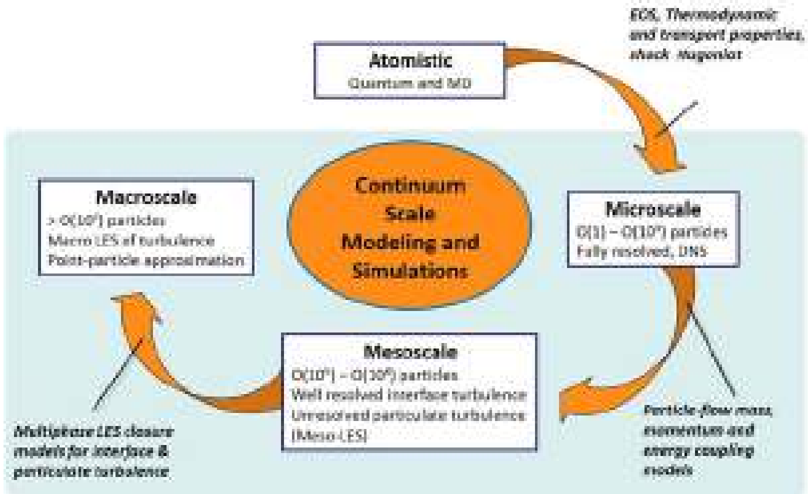
Multiscale Integration Strategy



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Multiphysics Scope (From Site Visit)

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

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Sources of Errors & Uncertainties

- T1: Detonation modeling
- T2: Multiphase turbulence modeling
- T3: Thermodynamics & transport properties
- T4: Particle-particle interaction modeling
- T5: Compaction modeling
- T6: Force coupling modeling
- T7: Thermal coupling modeling
- T8: Particle deformation and other complex physics

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

Key Focus

Advance state-of-the-art

- Multiphase turbulence

- Force coupling model

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Amendment to Scope

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

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

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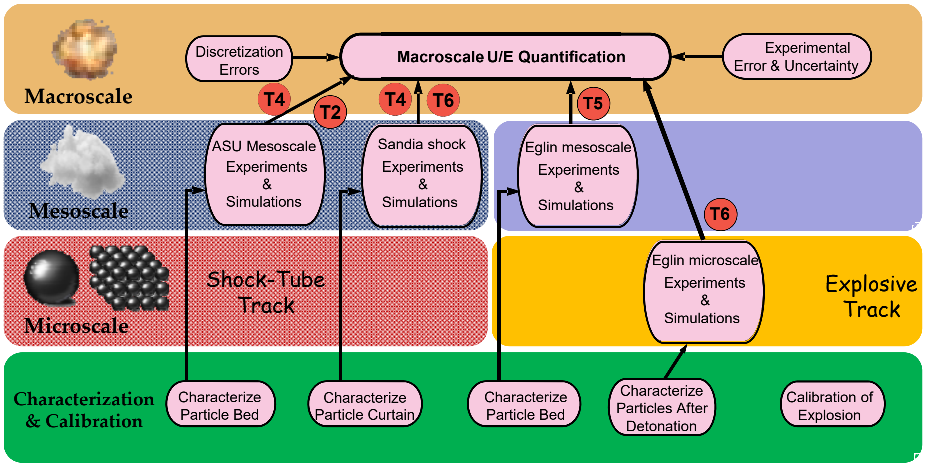
Uncertainty Budget – Overall Plan



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

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4 Micro/Meso Campaigns & Target Models

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

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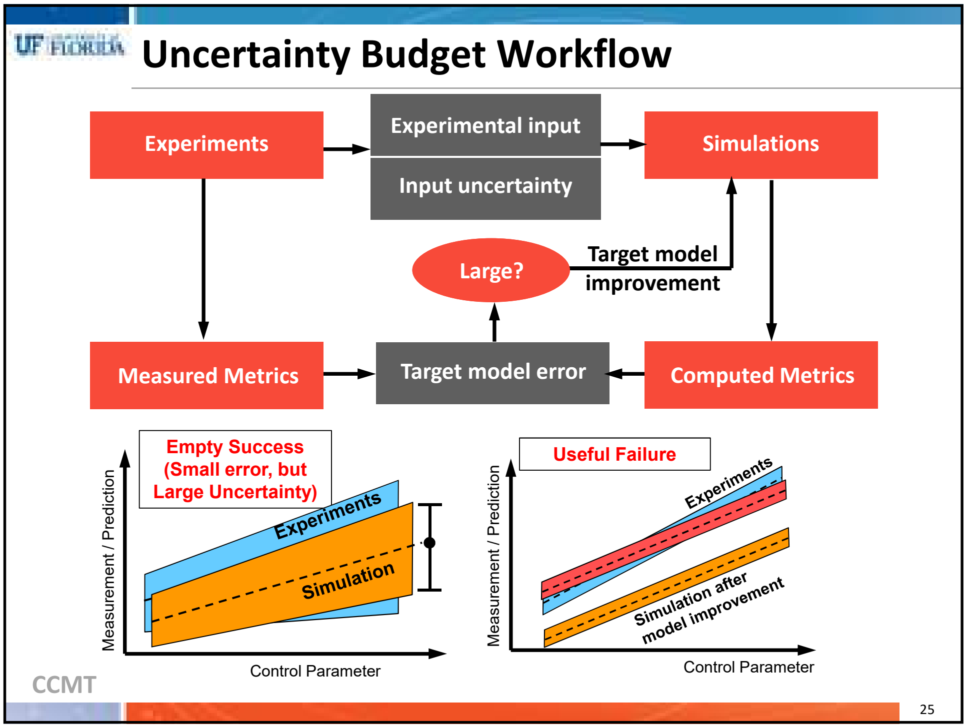
Uncertainty Budget Workflow
Experiments
Experimental input
Input uncertainty
Simulations
Large?
Target model
improvement
Measured Metrics
Target model error
Computed Metrics
Empty Success
(Small error, but
Large Uncertainty)
Experiments
Simulation
Measurement / Prediction
Control Parameter
Useful Failure
Experiments
Simulation after
model improvement
Measurement / Prediction
Control Parameter
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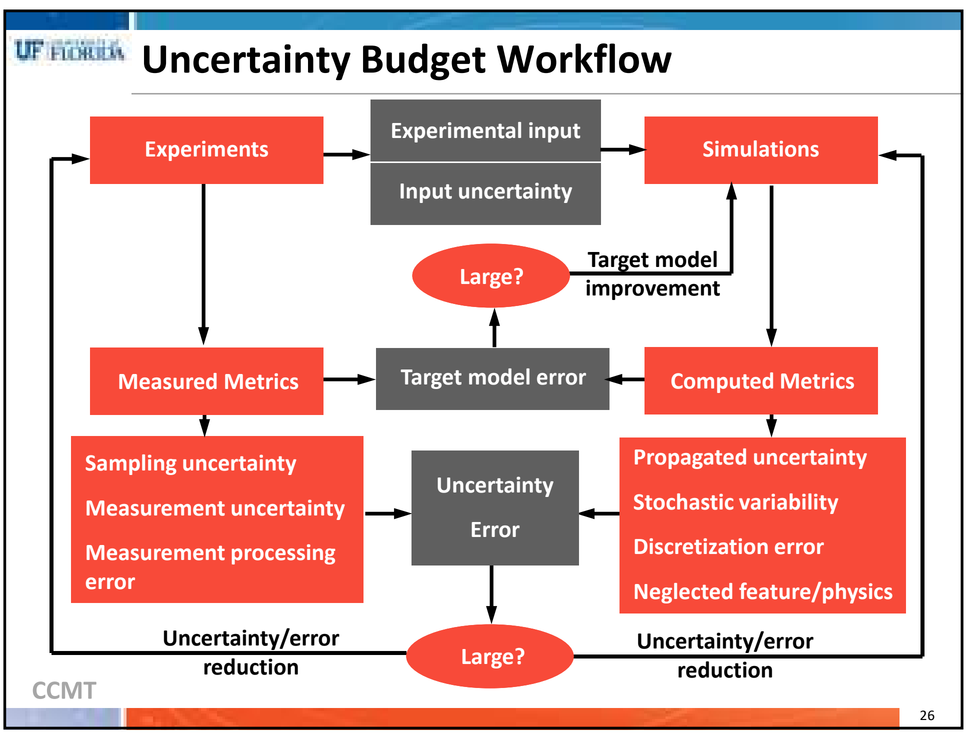
Uncertainty Budget Workflow
Experiments
Experimental input
Input uncertainty
Simulations
Large?
Target model
improvement
Measured Metrics
Target model error
Computed Metrics
Sampling uncertainty
Measurement uncertainty
Measurement processing
error
Uncertainty
Error
Propagated uncertainty
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error
reduction
Large?
Uncertainty/error
reduction
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UB Workflow - Experiment Worksheet

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

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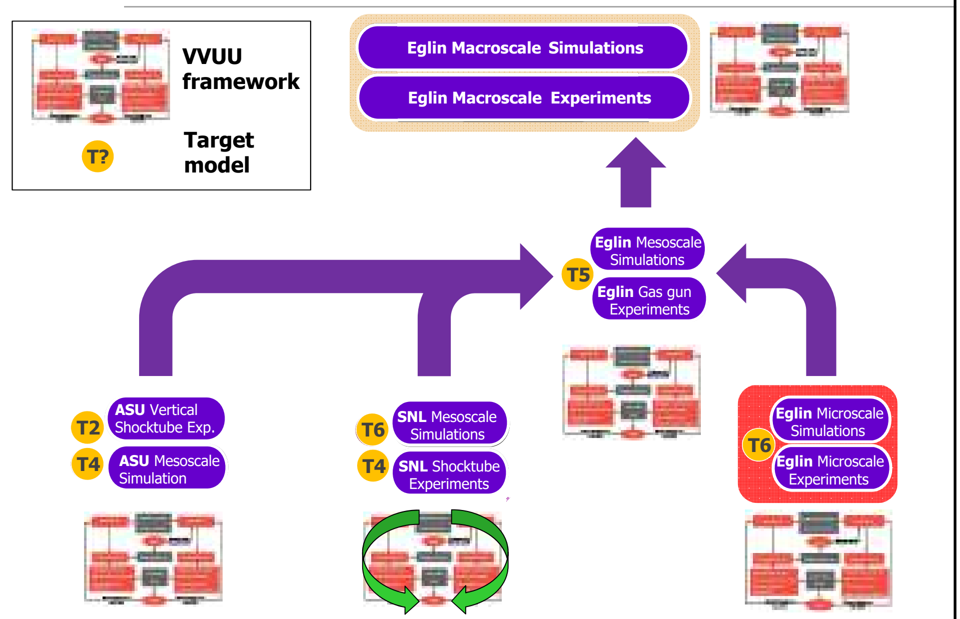
Hierarchical Error Estimation and UQ



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Other Simulation Campaigns

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

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Y4 Key Accomplishments

- Tight integration
- Empower students and staff
- PIEP model
- CMT-nek (O(10^6) core simulations)
- Culture of UQ integration
- BE framework and FPGA
- Dynamic load balancing

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Y4 Highlights

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

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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

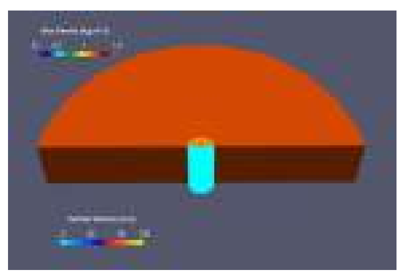
Year 4

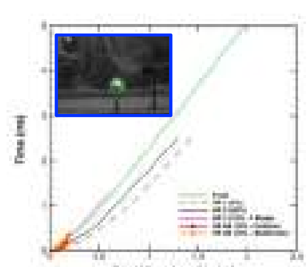
- Used existing code to perform largescale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)
- Develop capabilities for the hero runs: real gas EOS, reactive burn, collision modeling

Presentation

- Bertrand Rollin

3-D demonstration Simulations





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2: Blastpad Experiments

Goals

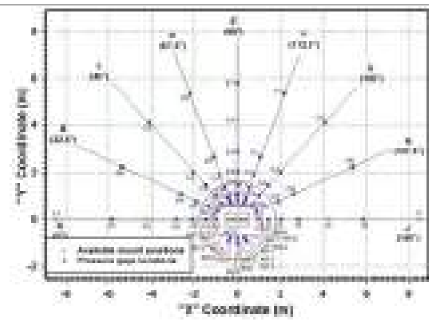
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

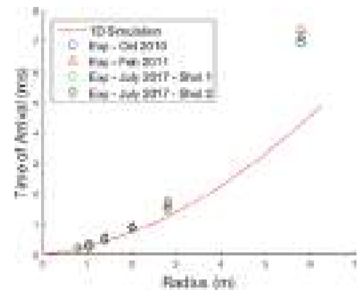
Year 4

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

Presentation

- Angela Diggs, Bertrand Rollin





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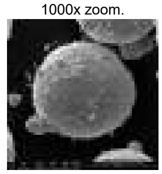
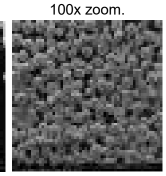
2: Blastpad Experiments

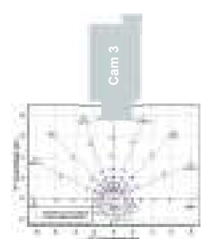
Input Parameter	Source
Explosive length [mm]	AFRL measurement
Explosive diameter [mm]	AFRL measurement at 5 locations
Explosive density [kg/m^3]	AFRL calculation
Explosive quality	AFRL X-ray
Particle diameter [mm]	CCMT measurement
Particle density [kg/m^3]	CCMT measurement
Particle volume fraction	AFRL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

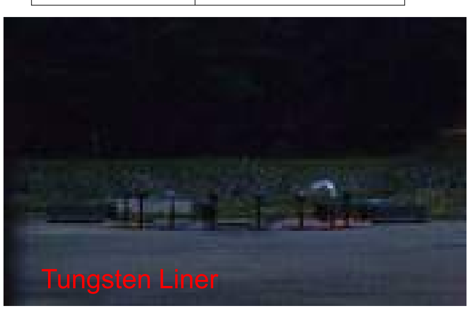
SEM of single steel particle at 1000x zoom.

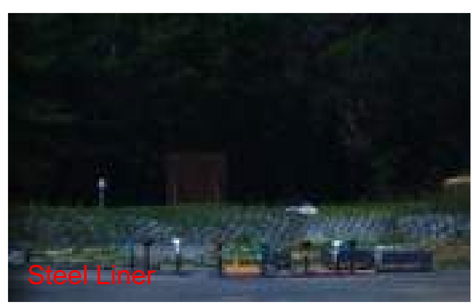


SEM of several steel particles at 100x zoom.









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2: Mesoscale Experiments

Goals

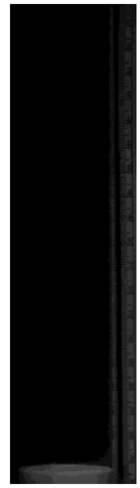
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

Year 4

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

Presentation

- Blair Johnson (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

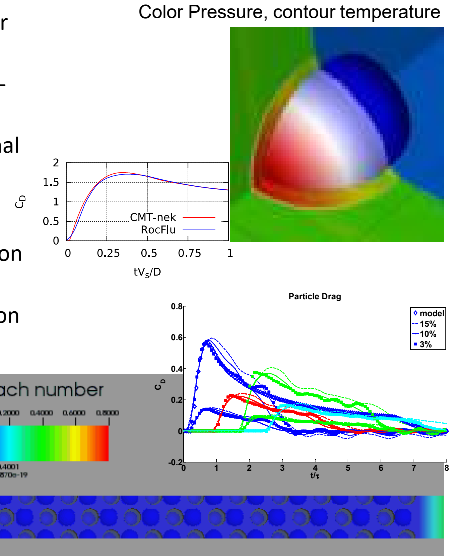
Year 4

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

Presentation

- Jason Hackl and David Zwick

Mach 3, γ = 1.4,
Color Pressure, contour temperature



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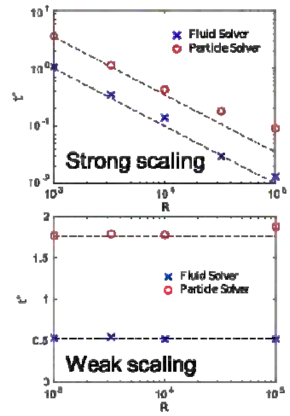
3. CMT-nek

- Capabilities
  - Viscous compressible N-S solver
  - DG spectral element (rigorous conservation)
  - Shock capturing with EVM
  - Spectrally accurate Lagrangian particle solver
  - 4-way coupling (Soft-sphere DEM, PIEP)
  - Scalable to O(10^6) cores and more



- Class of problems
  - Incompressible (Nek-5000) & compressible single phase
  - Incompressible & compressible dilute point-particle multiphase
  - Incompressible & compressible dense multiphase

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4: Mesoscale Simulations

Goal

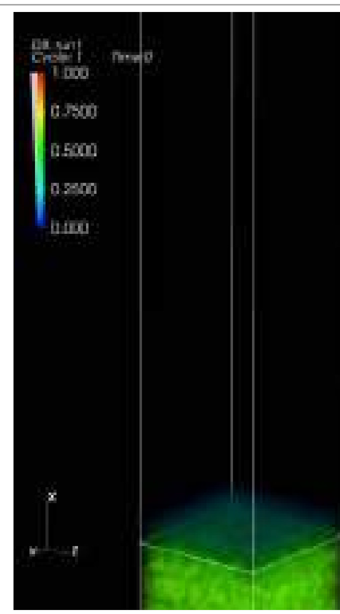
- Perform a hierarchy of mesoscale simulations to allow rigorous validation, uncertainty quantification and propagation to the demonstration problem

Year 4

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

Presentation

- David Zwick



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5: Microscale Simulations

Goals

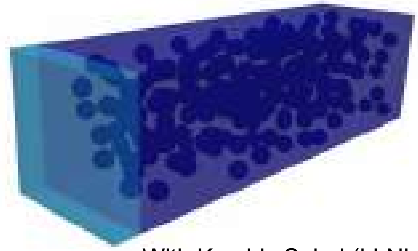
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation

Year 4

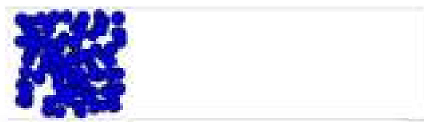
- Shock propagation over a structured array
- Shock propagation over a random array
- Shock + Contact + particles
- Shock over deformable particles

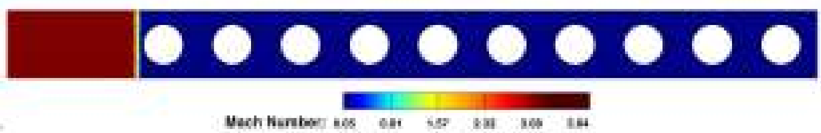
Presentation

- Brandon Osborne



With Kambiz Salari (LLNL)





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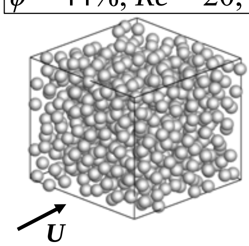
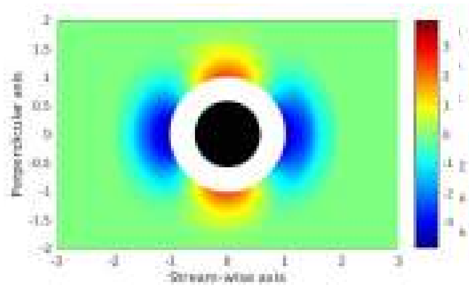
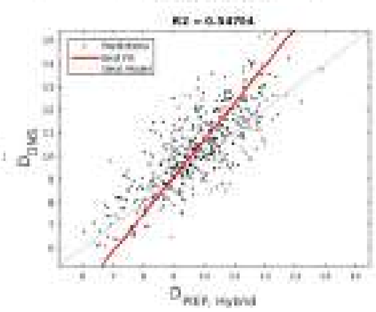
5: Extended Point Particle Model

$\phi = 44\%, Re = 20, \mathrm{N} = 459$





R² Values:		PIEP-Physics			PIEP-Hybrid		
ϕ	*Re*	Drag	Lift	Torque	Drag	Lift	Torque
0.1	40	0.70	0.68	0.75	0.72	0.75	0.79
0.1	70	0.65	0.68	0.65	0.67	0.72	0.72
0.1	173	0.35	0.59	0.45	0.44	0.60	0.58
0.2	16	0.38	0.34	0.48	0.66	0.74	0.71
0.2	89	0.50	0.48	0.72	0.62	0.63	0.77
0.45	21	0.01	0.09	0.47	0.55	0.59	0.76
0.45	115	0.21	0.19	0.51	0.63	0.57	0.65



CCMT **Presentation**: Chandler Moore

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6: UQ Workflow

Goals

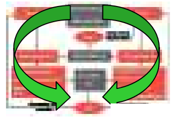
- Develop UB as the backbone of the Center
- Unified application of UB for both physics and exascale emulation

Year 4

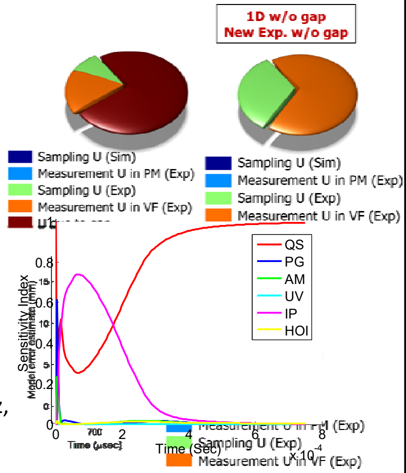
- Identify main uncertainty sources and quantify their contributions to the model uncertainty of the shock tube simulation
- Reduce uncertainty to focus on model error
- UQ and propagation in the context of exascale emulation
- JWL mixture-EOS surrogate for efficient computation

Presentation

- Rafi Haftka, Chanyoung Park, Giselle Fernandez, Fred Ouellet



UQ Workflow



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7: Exascale Emulation

Goal

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

Year 4

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

Presentation

- Herman Lam, Greg Stitt, Sai Chenna

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

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8: Dynamic Load Balancing

Goal

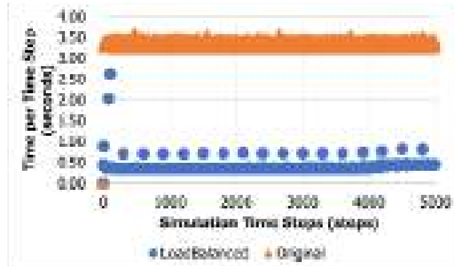
- Derive computationally intensive portions of the CMT-nek code and understand its performance, thermal and energy issues

Year 4

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

Presentation

- Sanjay Ranka



67,206 MPI ranks
1,867 nodes
36 cores per node
900,000 elements
1.125x10⁹ particles
Grid size: 5x5x5
Rarefaction test
8.3x improvement in performance

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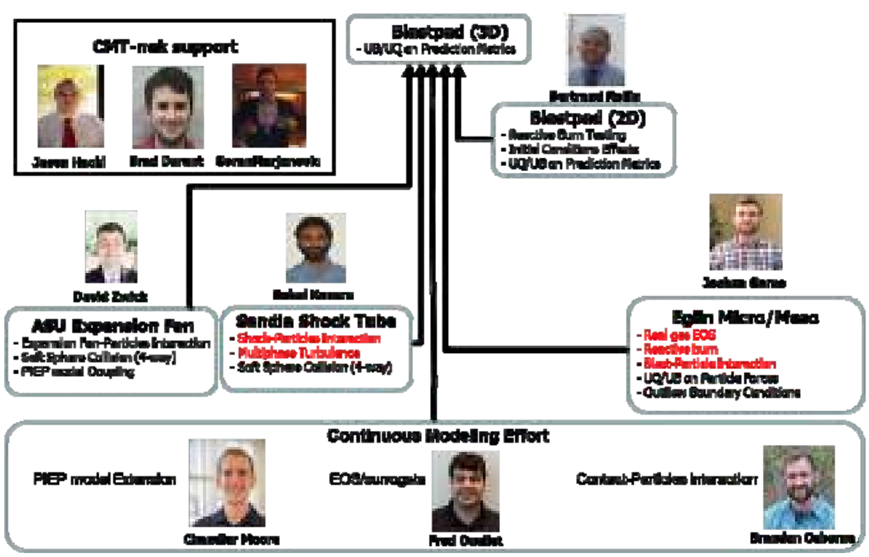
Transition to CMT-nek – Simulation Plan



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Transition to CMT-nek – CCMT Workshop

A Boot Camp on CMT-nek

November 29, 2017

Organizers: Bertrand Rollin, Jason Hackl

Agenda

- **CMT-nek: Anatomy of the Beast**
  Speaker: Jason Hackl | 12:00 pm – 1:30 pm
- **Lagrangian Particles in CMT-nek**
  Speaker: David Zwick | 1:30 pm – 2:30 pm
- **Running CMT-nek**
  Speakers: Goran Marjanovic and Brad Durant | 2:30 pm – 3:15 pm
- **Post-Processing and visualization in CMT-nek**
  Speakers: David Zwick and Brad Durant | 3:15 pm – 4:00 pm
- **Lesson Learnt from CCMT's Simulations**
  Spearkers: Fred Ouellet and Yash Mehta | 4:00 pm – 5:00 pm

Attendee list

Paul Crittenden
Brad Durant
Giselle Fernandez
Joshua Garno
Jason Hackl
Rahul Koneru
Yash Mehta
Goran Marjanovic
Chandler Moore
Fred Ouellet
Brandon Osborne
Bertrand Rollin
Prashanth Sridharan
David Zwick

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Transition to CMT-nek – Timeline

Task	Year4						Year5											
	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC	JAN	FEB	MAR	APR
Training with CMT-nek	W																	
Blastpad Simulation 3D (Hero Run)																		
Eglin Mesoscale Experiment (2D)																		
Eglin Mesoscale Experiment (3D)																		
Eglin Microscale Experiment (2D)																		
Eglin Microscale Experiment (3D)																		
Sandia Shock Tube Experiment																		
ASU Expansion Fan																		

W Workshop: "A Boot Camp on CMT-nek"

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CMT-nek – Blastpad Hero Runs

	Hero Run 6	Hero Run 7	Hero Run 8
Reactive burn	No	No	Yes
Equation of state	Ideal Gas	JWL	JWL
Initial Particle volume fraction	5 %	10 %	60 %
Particle bed perturbation	none	1 mode – (Notched Case)	Random
No. of computational particles	20 B	20 B	20 B
No. of Grid Points	1.8 B (1,025,000 Spectral Elements, 12x12x12 grid points/element)	1.8 B (1,025,000 Spectral Elements, 12x12x12 grid points/element)	14 B (8,200,000 Spectral Elements, 12x12x12 grid points/element)
No. of cores	131K	131K	393,216 (All of Vulcan - DAT)
Simulation Time	0.5ms	3.0ms	6.0ms

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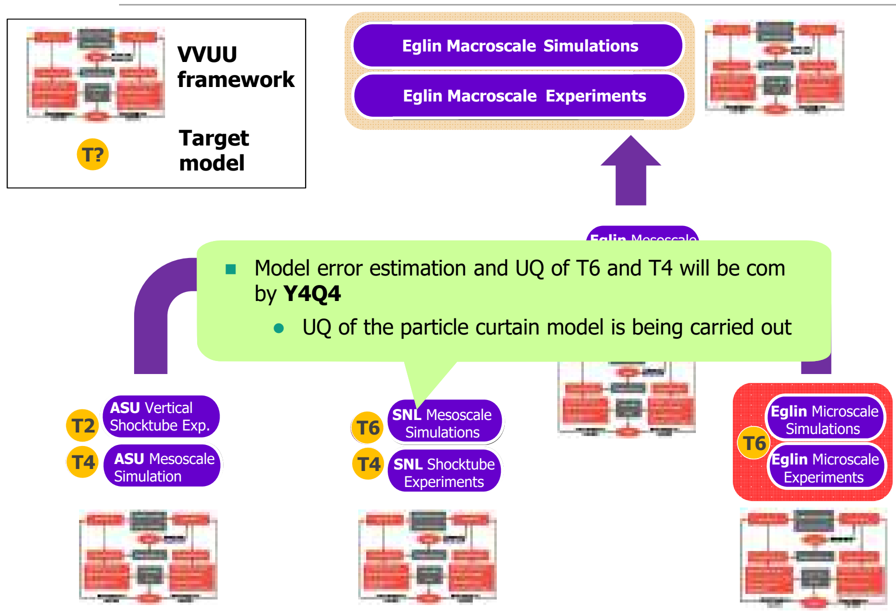
Hierarchical Error Estimation and UQ



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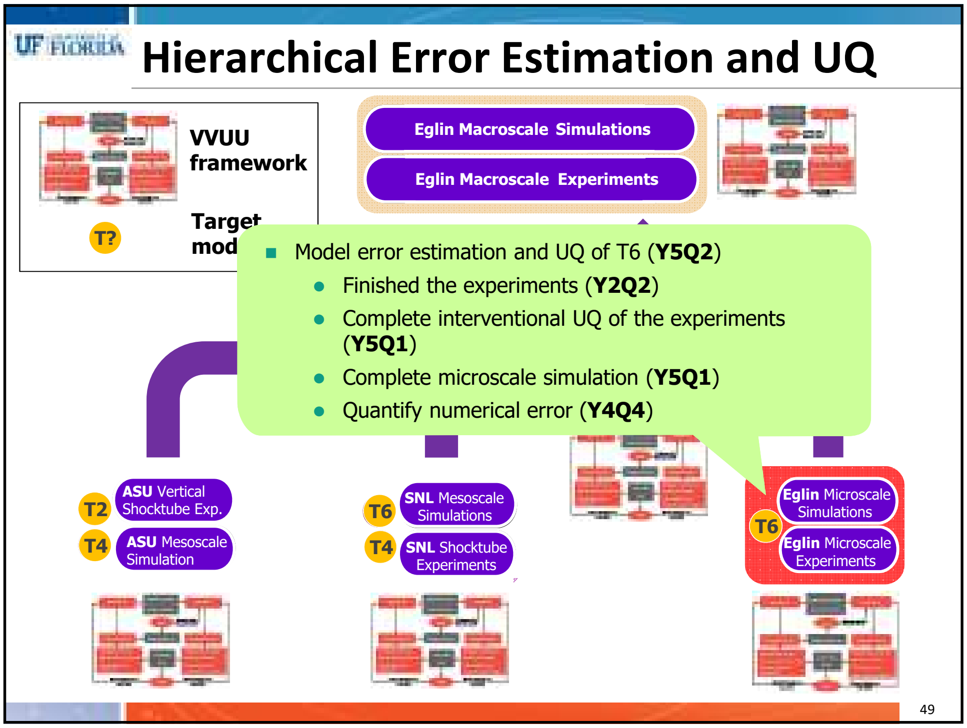
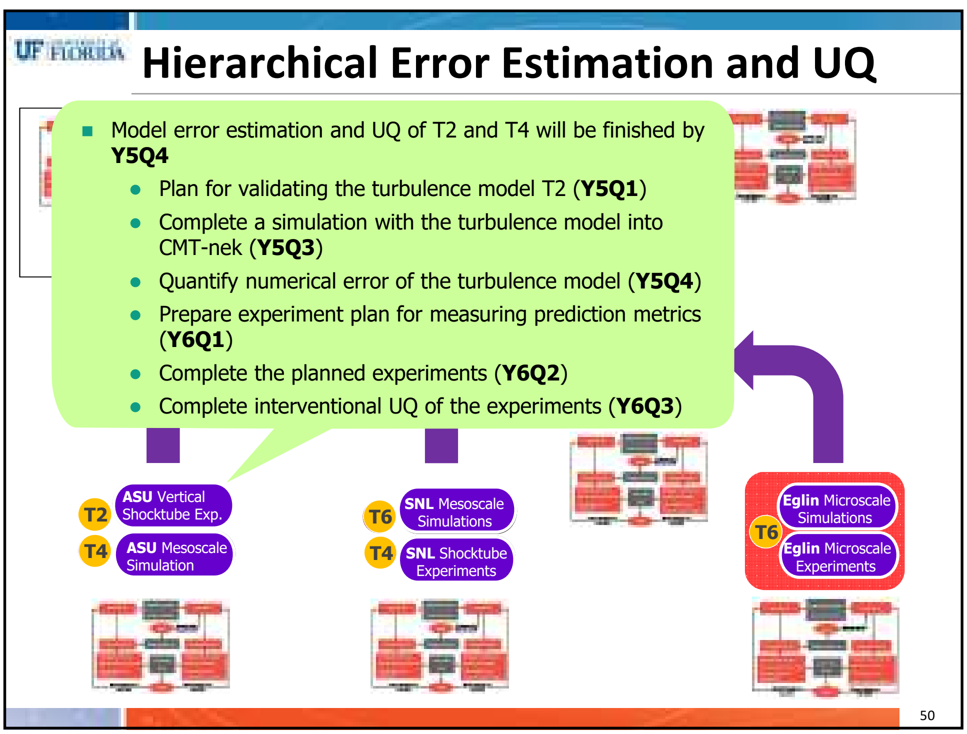

Hierarchical Error Estimation and UQ
VVUU
framework
Target
mod
T?
Eglin Macroscale Simulations
Eglin Macroscale Experiments
Model error estimation and UQ of T6 (Y5Q2)
Finished the experiments (Y2Q2)
Complete interventional UQ of the experiments (Y5Q1)
Complete microscale simulation (Y5Q1)
Quantify numerical error (Y4Q4)
T2
ASU Vertical Shocktube Exp.
T4
ASU Mesoscale Simulation
T6
SNL Mesoscale Simulations
T4
SNL Shocktube Experiments
T6
Eglin Microscale Simulations
Eglin Microscale Experiments
49


Hierarchical Error Estimation and UQ
Model error estimation and UQ of T2 and T4 will be finished by Y5Q4
Plan for validating the turbulence model T2 (Y5Q1)
Complete a simulation with the turbulence model into CMT-nek (Y5Q3)
Quantify numerical error of the turbulence model (Y5Q4)
Prepare experiment plan for measuring prediction metrics (Y6Q1)
Complete the planned experiments (Y6Q2)
Complete interventional UQ of the experiments (Y6Q3)
T2
ASU Vertical Shocktube Exp.
T4
ASU Mesoscale Simulation
T6
SNL Mesoscale Simulations
T4
SNL Shocktube Experiments
T6
Eglin Microscale Simulations
Eglin Microscale Experiments
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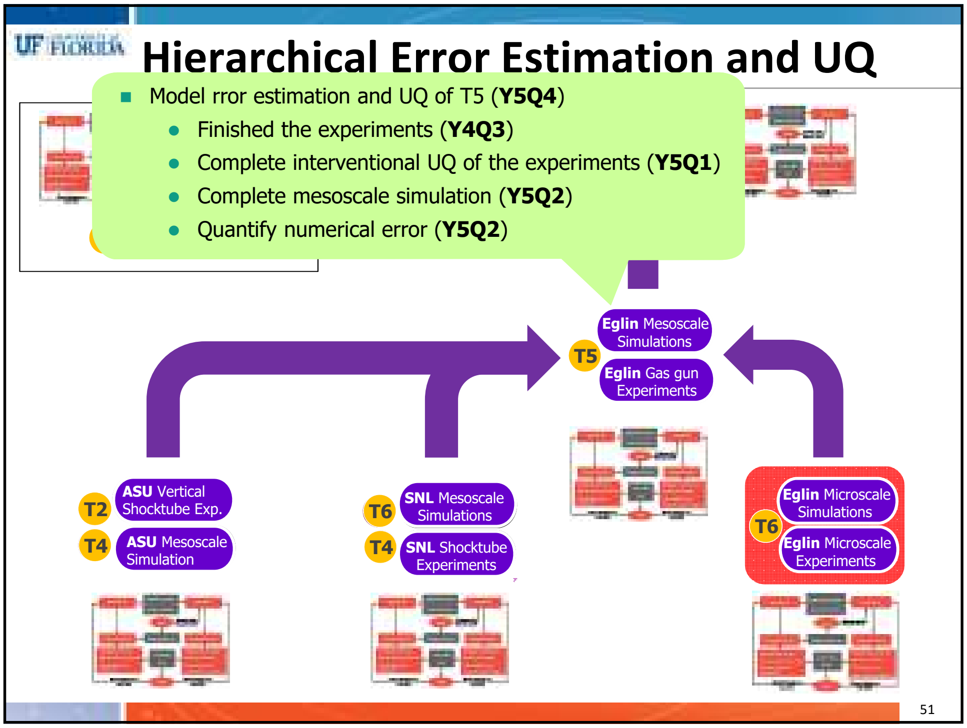
Hierarchical Error Estimation and UQ
Model rror estimation and UQ of T5 (Y5Q4)
Finished the experiments (Y4Q3)
Complete interventional UQ of the experiments (Y5Q1)
Complete mesoscale simulation (Y5Q2)
Quantify numerical error (Y5Q2)
T5
Eglin Mesoscale Simulations
Eglin Gas gun Experiments
T2
ASU Vertical Shocktube Exp.
T4
ASU Mesoscale Simulation
T6
SNL Mesoscale Simulations
T4
SNL Shocktube Experiments
T6
Eglin Microscale Simulations
Eglin Microscale Experiments
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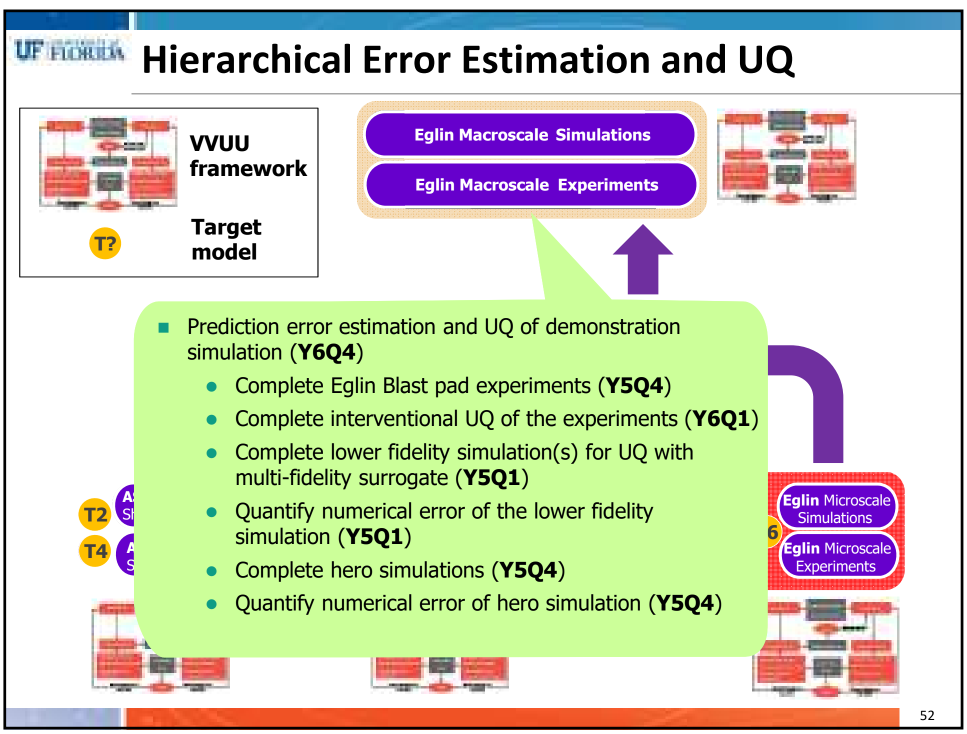
Hierarchical Error Estimation and UQ
VVUU framework
T?
Target model
Eglin Macroscale Simulations
Eglin Macroscale Experiments
Prediction error estimation and UQ of demonstration simulation (Y6Q4)
Complete Eglin Blast pad experiments (Y5Q4)
Complete interventional UQ of the experiments (Y6Q1)
Complete lower fidelity simulation(s) for UQ with multi-fidelity surrogate (Y5Q1)
Quantify numerical error of the lower fidelity simulation (Y5Q1)
Complete hero simulations (Y5Q4)
Quantify numerical error of hero simulation (Y5Q4)
T2
T4
Eglin Microscale Simulations
Eglin Microscale Experiments
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Timeline

◆: Coupling to Higher Scale

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Do you have any questions?


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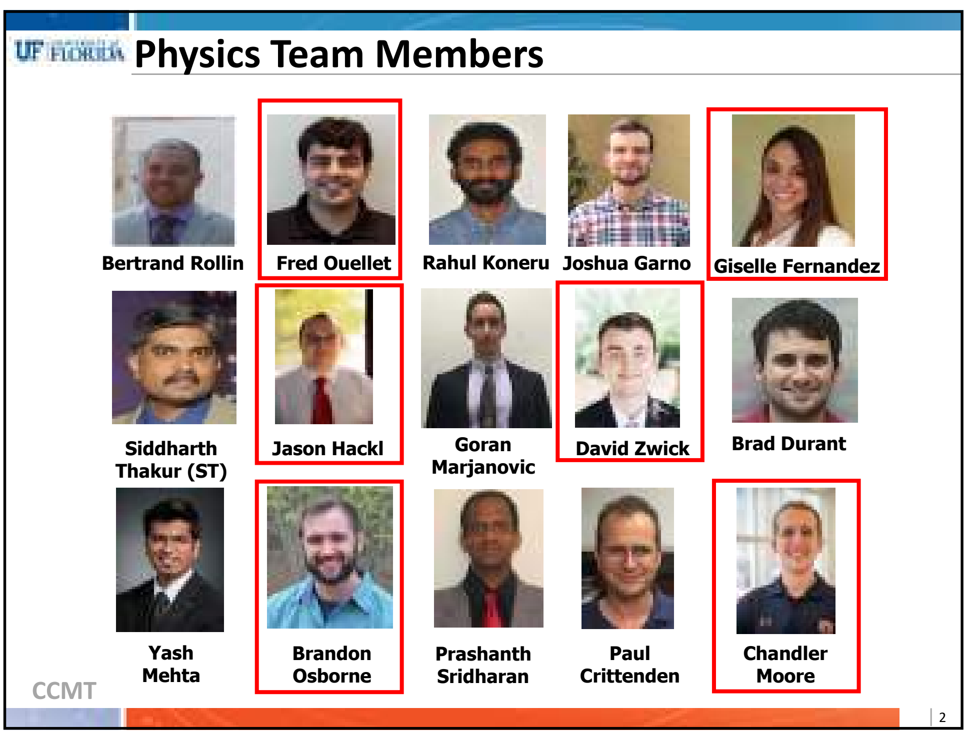
Full System Simulations
Bertrand Rollin
UF UNIVERSITY of FLORIDA
NNSA


UF FLORIDA
Physics Team Members
Bertrand Rollin
Fred Ouellet
Rahul Koneru
Joshua Garno
Giselle Fernandez
Siddharth Thakur (ST)
Jason Hackl
Goran Marjanovic
David Zwick
Brad Durant
Yash Mehta
Brandon Osborne
Prashanth Sridharan
Paul Crittenden
Chandler Moore
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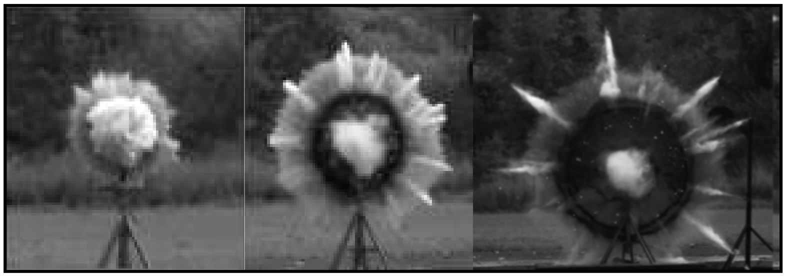
2

Explosive-Driven Particle-Laden Flows



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

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Outline

- **Demonstration Problems**
  - Frost's Experiment
  - Eglin's Blastpad Experiment
- **Micro and Mesoscale Campaigns**
  - Eglin Microscale Experiments
  - Eglin Mesoscale Experiments
  - SNL's Multiphase Shock Tube
  - ASU Expansion Fan

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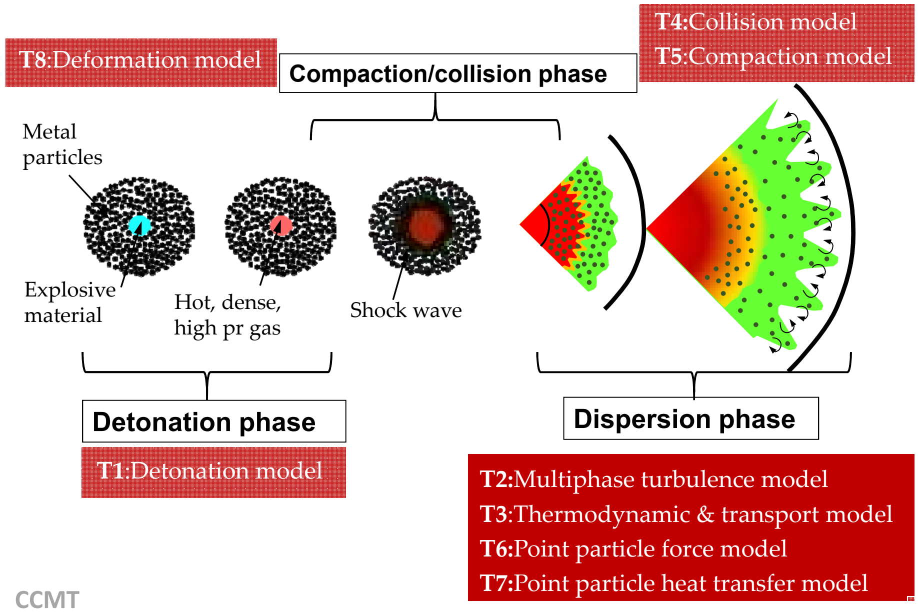
Physical Models – Sources of Error



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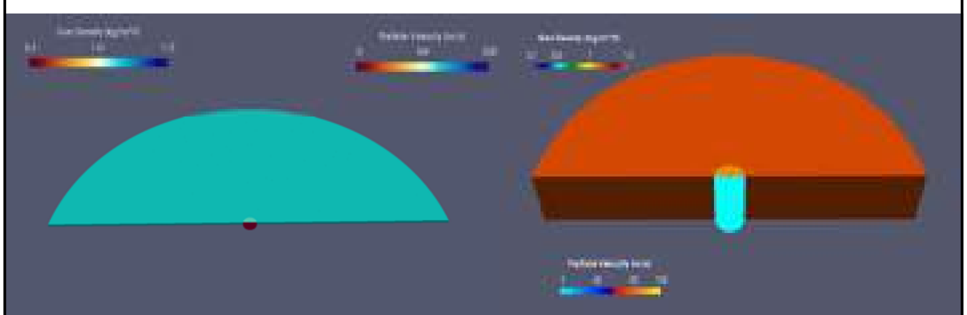
Hero Runs

HR 2 | HR 3



- Features:

HR 2:
- 30 Million computational cells
- 5 Million computational particles
- r_{max} = 4.00m
- t_{max} = 2.50ms
- 4096 cores

HR 3:
- 60 Million computational cells
- 15 Million computational particles
- r_{max} = 4.00m
- t_{max} = 1.40ms
- 5760 cores

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Hero Run: Evolution

	Hero Run 1	Hero Run 2	Hero Run 3	Hero Run 4A	Hero Run 4B	Hero Run 5
Reactive burn	No	No	Yes	Yes	Yes	Yes
Equation of state	Ideal Gas	JWL	JWL	JWL	JWL	JWL
Initial Particle volume fraction	5 %	40 % - Frozen	10 % - Frozen	10 % - Frozen	10 % - Frozen	10 % - Frozen
Particle bed perturbation	none	none	1 mode in azimuthal direction	none	4 mode in azimuthal direction + white noise	none
No. of computational particles	5 M	5 M	15 M	15 M	15 M	30 M
No. of elements	30 M	30 M	60 M	60 M	60 M	120 M
No. of cores	512	4096	5760	5760	5760	16384
Simulation Time	2.5ms	2.5ms	1.40ms	0.20ms	0.42ms	0.03ms

currently running

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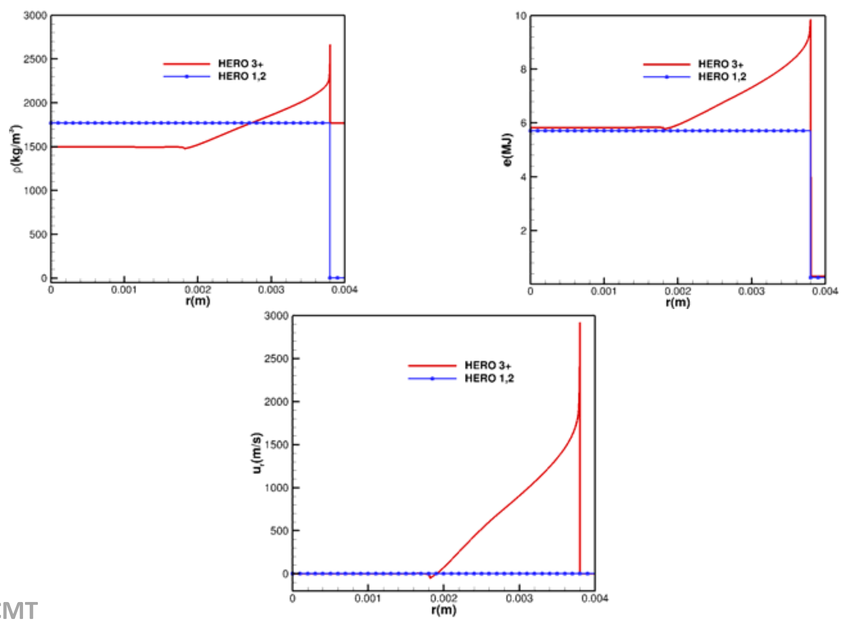
Hero Run 3: Reactive Burn Initial Conditions



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Hero Run 3: Equation of State Model

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

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

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

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

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

➤ "EoS Surrogate Modeling", Fred Ouellet

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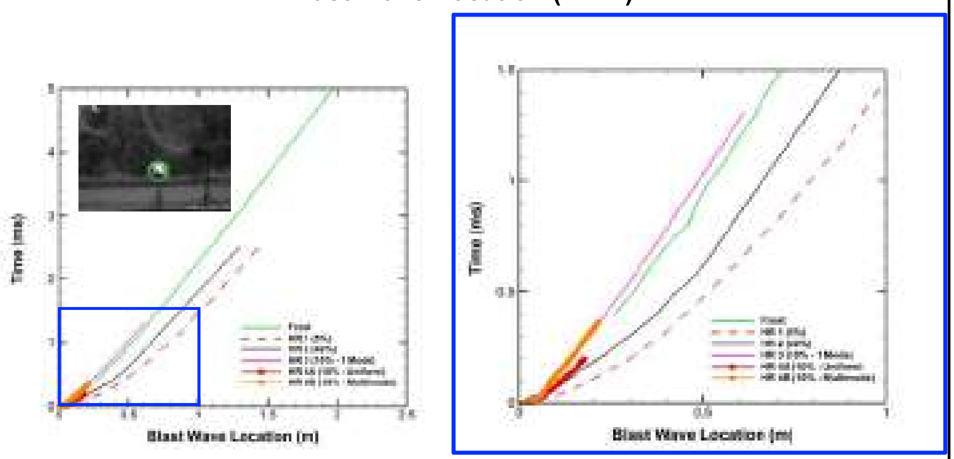
Demonstration Problem: Predictions

Blast Wave Location (PM-1)



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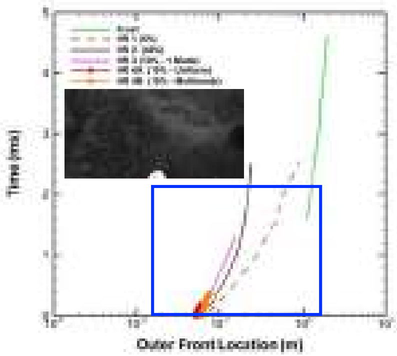
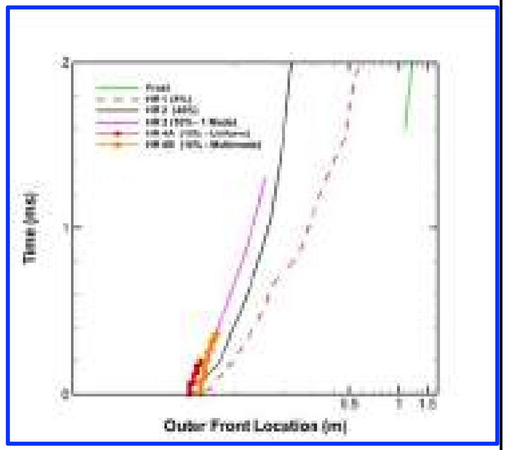
Demonstration Problem: Predictions

Particle Front Location (PM-2)





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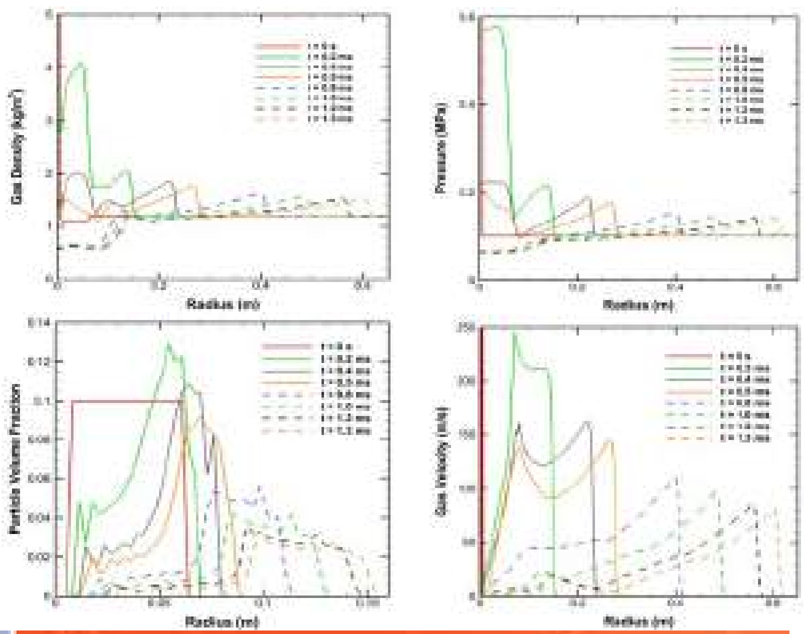
Hero Run 3 – A Closer Look



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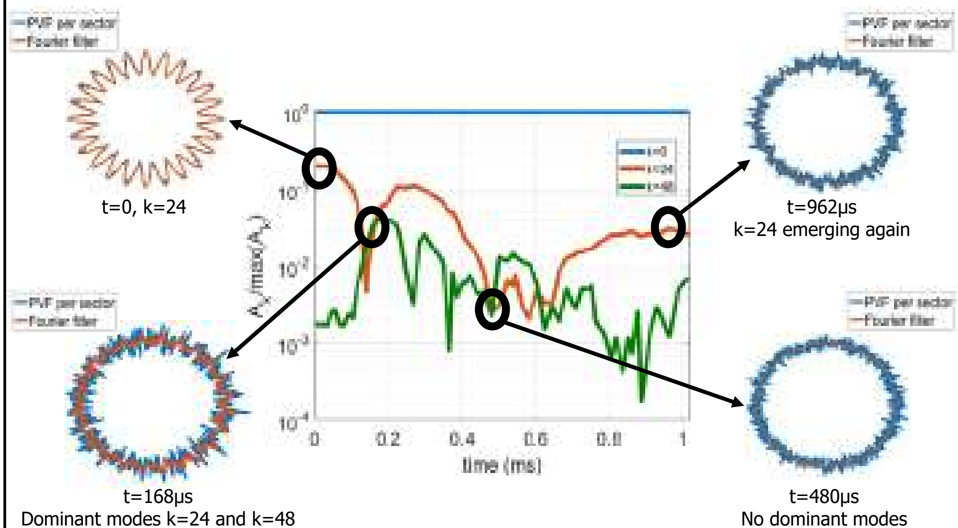
Hero Run 3 – A Closer Look



➢ "Multi-fidelity surrogate model for finding the fastest growing initial perturbation ", M. Giselle Fernandez-Godino

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Outline

- **Demonstration Problems**
  - Frost's Experiment
  - Eglin's Blastpad Experiment
- **Micro and Mesoscale Campaigns**
  - Eglin Microscale Experiments
  - Eglin Mesoscale Experiments
  - SNL's Multiphase Shock Tube
  - ASU Expansion Fan

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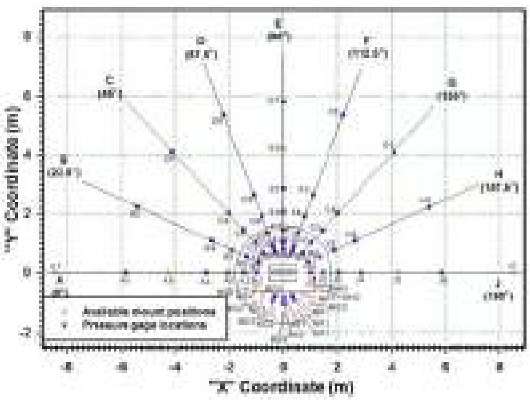
AFRL Blastpad Experimental Setup



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

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

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

➢ "Eglin Experiment", Angela Diggs

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Distribution A. Approved for public release. Distribution unlimited.

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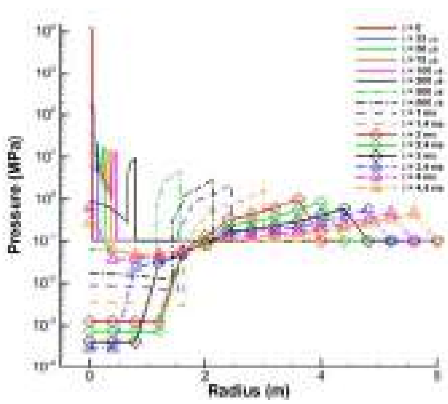
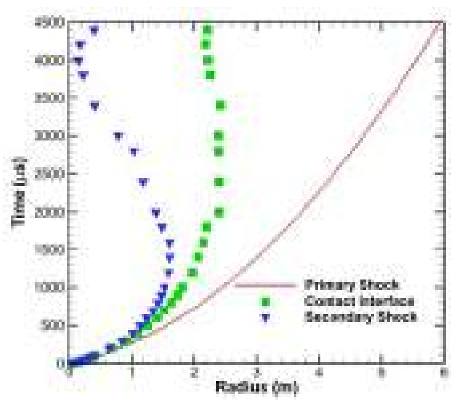
Blastpad Simulation (Bare charge 1d results)





1D Simulation Details:

- 100,000 cells in radial direction up to 6 m.
- Run using 16 cores up to a time of 4.5 ms
- 1 Equation JWL Model for Composition-B used for EoS

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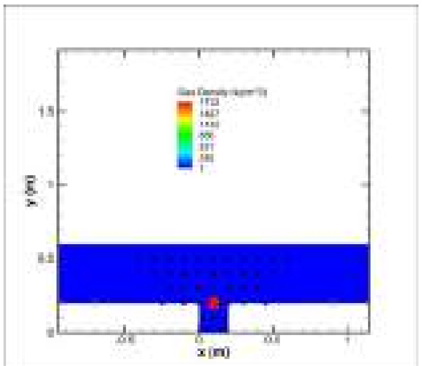
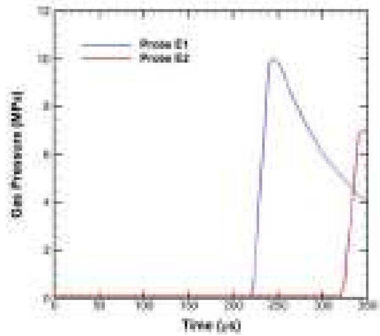
Blastpad Simulation Setup





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

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

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Outline

- **Demonstration Problems**
  - Frost's Experiment
  - Eglin's Blastpad Experiment
- **Micro and Mesoscale Campaigns**
  - Eglin Microscale Experiments
  - Eglin Mesoscale Experiments
  - SNL's Multiphase Shock Tube
  - ASU Expansion Fan

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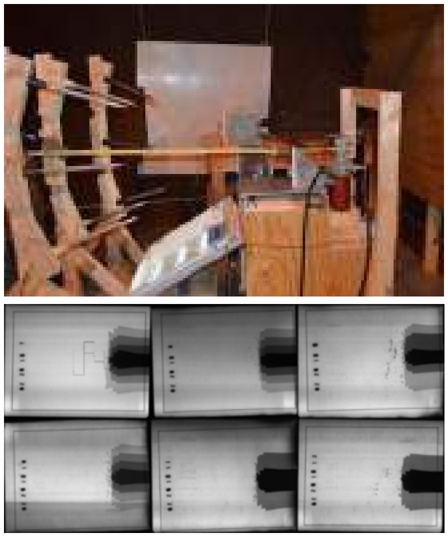
Eglin's Experiments



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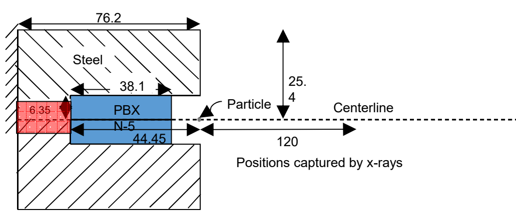
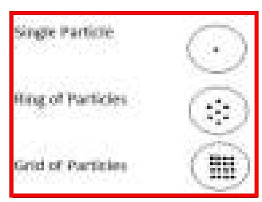
Eglin's Experiments





- Simulations implement the JWL equation of state and reactive burn initial condition for the explosive
- Plan for Uncertainty Quantification Analysis
  - Vary input parameters of particle density, particle diameter, and explosive mass for batch run (5 x 5 x 5 x 3 simulations) to construct surrogate model
  - Done for all variations of particle configuration
- Current geometry has a solid backwall for the explosive
  - In reality there is a sizable hole in the back of the explosive where the detonator attaches
  - Simulations will compare the effects of including this hole

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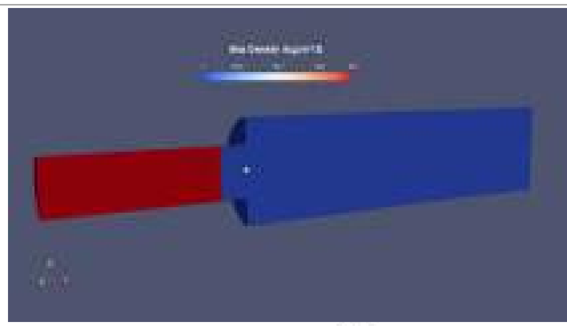
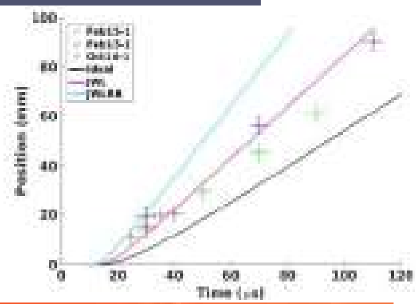
Simulation Results



Simulation Details:

- Axisymmetric
- Real gas equation of state (JWL)
- Point-particle model
- Explosive modeled with a reactive burn initial profile
- Time-shifted to align with experimental times
- 1-way coupled (1 Particle)



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Outline

- **Demonstration Problems**
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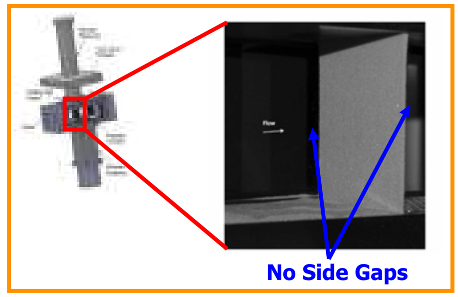
New Particle Curtain Experiments



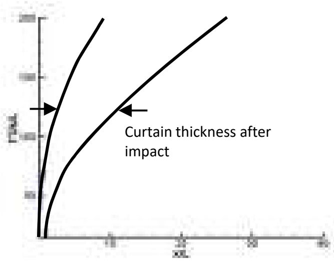


Table 1. Sandia Particle Curtain Data

Material	Particle Size (μm)	ϕ_p (%)	M_s
Soda Lime	106–125	21	1.24, 1.40, 1.45
	106–125	21	1.66, 1.92, 2.02†
	300–355	9	1.24, 1.40, 1.45
	850–1000	32	1.2, 1.33, 1.46, 1.60, 1.83, 2.48, 2.58‡

† From Wagner et al. and Ling et al.
‡ From Theofanous et al.

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Large-Scale Bundle Runs

- Comparison between mesoscale 1D/2D/3D simulations and the new SNL experiments with non-tophat initial particle volume fraction profile
  - Runs for:
    - 5 different Mach numbers: 1.24, 1.40, 1.45, 1.66, 1.92
    - Initial particle volume fraction
    - Random initial particle locations
    - Curtain thickness
  - 625 1D bundle runs with Dakota
  - 135 2D runs
  - 27 3D runs

➢ "Uncertainty Budget", Chanyoung Park

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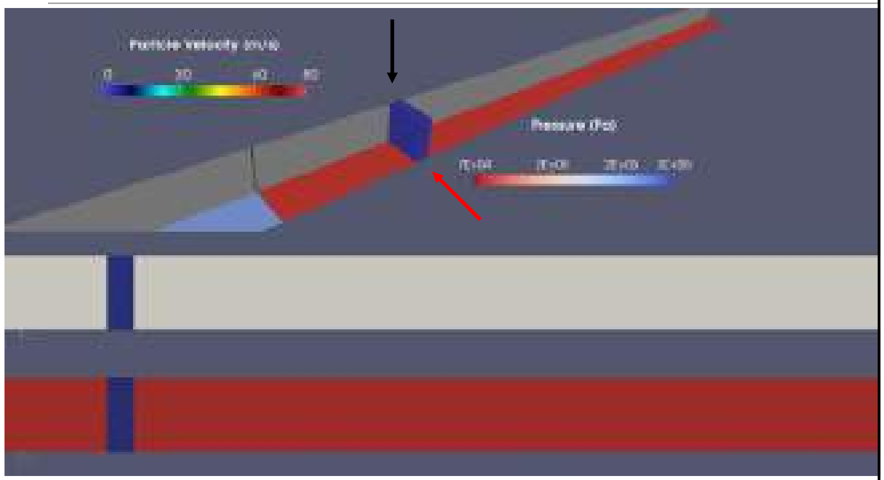
3D Particle Curtain Simulation



X-Y Plane

Y-Z Plane

- Features:
  - 18 Million computational cells
  - 6 Million computational particles
  - 2048 cores

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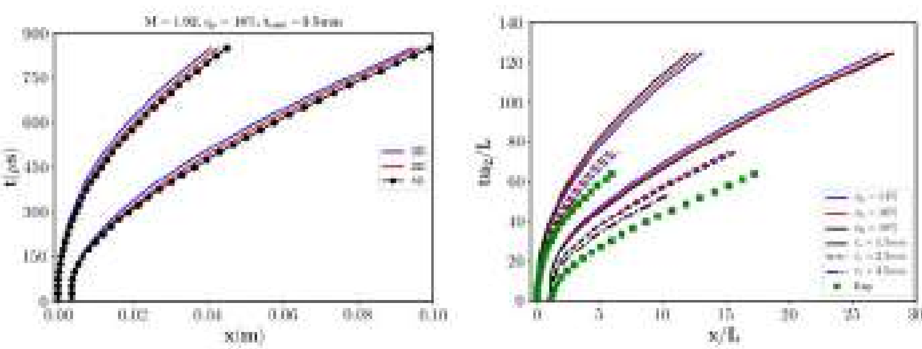
Shock Tube Results



- Particle fronts are defined as the locations of the trailing and leading 0.5% of particles

➢ "Uncertainty Budget", Chanyoung Park

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Outline

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  - ASU Expansion Fan

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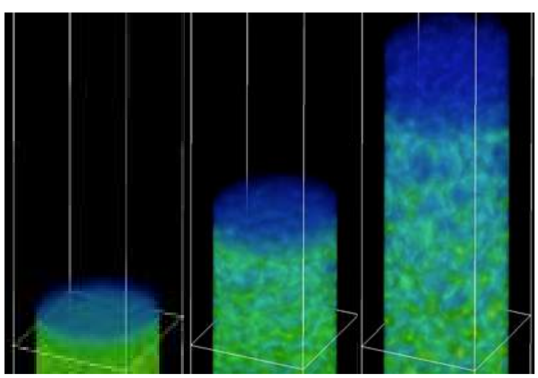
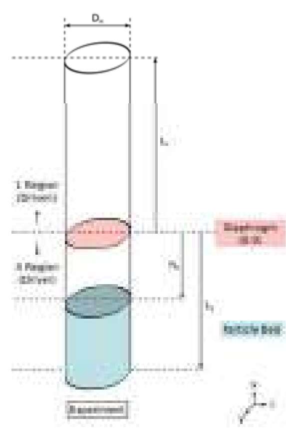
ASU Experiment

- Simulations are progressing with CMT-nek
  - "CMT-nek", Jason Hackl and David Zwick
  - "ASU Experiments", Blair Johnson





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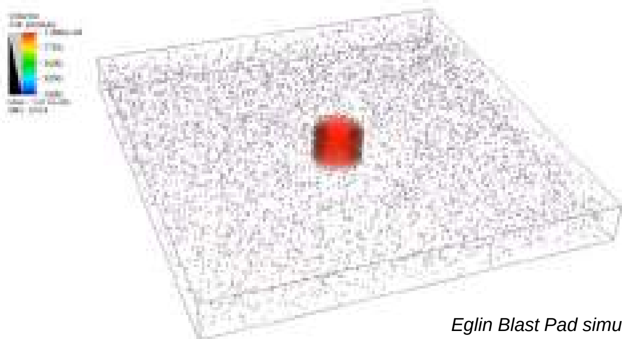
Do you have any questions?



Eglin Blast Pad simulation by CMT-nek

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CMT-nek Development and Application

Jason Hackl
David Zwick

UF UNIVERSITY of FLORIDA NNSA

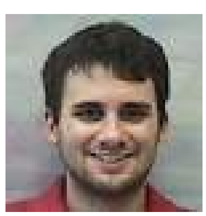
CMT-nek development team

Prof. Paul Fischer, UIUC

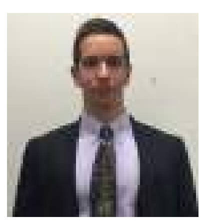
Jason Hackl, UF

David Zwick, UF

Li Lu, UIUC



Brad Durant, UF



Goran Marjanovic, UF

Rahul Koneru, UF

Postdoctoral fellow Nguyen Tri Nguyen arrives December 10th, 2017

CCMT 2

Outline

- CMT-nek hydrodynamics
  - Discontinuous Galerkin spectral element method
  - Euler equations + entropy viscosity method (EVM)
- Microscale release
  - Shock waves and interactions of waves with spheres
- CMT-nek particles
  - Multiphase source terms
  - Algorithms and parallelization
- Mesoscale release
  - ASU experiment

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3

Discontinuous Galerkin SEM

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

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

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

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

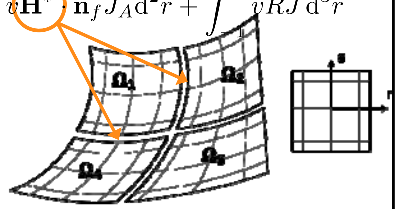
$$\frac{\partial}{\partial x_i} = \frac{\partial r_k}{\partial x_i}\frac{\partial f}{\partial r_k} \approx [\mathbf{r}_{k,\mathbf{x}_i}][\mathbf{D}_k \mathbf{f}]$$

Matrix ops within Ω_e

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

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

5. Approximate integrals with quadrature
6. Approximate U & v with Lagrange polynomials
   - N Gauss-Legendre-Lobatto (GLL) nodes
   - Nested tensor product ~ $O(N^4) < N^3 \times N^3$
     $N \times N$ matrices applied N^2 times



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

Convective terms in DGSEM

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

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

E : Restriction op
D : Differentiation op
B : Mass matrix

Volume fractions of ***g***as…

$\phi_g \equiv 1 - \phi_p$

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

…and ***p***articles

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

Convective fluxes of

Mass

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

Thermodynamic state

Temperature T

Pressure $p(\rho, T)$

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

Momentum

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

Energy

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

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

5

Artificial viscosity

flux = convective + diffusive

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

Artificial stress tensor[1] (**NOT** Navier-Stokes) with AV that tracks the **entropy residual**
NOT weighted by volume fraction ϕ_g

Diffusive flux of…

Mass

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

Momentum

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

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

Energy

$$\mathbf{H}_5^d = -\left[\rho\, \nu_s \mathbf{u} : \underline{\sigma} + \kappa_s \times \left(\nabla(\rho e) + \frac{1}{2}|\mathbf{u}|^2 \nabla \rho\right)\right]$$

due to **entropy viscosity**

$$\nu_* = c_E h^2 \frac{|R_s|}{||s - \langle s \rangle||_\infty}$$

$$\nu_{\max} \equiv c_{\max} h \max_{\Omega_e}\left(|\mathbf{u}| + c\right)$$

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

$$\kappa_s = \mathcal{P}\nu_s$$

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

R_s approx by finite diff between RK3 stages' s

$$s = \rho\, c_v \log\left(p\rho^{-\gamma}\right)$$

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

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

[1]Guermond & Popov (2014) "Viscous regularization of Euler eqn and entropy principles" *J. Appl. Math.* **74**:284-305
Guermond, Pasquetti & Popov (2011) *J. Comp. Phys.* **230**:4248-4267

Diffusive terms in DGSEM

Quasi-linear flux Jacobian *A*
Primal form
NOT weighted by volume fraction ϕ_g

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

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

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

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

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

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

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

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

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

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

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

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

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CMT-nek: final form of DGSEM

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

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

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

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

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

Right-hand-side for fully explicit[1] TVDRK3 = Surface ops + Volume ops

T 7 : CS
(2:30 PM)

Restrictive time step due to diffusion number $D = \frac{\kappa_s \Delta t}{h^2}, \quad \min(D, \text{CFL}) < 1$

Mass matrix is diagonal; all other matrices are element block-diagonal
- Locality, scaling

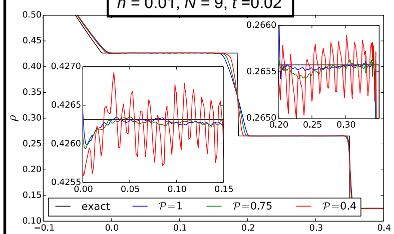
Diagonal mass matrix means LHS is ***not*** exactly integrated ("variational crime")
- Dealiased convective terms via interpolator **I** to M=3(N-1)/2 Gauss-Legendre nodes[2]
- Tensor-nesting saves M^2 factor in cost of volume operations

[1]Gottlieb & Shu (1998) *Math. Comp.* **67**:73-85
[2]Canuto, Hussaini, Quateroni & Zang (2007) *Spectral Methods* Springer
Banerjee *et al* (2016) *IEEE 23rd Int. Conf. HiPC* (2017) *Sustainable Computing, Informatics and Systems*
Hackl, Shringarpure, Koneru, Delchini & Balachandar (2017) submitted to *Computers & Fluids*

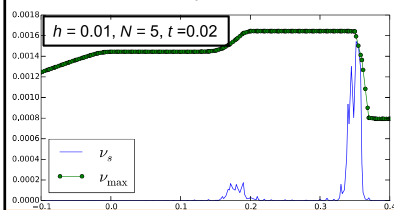
8

Shock capturing in CMT-nek

Calibrated P, c_E, c_{max} in Sod[1] shock tube

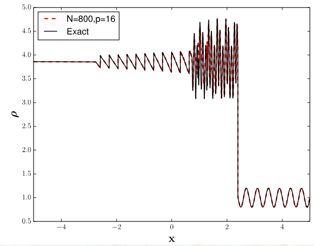


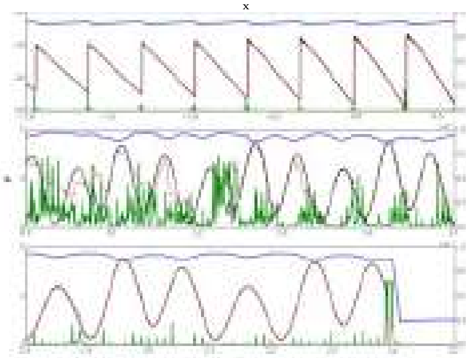
- ν_* reaches ν_{max} at shock wave
- Less oscillatory than other HODG[3]



[1]Sod (1978) *J. Comp. Phys.* **27**:1-31
[2]Shu & Osher (1989) *J. Comp. Phys.* **83**:32-78
[3]Lv, See & Ihme (2016) *J. Comp. Phys.* **322**:448-472

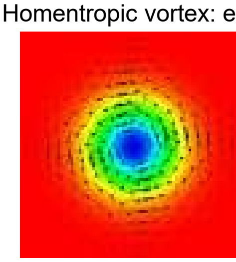
Shu-Osher[2] 1D shock-turbulence surrogate

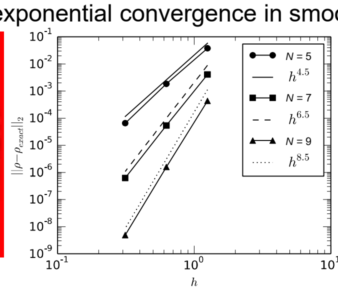


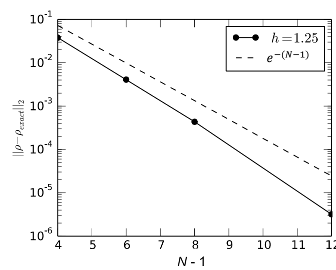


CMT-nek convergence and validation

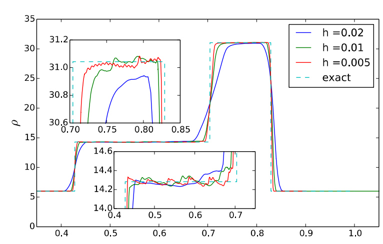
Homentropic vortex: exponential convergence in smooth flow

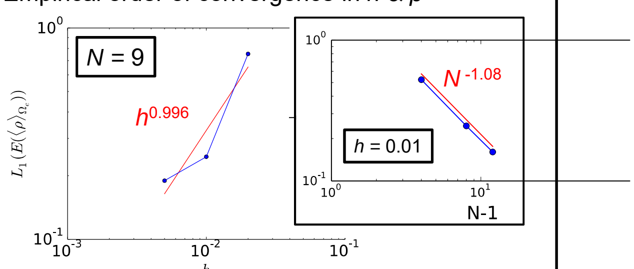






Two-shock collision, t = 0.035: O(1) Empirical order of convergence in h & p





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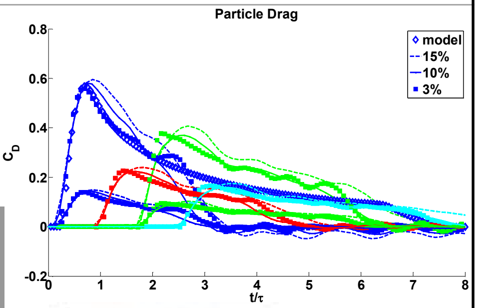
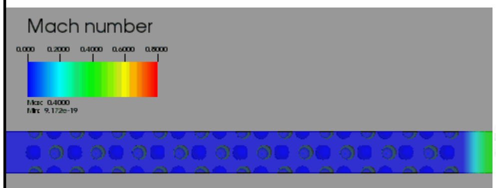
Microscale: Potential flow over spheres

Tests generalized Faxen theorem[1]

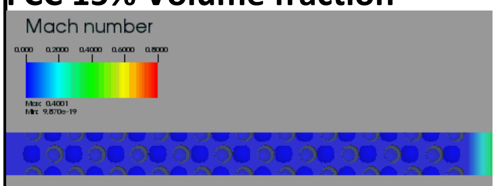
$$\mathbf{F}^{GF}(t) = \frac{4}{3}\pi R^3 \rho^m \overline{\frac{D\mathbf{u}}{Dt}}^{0S'} + 4\pi R^3 \int_{\xi=-\infty}^{t} K_{vu}(t-\xi; M)\left[\frac{D}{Dt}\overline{(\rho\mathbf{u}_c)}^{0S}\right]_{t=\xi} d\xi$$

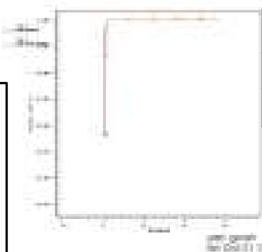


FCC 10% Volume fraction



FCC 15% Volume fraction





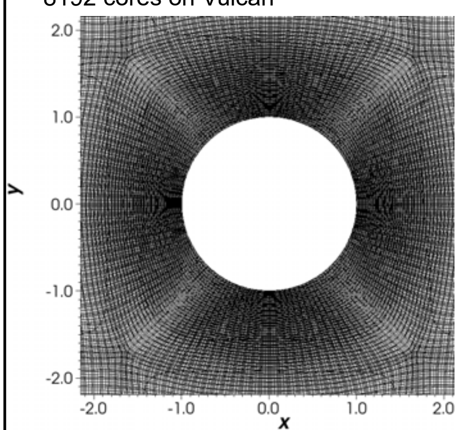
N_{elem}	23424
Spheres	95
Rows	21

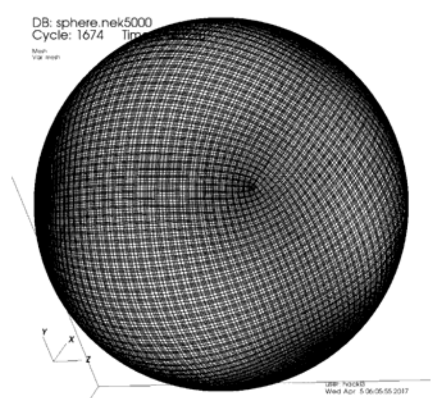
CMT-nek supports model dev

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

Microscale: Mach 3 shock-sphere

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





c_E	c_{max}	P	Δt
40	0.5	0.75	2.5e-6

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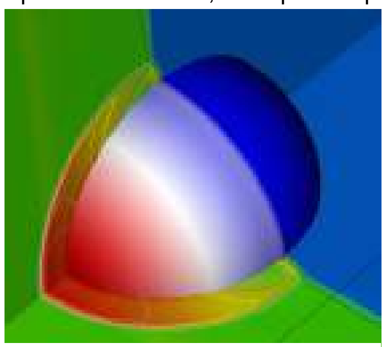
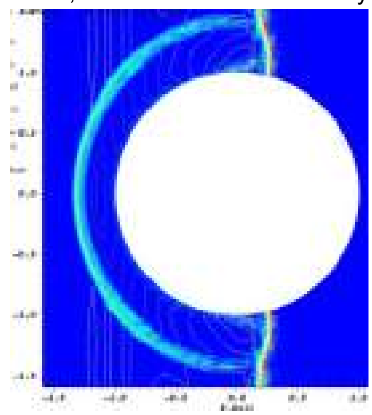
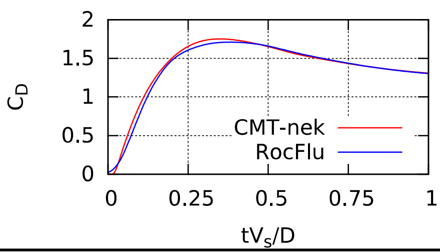
Microscale: Mach 3 shock-sphere

Temperature contours; color plots of pressure, artificial kinematic viscosity







Triple point

- Bryson & Gross (1960) *JFM*

Drag coefficient

- Mehta *et al* (2016) *J. Appl. Phys.*

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CMT-nek transition plan

- ASU expansion fan (David)
  - Without 4-way coupling (underway)
  - 4-way coupled (CMT-nek runs with PIEP, collision)
- Sandia shock tube (Rahul)
  - Test shock-particle interaction at mesoscale
- Eglin micro/meso (Josh, Brandon)
  - Real-gas EOS
  - Reactive burn
  - Problem setup
- Demonstration problem (Josh, Rahul, Fred)

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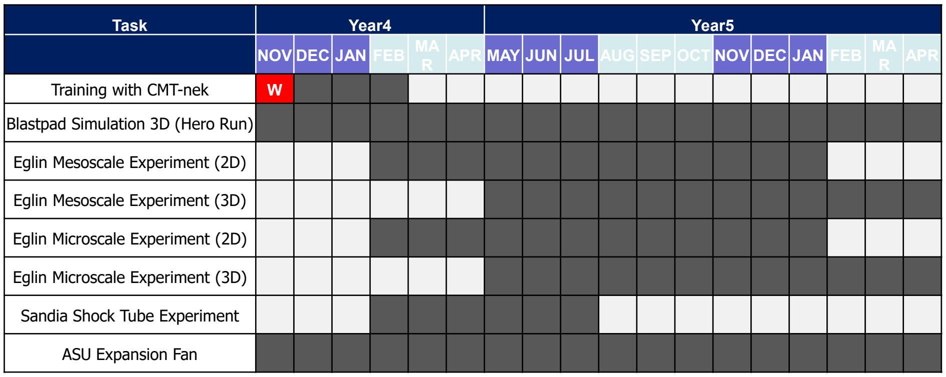
Transition to CMT-nek – Timeline



W Workshop: "A Boot Camp on CMT-nek"

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Transition to CMT-nek – CCMT Workshop

A Boot Camp on CMT-nek

November 29, 2017

Organizers: Bertrand Rollin, Jason Hackl

Agenda

- **CMT-nek: Anatomy of the Beast**
  Speaker: Jason Hackl | 12:00 pm – 1:30 pm
- **Lagrangian Particles in CMT-nek**
  Speaker: David Zwick | 1:30 pm – 2:30 pm
- **Running CMT-nek**
  Speakers: Goran Marjanovic and Brad Durant | 2:30 pm – 3:15 pm
- **Post-Processing and visualization in CMT-nek**
  Speakers: David Zwick and Brad Durant | 3:15 pm – 4:00 pm
- **Lesson Learnt from CCMT's Simulations**
  Spearkers: Fred Ouellet and Yash Mehta | 4:00 pm – 5:00 pm

Attendee list

Paul Crittenden
Brad Durant
Giselle Fernandez
Joshua Garno
Jason Hackl
Rahul Koneru
Yash Mehta
Goran Marjanovic
Chandler Moore
Fred Ouellet
Brandon Osborne
Bertrand Rollin
Prashanth Sridharan
David Zwick

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Multiphase Flow in CMT-nek

- CMT-nek is built on single-phase nek5000
- While not fully resolved, Eulerian-Lagrangian method can simulate a realistic (~10^9) particles
- Difficulties related to particle-fluid coupling
  - Physics
  - Numerics
  - Computer Science
- Outline
  - Particle implementation in CMT-nek/nek5000
  - ASU experiment application

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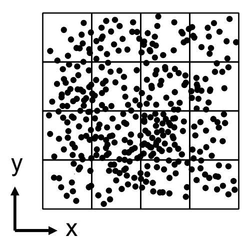
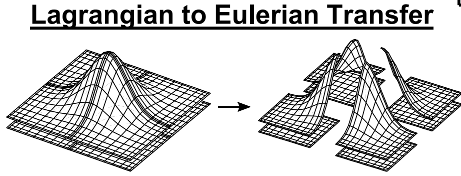
Multiphase Source Terms

$$\mathbf{R} = \begin{bmatrix} 0 \\ \mathbf{f}_{pg} \\ \sigma_g : \nabla(\phi_p \mathbf{v}) + g_{pg} + q_{pg} \end{bmatrix}$$

Reference Frames



Lagrangian to Eulerian Transfer



Particle-fluid force coupling and energy contribution

Particle-fluid energy coupling

Eulerian particle velocity

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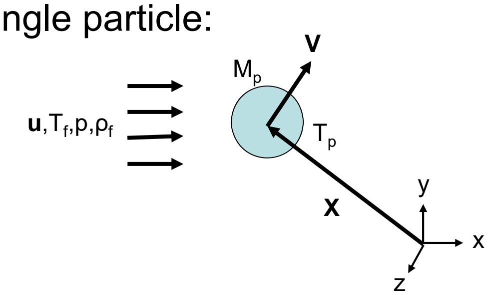
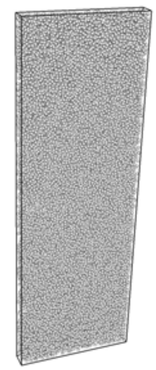
Dispersed Phase

- For a single particle:





Position:

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

Momentum:

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

Energy:

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

Hydrodynamic force | Collisional force | Body force | Hydrodynamic heat transfer

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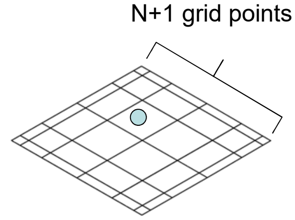
Interpolation

- Fluid properties need to be evaluated at particle location
- Quasi-steady force:

$$\mathbf{F}_{qs} = \frac{1}{2}\rho_f(\mathbf{u} - \mathbf{V})^2 A_p C_D$$

- Interpolation choices:

Method	Accuracy	Scalability
Linear	$O(1/N^2)$	O(1) – O(N)
Cubic	$O(1/N^4)$	O(N) – $O(N^2)$
Lagrange	$O(1/N^{N+1})$	$O(N^6)$
Barycentric Lagrange	$O(1/N^{N+1})$	$O(N^3)$



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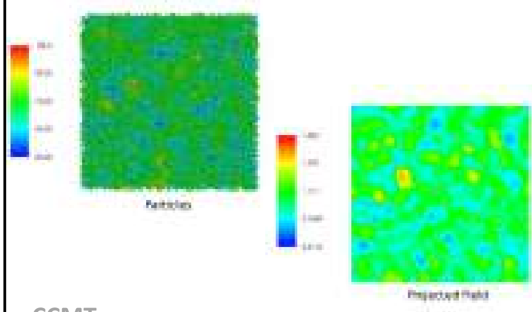
Projection

- Process of spreading Lagrangian quantities to the Eulerian reference frame
- Arises from volume filtering used to get multiphase governing equations
- Here, a Gaussian filter is used



$$a(\mathbf{x}) = A(\mathbf{X}) g_{\mathcal{M}}(|\mathbf{x} - \mathbf{X}|)$$

A (Lagrangian)	a (Eulerian)
$-\mathbf{F}_{pg}$	$\mathbf{f}_{pg}$
$-G_{pg}$	g_{pg}
$-Q_{pg}$	q_{pg}
V_p	Φ_p
$V_p\mathbf{V}$	$\Phi_p\mathbf{v}$

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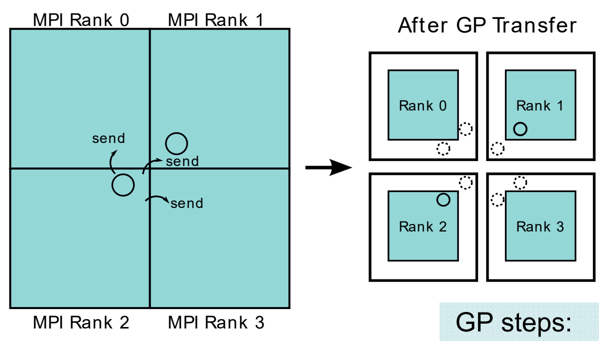
Ghost Particles

Idea:

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



GP steps:
1. Create GP
2. Send GP

(Ghost particles shown in orange boxes)

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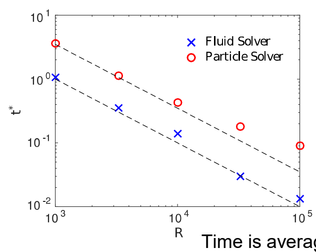
Algorithmic Scaling

Ideal Setup:

- Uniform flow in a periodic box
- Particle time scale is 10 time steps
- One particle per grid point
- N = 5 grid points in each direction
- Vulcan (LLNL)
- CS Team will show load-imbalanced cases

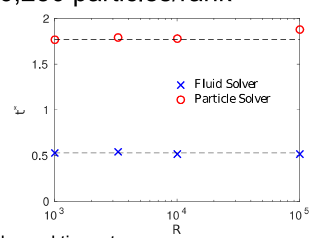
Strong Scaling:

- 13 million grid points
- 13 million particles



Weak Scaling:

- 6,250 grid points/rank
- 6,250 particles/rank



Time is averaged over MPI ranks and time steps

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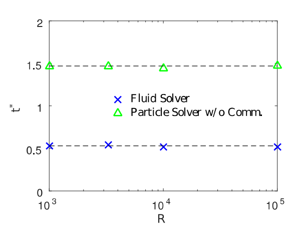
Algorithmic Scaling

- Strong scaling diverges from ideal due to:
  - 1 element/rank
  - Ghost particles
- Weak scaling diverges from ideal due to:
  - Inter-processor communication from sending particles

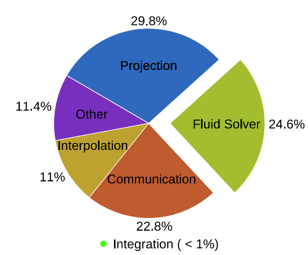
Weak Scaling

(without GP Comm.)



Example Profiling

(10,000 rank case from strong scaling)



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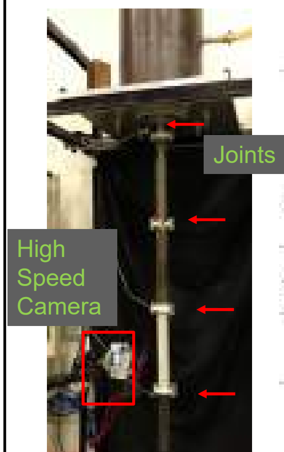
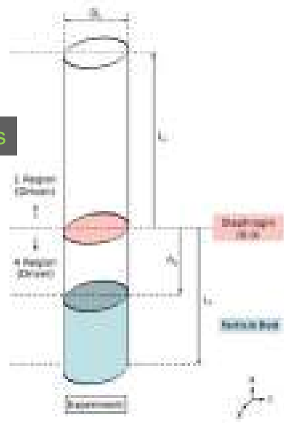
Particles in Expansion Waves

- Simulation of vertical shock tube with particle bed at bottom





- When diaphragm bursts, particle bed will swell upwards
- ASU team will provide more detail
- Main goals:
  1. Uncertainty study
  2. Physics
  3. High resolution

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Prediction (Validation) Metrics

Prediction metrics:

- Bed height
- Fluid pressure

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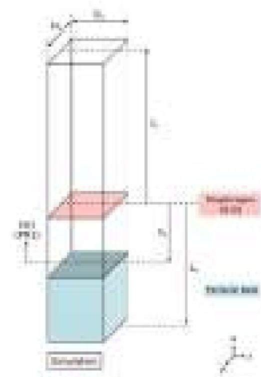
Detailed Simulation

Geometry

	Experiments	Simulations
$L_1[m]$	0.64	5.76
$L_4[m]$	0.64	0.64
$D_H[m]$	0.04	0.04
$h_0[m]$	-0.3	-0.3



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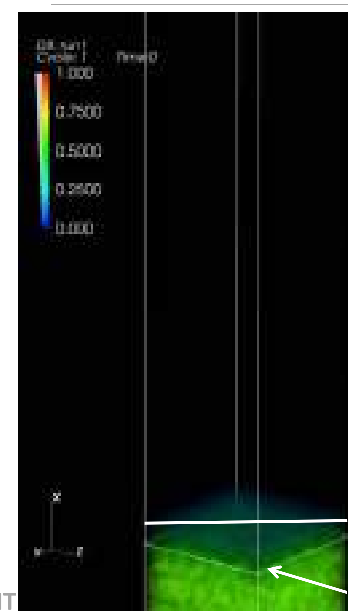
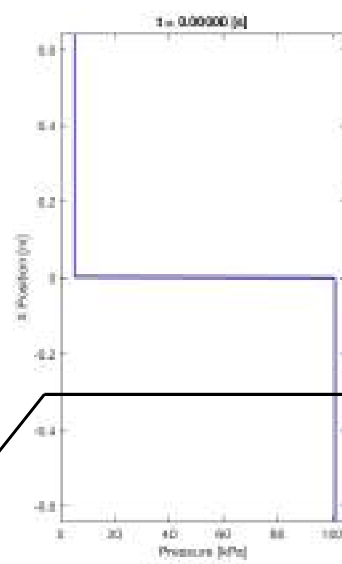
Initial Results





Initial Bed Height (x = -30 cm)

Experimental Tube Joint (x = -32 cm)

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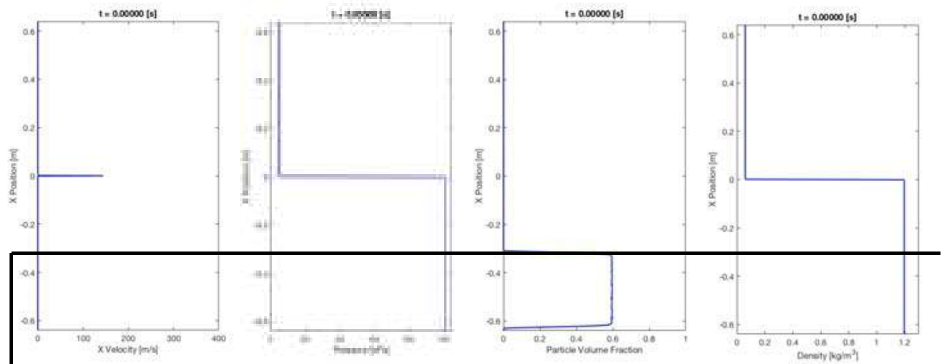
Planar Averaged Profiles



Initial Bed Height (x = -30 cm)

Observations:

- Reflected/transmitted expansion wave when incident expansion wave head hits bed
- Pressure ahead of bed is nearly constant but lower than standard shock tube
- Possible clustering of particles

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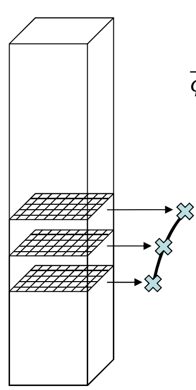
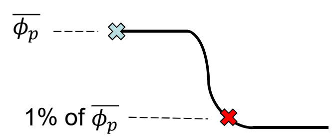
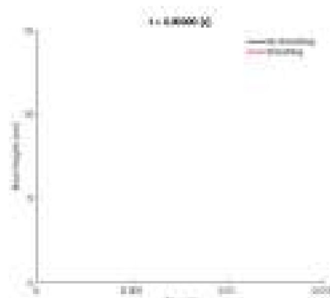
Bed Height

Planar Averaging

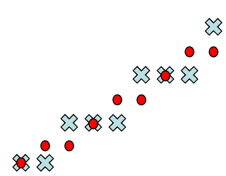


Threshold





Box Filter



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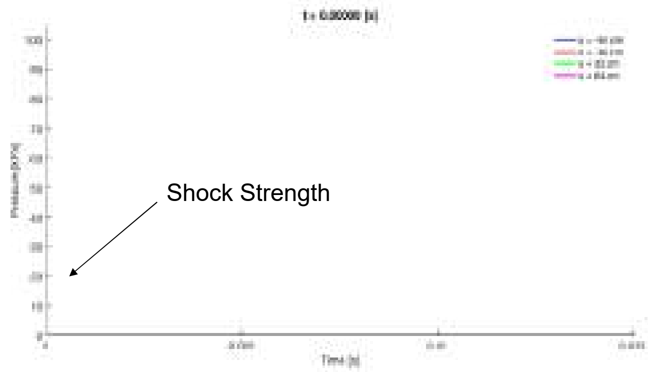
Fluid Pressure Traces

- At the four joints (excluding diaphragm) along the tubes in the experiment we have pressure sensors



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Future Work

- Uncertainty quantification
  - Sensitivity of force models, collision models, diameter distributions
- Physics
  - Effect of bed height, pressure ratio, diameter ranges
- High resolution
  - From results a small number of high resolutions simulations will be run
- Numerics
  - Quadrature effects on small-scale resolution
  - Implicit time marching and artificial viscosity
  - Particle initial conditions

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Do you have any questions?

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High Resolution Simulation

Geometry

	Experiments	Simulations
$L_1[m]$	0.64	5.76
$L_4[m]$	0.64	0.64
$D_H[m]$	0.04	0.04
$h_0[m]$	-0.3	-0.3

Particles

	Experiments	Simulations
$D_p[\mu m]$	[44,88]	[44,88]
$\rho_p[\text{kg}/m^3]$	2,460	2,460
N_p	5,033,861,327	73,440,000

Initial Conditions

	Experiments	Simulations
$P_1[kPa]$	5	5
$T_1[K]$	294	294
$P_4[kPa]$	101	101
$T_4[K]$	294	294
ϕ_f	40%	40%

Grid

	Simulations
N_e	1,280,000
N_{ex}	3,200
N_{ey}, N_{ez}	20
N	6
Δx	0.0003
Ranks	131,072

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Uncertainty Quantification

- Full factorial design

Configuration	Force Model
1	$F_{un} + F_{qs}$
2	$F_{un} + F_{qs} + F_{am}$
3	F_{PIEP}

Configuration	Collision Model
1	Off
2	Walls Only
3	Particles Only
4	Walls & Particles

Configuration	Diameter Distribution
1	Monodisperse
2	Polydisperse

- Soft-sphere collision model
- 72 total simulations (3 repeats)

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Physics Simulations

- Full factorial design

Configuration	Bed Height
1	-30 cm
2	−20 cm
3	−10 cm
4	0 cm

Configuration	Pressure Ratio
1	5
2	10
3	20
4	40

Configuration	Diameter Range
1	[44,88] μm
2	[89,149] μm

- Parameters chosen to compare to experiments:
  - ASU
  - Literature (Chojnicki et al., 2006)
- 96 total simulations (3 repeats)

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Experimental Studies of Gas-Particle Mixtures Under Sudden Expansion

Blair Johnson, Ph.D., Heather Zunino

Ronald Adrian, Ph.D., Amanda Clarke, Ph.D.

Arizona State University

Outline

- Research Objectives
- Experimental Setup & Measurement Techniques
  - Installation of new pressure sensors
  - Synchronization to optical measurements
  - High speed video of particle bed evolution
  - Particle image velocimetry (PIV) of gas
- Results
  - Pressure analysis
  - Particle bed motion
  - Gas velocity
- Summary & Upcoming Work

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Research Objectives

- Provide data for validation of numerical simulations developed by CCMT.
- Measure shock wave, expansion wave, incipient particle bed motion and gas flow, and particle motion in 0 < z < D (near field), 0 < z < 7D (far field),and z < 0 (within bed).
- Coordinate with UQ, UB teams to quantify experimental error and gain insight for potential improvements to experimental facility.

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Experimental Plan

Particle size (μm)	Pressure Ratio P_4 / P_1	Bed Height (cm)	Measurement Type	# of tests
44 – 90	20	37.9	FV	10
		32+	EXP	∞
		10.0	PIV	∞
	15	37.9	FV	2
	10	37.9	FV	2
90 – 150	20	37.9	FV	2
		32+	EXP	∞
	15	37.9	FV	2
	10	37.9	FV	2
150+	20	10.0	PIV	∞

FV = Front Rise Velocity
EXP = Bed Expansion Video of Crack/Void Evolution
PIV = Particle Image Velocimetry for gas velocity

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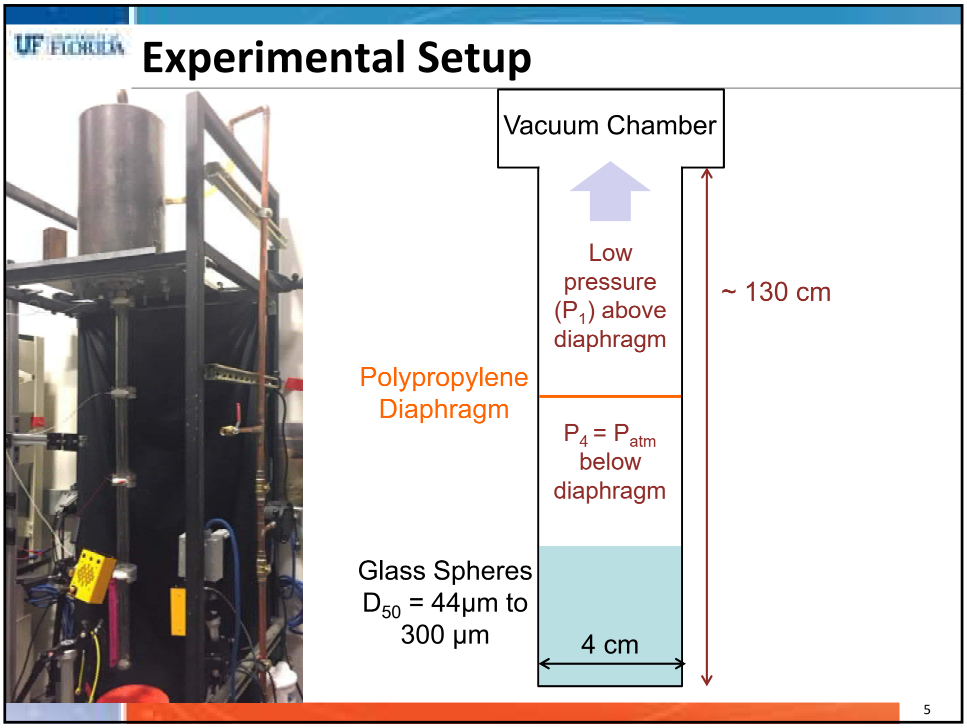
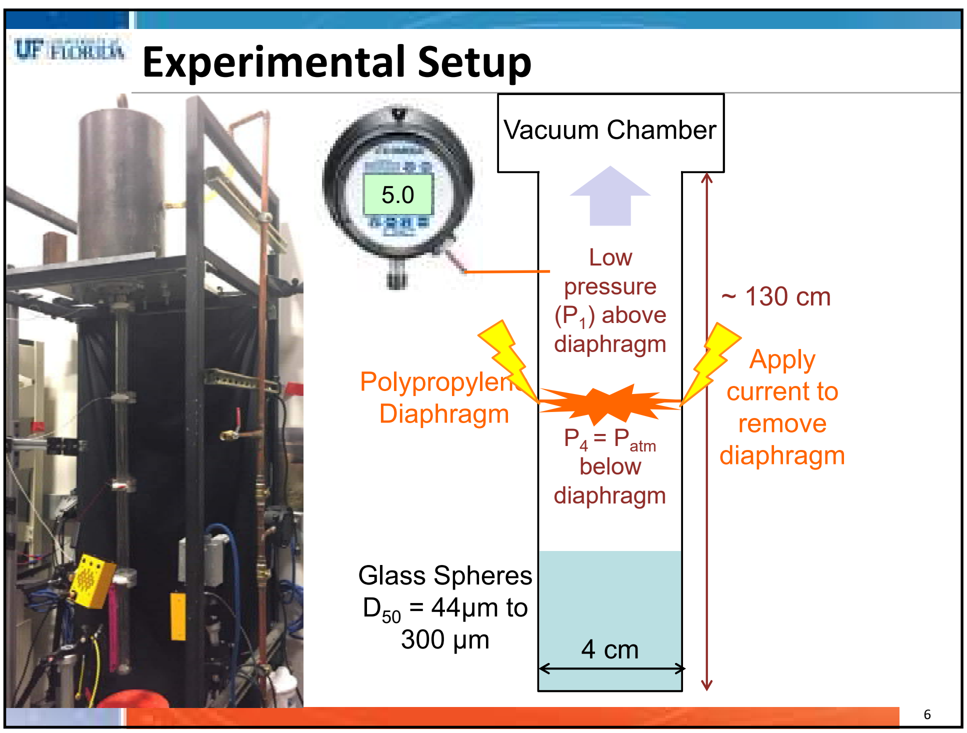
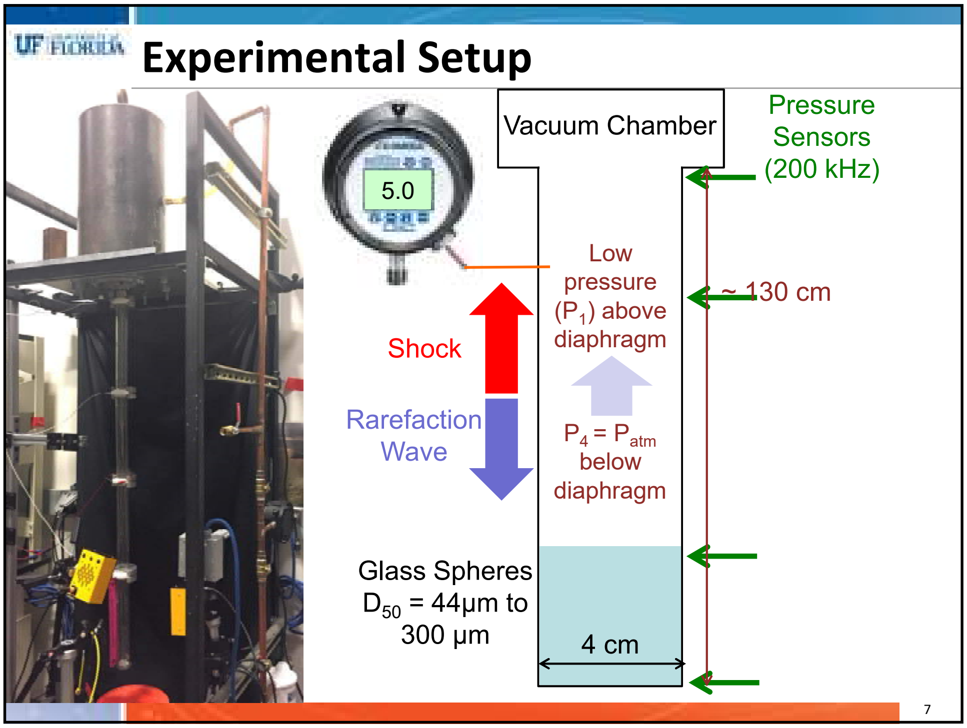
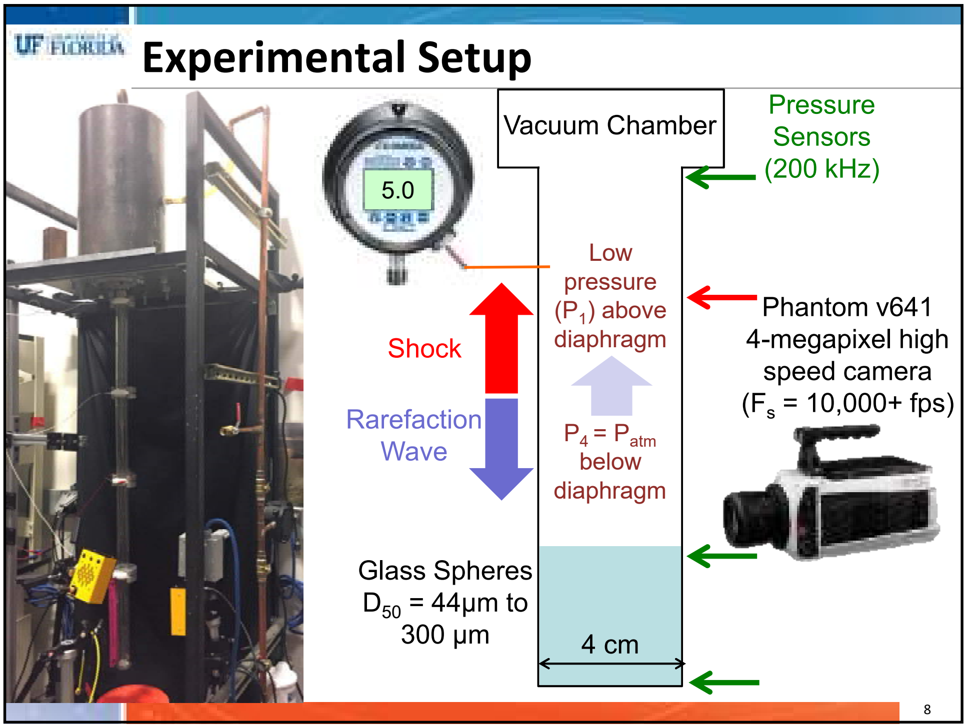
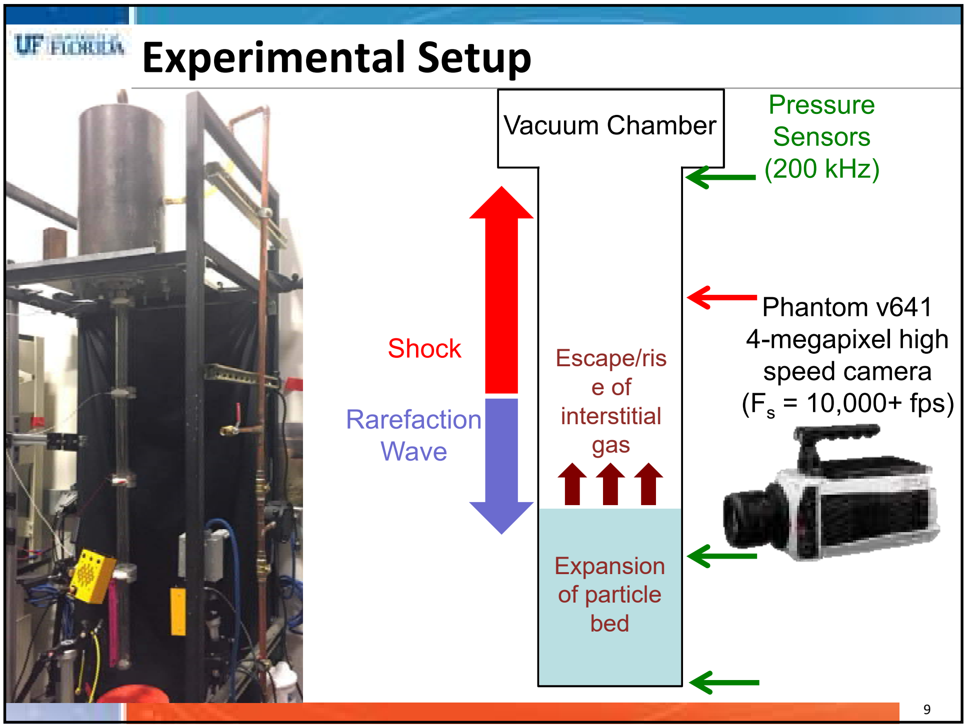
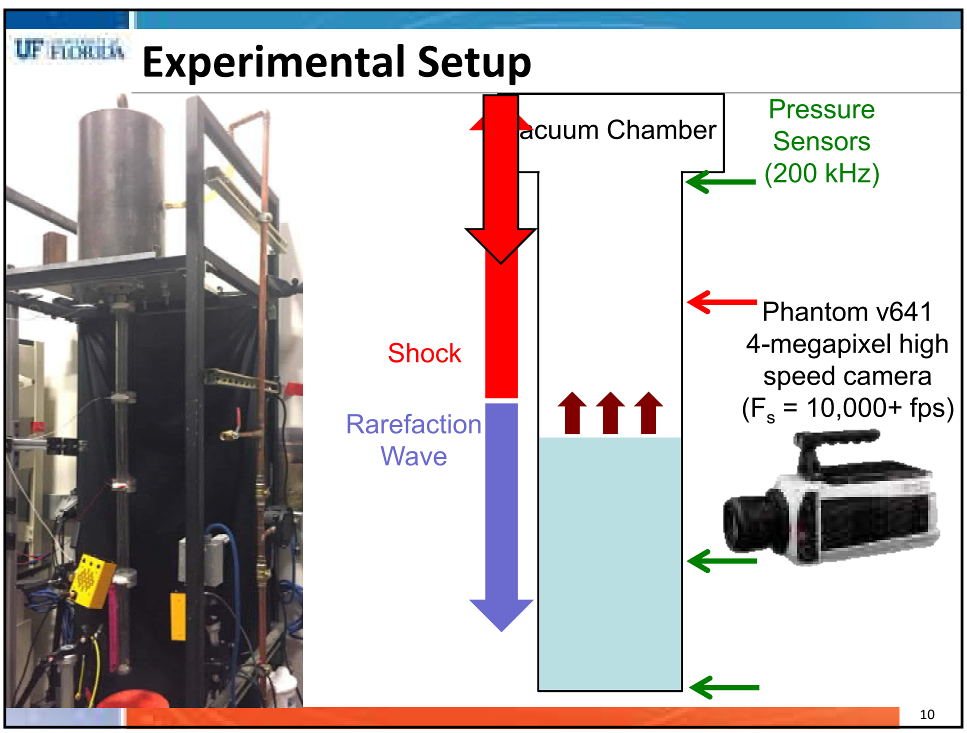

Experimental Setup
Vacuum Chamber
Low pressure (P_1) above diaphragm
~ 130 cm
Polypropylene Diaphragm
$P_4 = P_{atm}$ below diaphragm
Glass Spheres D_{50} = 44μm to 300 μm
4 cm
5


Experimental Setup
Vacuum Chamber
5.0
Low pressure (P_1) above diaphragm
~ 130 cm
Polypropylene Diaphragm
Apply current to remove diaphragm
$P_4 = P_{atm}$ below diaphragm
Glass Spheres D_{50} = 44μm to 300 μm
4 cm
6


Experimental Setup
5.0
Vacuum Chamber
Pressure Sensors (200 kHz)
Low pressure (P_1) above diaphragm
~ 130 cm
Shock
Rarefaction Wave
$P_4 = P_{atm}$ below diaphragm
Glass Spheres D_{50} = 44µm to 300 µm
4 cm
7


Experimental Setup
5.0
Vacuum Chamber
Pressure Sensors (200 kHz)
Low pressure (P_1) above diaphragm
Phantom v641 4-megapixel high speed camera (F_s = 10,000+ fps)
Shock
Rarefaction Wave
$P_4 = P_{atm}$ below diaphragm
Glass Spheres D_{50} = 44µm to 300 µm
4 cm
8


Experimental Setup
Vacuum Chamber
Pressure Sensors (200 kHz)
Shock
Rarefaction Wave
Escape/rise of interstitial gas
Expansion of particle bed
Phantom v641 4-megapixel high speed camera (F_s = 10,000+ fps)
9


Experimental Setup
acuum Chamber
Pressure Sensors (200 kHz)
Shock
Rarefaction Wave
Phantom v641 4-megapixel high speed camera (F_s = 10,000+ fps)
10

Measurement Techniques

- Pressure sensors
- High-speed (10 kfps) video
  - Particle bed expansion
  - Front velocity
- Particle image velocimetry (PIV) of gas in expansion region at top of particle bed

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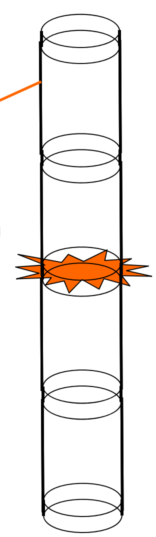
Dynamic Pressure Sensors

- Static pressure sensor Omega DPG9145-15 pressure above diaphragm (below ~ atmospheric)

- Holes built into diaphragm joint ensure $P_4 = P_{atm}$



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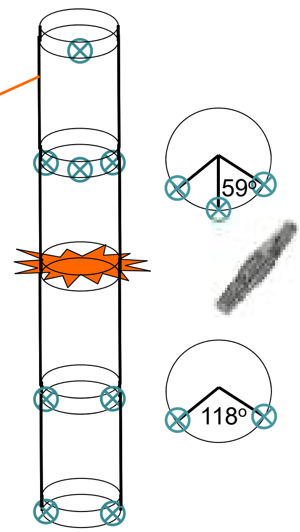
Dynamic Pressure Sensors

- Static pressure sensor Omega DPG9145-15 pressure above diaphragm (below ~ atmospheric)
- Dynamic sensors PCB113B28, F_s = 200 kHz
- Use shock to trigger/sync optical measurements
- Detect lateral variations of shock and expansion waves (UQ, simulation)



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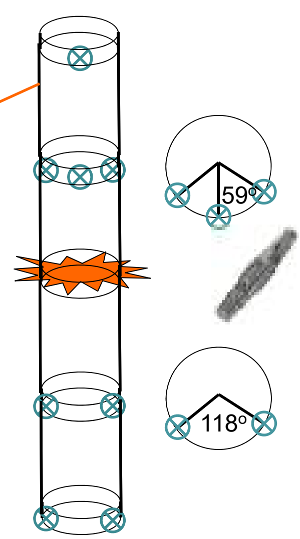
Dynamic Pressure Sensors

- Static pressure sensor Omega DPG9145-15 pressure above diaphragm (below ~ atmospheric)
- Dynamic sensors PCB113B28, F_s = 200 kHz
- Use shock to trigger/sync optical measurements
- Detect lateral variations of shock and expansion waves (UQ, simulation)



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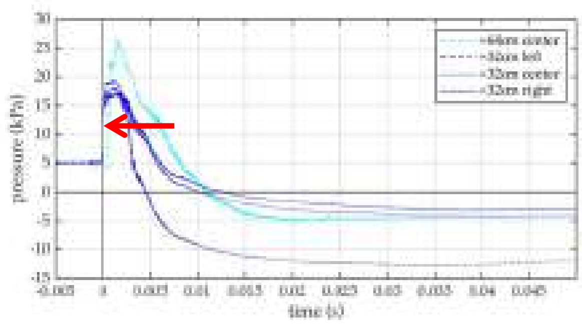
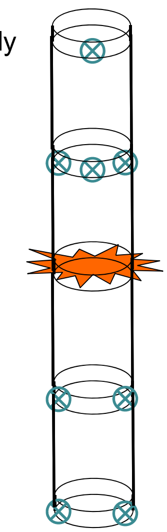
Pressure Sensors / Synchronization

- 8 pressure sensors (PCB 113B28) read simultaneously into LabView via PXIe-4492
- Pressure threshold set in LabView (UQ, simulation)
  - Shock trigger for particle bed measurements
  - Expansion trigger for gas PIV





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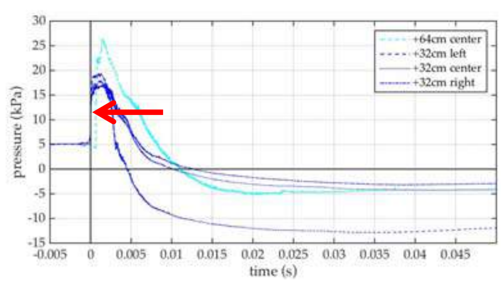
Pressure Sensors / Synchronization



- Hardware trigger sent from PXIe-4492 to PXIe-6341, to BNC-2120, to BNC 565 pulse/delay generator, and to Phantom v641 camera
- Trigger received by camera to initiate optical recording

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High speed video

Left: Bed rise

Right: Void development

F_s = 10,000 fps

Particle Image Velocimetry (PIV)

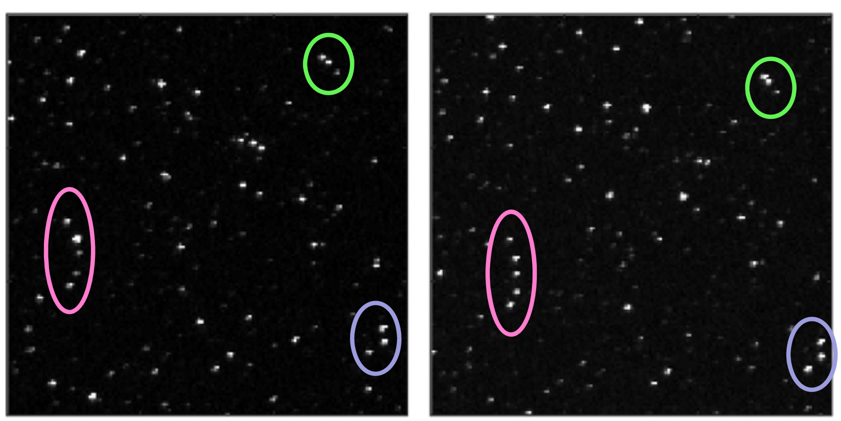
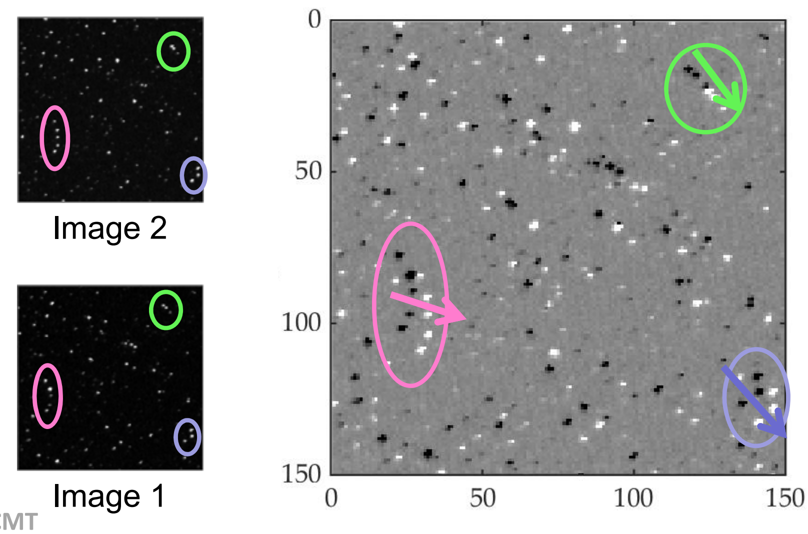


Image 1 Δt = 80 μs Image 2

Particle Image Velocimetry (PIV)



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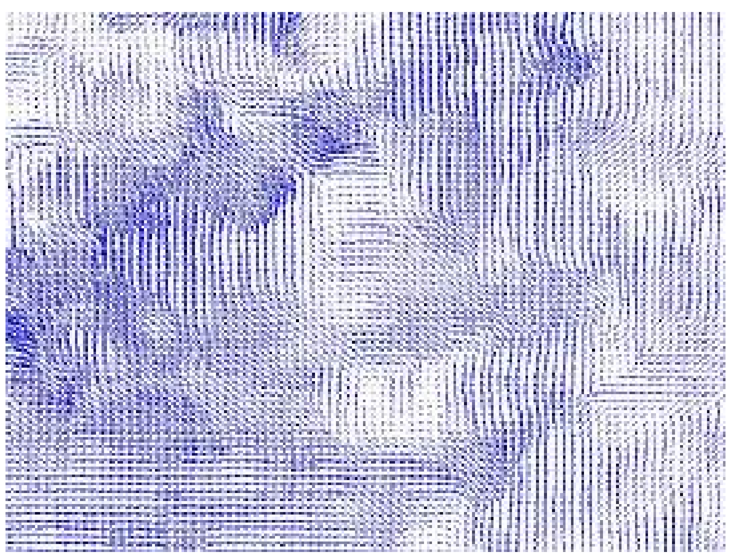
Particle Image Velocimetry (PIV)



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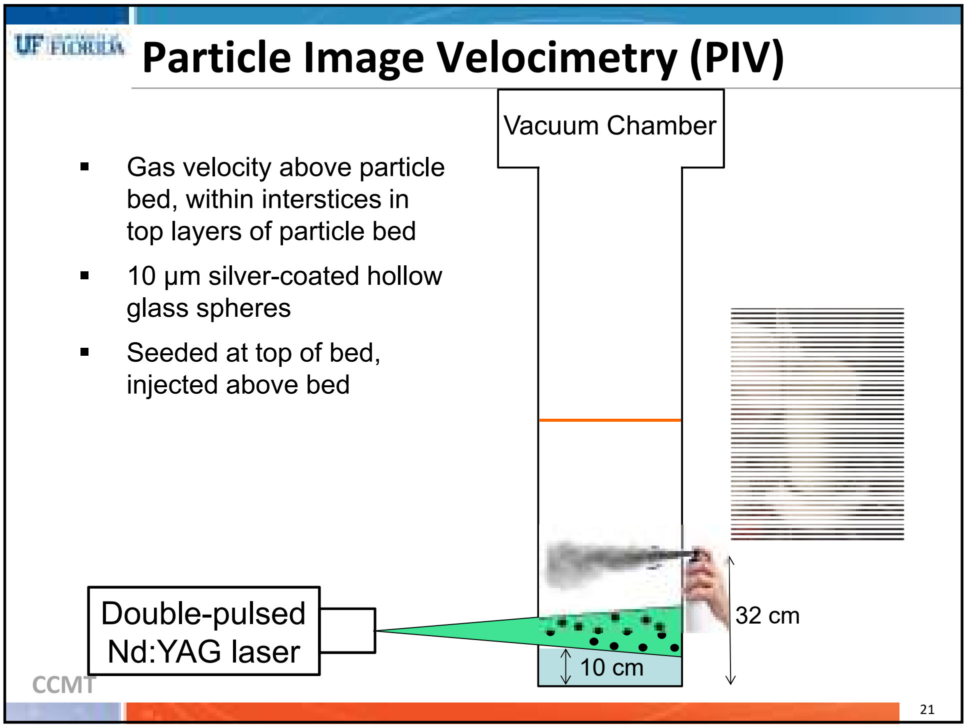
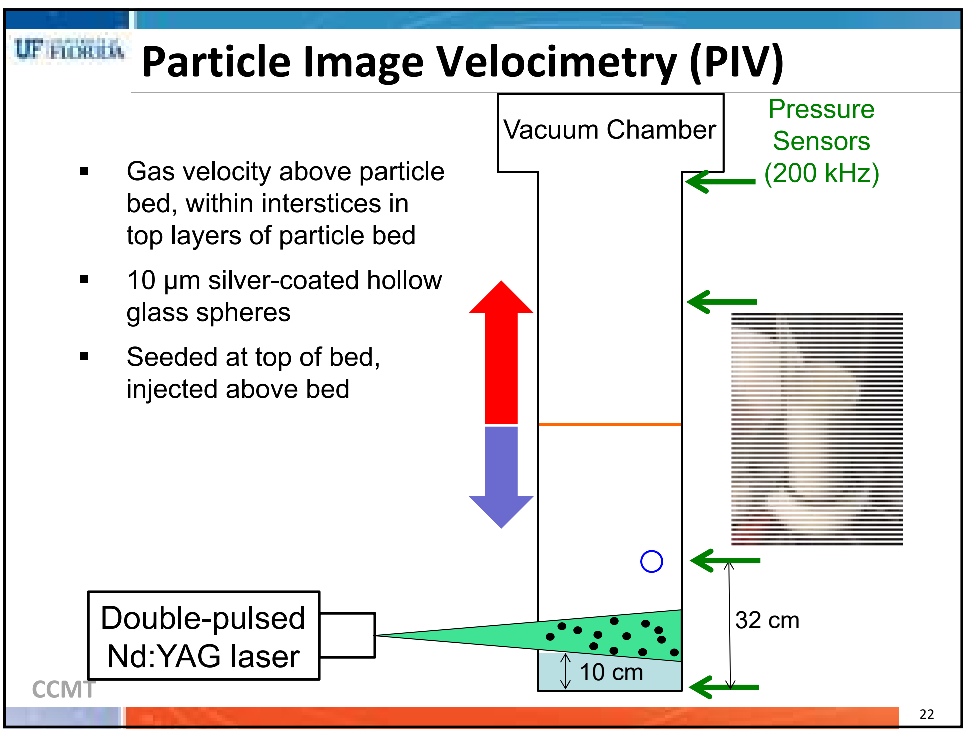

Particle Image Velocimetry (PIV)
Gas velocity above particle bed, within interstices in top layers of particle bed
10 µm silver-coated hollow glass spheres
Seeded at top of bed, injected above bed
Vacuum Chamber
Double-pulsed Nd:YAG laser
32 cm
10 cm
CCMT
21


Particle Image Velocimetry (PIV)
Gas velocity above particle bed, within interstices in top layers of particle bed
10 µm silver-coated hollow glass spheres
Seeded at top of bed, injected above bed
Vacuum Chamber
Pressure Sensors (200 kHz)
Double-pulsed Nd:YAG laser
32 cm
10 cm
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22

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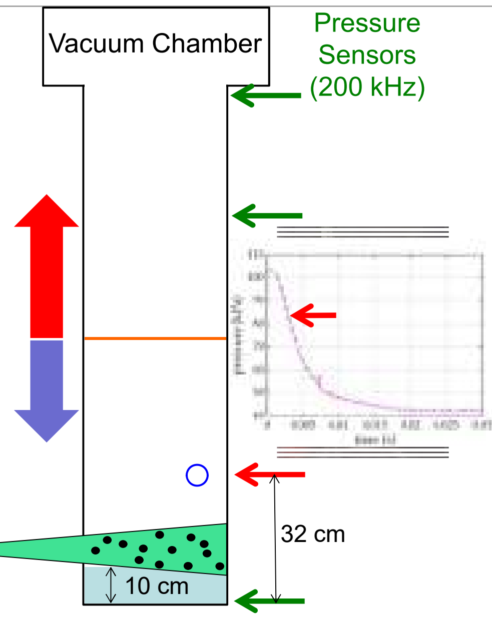
Particle Image Velocimetry (PIV)

- Gas velocity above particle bed, within interstices in top layers of particle bed
- 10 μm silver-coated hollow glass spheres
- Seeded at top of bed, injected above bed
- Triggered in expansion
- Synchronization via BNC 565 pulse/delay generator



Double-pulsed Nd:YAG laser

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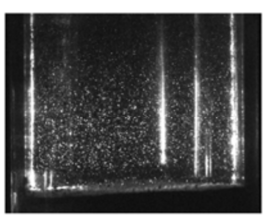
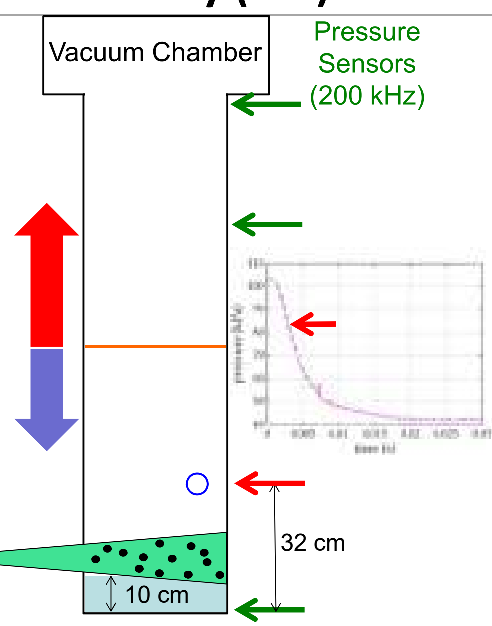
Particle Image Velocimetry (PIV)

- Field of view: 4 cm x 4 cm, above 10cm bed
- Δt ~ 80 μs
- F_s = 14 Hz (limited by laser)





Double-pulsed Nd:YAG laser

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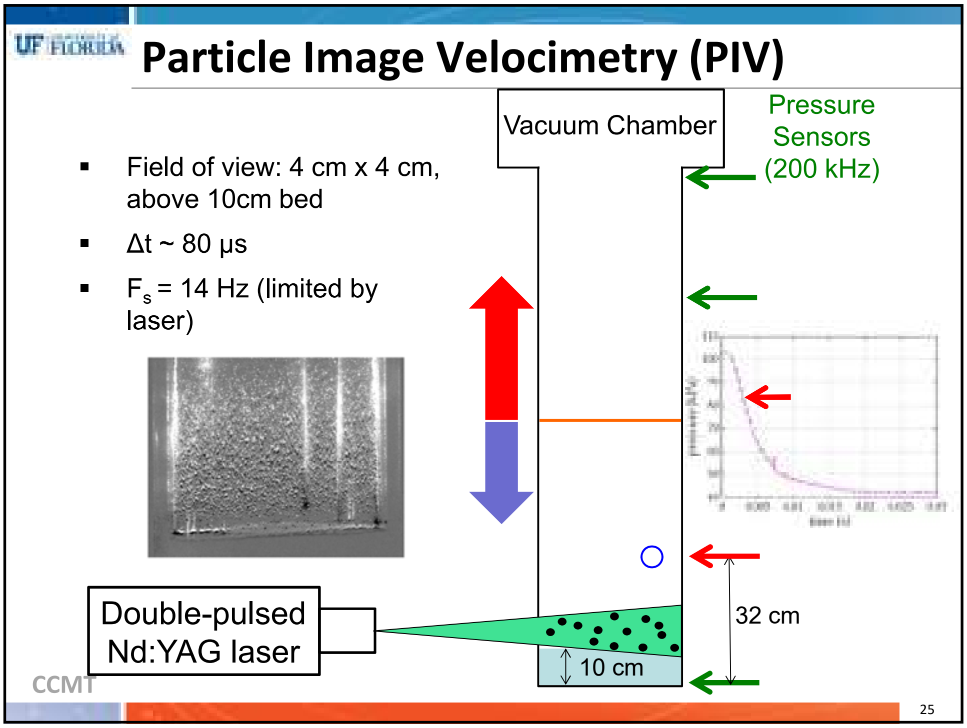
Particle Image Velocimetry (PIV)
Field of view: 4 cm x 4 cm, above 10cm bed
Δt ~ 80 μs
F_s = 14 Hz (limited by laser)
Vacuum Chamber
Pressure Sensors (200 kHz)
32 cm
10 cm
Double-pulsed Nd:YAG laser
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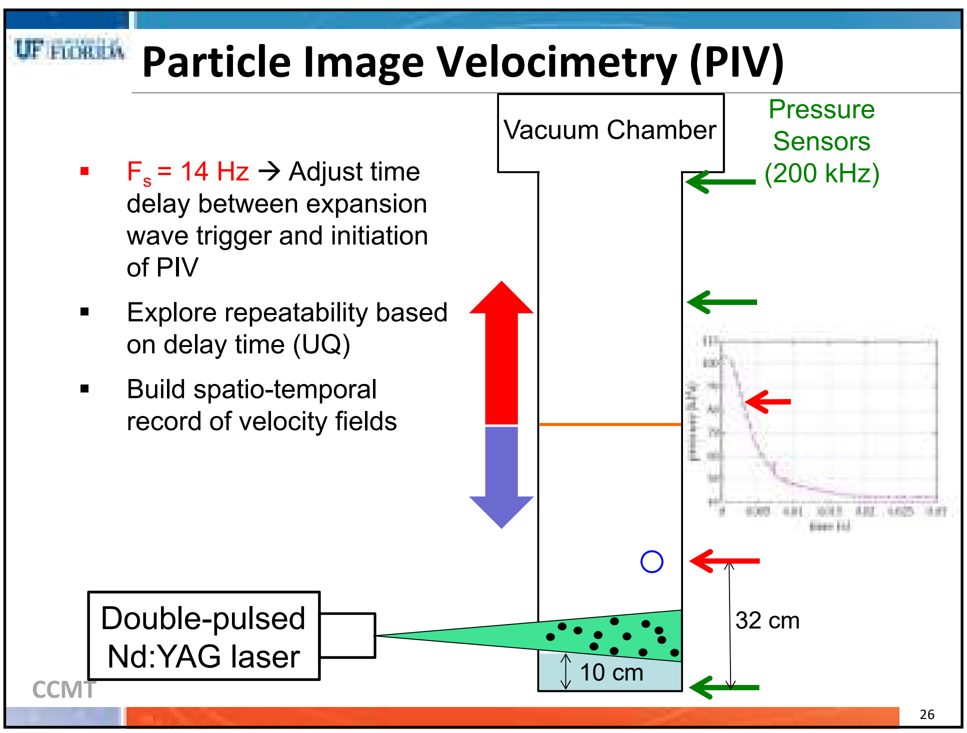
Particle Image Velocimetry (PIV)
F_s = 14 Hz → Adjust time delay between expansion wave trigger and initiation of PIV
Explore repeatability based on delay time (UQ)
Build spatio-temporal record of velocity fields
Vacuum Chamber
Pressure Sensors (200 kHz)
32 cm
10 cm
Double-pulsed Nd:YAG laser
CCMT
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Outline

- Research Objectives
- Experimental Setup & Measurement Techniques
  - Installation of new pressure sensors
  - Synchronization to optical measurements
  - High speed video of particle bed evolution
  - Particle image velocimetry (PIV) of gas
- Results
  - Pressure analysis
  - Particle bed motion
  - Gas velocity
- Summary & Upcoming Work

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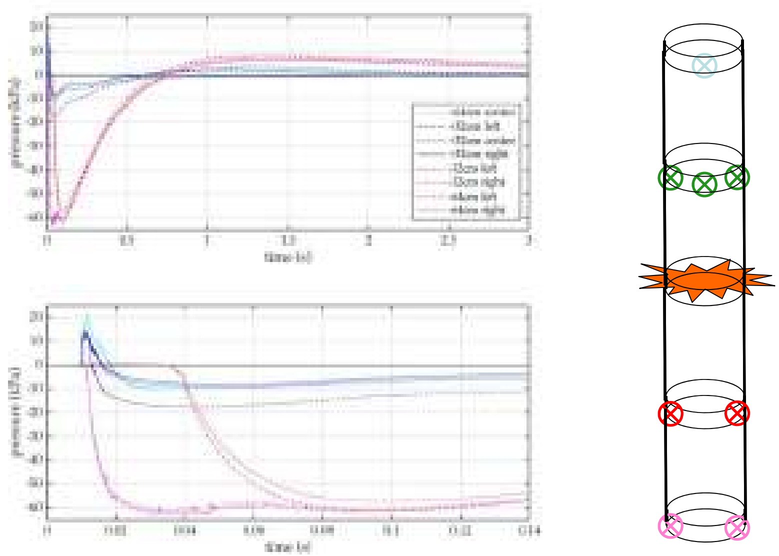
Results – Pressure Sensors



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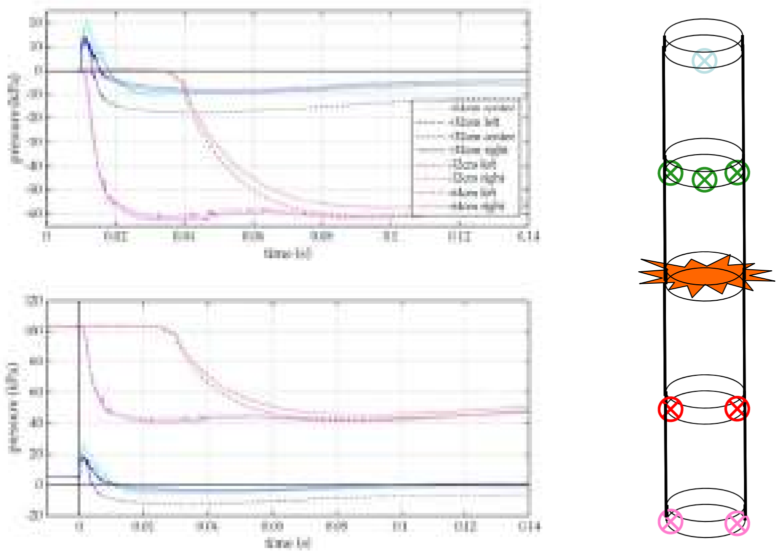
Results – Pressure Sensors



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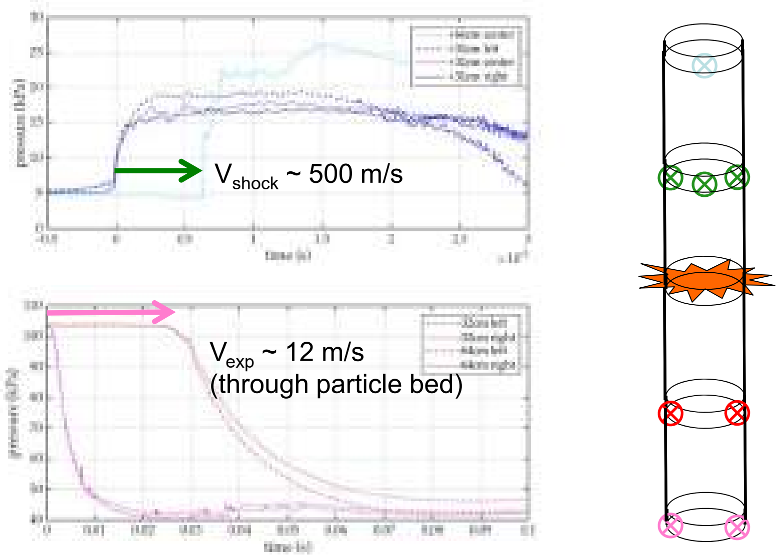
Results – Wave Speeds



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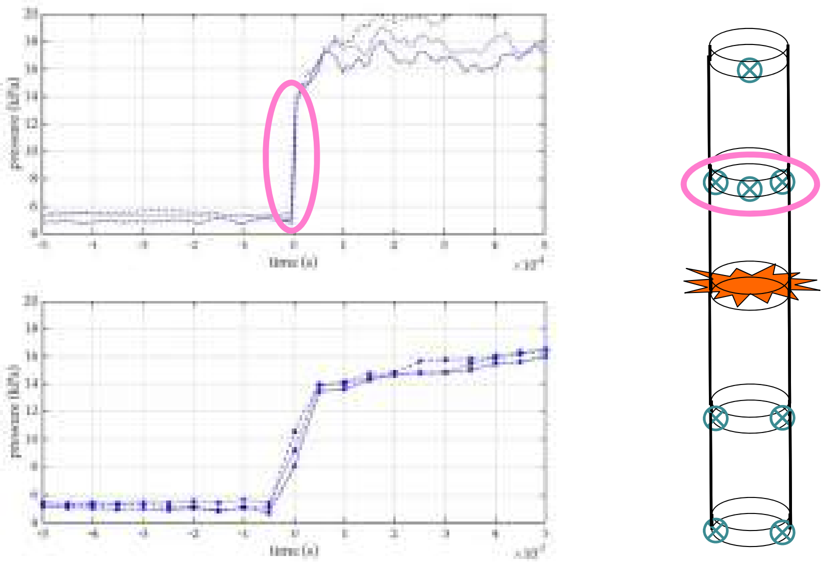
Results – Flatness of Shock



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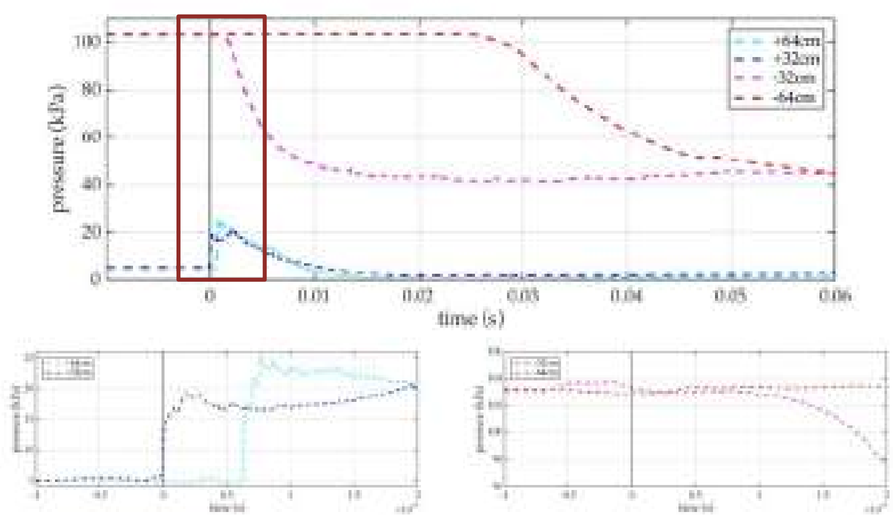
Results – Pressure Sensors



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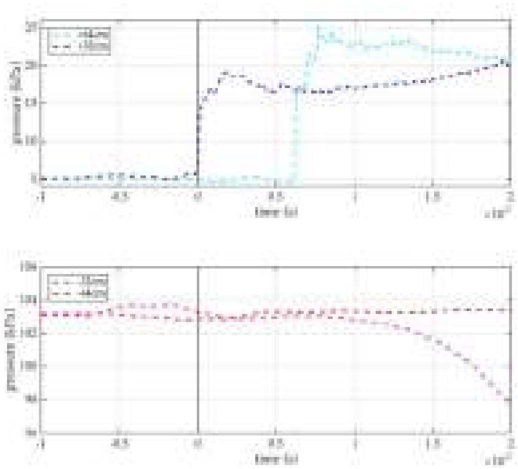
Results – Pressure Sensors



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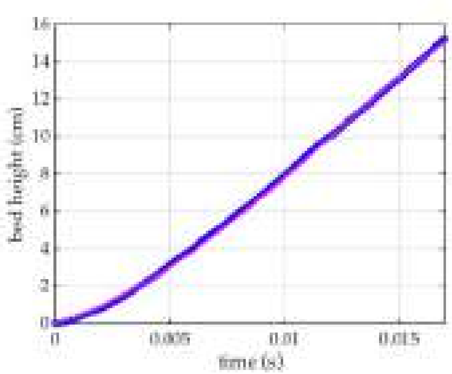
Results – Particle Bed Front Velocity



- P_4/P_1 = 20; P_1 ~ 5 kPa
- Track bed height as a function of time, ~60% intensity
- Cubic fit to experimental data

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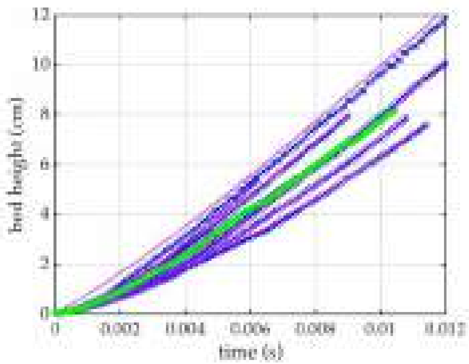
Results – Particle Bed Front Velocity



- $P_4/P_1 = 20$; $P_1 \sim 5$ kPa
- 8 experiments of identical conditions

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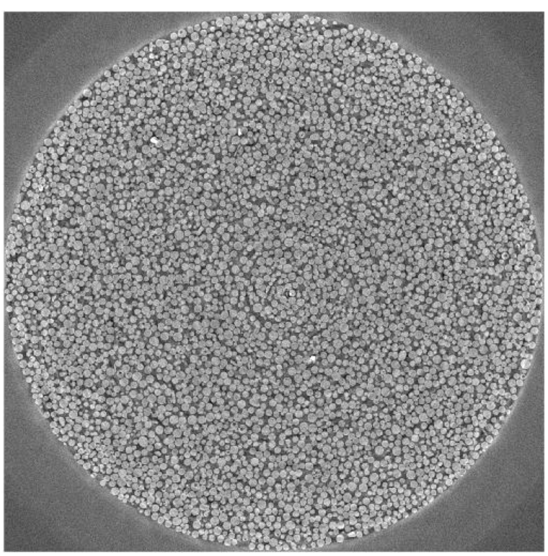
Results – Particle Bed Packing



- Able to measure mass/volume in laboratory, but not packing density, porosity, etc.
- Volume fraction of particles
- Segregation of particles by size

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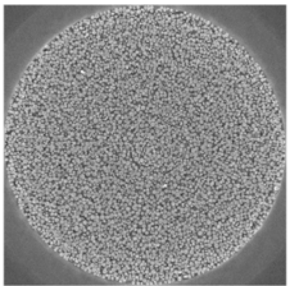
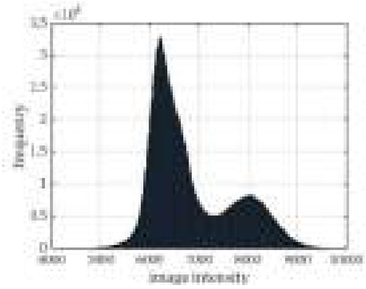
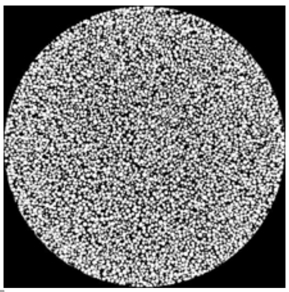
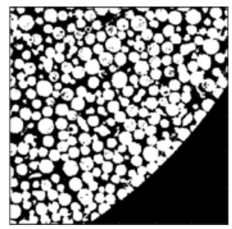
Results – Particle Bed Packing







- Threshold method suggests ~59% packing density
- Previously estimated 61%



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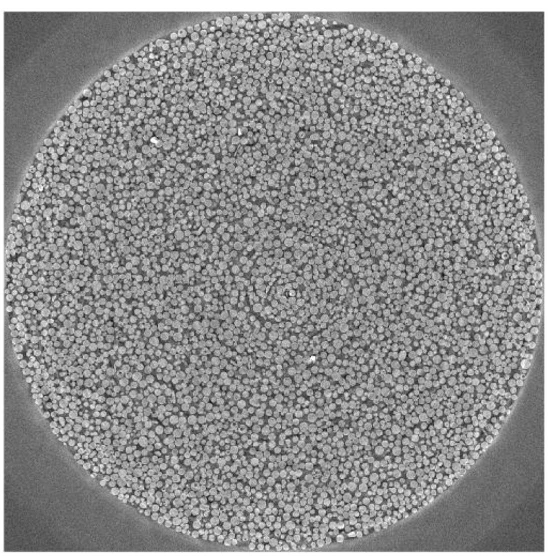
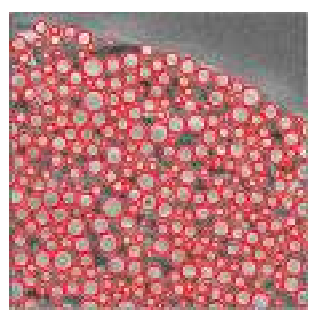
Results – Particle Bed Packing





- Identifies location and radius of each particle
- Volume fraction ~53%

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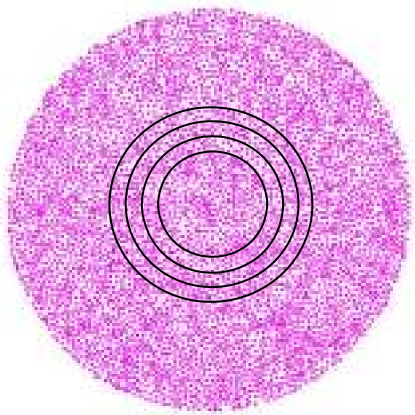
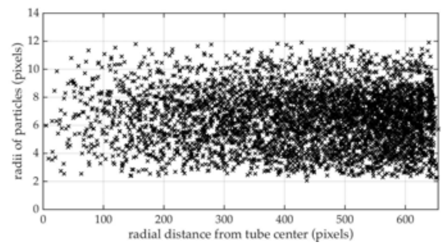
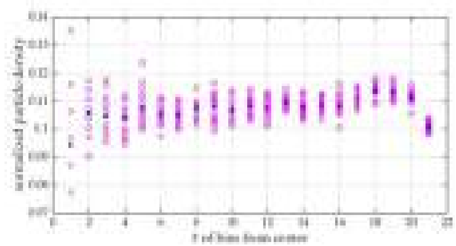
Results – Particle Bed Packing







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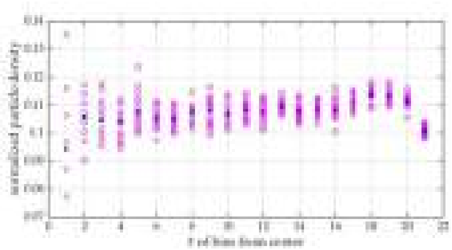
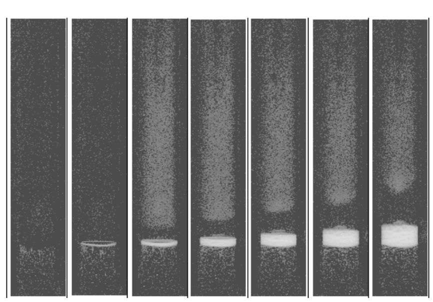
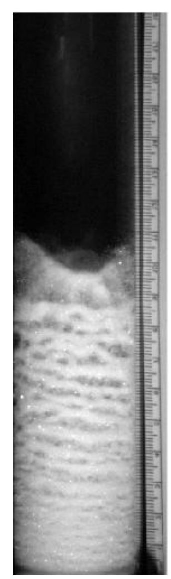
Results – Particle Bed Packing





- Faster bed rise near edges of shock tube
- Faster escape of “cloud” particles in gas velocity near edges
- Lower packing density near walls *could* explain faster air flow, both gas/particle velocities



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Results - Gas Velocity

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Outline

- Research Objectives
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  - Gas velocity
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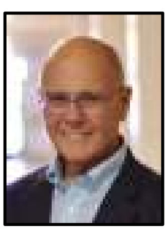
Summary & Upcoming Work

- Synchronization between pressure sensors (via shock or expansion waves) successful with optical measurements (high-speed video, PIV)
- Bed motion can be observed prior to shock wave
- Shock wave self-corrects and shows no lateral variation at pressure sensors 32 cm above diaphragm
- Still pursuing bed packing structure near walls; impact on particle & gas velocity differences at walls
- Possible future experimental update: replace one glass segment with acrylic tube to measure evolution of expansion wave speed

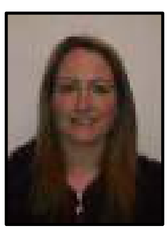
ASU Experimental Team

Heather Zunino

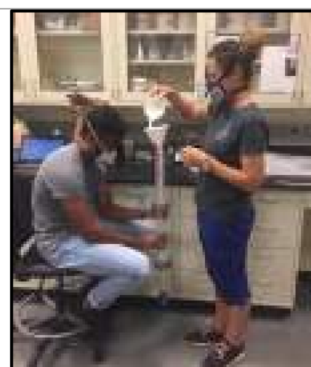
Blair Johnson

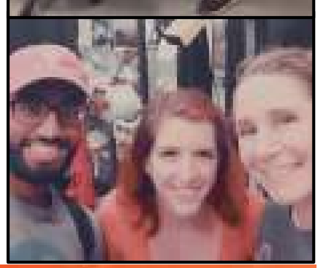


Ron Adrian



Amanda Clarke



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Do you have any questions?

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AFRL/RW Experiments

Angela Diggs

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Outline

- FY17 Macroscale Experiment
  - Test Set-up & Instrumentation
  - Results & Analysis
    - High Speed Video
    - Pressure Transducers
  - Future Work
- FY18 Microscale Experiment
  - Test Set-up
  - Instrumentation

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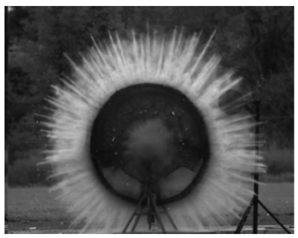
| 2

Motivation

- Frost [1]
  - Instrumentation
    - High speed cameras
    - Far field pressure probes
  - Detonation
    - Charge mass = 2.4g
    - Glass mass = 240g
      M/C = 100
    - Steel mass = 10.5kg
      M/C = 4400



- Desired
  - Instrumentation
    - High fidelity data for model development and validation
    - Large quantity of data collected at near field
  - Proposed solution
    - AFRL/RW Blast Pad: pressure probes, high speed cameras, additional instrumentation for momentum
    - Match legacy Comp B charges for cost savings
      - Charge mass = 8.55lb

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Outline

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  - Test Set-up
  - Instrumentation

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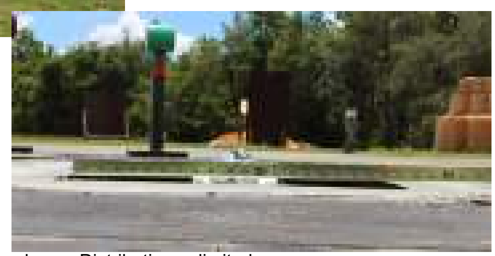
AFRL Blastpad Experimental Setup

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



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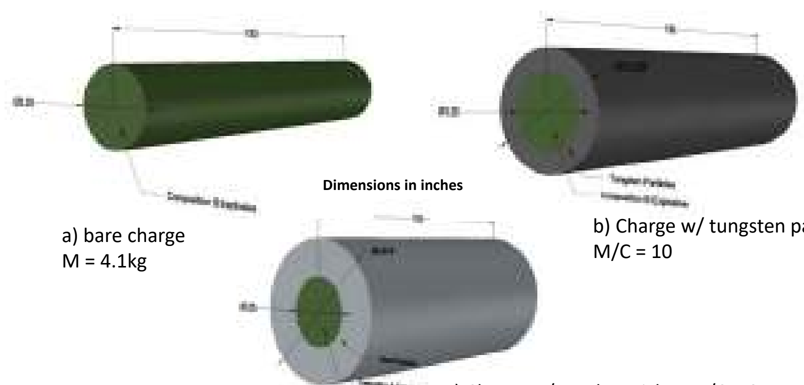
Blastpad Test Articles

- The ratio of the mass of the particles to the mass of the charge (M/C ratio) is critical to expected behavior
- Literature review (Frost, Zhang) indicates instabilities will be present for M/C ≥ 10
- The charge mass matches legacy blastpad data (released to UF for UQ analysis)



a) bare charge
M = 4.1kg

b) Charge w/ tungsten particles
M/C = 10

c) Charge w/ steel particles, M/C=13

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Test Article Casing

- Case fracture may be a possible mechanism for jetting instability [Zhang et al. 2001, Xu et al. 2013]
- Case influence was minimized by using 3/16" phenolic tubing (notches were 1/32")

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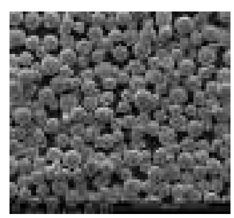
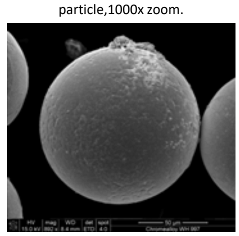
Preliminary Particle Characterization

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

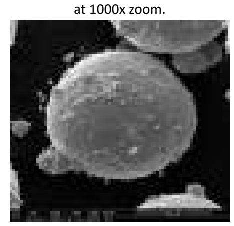
SEM of several steel particles at 100x zoom.



SEM of single tungsten particle,1000x zoom.



SEM of single steel particle at 1000x zoom.



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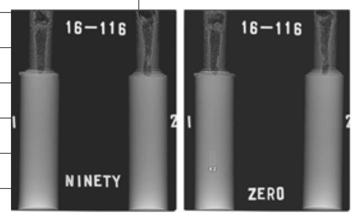
Uncertainty Quantification

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



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

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  - Instrumentation

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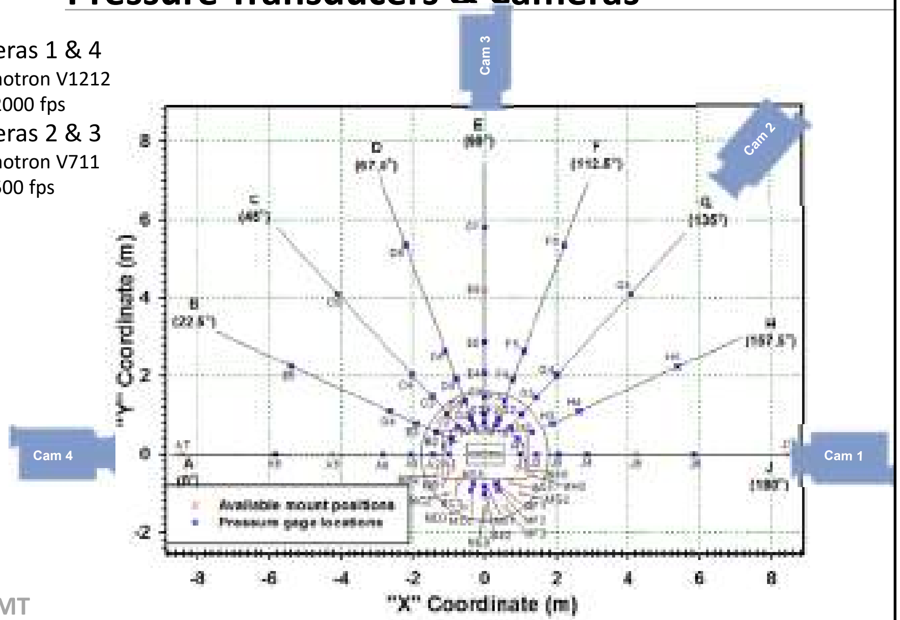
Pressure Transducers & Cameras

Cameras 1 & 4
- Photron V1212
- 12000 fps

Cameras 2 & 3
- Photron V711
- 7500 fps



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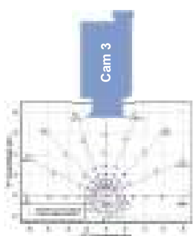
Bare Charge Video



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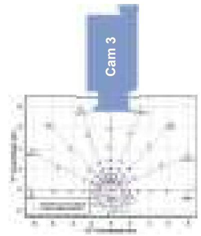
Tungsten & Steel Liner Videos

- Tungsten Liner
  - Instabilities present
  - Luminosity from particles
- Tungsten Particles
  - Instabilities present



Tungsten Liner

Steel Liner

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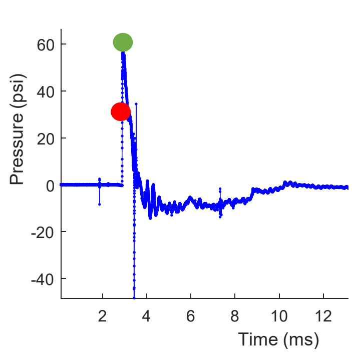
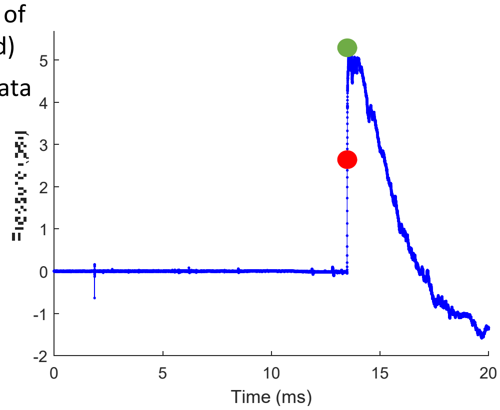
Pressure Transducer Analysis

- Peak pressure (PP) recorded for each pressure transducer (green)
- Shock time of arrival (TOA) when 50% of the maximum pressure is reached (red)
- Manual corrections applied to noisy data





E line pressures (perpendicular) for position 1 (near, left) & 7 (far, right).

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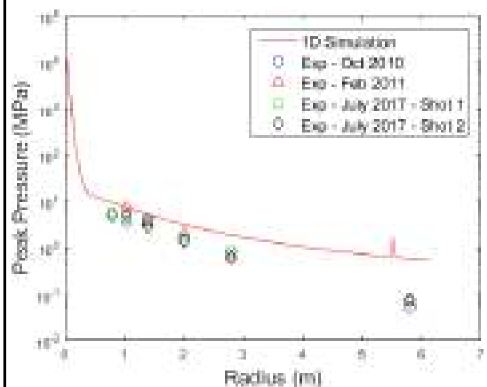
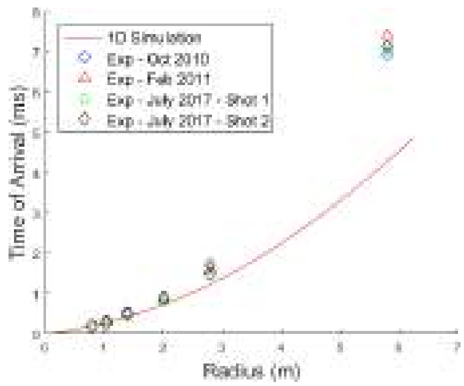
Legacy Data

- Comparison performed along the E line (perpendicular)
- Constant shape and weight of Comp B





Legacy data may be used to calculate uncertainties with confidence.

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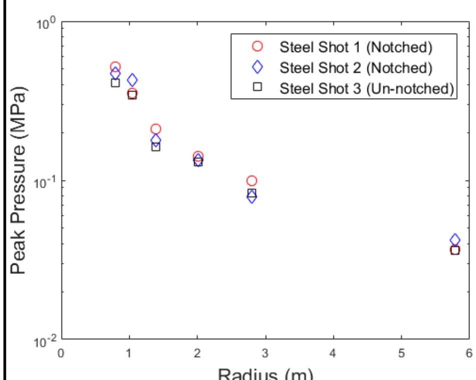
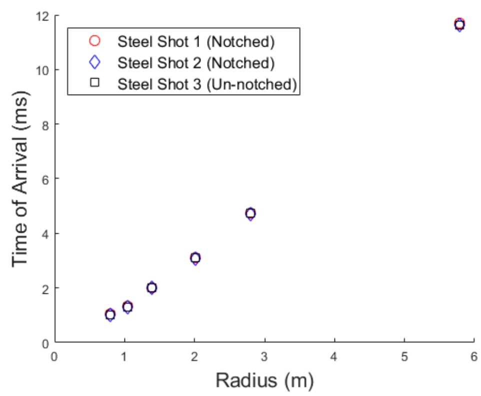
Effect of Notched Casing

- Some variability
- No clear, consistent trends





Case notches do not appear to have an effect. Analysis may assume 3 repeats of steel liner shots.

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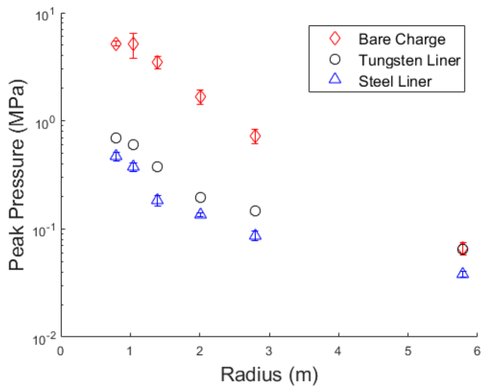
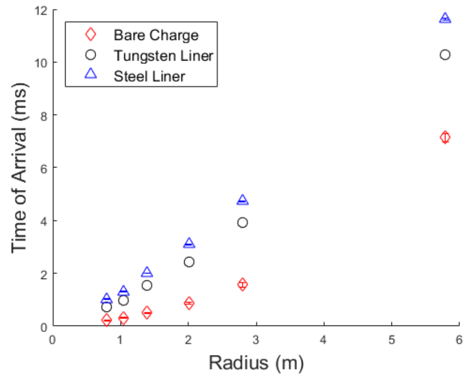
Shot Comparison

- Data point = average
- Vertical error bars = 1σ
- Steel = 3 repeated shots
- Bare charge = 4 repeated shots





Momentum transfer to particles lowers peak pressure in near field and slows the shock speed.

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Outline

- FY17 Macroscale Experiment
  - Test Set-up & Instrumentation
  - Results & Analysis
    - High Speed Video
    - Pressure Transducers
  - Future Work
- FY18 Microscale Experiment
  - Test Set-up
  - Instrumentation

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Additional Blastpad Analysis

- High Speed Video
  - Shock front tracking
  - Particle front tracking
  - Analysis of instabilities
- Pressure Transducers
  - Pressure contours
  - Impulse calculations
- Unconfined momentum traps
  - Particle & gas momentum
- Optical linear encoders
  - Particle & gas momentum

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Outline

- FY17 Macroscale Experiment
  - Test Set-up & Instrumentation
  - Results & Analysis
    - High Speed Video
    - Pressure Transducers
  - Future Work
- FY18 Microscale Experiment
  - Test Set-up
  - Instrumentation

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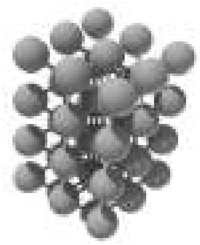
Future Experiments

- Previous feedback from AST/TST shows concern with modeling the compaction regime
- Future experiments at lower volume fraction will allow a focus on multi-disperse effects, vice compaction
  - 20% volume fraction explosive experiments
  - Motivated by Multiphase Shock Tube at Sandia, but explosively driven
  - Additively manufacture test articles to achieve low volume fraction
  - Microscale experiments due to AFRL budget constraints



Additively-manufactured particle bed concept. (Flater)

Future Experiments

- Instrumentation
  - High Speed Videos
  - Pressure Transducers
  - X-rays
  - Schlieren Imaging

Conclusions

- Blastpad data analysis ongoing
- AFRL/RW approved funding for FY18 microscale experiments
- Close coordination between UF and AFRL/RW ensures relevant experimental data is collected for model development and validation

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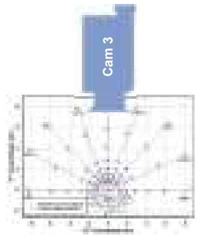
Do you have any questions?

Bare Charge Video



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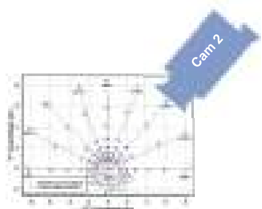
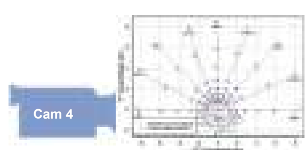
Bare Charge Video (Backup)





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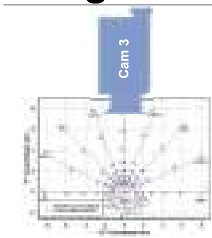
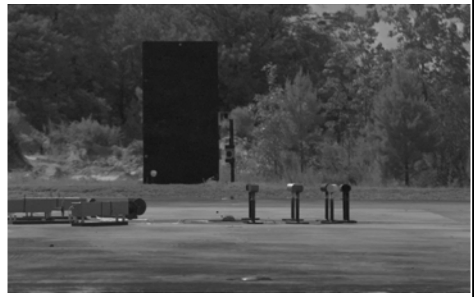
Tungsten Liner Video





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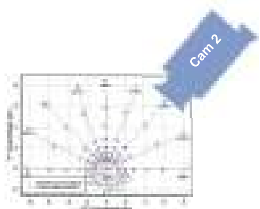
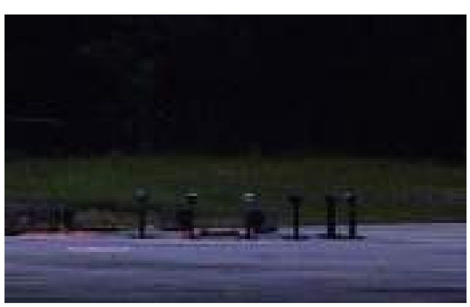
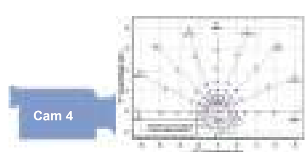
Tungsten Liner Video (Backup)







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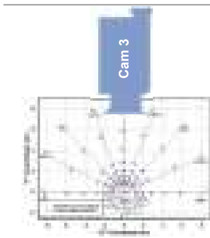
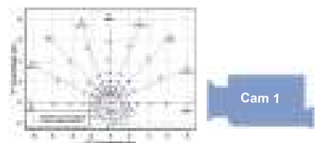
Steel Liner Video





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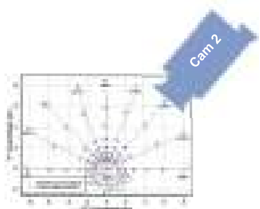
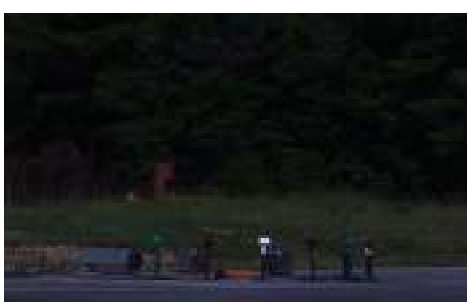
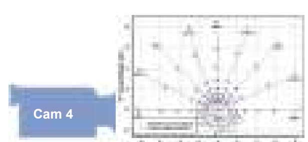
UF FLORIDA

Steel Liner Video (Backup)







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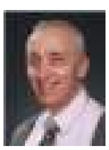
Uncertainty Budget

Validation and Uncertainty Reduction

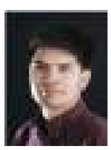
Chanyoung Park, Raphael (Rafi) T. Haftka and Nam-Ho Kim

Department of Mechanical & Aerospace Engineering, University of Florida

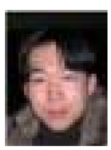
Integrated Uncertainty Budget Team



Raphael T. Haftka, PhD

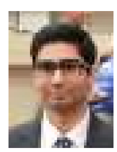


Nam-Ho Kim, PhD

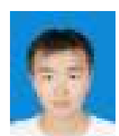


Chanyoung Park, PhD

Kyle Hughes



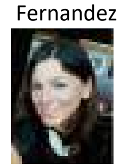
Samaun Nili



Yiming Zhang

Giselle Fernandez

Justin T. Mathew



Shirly Spath (Undergrad)

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

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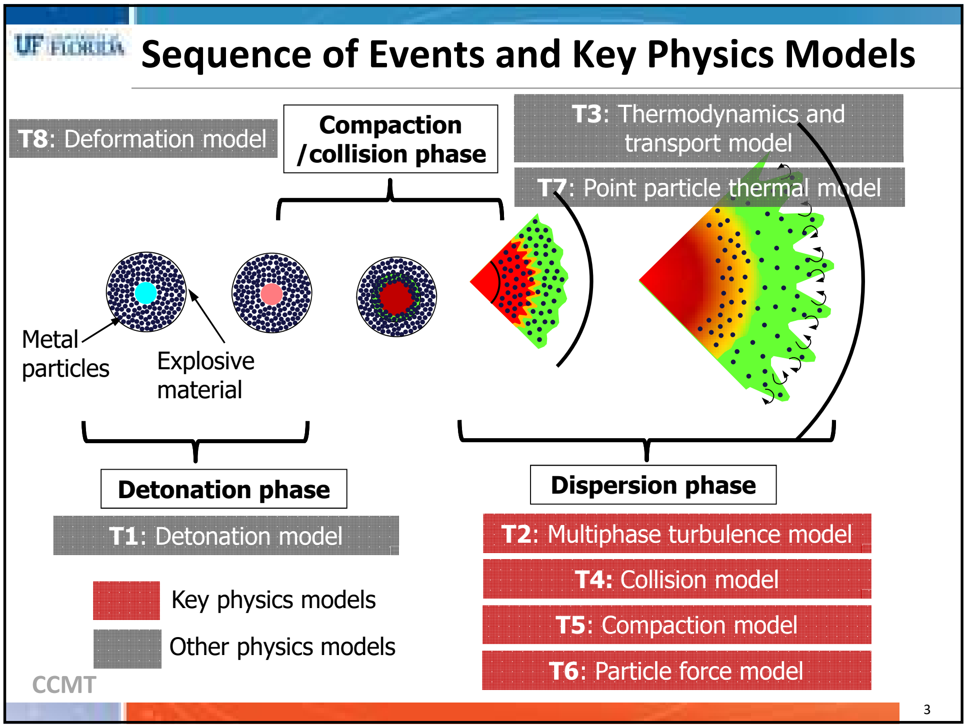
Sequence of Events and Key Physics Models
T8: Deformation model
Compaction /collision phase
T3: Thermodynamics and transport model
T7: Point particle thermal model
Metal particles
Explosive material
Detonation phase
T1: Detonation model
Dispersion phase
T2: Multiphase turbulence model
T4: Collision model
T5: Compaction model
T6: Particle force model
Key physics models
Other physics models
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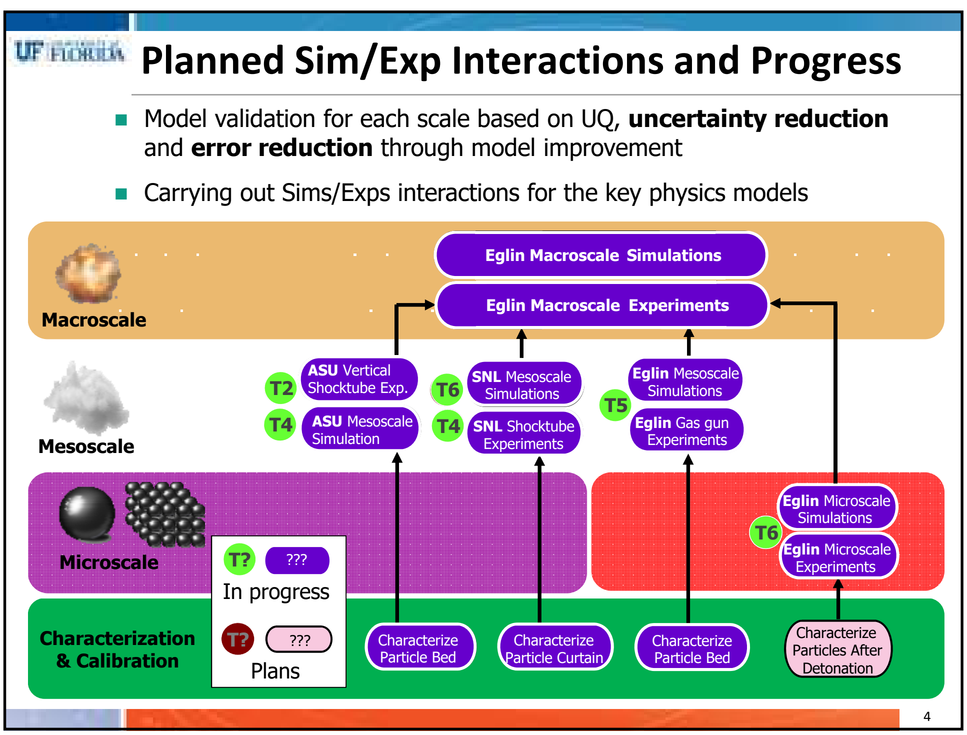
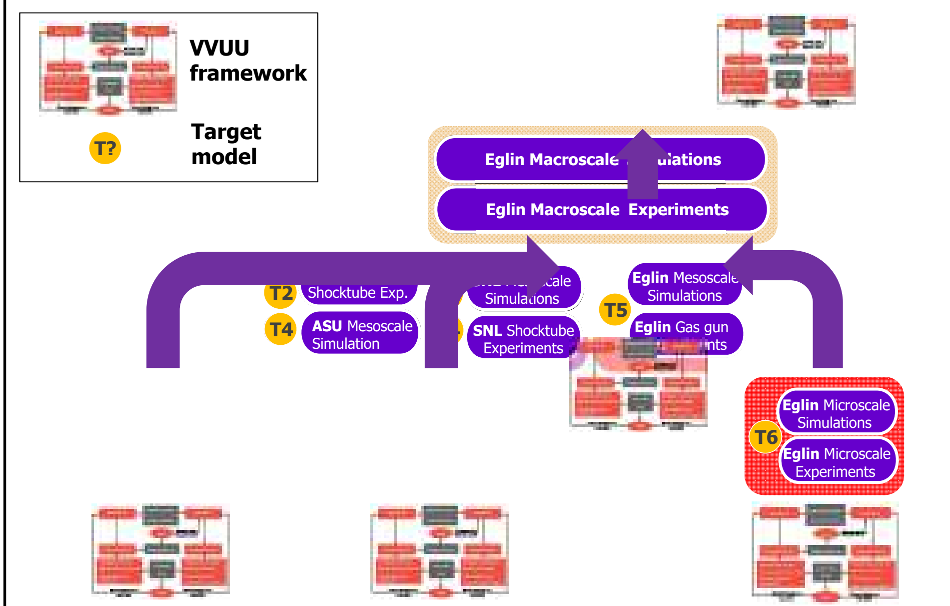
3


Planned Sim/Exp Interactions and Progress
Model validation for each scale based on UQ, uncertainty reduction and error reduction through model improvement
Carrying out Sims/Exps interactions for the key physics models
Macroscale
Eglin Macroscale Simulations
Eglin Macroscale Experiments
Mesoscale
T2
ASU Vertical Shocktube Exp.
T4
ASU Mesoscale Simulation
T6
SNL Mesoscale Simulations
T4
SNL Shocktube Experiments
T5
Eglin Mesoscale Simulations
Eglin Gas gun Experiments
Microscale
T6
Eglin Microscale Simulations
Eglin Microscale Experiments
T?
???
In progress
T?
???
Plans
Characterization & Calibration
Characterize Particle Bed
Characterize Particle Curtain
Characterize Particle Bed
Characterize Particles After Detonation
4

Hierarchical Validation and U Propagation



5

Integrated UQ Accomplishments

- **UQ of experimental measurement processing**
  - Propagating uncertainty when desired measurements are obtained by processing proxy data
  - Planning experiment to better expose uncertainty in measurements
  - Involvement of UQ team in measuring uncertainty in experiments
- **Help verification by enabling convergence**
  - Achieving convergence of the mesoscale multiphase flow simulation by modeling effect of finite size of particles
- **Preparation for UQ of macroscale simulation**
  - Multi-fidelity surrogate
  - **Also useful for exascale behavioral emulation**

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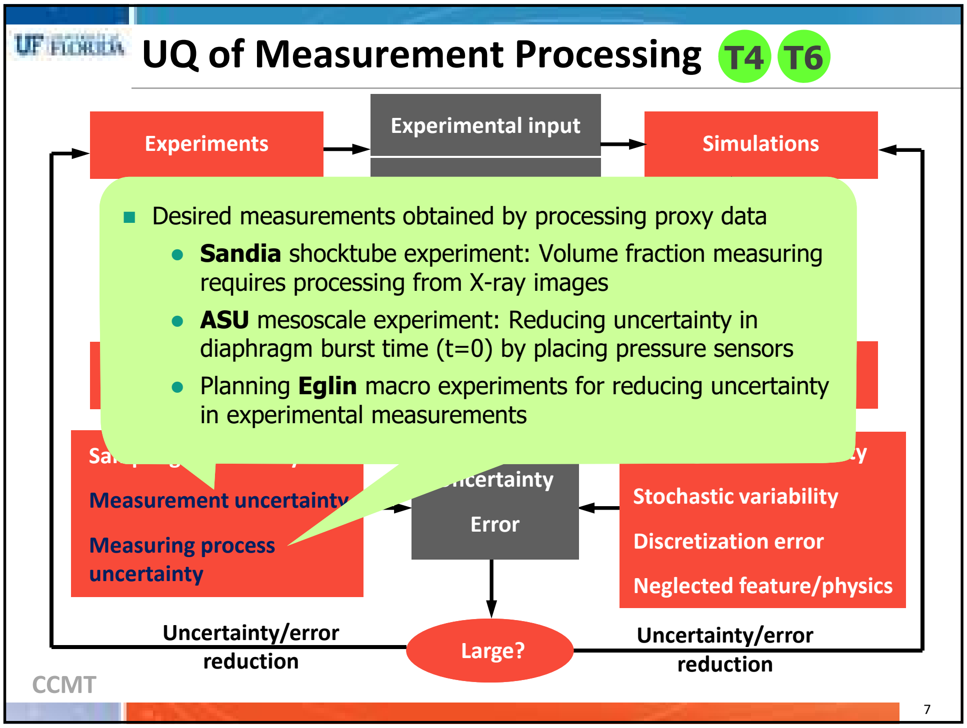
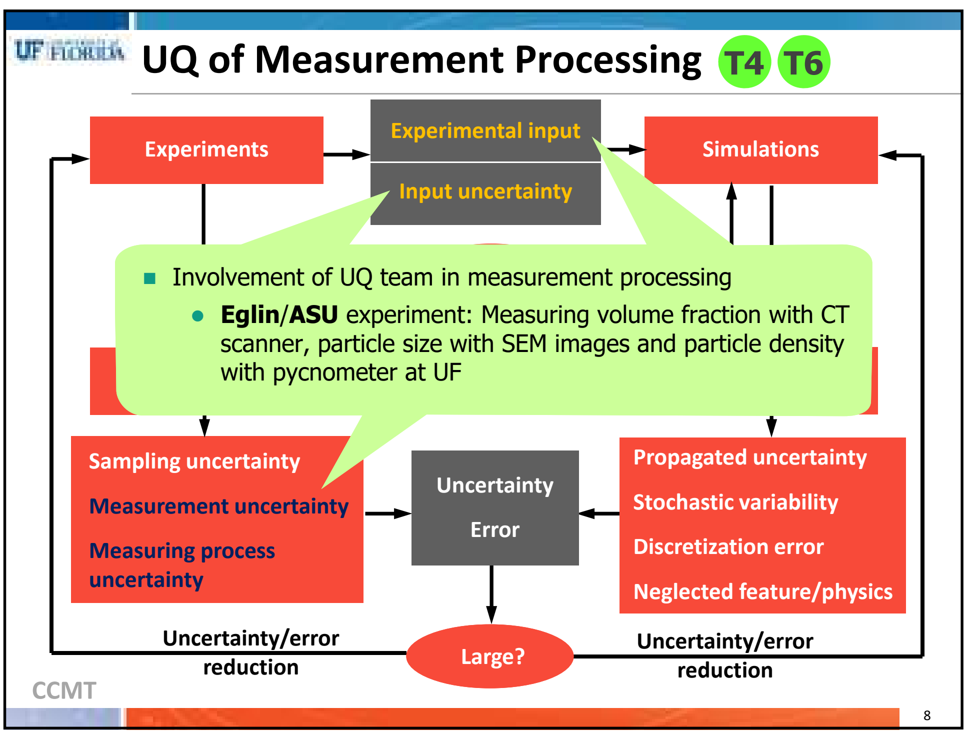
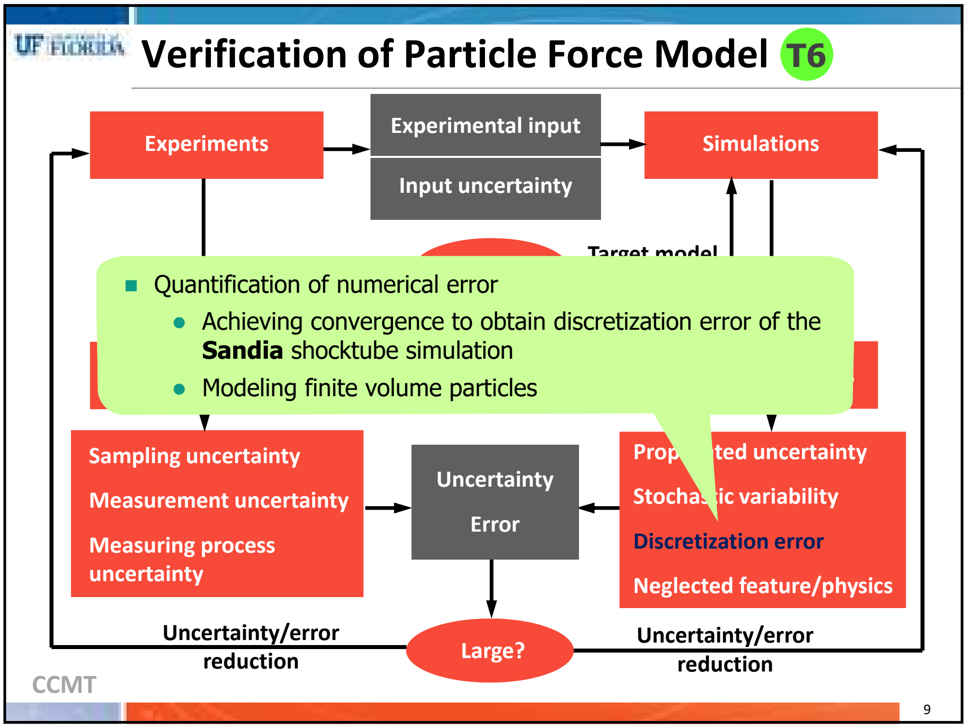
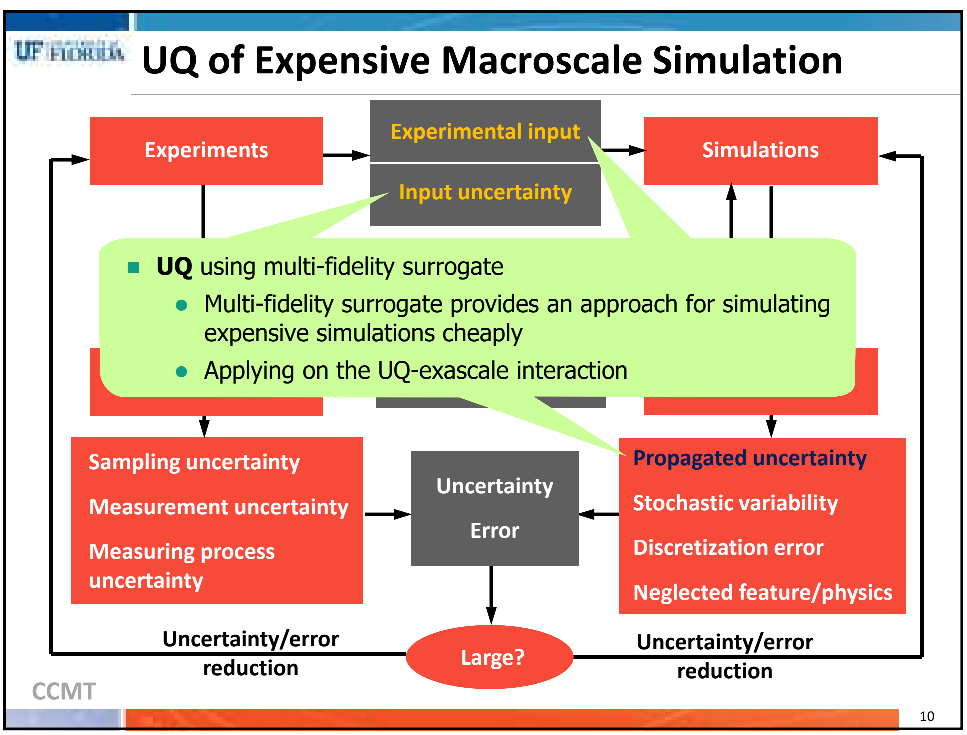

UQ of Measurement Processing
T4
T6
Experiments
Experimental input
Simulations
Desired measurements obtained by processing proxy data
Sandia shocktube experiment: Volume fraction measuring requires processing from X-ray images
ASU mesoscale experiment: Reducing uncertainty in diaphragm burst time (t=0) by placing pressure sensors
Planning **Eglin** macro experiments for reducing uncertainty in experimental measurements
Measurement uncertainty
Measuring process uncertainty
Error
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
CCMT
7


UQ of Measurement Processing
T4
T6
Experiments
Experimental input
Input uncertainty
Simulations
Involvement of UQ team in measurement processing
Eglin/ASU experiment: Measuring volume fraction with CT scanner, particle size with SEM images and particle density with pycnometer at UF
Sampling uncertainty
Measurement uncertainty
Measuring process uncertainty
Uncertainty
Error
Propagated uncertainty
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
CCMT
8


Verification of Particle Force Model
T6
Experiments
Experimental input
Input uncertainty
Simulations
Quantification of numerical error
Achieving convergence to obtain discretization error of the **Sandia** shocktube simulation
Modeling finite volume particles
Sampling uncertainty
Measurement uncertainty
Measuring process uncertainty
Uncertainty
Error
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
CCMT
9


UQ of Expensive Macroscale Simulation
Experiments
Experimental input
Input uncertainty
Simulations
UQ using multi-fidelity surrogate
Multi-fidelity surrogate provides an approach for simulating expensive simulations cheaply
Applying on the UQ-exascale interaction
Sampling uncertainty
Measurement uncertainty
Measuring process uncertainty
Uncertainty
Error
Propagated uncertainty
Stochastic variability
Discretization error
Neglected feature/physics
Uncertainty/error reduction
Large?
Uncertainty/error reduction
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UQ of Measurement Processing

UQ involvement in experiments

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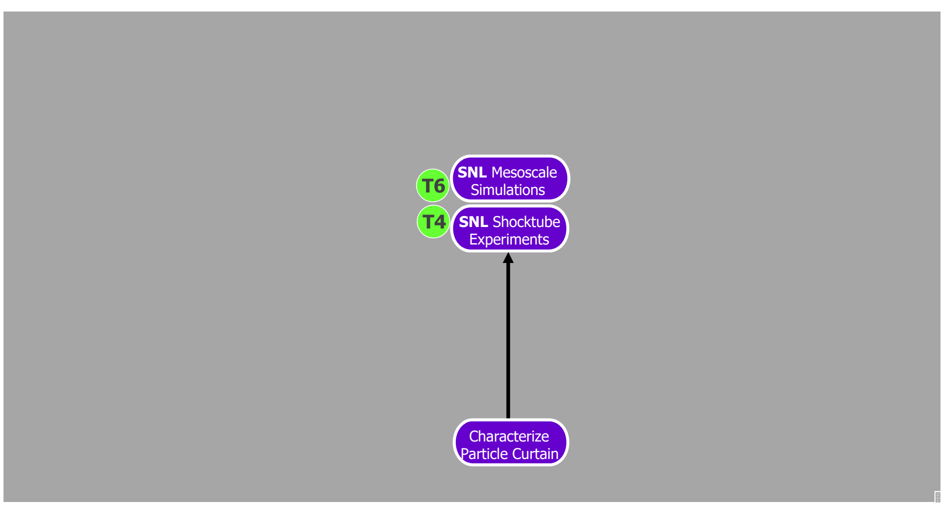
UQ of Measurement Processing



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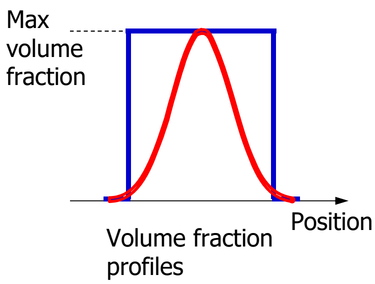
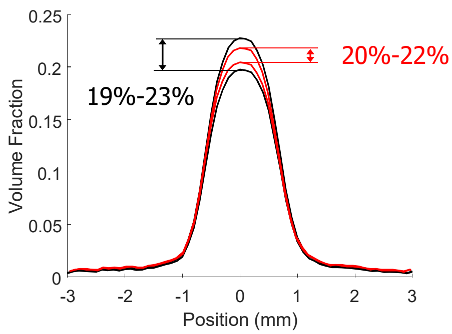
UQ in VF Measuring Process (Sandia)

- **Goal:** Quantifying and modeling uncertainty in the measuring process of initial volume fraction and profile shape (**Justin Mathew**)
- We found that the maximum volume fraction was used with 'top-hat' profile in the **Sandia** shock tube simulations
- Dominant uncertainty in the maximum volume fraction
- Bell shaped profiles (Little uncertainty in the symmetricity)
- Reduced the uncertainty in the maximum volume fraction





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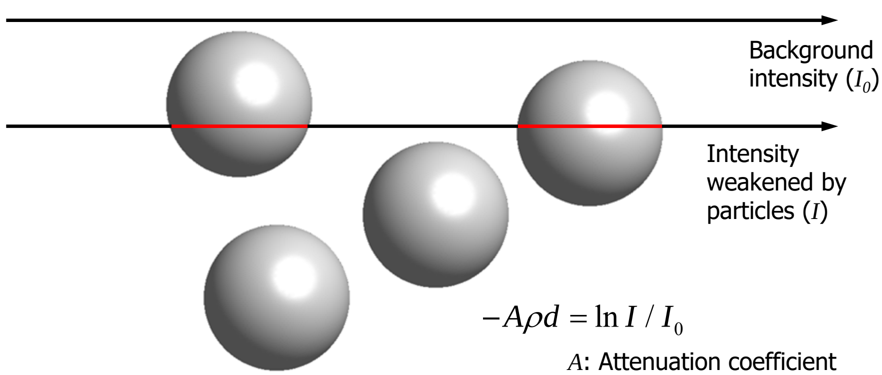
Measuring VF from X-ray Images

- Volume fraction was calculated based on intensity ratio using the Beer-Lambert law and calibration experiment



$$-A\rho d = \ln I / I_0$$

A: Attenuation coefficient

ρ: Particle density

d: Distance through particles

$$d = \varphi t$$

t: Curtain thickness

φ: Volume fraction

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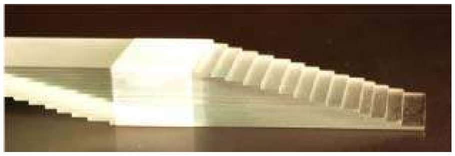
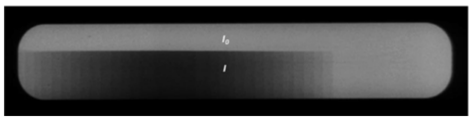
Calibration of A for Measuring VF

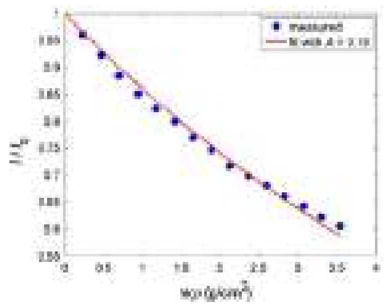




Wagner et. al (2015)

- **Goals:** Estimating the true trend and quantifying the uncertainty in the prediction

- A constant attenuation coefficient does not fit the measured data well due to beam hardening



$$A(I/I_0) = \frac{\ln I/I_0}{-\rho d}$$

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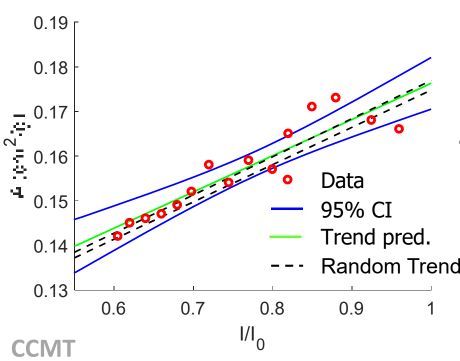
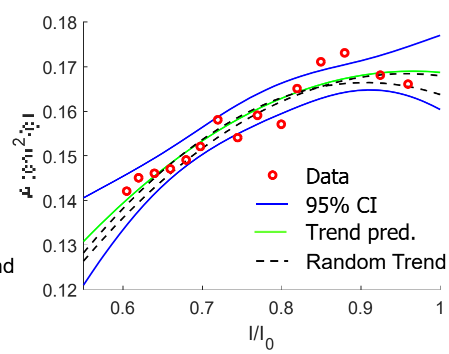
15

Calibrated *A* for Measuring VF

- Assumed correlated **noise in the data**
- Made prediction of A and its uncertainty using a Gaussian process model
- Considered linear and quadratic polynomial models (model form uncertainty)
- Obtained random attenuation curves based on the correlated noise model with Monte Carlo simulations





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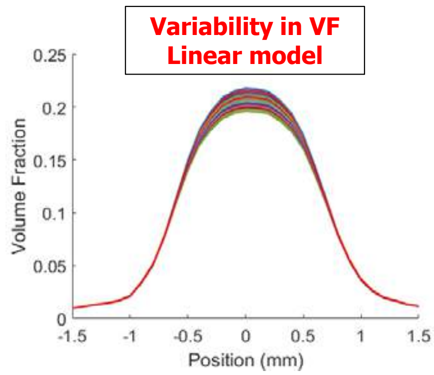
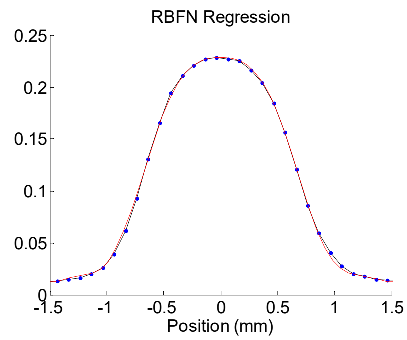
Uncertainty in Initial Volume Fraction

- Two models gave similar results: little model form uncertainty
- The uncertainty in the attenuation coefficient was propagated mostly in the uncertainty of the maximum volume fraction
- The uncertainty in the volume fraction profile was modeled with radial basis function networks (RBFN)





- **Implementing the bell shaped profile for simulations**

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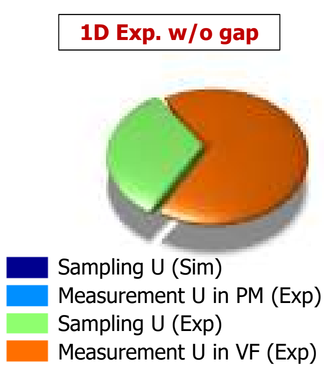
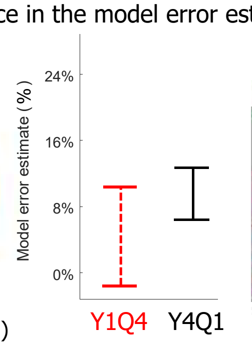
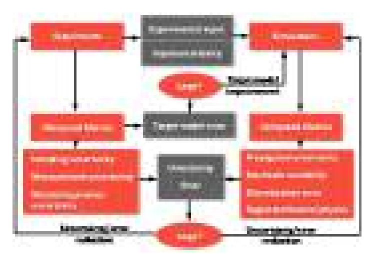
Summary of Sandia Mesoscale Campaign

- **Sandia** campaign has been almost completed
- Found and reduced 1) the hidden error due to the use of AUSM+ and 2) the uncertainty due to the gaps
- Uncertainty in the initial volume fraction is the currently largest uncertainty source in the model error estimate (down stream position)





(80mm DFP from experiment)



- Implementing the bell shaped profile for simulations

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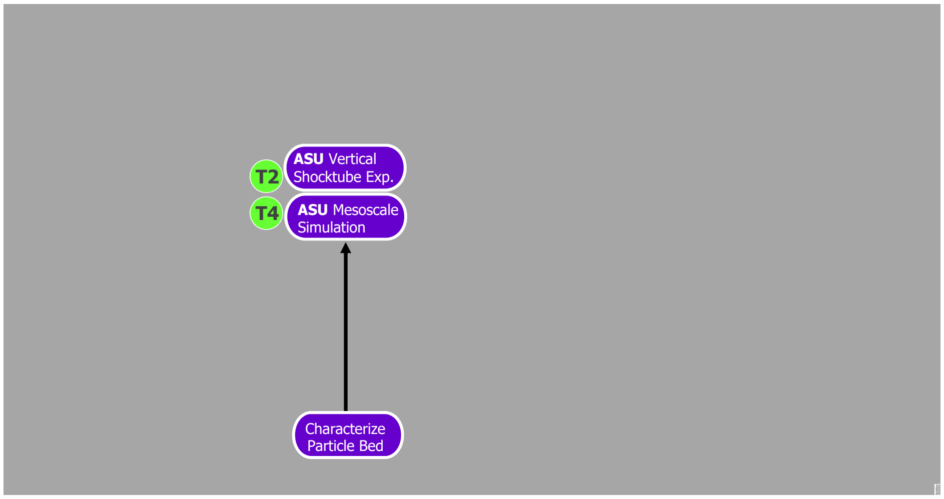
UQ of Measurement Processing



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UQ Involvement in ASU Experiment

2

Diaphragm

3

4

- **Goals:**
  - Plan new validation experiments that consider simulation limitations and uncertainty quantification goals (**Justin Mathew**)
  - **Identify** sources of experimental uncertainty, **quantify** those suspected to have a greatest influence on simulation inputs (**Justin Mathew, Kyle Hughes**)
  - UQ is involved in the experiment
- Shock tube overview:
  - Four 32cm length segments
  - Particle diameter: 45-90 microns
  - Pressure ratio: ~20
  - Initial bed height: 32 cm

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Uncertain Experimental Parameters

Parameter	Quantity	Method
Diaphragm burst time	?	Pressure sensor
Volume of particle bed	383.5-385.6 cm^3	
Initial volume fraction	59-65%	CT scanner
Initial mean volume fraction	60-61%	$\varphi_{mean} = \frac{m}{hA} * \frac{1}{\rho_{glass}}$ (Justin)
Particle diameter (before)	67±8 µm	SEM
Particle diameter (after)	68±22 µm	SEM
Particle density	2.44±0.006 g/cm^3	Pycnometer
Driver section pressure	100.68±? kPa	
Driven section pressure	5.5±? kPa	
Tube geometry	Negligible	

- **Justin Mathew** and **Kyle Hughes** actively involved in measuring the uncertainties

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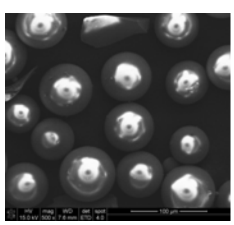
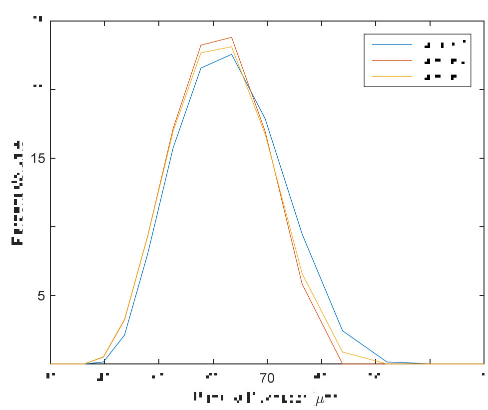
Particle Characterization – Shape/Size

- Glass particles: 45-90 microns in diameter, 2.44±0.006 g/cm^3 (**Kyle Hughes** and **Justin at UF**)
- Scanning electron microscope (SEM) Images show largely homogenous groups of particles with no apparent source of significant variation (**Kyle**)



Scanning SEM images of particles after the experiment



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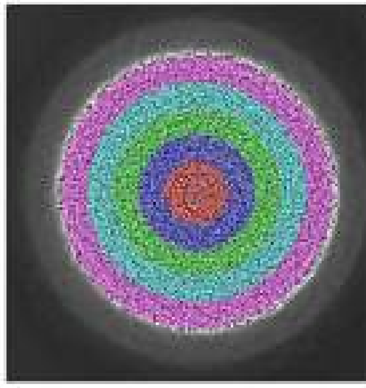
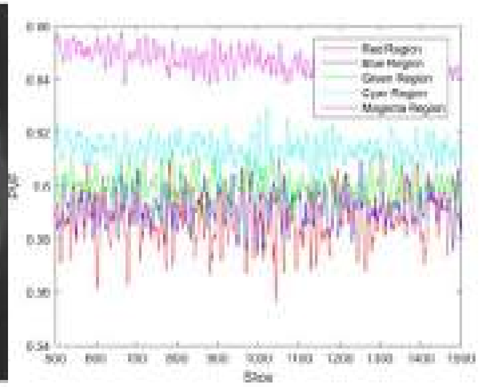
Particle Bed Characterization – Initial VF

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





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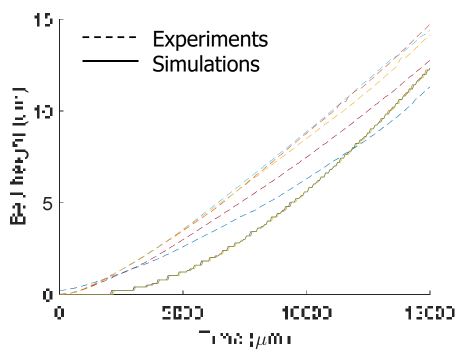
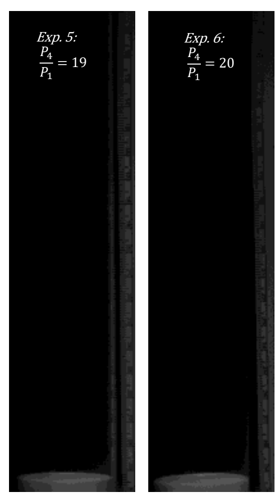
Preliminary Comparison and UQ

- There is inconsistency in measuring the bed heights
- The height data from the experiments is based on high speed camera image while the simulation predicts height data based on volume fraction prediction
- The uncertainty in t=0 has to be quantified accurately





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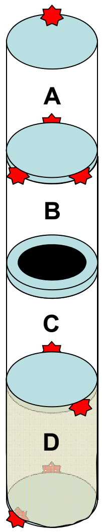
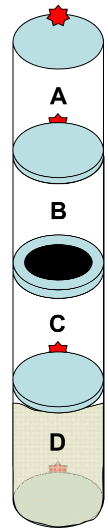
New Experiment Planning



- New experiments are conducted considering simulation limitations and UQ goals
  - Usage of smaller particle sizes (45-90 micron) **to speed up simulation time**
  - Pressure probes distributed **to reduce uncertainty in diaphragm burst timing**
    - 1-3-2-2 distribution of pressure probes
    - The lesson learned from UQ of the Eglin microscale experiment
  - Additional 2-3 cm of bed height added above the clamp for better optical range



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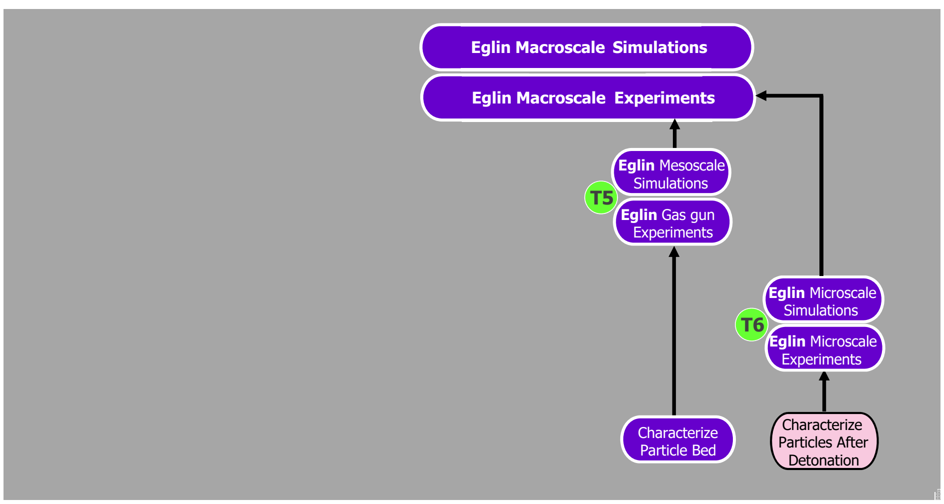
UQ of Measurement Processing



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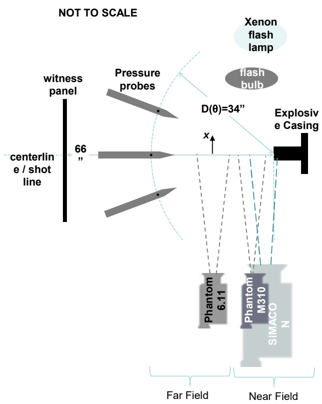
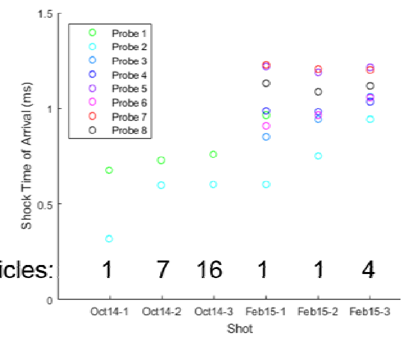
Eglin Microscale Experiments



Schematic top-view of the test set-up.

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



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

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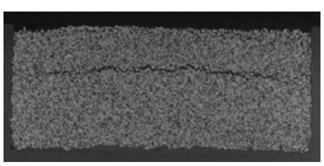
UF Analysis of Particles Used in Eglin

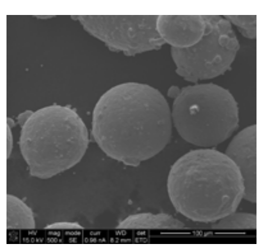


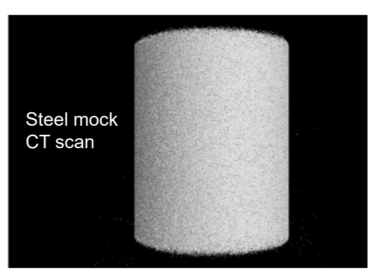
CT scans of particle packet for the Eglin mesoscale gas gun experiment

- Eglin mesoscale gas gun experiment
  - CT scans of particle packet, SEM of particles, particle density via pycnometer
  - Simacon and X-ray images to track particle cloud movements
- Eglin macroscale blastpad experiment
  - SEM of particles and particle density via pycnometer
  - Steel mock CT scan
  - Comp B X-rays

SEM of several steel particles at 500x zoom.

75-125 µm Steel





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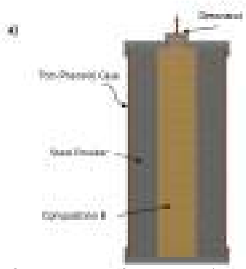
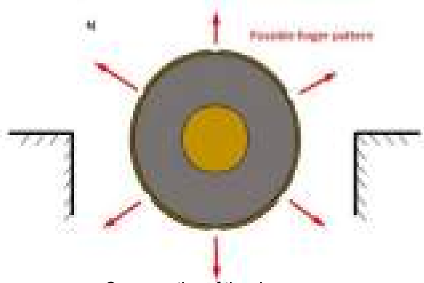
Controlling Casing Influence

- Casing fracture may be a possible mechanism for jetting instability
- No significant effect from analytical estimation
- Steps taken to reduce the influence of the casing:
  - Thin phenolic tubing (3/16") for the casing
    - Failure energy ~0.06% of explosive energy
  - No casing between the explosive and particles
  - Casing notched on outer surface to control case failure

Shot	Liner	Notched?
1	-	-
2	-	-
3	Tungsten	Y
4	Steel	Y
5	Steel	Y
6	Steel	N



Cross-section of the charge (side view) showing no inner casing



Cross-section of the charge (axial view) showing alignment of the notches with the pad surface

Side view of the tungsten (left) and steel (right) casing with notches

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Quantification of Numerical Error

Achieving convergence by modeling finite size particles

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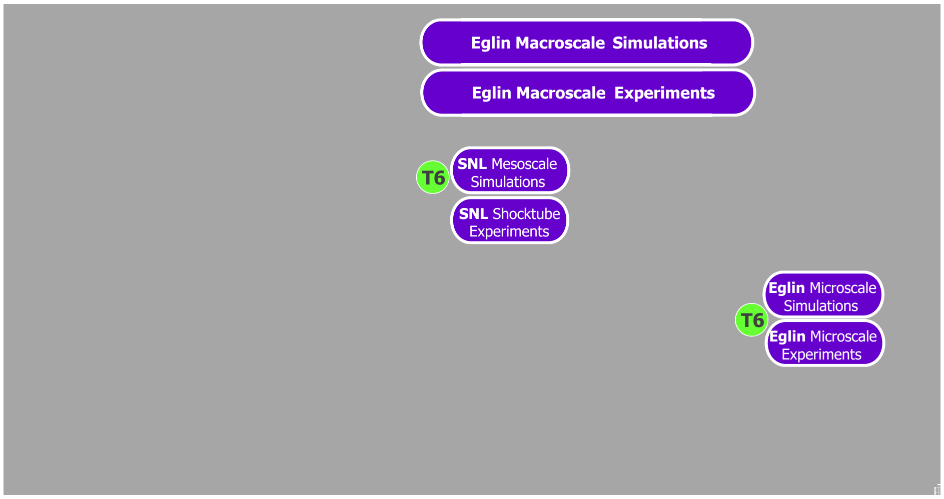
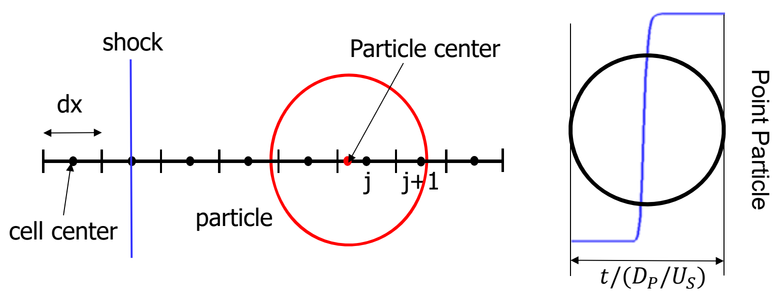
Quantification of Numerical Error



Summary and Overview

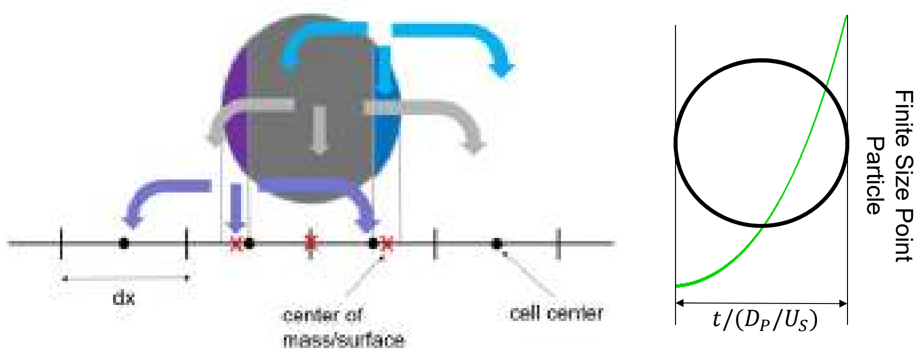
- **Goal:** To achieve force convergence in a two-way coupled point particle Euler-Lagrange simulation using the finite size of the particles and to estimate the numerical error in the point-particle force (Samaun Nili)



- In the point particle method, the particle feels the shock only if the shock reaches to the cell where particle center is located
- When the particle diameter is larger than the grid size, the particle force shows an unrealistic jump at the center
- The peak force increases as we reduce the grid size

Proposed Solution

- The inhomogeneous flow felt by the particle represented by average over the surface or volume of the particle (Faxen theorem)
- Computing the average volume and surface gas quantities and forces
- The numerical solution compared against the analytical solution



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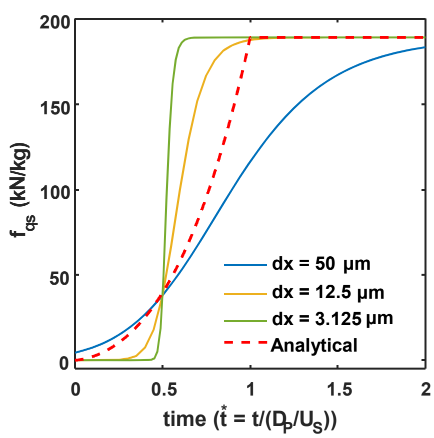
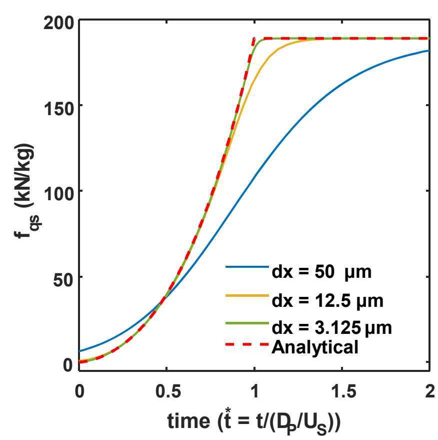
QS Force with Single Particle (115µm)

Point particle



Finite size particle



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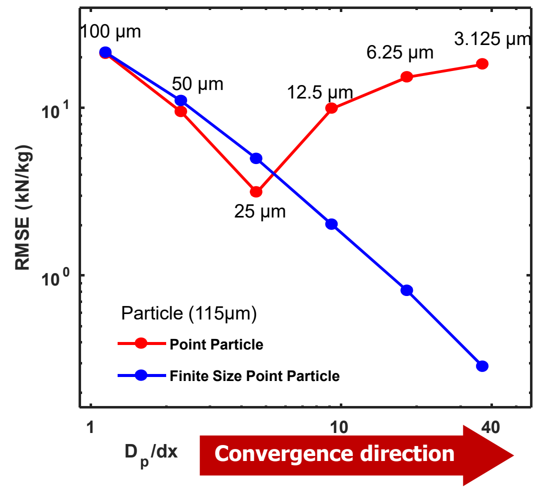
Quasi-Steady Force Convergence



- RMSE measures the difference between analytical solution and finite size point particle model
- RMSE decreases exponentially

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Preparation for UQ of Macroscale Simulation

With Multi-Fidelity Surrogate

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Preparation for UQ of Macroscale Simulation

Eglin Macroscale Simulations

Eglin Macroscale Experiments

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Multi-Fidelity Surrogate for UQ

- UQ often computationally expensive since it requires numerous simulation runs
- Surrogates often provide good approximations based on several dozens of samples but even sampling for building a surrogate is not affordable for expensive simulations
- **Multi-fidelity surrogate**: Approximating an expensive high fidelity simulation behavior by combining a few expensive high fidelity samples with cheap low fidelity samples
- **Low fidelity model selection**: There are multiple lower fidelity models and selection is another questions to be answered
- This technique is used for the collaboration with the **exascale team** to approximate the CMT-bone with CMT-bone-BE and BE emulation

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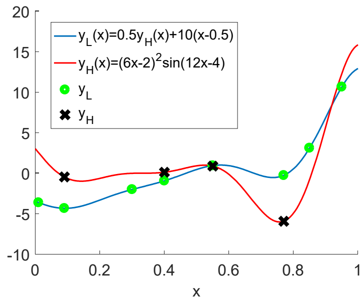
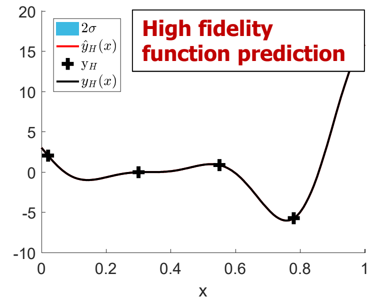
Introduction to Multi-Fidelity Surrogate





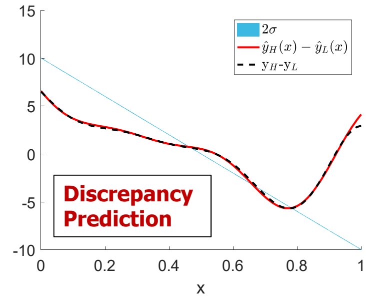
- **Goal:** Approximating the **high fidelity response** based on a few high fidelity samples with low fidelity samples

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

$\hat{y}_H(\mathbf{x})$: High fidelity simulation prediction

$\hat{y}_L(\mathbf{x})$: Low fidelity simulation prediction

$\hat{\delta}(\mathbf{x})$: Discrepancy prediction



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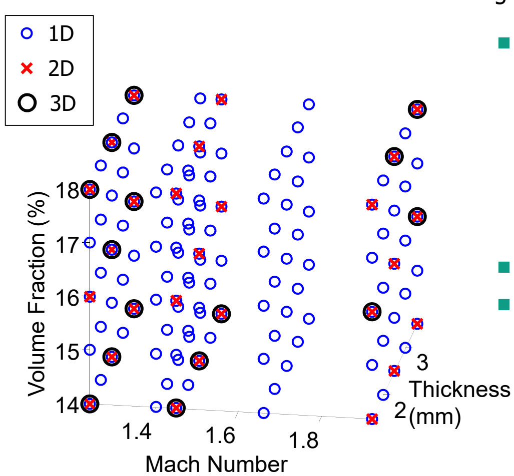
MFS for UQ of 3D Sandia Shocktube Sim.

- **Goal:** Approximating the 3D simulation for predicting front positions using 1D and/or 2D simulations
- The simulations have the same grid resolution



- Simulation parameters:
  - Volume fraction
  - Curtain thickness
  - Mach number
  - Random initial particle position
- 15 (3D) / 135 (2D) / 625 (1D)
- Computational cost ratios:
  - A single 3D run is equal to 25000 1D runs or 100 2D runs
  - A single 2D run is equal to 250 1D runs

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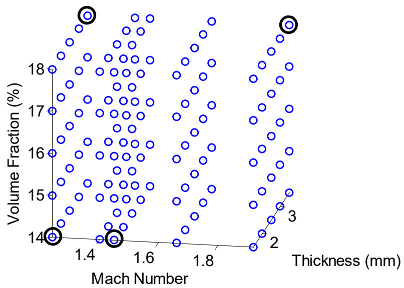
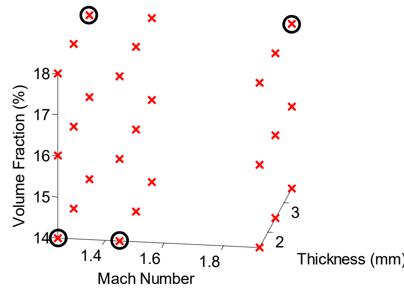
MFS Accuracies with 1D+3D and 2D+3D

- Predicting **downstream front position** at 700 μs
- Using 11 other 3D runs to evaluate accuracy in terms of **relative RMSE** (RMSE/max value)
  - 0.025 (1D+3D) and 0.0875 (1D only)
  - 0.0125 (2D+3D) and 0.0375 (2D only)
  - 0.0638 (3D only)



DOE: 1D (125) +3D (4)



DOE: 2D (27) +3D (4)

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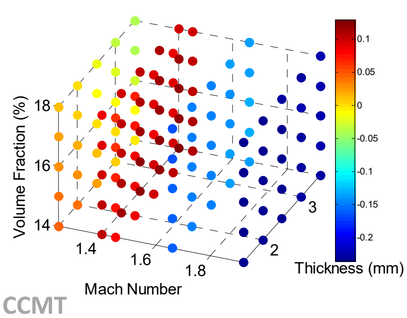
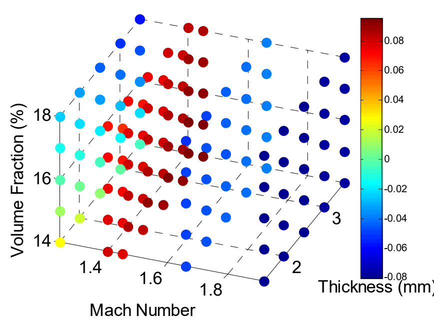
Difference Between 1D/2D/3D

- MFS prediction allows to **predict difference** between models of different fidelities
- For the shock tube simulation, the difference is most sensitive to Mach number
- The difference between 3D and 1D is higher than that between 3D and 2D

Relative error in 1D



Relative error in 2D



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Summary

- Involvement of physics and UQ for experimental data extraction through measurement processing
  - The initial volume fraction of the Sandia shock tube experiment extracted from X-ray images using a X-ray attenuation model
  - Rigorous UQ has reduced the initial uncertainty by 50%
- Involvement of UQ team in measurement processing
  - UQ of the ASU and Eglin experiments
  - Planning those experiments for reducing measurement uncertainty
- Quantifying numerical error in the particle force model by modeling finite size particles
- Carrying out a study on Multi-fidelity surrogate for UQ and parametric study of hero simulations and BE emulation development

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Do you have any questions?

Computation Cost

- 3D
  - dx=dy=dz=125μm
  - Legnth x Width x Height = 0.35 0.04 0.01 (M=1.45, 1.24)
  - Legnth x Width x Height = 0.38 0.04 0.01 (M=1.92)
  - 6 million particles
  - Quartz 2048 cores wall time 24 hrs (max), 23 hrs+-20 mins
- 2D
  - dx=dy=dz=125μm
  - Legnth x Width x Height = 0.35 0.04 125μm (M=1.45, 1.24)
  - Legnth x Width x Height = 0.38 0.04 125μm (M=1.92)
  - 600,000 particles
  - Vulcan 128 cores wall time 40 hrs
- 1D
  - dx=125μm
  - Legnth = 0.35 (M=1.45, 1.24)
  - Legnth = 0.38 (M=1.92)
  - 5000 particles
  - Hipergator 4 cores wall time 20-30 mins

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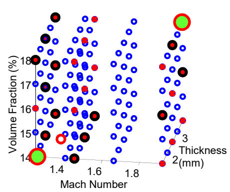
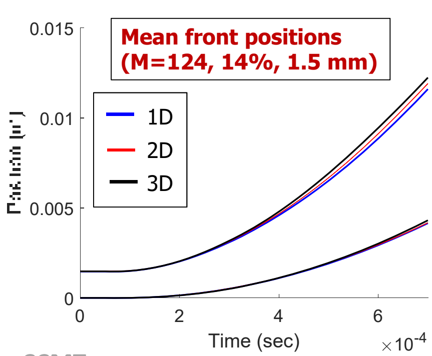
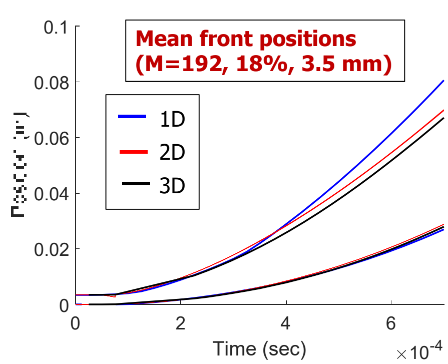
1D/2D/3D Front Position Comparisons



- Comparing 1D/2D/3D for two extreme combinations in terms of prediction metric (mean front positions)
- M=1.24, 14%, 1.5 mm and M=192, 18%, 3.5 mm
- Variability due to initial particle positions is small for 1D and negligible for 2D





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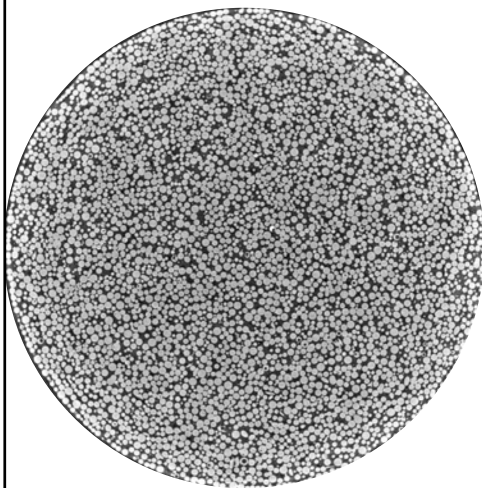
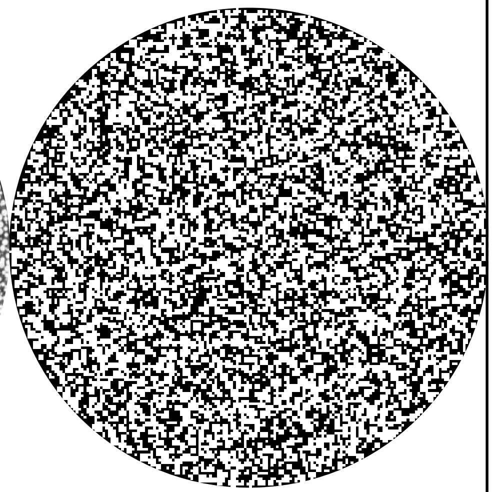
Slices from CT scan vs Rocpack



Mock Bed - CT



Rocpack - CT

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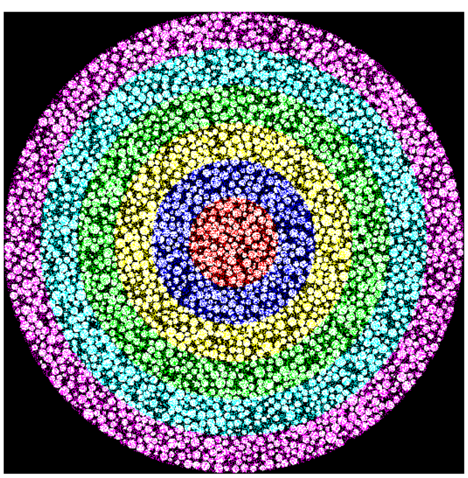
PVF Calculated Along Circular Region



Region	PVF
Red	0.566
Blue	0.544
Yellow	0.568
Green	0.557
Cyan	0.562
Magenta	0.540

Nominal PVF = 0.54

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CMT-nek: CS Update

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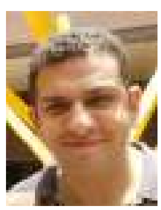
Members

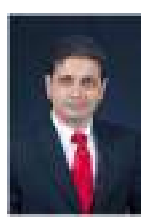


Keke Zhai

Mohamed Gadou

Adeesha Malavi

Tania Banerjee



Aravind Neelakantan

Sai Chenna

Sanjay Ranka

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Key Accomplishments (past year)

- Dynamic load balancing of CMT-nek
- Hybrid Multicore Computing using DVFS
- Multi-level Memories and performance impact

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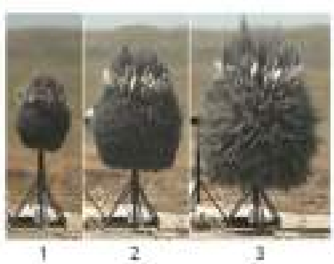
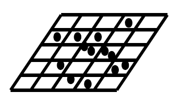
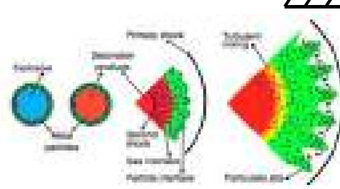
Exascale Simulation: CS Challenges

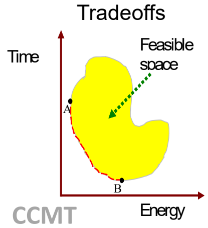


Dynamic Load Balancing





Energy and Performance Tradeoffs



Future Architectures and Hybrid Processors

Parallelization on a million+ processors

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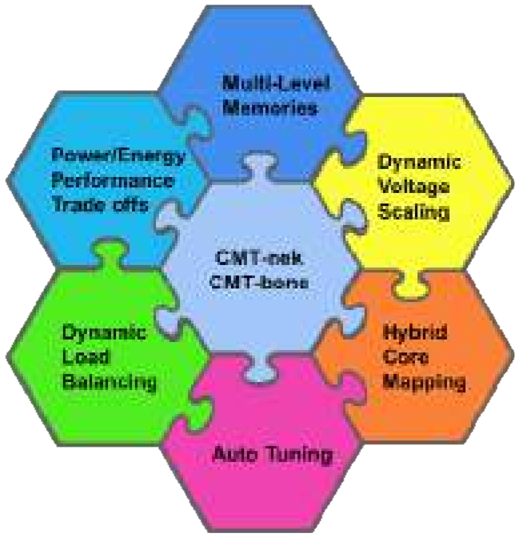
Talk Overview

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



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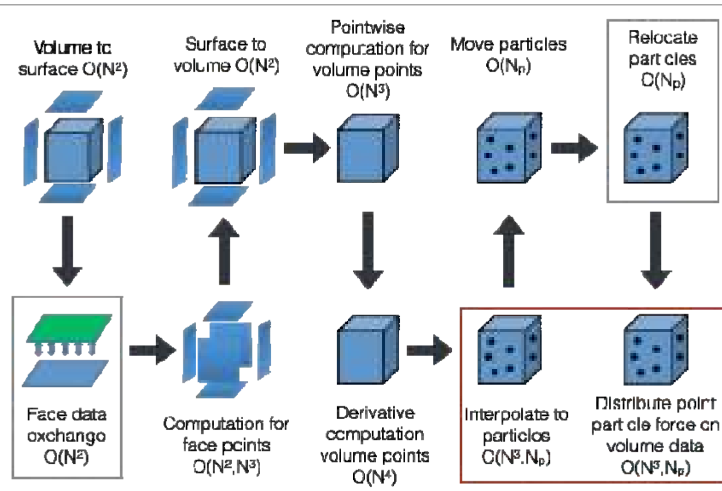
CMT-bone

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



CMT-bone -- A Proxy Application for Compressible Multiphase Turbulent Flows, Jason Hackl, Mrugesh Sringarpure, Tania Banerjee, Tanzima Islam, S. Balachandar, Thomas Jackson, Sanjay Ranka, HiPC 2016, December 2016.

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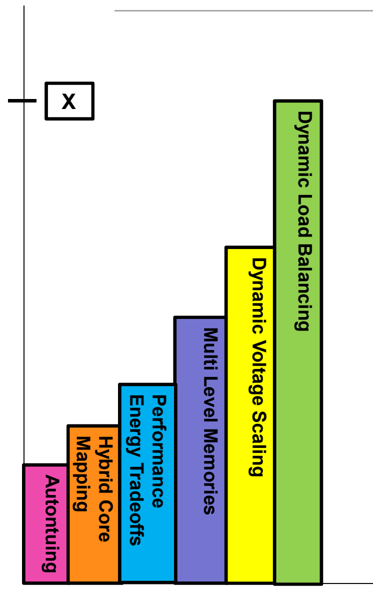
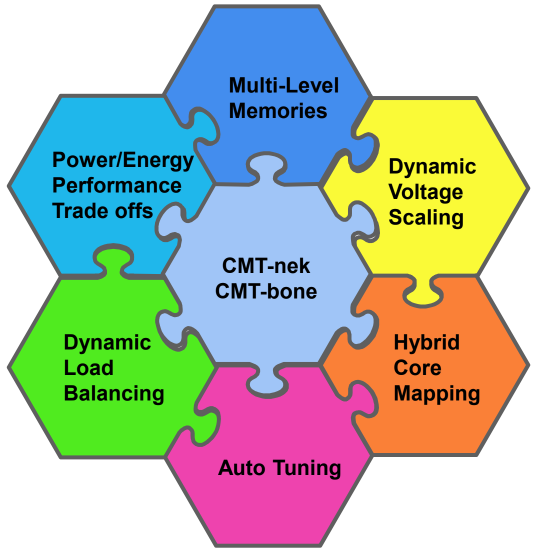
Performance per Watt Improvement





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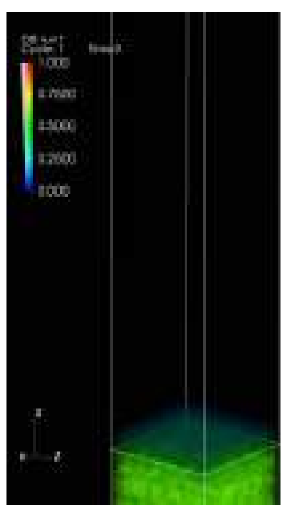
Dynamic Load Balancing: Expansion Fan



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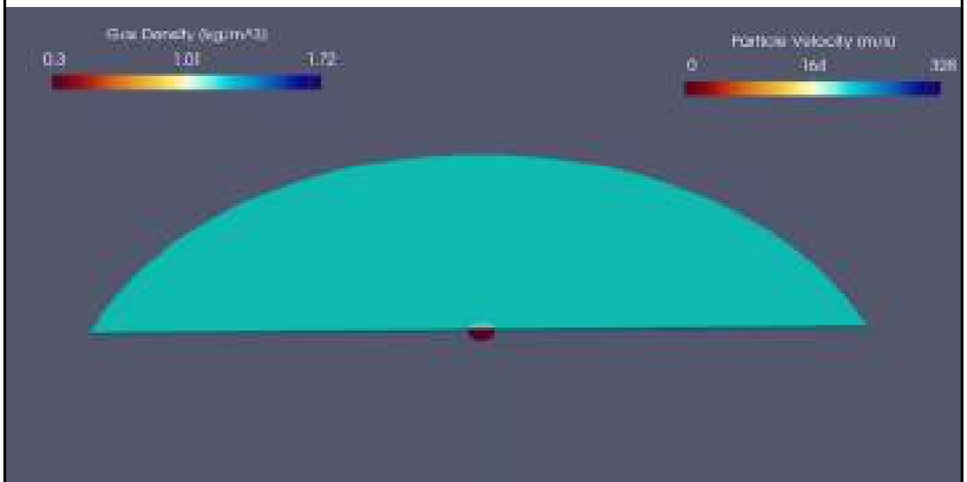
Hero Run 2



CCMT

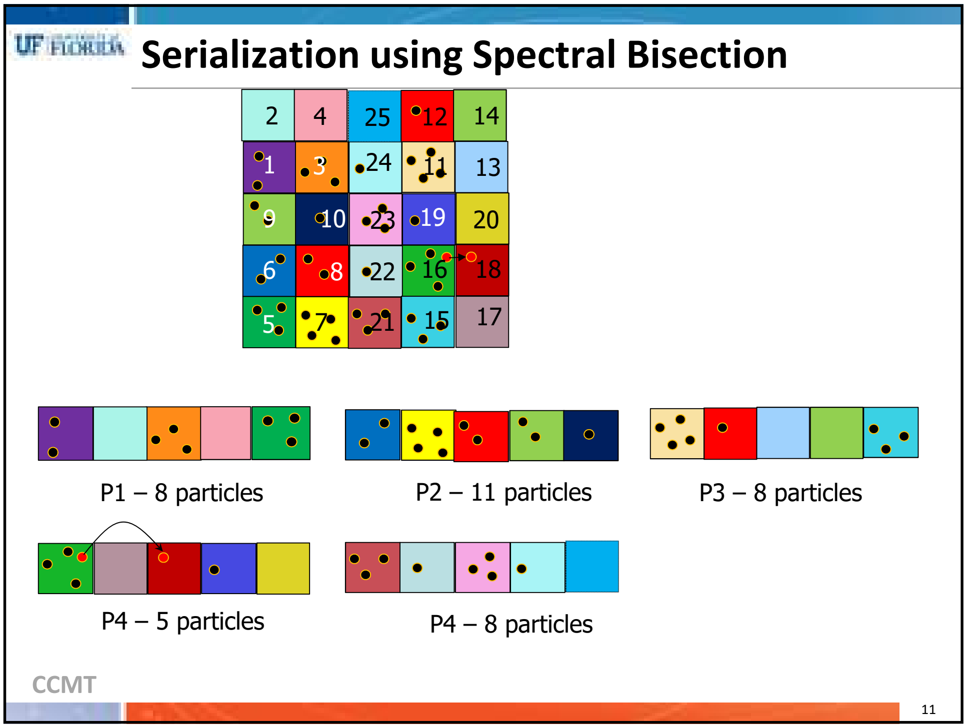
9

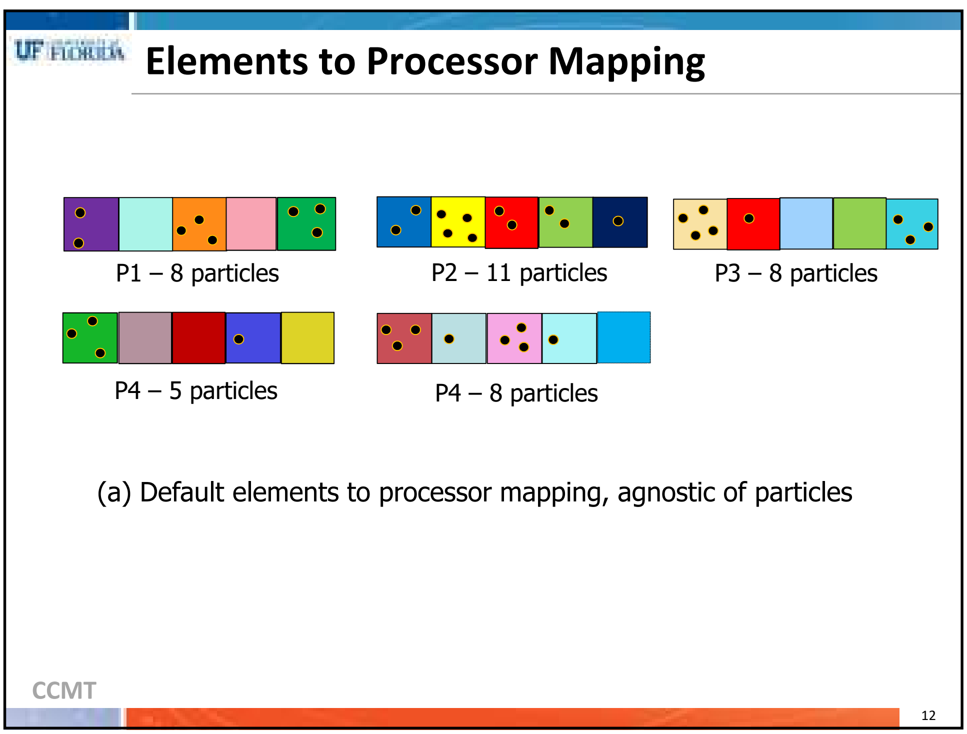
Dynamic Load Balancing

- Initialization
  - Elements to processor mapping
- Repeat the following steps
  - Decide when to trigger a remap
    - Rebalance after every **k** time steps
    - Rebalance when processing time per step gets higher beyond a threshold
  - If remap trigger = yes
    - Derive new elements to processor mapping
  - Transfer elements and particles and reset other data structures
    - Serialize
    - Communication
    - Deserialize
- Final Steps

CCMT

10


Serialization using Spectral Bisection
2 4 25 12 14
1 3 24 11 13
9 10 23 19 20
6 8 22 16 18
5 7 21 15 17
P1 – 8 particles
P2 – 11 particles
P3 – 8 particles
P4 – 5 particles
P4 – 8 particles
CCMT
11


Elements to Processor Mapping
P1 – 8 particles
P2 – 11 particles
P3 – 8 particles
P4 – 5 particles
P4 – 8 particles
(a) Default elements to processor mapping, agnostic of particles
CCMT
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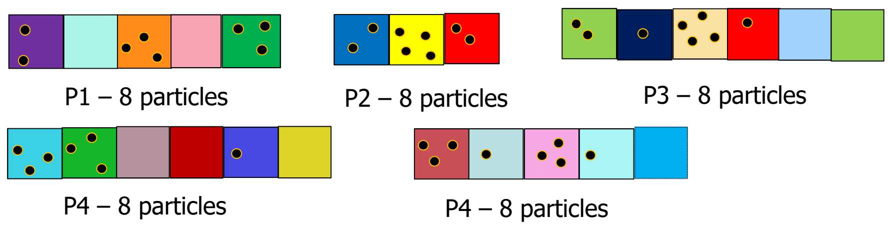
Elements to Processor Mapping

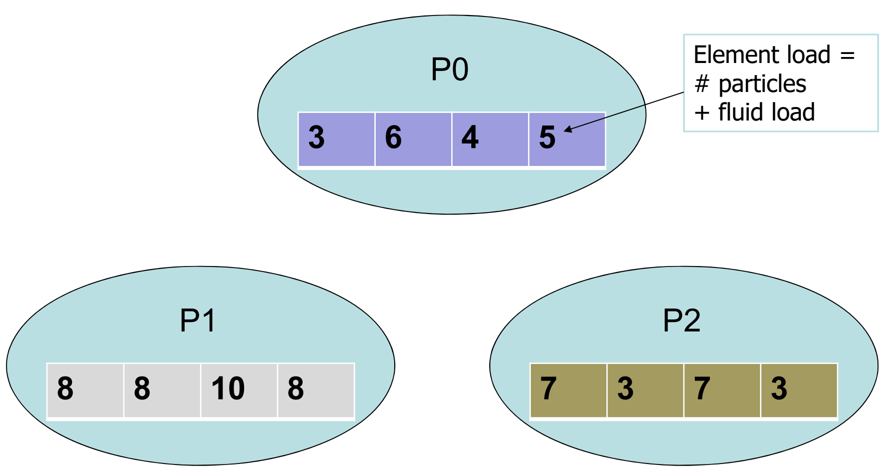


(b) Elements to processor mapping, after taking into account both elements and particles

CCMT 13

The Centralized Algorithm

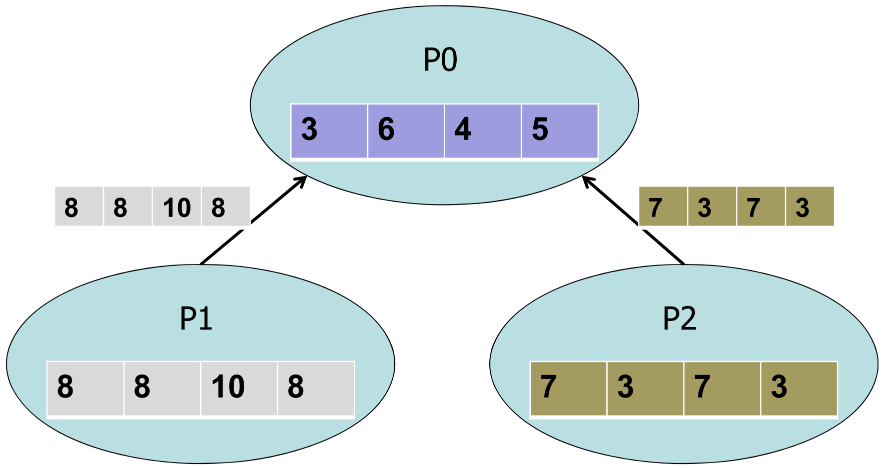
Initially, each processor has an element load array



CCMT 14

The Centralized Algorithm

Each processor sends element load array to P0

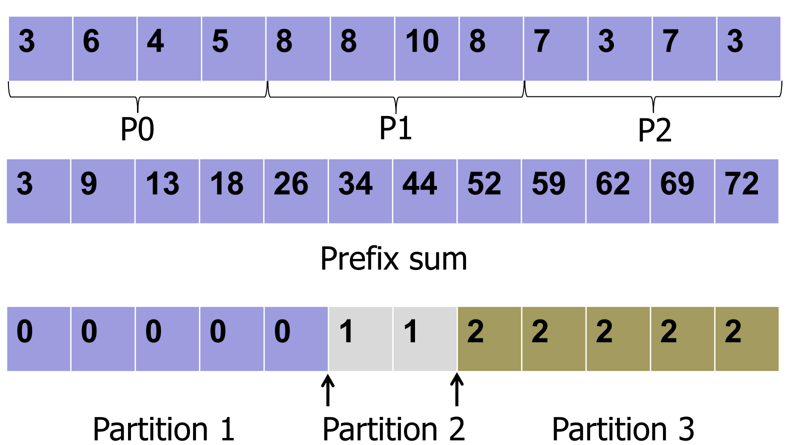


CCMT

15

The Centralized Algorithm

P0 receives and concatenates the element load array, computes the prefix sum, divides prefix sum by average load



CCMT

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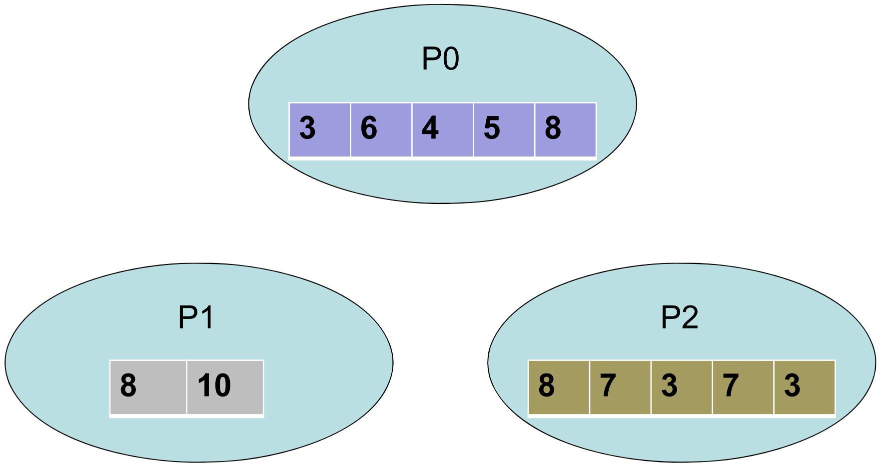
The Centralized Algorithm

P0 distributes the assignment to other processors, and each processor gets the new elements

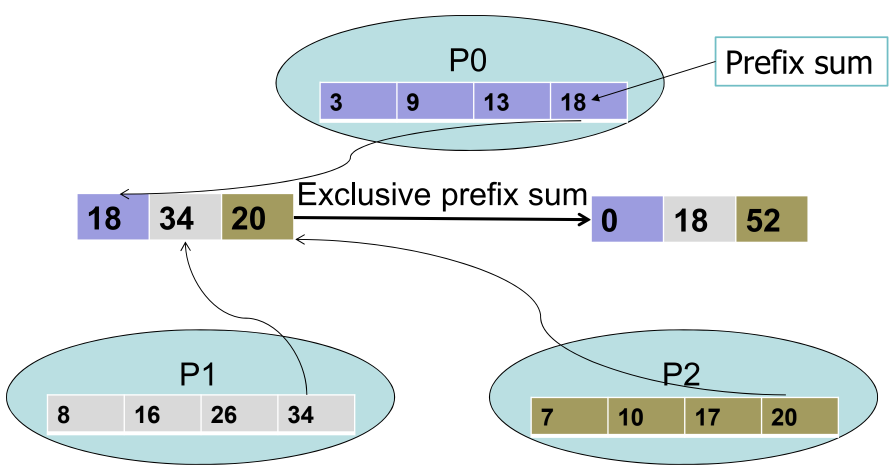


CCMT

17

The Distributed Algorithm

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

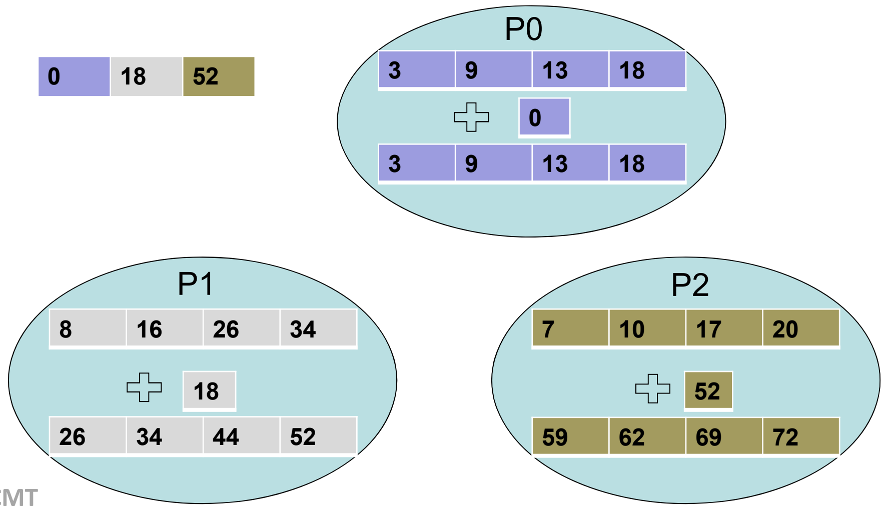


CCMT

18

The Distributed Algorithm

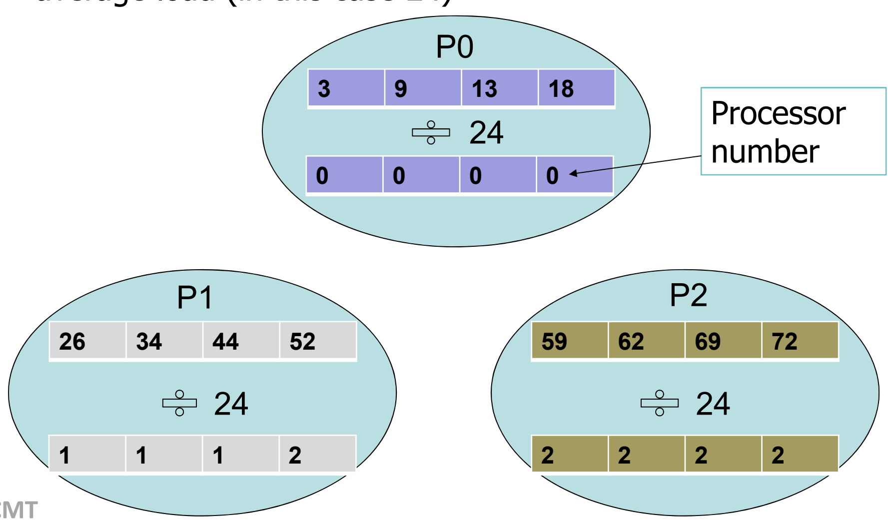
Each processor adds the exclusive prefix sum to local prefix sum array to get the global prefix sum of element load array



CCMT 19

The Distributed Algorithm

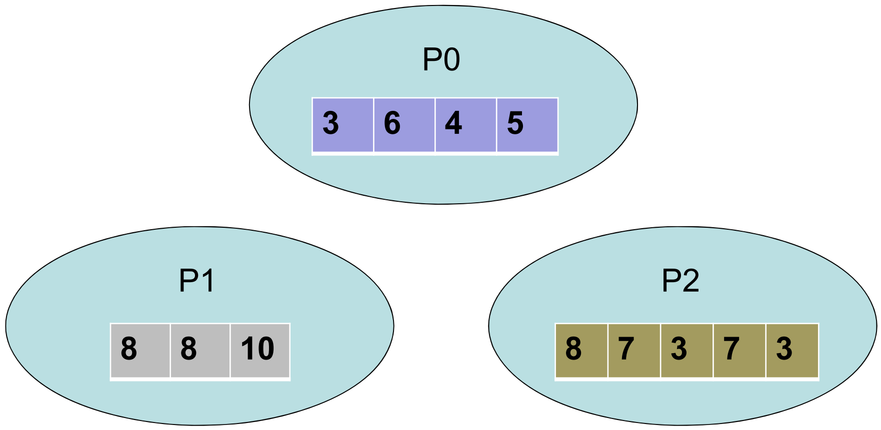
Each processor divides the global prefix array with the average load (in this case 24)



CCMT 20

The Distributed Algorithm

Each processor keeps the elements that belong to them, and sends the remaining elements to the target processor

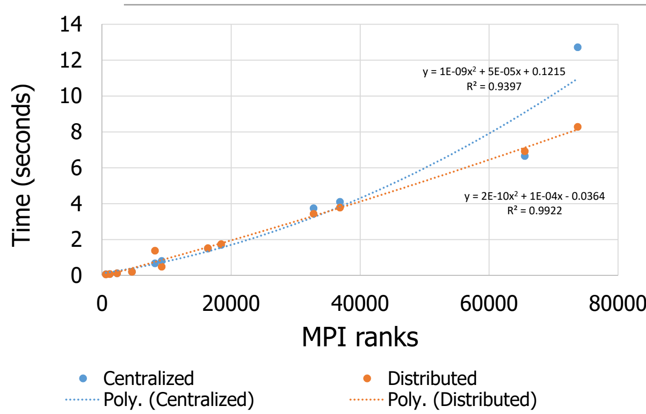


Dynamic Load Balancing for Compressible Multiphase Turbulence, Keke Zhai, Tania Banerjee, David Zwick, Jason Hackl and Sanjay Ranka, submitted to IPDPS 2018

CCMT

21

Rebalancing Time: Total Overhead (Quartz)



CMT-nek

Max: 73,728 MPI ranks
4 elements / rank
343 particles / element
Grid size: 5x5x5
Rarefaction test

- Overhead is about 220 and 121 time steps upon using centralized and distributed algorithms respectively
- When extrapolated to a million ranks, centralized algorithm will take about 2300 time steps, whereas distributed algorithm will take 1800 time steps

CCMT

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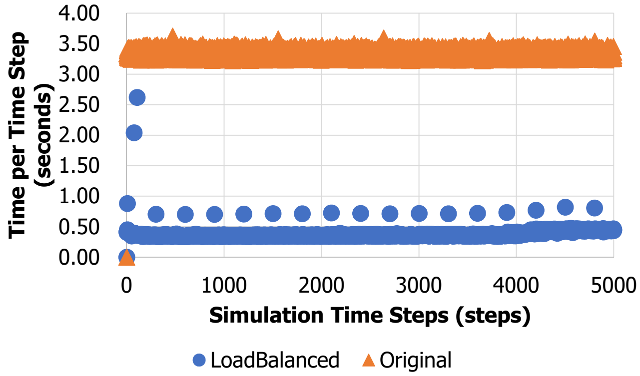
Expansion testcase: CMT-nek on Quartz



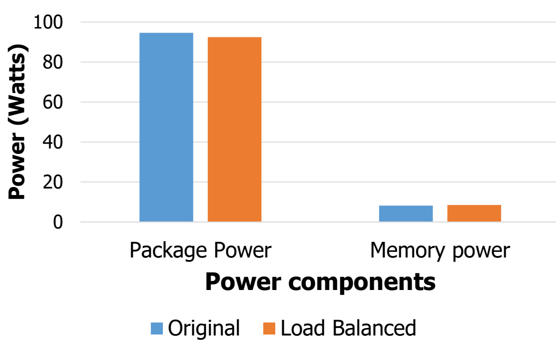
CMT-nek

67,206 MPI ranks
1,867 nodes
36 cores per node
900,000 elements
1.125×10^9 particles
Grid size: 5x5x5
Rarefaction test
8.3x improvement in performance

- Total time taken by CMT-nek is 4.62 hours
- Total time taken by load balanced code is 33 minutes
- Time per time step: 3.33 s for the original versus 0.4 s for the load balanced code (balancing done every 300 s)
- Adaptive load balancing takes about 31 minutes total and 0.37 seconds per time step

CCMT 23

Expansion testcase: Power consumption on Quartz (using Libmsr)



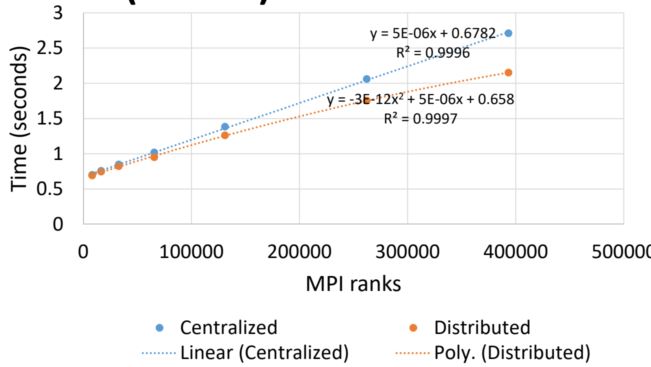
CMT-nek

67,206 MPI ranks
1,867 nodes
36 cores per node
900,000 elements
1.125×10^9 particles
Grid size: 5x5x5
Rarefaction test
8.3x improvement in performance

- Power consumption is comparable

CCMT 24

Rebalancing Time: Total Overhead Time (Vulcan)



CMT-nek

Max: 393,216 processors
2 elements / rank
343 particles / element
Grid size: 5x5x5
Rarefaction test

- When extrapolated to a million ranks, centralized algorithm will take 5.68s, whereas distributed algorithm will take 2.66s
- Overhead is approximately is 9 time steps with centralized and 7 with distributed when 393,216 cores are used

CCMT

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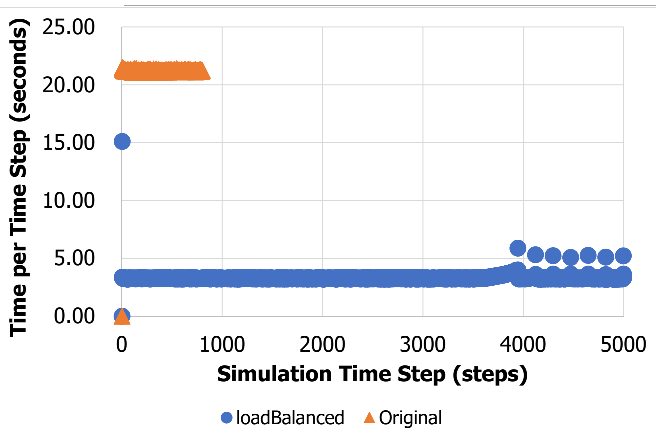
Expansion testcase: CMT-nek on Vulcan



CMT-nek

32,768 MPI ranks
8192 nodes
4 cores per node
460,800 elements
756,000,000 particles
Grid size: 5x5x5
Rarefaction test
6.4x improvement in performance

- The original CMT-nek finished 800 steps in 5 hours
- Total time taken by load balanced code is 4.57 hours
- Time per time step: 21.2 seconds for the original versus 3.3 for the load balanced code

CCMT

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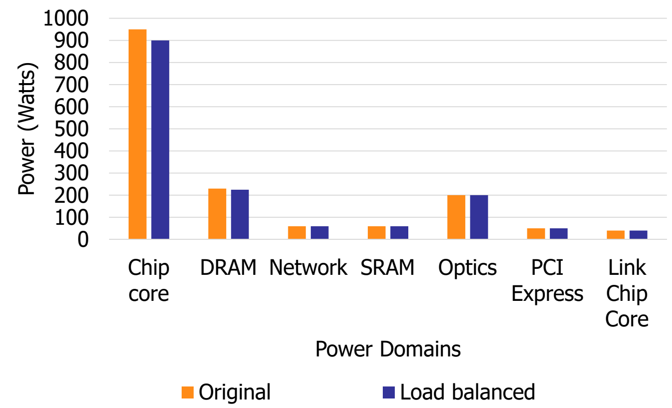
Expansion testcase: Power consumption on Mira (Using MonEQ)

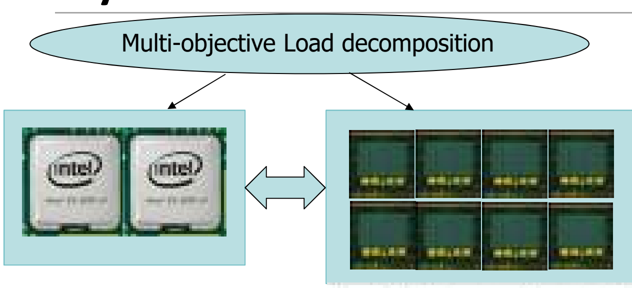


CMT-nek

4,608 processors
73,728 elements
86,400,000 particles
Grid size: 5x5x5
Rarefaction test

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

Hybrid Multicore Architectures



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

GPU Attribute	Description
Manufacturer	NVIDIA
Model	Tesla K40m (Kepler)
Number of GPUs	8
Number of SMs/GPU	15
Number of Cores/SM	192
Global Memory(GB)	12
L2 Cache(KB)	1536
Shared Memory/SM (KB)	48
L1 cache/SM (KB)	16
Number of Registers/SM	65K
Peak performance(GFlops)	3430

Multi-objective Optimization on Hybrid Systems using DVFS, Mohamed Gadou, Sankeerth Mogili, Tania Banerjee, Sanjay Ranka, submitted to IPDPS 2018

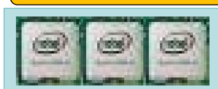
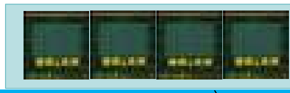
Theoretical formulation

Minimize $E(n, m, f, g, S)$
Subject to $T(n, m, f, g, S) <= T_1 - O(n, m, f, g, S)$
$n <= N$ → 24
$m <= M$ → 8
$f \in F$ → 12
$g \in G$ → 7

16128 S

X | S-X

n CPU cores, freq f | m GPU cores, freq g

Minimize $E_{CPU}(n, f, X) + E_{GPU}(m, g, S\text{-}X)$
Subject to $T_{CPU}(n, f, X) <= T_1 - C_o(m+n, S)$
$T_{GPU}(m, g, S\text{-}X) <= T_1 - C_o'(m, S\text{-}X)$
$n <= N$ → 24
$m <= M$ → 8
$f \in F$ → 12
$g \in G$ → 7

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

$T_{CPU}(n, X)/f \times P_{CPU}(n, f)$ | 344+32S | $T_{GPU}(m, S\text{-}X) /g \times P_{GPU}(m, g)$

E : Energy consumed
n : Number of CPUs
m : Number of GPUs
f : CPU Frequency
g : GPU Frequency
S : Problem size
T : Computation Time
T_1 : Constrained time
O: Communication overhead
N : Total available CPUs
M : Total available GPUs
F : Set of available CPU frequencies
G : Set of available GPU frequencies

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CPU Experiments

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

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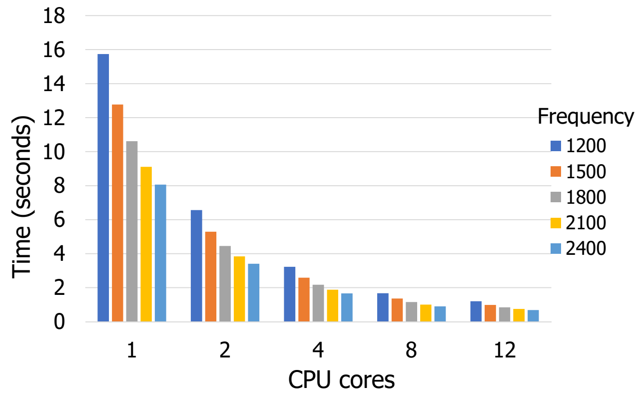
CPU Experiments



CMT-bone

8,192 elements
256,000 particles
Grid size: 7x7x7

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

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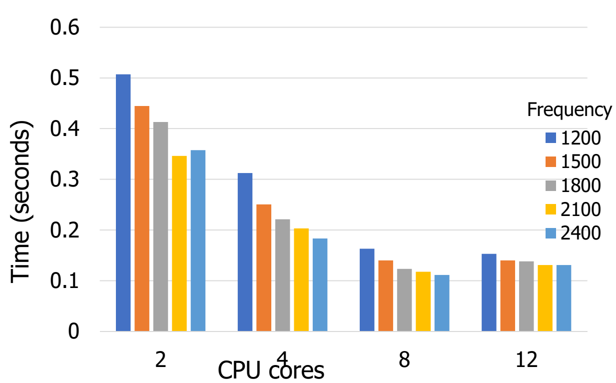
CPU Experiments



CMT-bone

8,192 elements
256,000 particles
Grid size: 7x7x7

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

CCMT

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Assumptions

- Performance using lower clock frequencies may be derived from that using the highest clock frequency
  - $T_{CPU}(n, f, x) = k \times \frac{f_{max}}{f} \times TCPU(n, fmax, x)$
- Power consumption does not depend on problem size
  - $P_{CPU}\ (n, f, x) = PCPU\ (n, f)$
- n = CPU count, f = CPU frequency, x = problem size
- Example: Power lookup table:

f \ n	1	2	4	8	12
1200	93.24	97.33	101.32	114.46	127.50
1500	96.67	100.78	108.32	122.95	136.79
1800	98.14	102.88	111.53	131.86	148.45
2100	100.69	106.31	117.11	138.72	160.84
2400	102.65	108.12	123.94	145.54	167.08

CMT-bone

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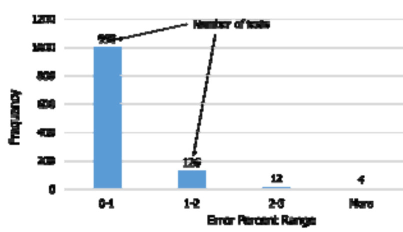
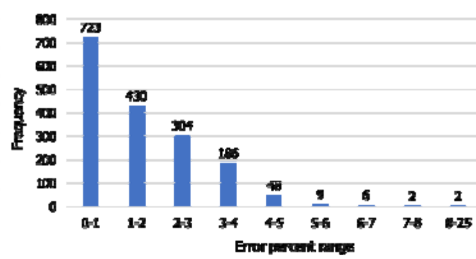
Prediction Error

Performance



- Prediction error is within 3% for 99% of the tests

Power



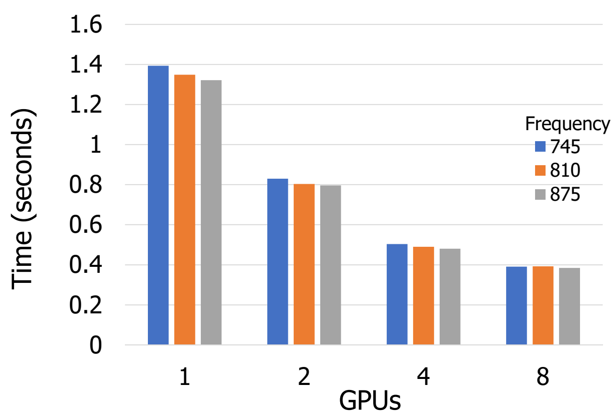
- Prediction error is within 5% for 99% of the tests

CCMT

GPU Experiments

Parameters	Values
y, problem size in terms of number of elements (57)	Same problem sizes as described for CPUs.
g, frequency in MHz (3)	875, 810, 745
m, number of GPUs (4)	1, 2, 4, 8

GPU Experiments

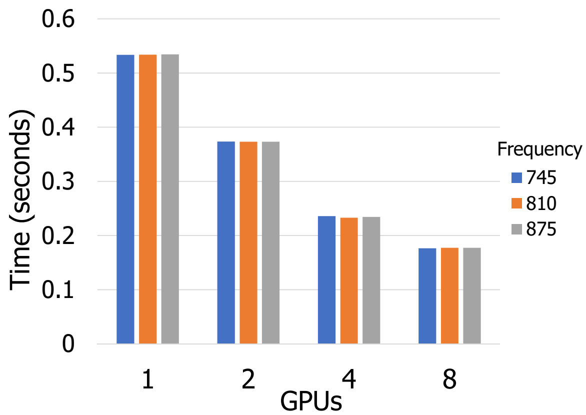


CMT-bone

8,192 elements
256,000 particles
Grid size: 7x7x7

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

GPU Experiments



CMT-bone

8,192 elements
256,000 particles
Grid size: 7x7x7

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

CCMT 37

Assumptions

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

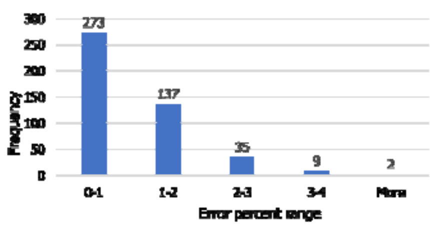
g \ m	1	2	4	8
745	89.79	169.91	314.53	550.91
810	93.51	176.05	324.59	567.11
875	98.80	185.46	341.26	589.41

CMT-bone

CCMT 38

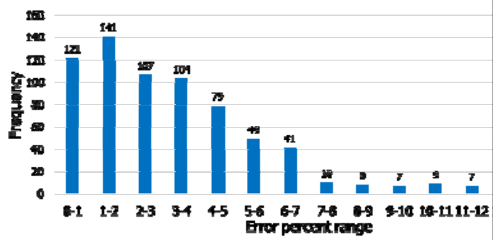
Prediction Error

Performance



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

Power



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

CCMT

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Summary of CPU and GPU experiments

- The following assumptions are experimentally verified
  - Performance at lower clock frequencies may be derived from the performance of the application at the highest clock frequency holds both for CPUs and GPUs
  - Power consumption does not depend on problem size holds for both CPUs and GPUs
- The above assumptions help to reduce the number of required experiments further

CMT-bone

CCMT

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Hybrid Experiments

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

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Hybrid Experiments

CPU			GPU			Predicted Energy (J)	Actual Energy (J)	Error %
elements	**count**	**GHz**	**elements**	**count**	**MHz**			
2540	8	2.4	5652	2	875	225.25	232.87	3.27
2621	8	2.4	5571	2	810	226.05	235.01	3.81
2621	8	2.4	5571	2	875	227.13	237.77	4.48
2540	8	2.4	5652	2	810	228.61	227.14	0.65
2293	8	2.4	5899	2	875	229.86	227.72	0.94
1474	4	2.4	6718	2	875	230.35	236.19	2.47

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

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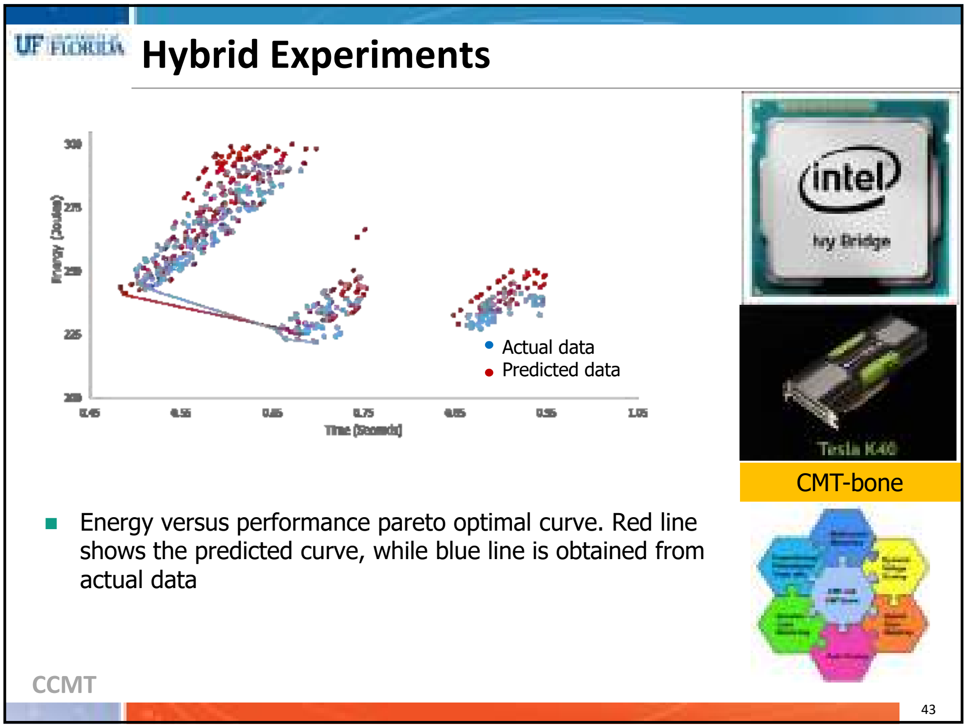
Hybrid Experiments
Actual data
Predicted data
Time (Seconds)
Energy (Joules)
intel
Ivy Bridge
Tesla K40
CMT-bone
Energy versus performance pareto optimal curve. Red line shows the predicted curve, while blue line is obtained from actual data
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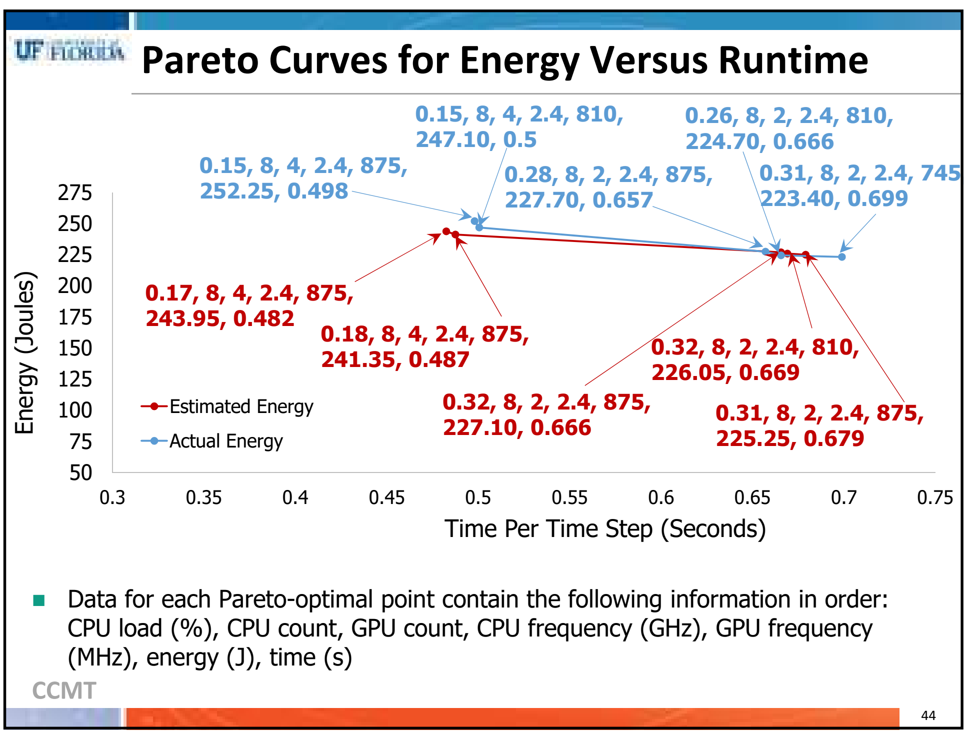
Pareto Curves for Energy Versus Runtime
0.15, 8, 4, 2.4, 810, 247.10, 0.5
0.26, 8, 2, 2.4, 810, 224.70, 0.666
0.15, 8, 4, 2.4, 875, 252.25, 0.498
0.28, 8, 2, 2.4, 875, 227.70, 0.657
0.31, 8, 2, 2.4, 745 223.40, 0.699
0.17, 8, 4, 2.4, 875, 243.95, 0.482
0.18, 8, 4, 2.4, 875, 241.35, 0.487
0.32, 8, 2, 2.4, 810, 226.05, 0.669
0.32, 8, 2, 2.4, 875, 227.10, 0.666
0.31, 8, 2, 2.4, 875, 225.25, 0.679
Estimated Energy
Actual Energy
Energy (Joules)
275
250
225
200
175
150
125
100
75
50
0.3
0.35
0.4
0.45
0.5
0.55
0.6
0.65
0.7
0.75
Time Per Time Step (Seconds)
Data for each Pareto-optimal point contain the following information in order: CPU load (%), CPU count, GPU count, CPU frequency (GHz), GPU frequency (MHz), energy (J), time (s)
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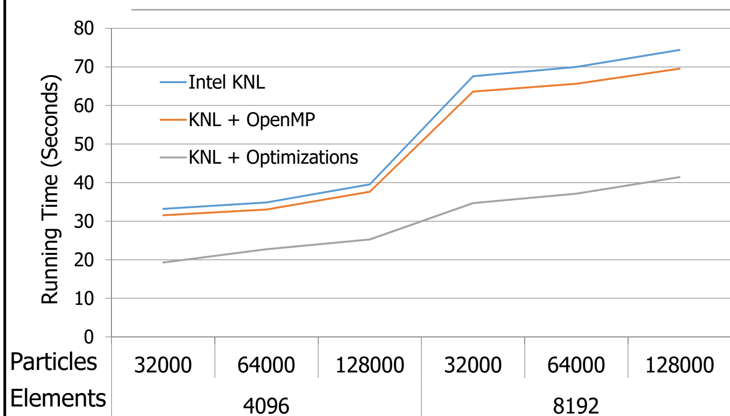
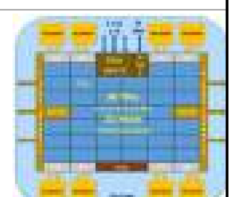
Multi-Level Memories

CCMT

CMT-bone on Intel KNL





Single node

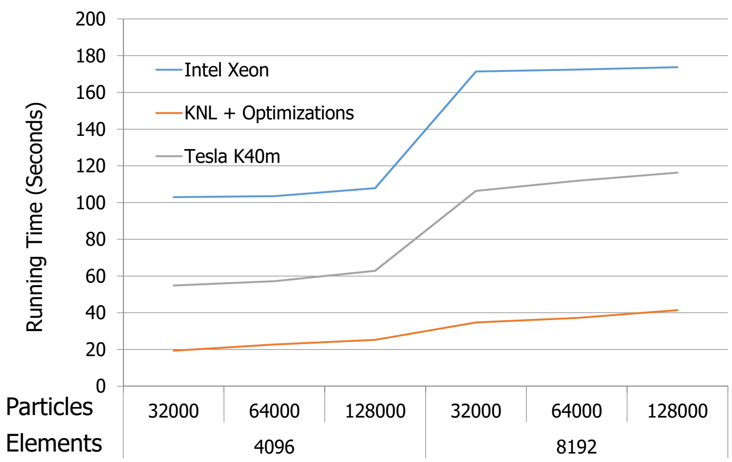
CMT-bone

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

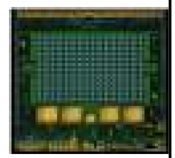
- Running time is total time taken to complete 100 time steps
- Optimizations on KNL include autotuning, vectorization AVX-512 instructions, using OpenMP + MPI, using MCDRAM as cache

CCMT

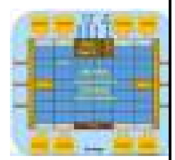
CMT-bone on Different Platforms



TDP: 150W



TDP: 245W



TDP: 215W

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

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Publications

1. Tania Banerjee and Sanjay Ranka, Genetic Algorithm based Autotuning Approach for Performance and Energy Optimization, Proceedings of International Green and Sustainable Computing, 2015
2. Tania Banerjee, Mohammed Gadou, Sanjay Ranka, A Genetic Algorithm based Approach for Multi-objective Hardware/Software Co-optimization, Journal of Sustainable Computing, Vol 10, June 2016, 36 – 47.
3. Tania Banerjee, Jacob Rabb and Sanjay Ranka, Multi-objective Optimization of Spectral Solvers on Hybrid Multicore Platforms, Journal of Sustainable Computing, Vol 12, Dec 2016, 10 - 20.
4. Tania Banerjee, Jason Hackl, Mrugesh Sringarpure, Tanzima Islam, S. Balachandar, Thomas Jackson, Sanjay Ranka, CMT-bone -- A Proxy Application for Compressible Multiphase Turbulent Flows, Proceedings of HiPC, 2016
5. Mohamed Gadou, Tania Banerjee, Sanjay Ranka, Multi-objective Optimization of CMT-bone on Hybrid Processors, Proceedings of IGSC 2016
6. Tania Banerjee, Jason Hackl, Mrugesh Sringarpure, Tanzima Islam, S. Balachandar, Thomas Jackson, Sanjay Ranka, A New Proxy Application for Compressible Multiphase Turbulent Flows. Sustainable Computing: Informatics and Systems, 2017
7. Mohamed Gadou, Tania Banerjee, Meena Arunachalam, Sanjay Ranka, Multiobjective evaluation and optimization of CMT-bone on multiple CPU/GPU systems, Journal of Sustainable Computing: Informatics and Systems, 2017
8. Keke Zhai, Tania Banerjee, David Zwick, Jason Hackl and Sanjay Ranka, Dynamic Load Balancing for Compressible Multiphase Turbulence, submitted to IPDPS 2018
9. Mohamed Gadou, Sankeerth Mogili, Tania Banerjee, Sanjay Ranka, Multi-objective Optimization on Hybrid Systems using DVFS, submitted to IPDPS 2018
10. Mohamed Gadou, Meena Arunachalam, Tania Banerjee, Sanjay Ranka, Multiobjective evaluation and optimization of CMT-bone on Intel Knights Landing, in preparation.

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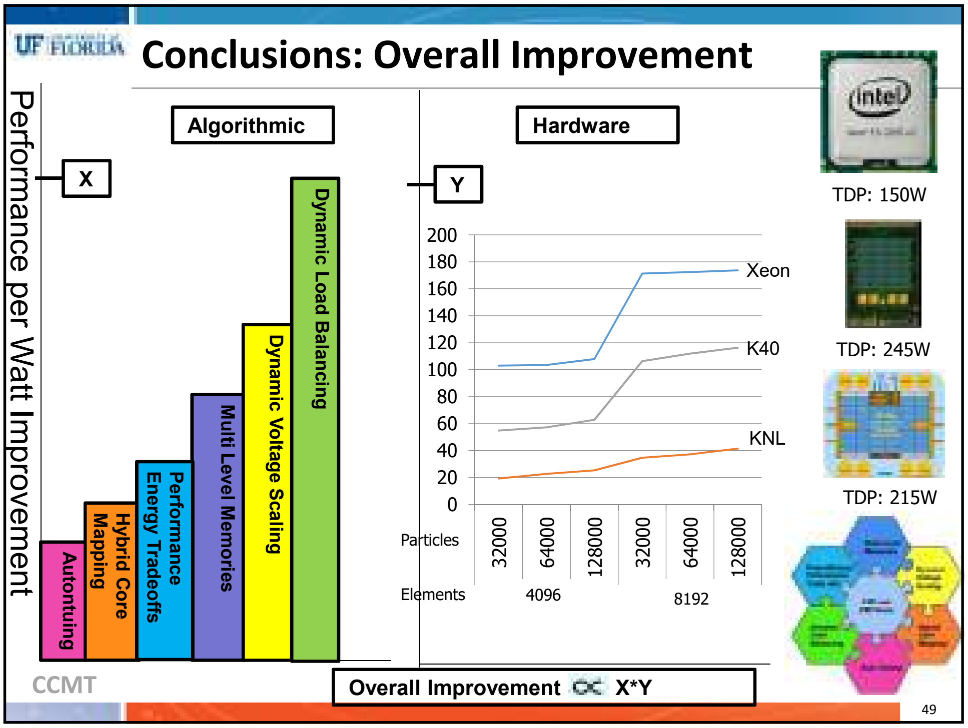
Conclusions: Overall Improvement
Performance per Watt Improvement
Algorithmic
Hardware
X
Y
Autontuing
Hybrid Core Mapping
Performance Energy Tradeoffs
Multi Level Memories
Dynamic Voltage Scaling
Dynamic Load Balancing
Xeon
K40
KNL
Particles
Elements
4096
8192
TDP: 150W
TDP: 245W
TDP: 215W
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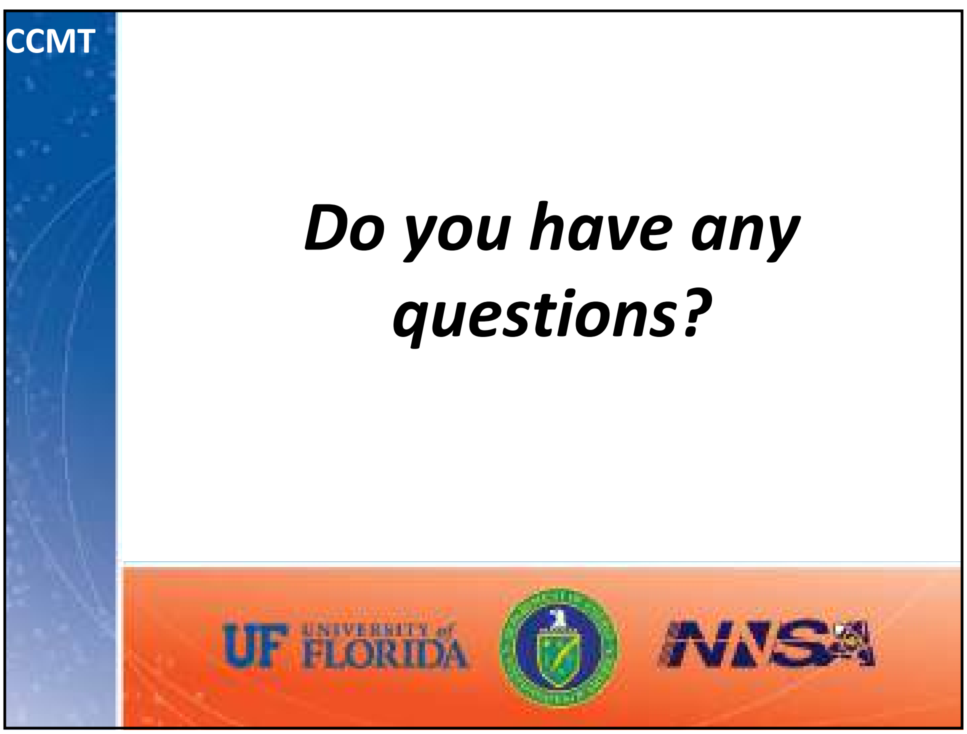
Overall Improvement ∝ X*Y
49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Do you have any questions?

CPU Experiments

- Constant of proportionality, for total execution time

f \ n	1	2	4	8	12
1200	0.975	0.965	0.965	0.935	0.905
1500	0.985	0.985	0.975	0.955	0.915
1800	0.995	0.995	0.990	0.985	0.975
2100	0.990	0.990	0.990	0.990	0.970

- Constant of proportionality, for communication time

f \ n	1	2	4	8	12
1200	0.82	0.88	0.82	0.72	0.62
1500	0.86	0.86	0.86	0.77	0.70
1800	0.90	0.90	0.90	0.83	0.80
2100	0.95	0.95	0.95	0.92	0.90

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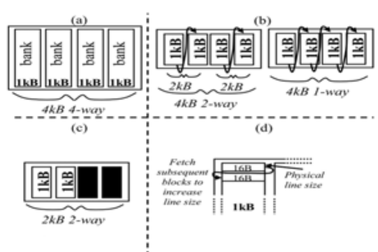
Hardware-Software Autotuning

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

Algorithm: *dudr-4loop-fused*
do k = 1, $N_z * N_y$
do i = 1, N_x
do l = 1, N_x
*dudr(l, k) = dudr(l, k) + a(i, l) * u(l, k, ie)*
enddo
enddo
enddo



Total number of variants = 20

Algorithm: *dudr-4loop-permuted-and unrolled*
do k = 1, N_z
do i = 1, N_x
do j = 1, N_y
do l = 1, N_x,2
*dudr(l, j, k) = dudr(l, j, k) + a(i, l) * u(l, j, k, ie)*
*dudr(l+1, j, k) = dudr(l+1, j, k) + a(i, l+1) * u(l+1, j, k, ie)*
enddo
enddo
enddo
enddo

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

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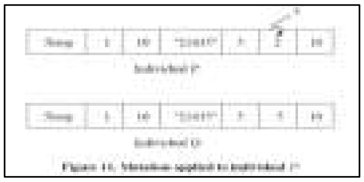
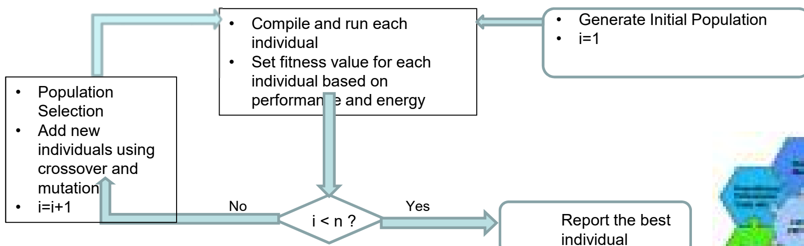
Genetic Algorithm





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Comparison of GA with Exhaustive Approach

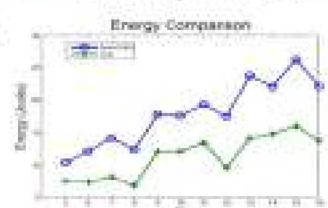
Comparison of performance by platform

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

Comparison of energy consumption by platform

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

Results (AMD Fusion @ Sandia)



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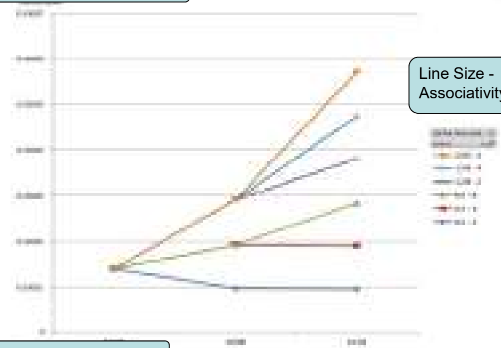
Performance (varying hardware parameters)

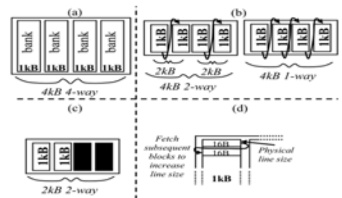
Best Time (seconds)



Line Size - Associativity

Cache size

Associativity Tuning



Capacity Tuning

Line Size Tuning

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

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

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

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Exascale Behavioral Emulation

Principal Investigators:

Herman Lam, Greg Stitt

Center for Compressible Multiphase Turbulence (CCMT)

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

Exascale Behavioral Emulation (BE) Team

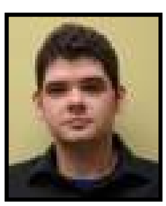

Ryan Blanchard
FPGA Acceleration


Sai Chenna
BE Design Space Exp.


Trokon Johnson
BE Tools

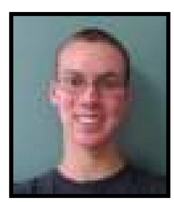

Aravind Neelakantan
BE Methods


Nalini Kumar
BE Methods


Carlo Pascoe
FPGA Acceleration


Raj Rajagoplan
BE-SST


Ben Reynolds
Thermal Modeling


Chad Saunders
FPGA Acceleration

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Outline

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

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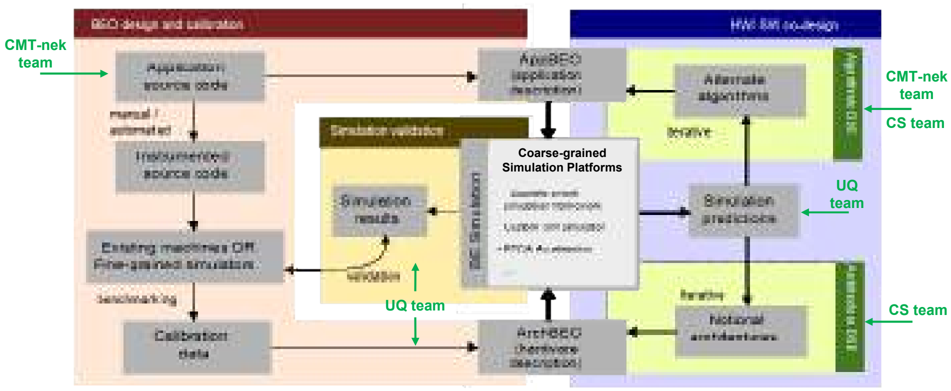
Co-Design Using *Behavioral Emulation*



* BEO – Behavioral Emulation Object

HW/SW co-design

- Algorithmic & architectural design-space exploration (DSE)

Coarse-grained BE simulation

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

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  - CMT-nek d
  - Acceleratio
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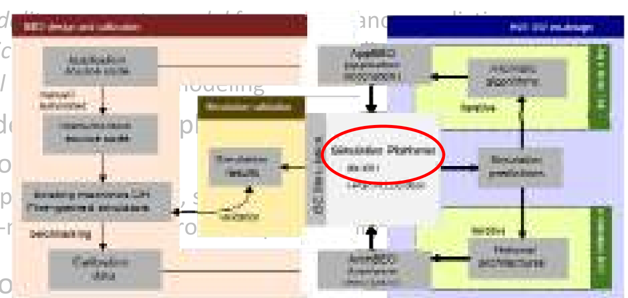
    - Of CMT-n
- Summary, co



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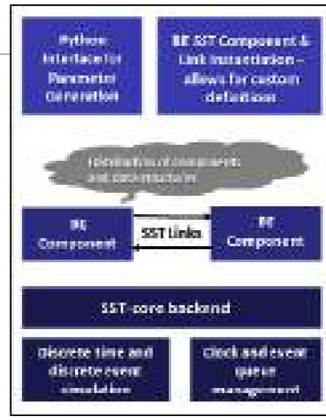
BE-SST Simulator*

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



* A. Ramaswamy, N. Kumar, H. Lam, and G. Stitt, "Scalable Behavioral Emulation of Extreme-Scale Systems Using Structural Simulation Toolkit", submitted to the International Parallel and Distributed Processing Symposium (IPDPS), Vancouver, CA., May 21-25, 2018.

** From Sandia National Labs

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BE-SST Enhancements

- Developed interpolation API
  - To select appropriate interpolation techniques (e.g., Linear interpolation, polynomial interpolation)
- Since AST review 2017: support for symbolic regression
  - Improve accuracy (More details later)
- Able to support trace-driven simulation*
  - For time-dependent simulations
  - To mimic CMT-nek with particles more accurately
- Inclusion of collective-communication operations
  - MPI_ISEND, MPI_IRECV, MPI_WAITALL
- Communication model
  - Replaced static routing method with dynamic routing
- Leverage parallel capabilities of SST for BE-SST

* More details in Sai Chenna's presentation on Tuesday

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Dynamic Routing

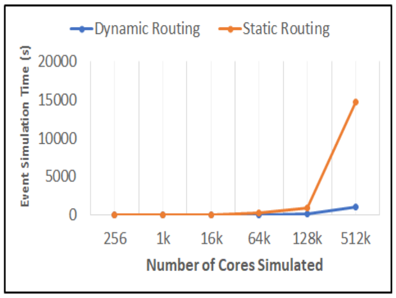

Fig. 1 Static vs. Dynamic Routing

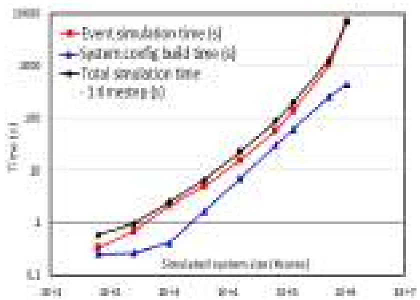

Fig. 2 BE-SST parallelized on 64 cores on HiPerGator @UF

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

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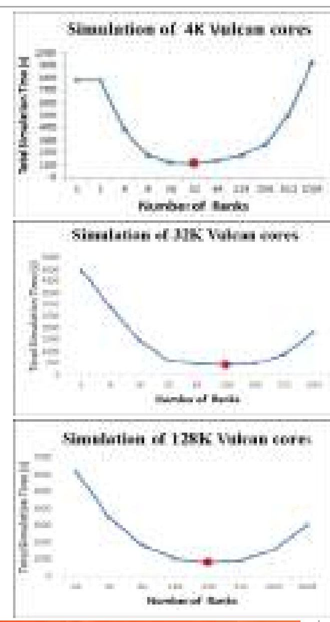
Parallel Performance of BE-SST

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



* Run using BE-SST installed on Titan

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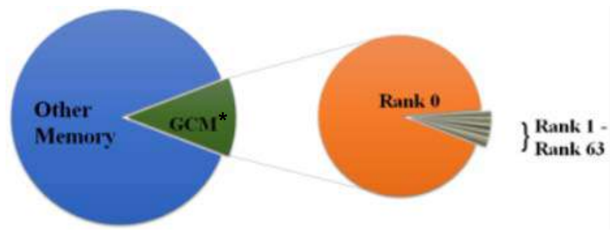
BE-SST Scalability

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

*** GCM**
Graph Construction Memory: initial memory allocation before simulation



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

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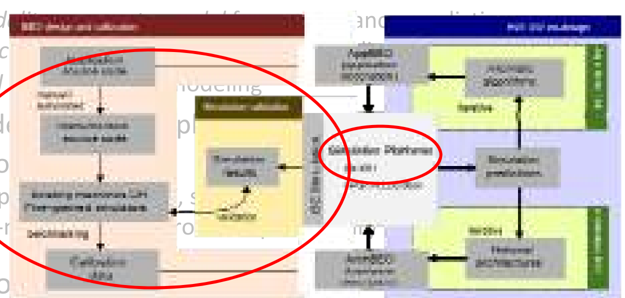

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BE simulations of HPC systems

- Titan @ ORNL

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

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

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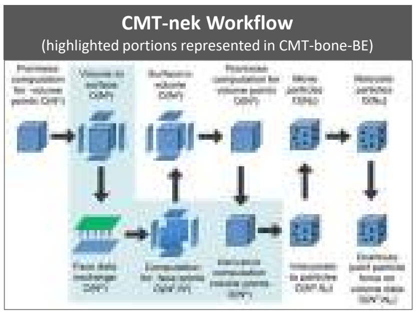
Application Case Study: CMT-bone-BE

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



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

* design-space exploration

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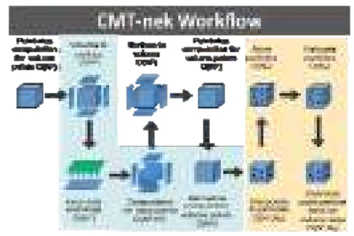
Experiment Setup

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



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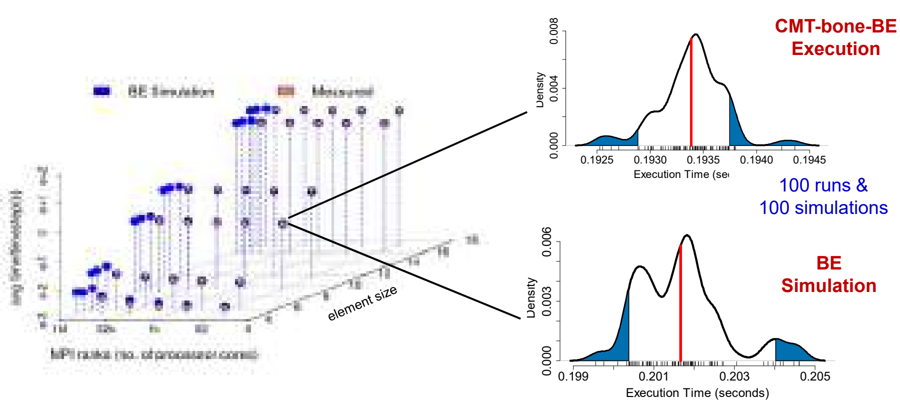
BE Simulations of CMT-bone-BE on Titan+



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

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

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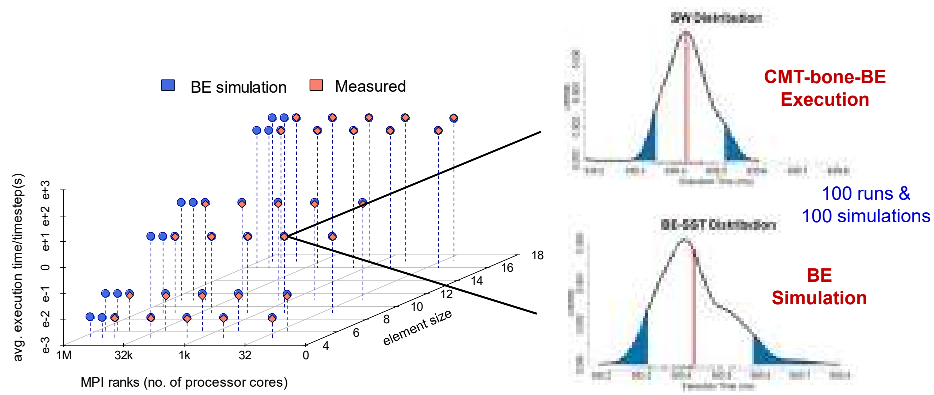
BE Simulations of CMT-bone-BE on Vulcan+



- Simulating a bigger system than Vulcan (512k cores)
- Average % error between CMT-bone-BE simulation and execution time is 4%
- Maximum error is 9%

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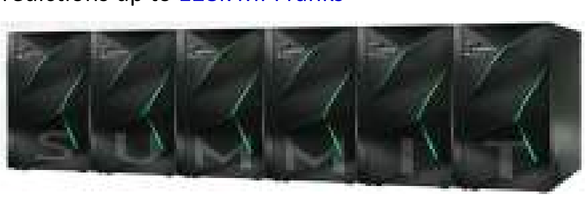
BE Simulations of CMT-bone-BE on Notional Architecture

- Notional architecture
  - IBM POWER architecture
  - 48 cores/node
  - Non-blocking fat-tree topology
  - Tending towards Summit @ ORNL
- Initial methodology
  - OSU n/w benchmark* of Cab (fat-tree topology)
  - Lookup tables of Vulcan (POWER architecture)
  - Predictions up to 128k MPI ranks



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Work in progress

*developed in Ohio State University

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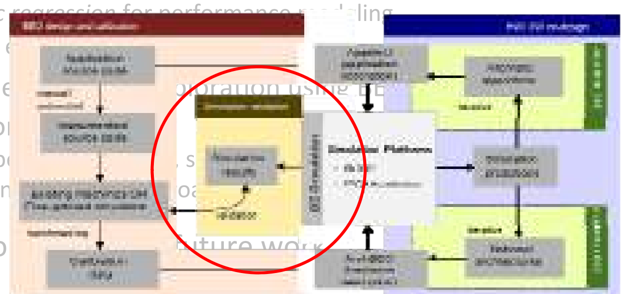
    - *Multi-fidelity surrogate model* for performance prediction
    - *Symbolic regression for performance mod*...*ling*
    - *Thermal* ...
  - CMT-nek de... ...oration using BE
  - Acceleration...
    - Of BE: sp... ...s
    - Of CMT-n... ...oa...
- Summary, co... ...uture work



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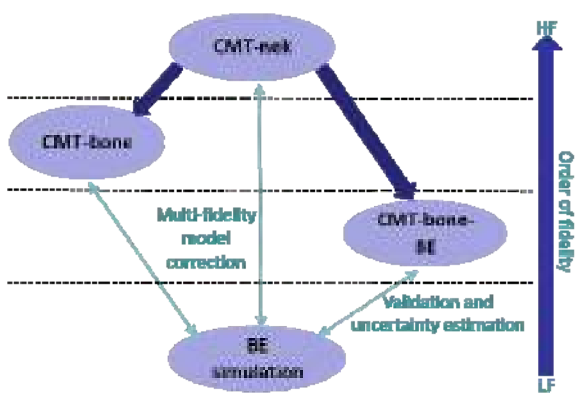
Behavioral Emulation with UQ

w/ UB

Goal: Improve BE models via validation and uncertainty estimation

- Reduce computational budget by fitting BE simulation to CMT-nek using Multi-Fidelity Surrogate (MFS)
- Extrapolation of CMT-nek towards large-scale runs using BE and MFS



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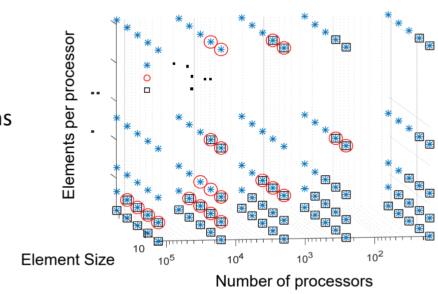
Multi-fidelity Prediction of CMT-nek

w/ UB

Experimental setup

- Design of experiment (DOE)
  - Element size (ES) = 5,9,13,17,21
  - Elements per processor (EPP) = 8,32,64,128,256
  - Number of processors (NP) = 16,256,2048,16384,131072
- 125 total data points
  - ∗ BE simulation: all 125 runs
  - ○ CMT-nek: 22 runs
  - □ CMT-bone: 67 runs



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

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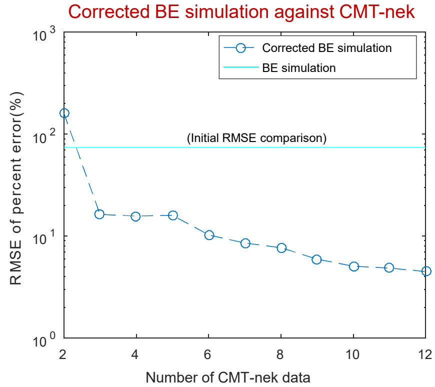
Multi-fidelity Prediction of CMT-nek

w/ UB

Initial RMSE comparison:

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

Corrected BE simulation against CMT-nek



Accuracy of corrected BE sim.

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

Y. Zhang, A. Neelakantan, N. Kumar, C. Park, R. Haftka, N. H. Kim, and H. Lam, "Multi-fidelity Surrogate Modeling for Application/Architecture Co-design", accepted to Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS17), Denver, CO, Nov. 13, 2017.

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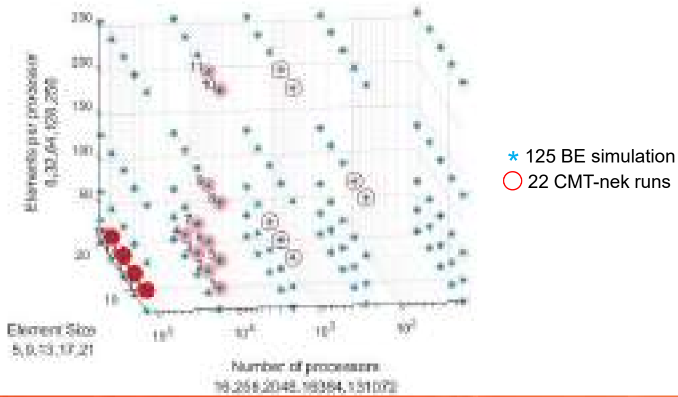
Extrapolation Towards Large-scale Runs

w/ UB

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



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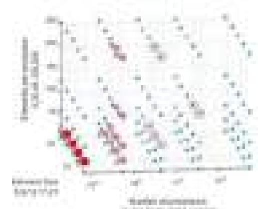
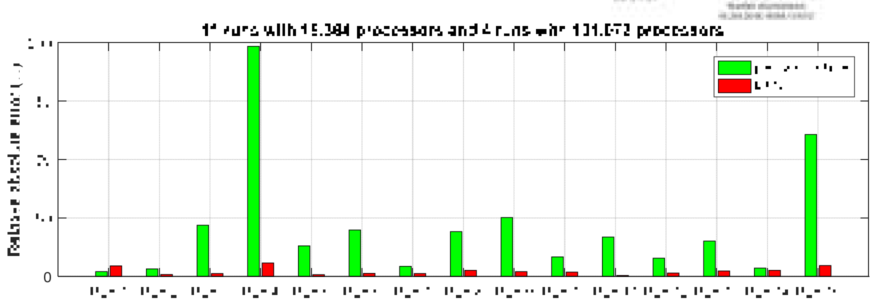
Extrapolation: Validation

w/ UB

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





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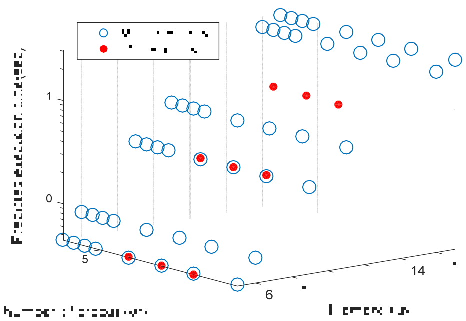
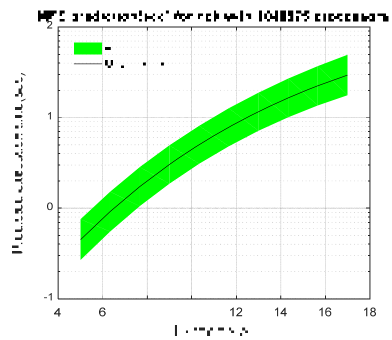
Extrapolation: Prediction of CMT-nek

w/ UB

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





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Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thrusts & achievements

- BE-SST simulator & tools, experimental results
- BE method enhancements
  - *Multi-fidelity surrogate model* for performance prediction
  - *Symbolic regression* for performance modeling
  - *The*
- CMT-r
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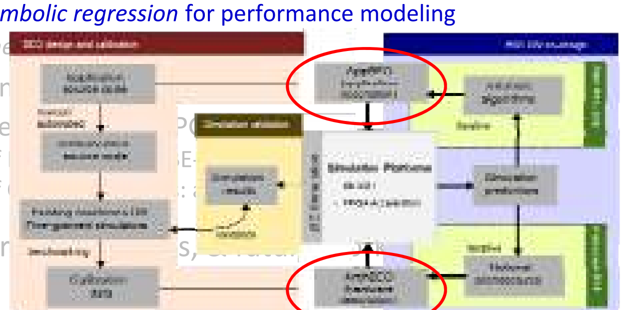

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Symbolic Regression: Motivation

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

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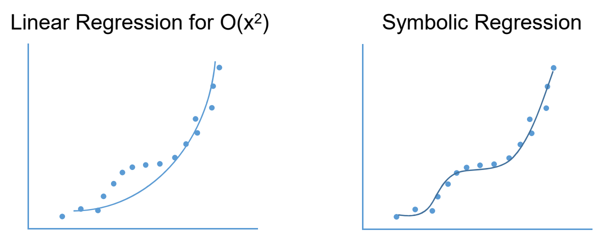
Symbolic Regression



- Advantages:
  - Captures machine-specific performance behaviors
  - Enables tradeoffs between accuracy and computational complexity
    - Can maximize performance for a given error constraint
  - Requires no prior knowledge of the kernel
- Approach: custom genetic-programming tool
  - Evolves "trees" from mathematical primitives
  - Multiple optimization goals: minimize error, minimize error given tree size constraint, minimize tree size given error constraint, etc.

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Symbolic Regression: Results

Particle solver kernel	Linear Regression		Symbolic Regression		Error Improvement
	RMSE	MAPE	RMSE	MAPE	$MAPE_{Linear}/MAPE_{symbolic}$
Compute1	4.43E-06	3.5%	1.08E-05	1.5%	2.4x
update_particle_location	1.26E-05	10.8%	1.26E-05	1.6%	6.8x
particles_in_nid	1.17E-02	76.4%	1.27E-02	31.1%	2.5x
interp_props_part_location	4.51E-01	902.6%	3.67E-01	10.0%	90.7x
upd_vel_and_pos_rk3_stage1	8.22E-04	399.0%	5.43E-04	9.0%	44.2x
upd_vel_and_pos_rk3_stage3	1.06E-04	19.4%	6.50E-05	9.7%	2.0x
upd_vel_and_pos_rk3_allstage	7.34E-03	27.3%	7.57E-04	6.8%	4.0x
upd_vel_and_pos_bdf	5.38E-04	20.0%	1.21E-03	4.9%	4.1x
red_interp	9.33E-02	4.7%	2.94E-02	4.3%	1.1x
usr_particles_forces	8.80E-05	6.3%	6.85E-05	2.1%	2.9x
tri_interp	1.58E-04	1.4%	5.34E-05	0.7%	1.9x
Average	5.14E-02	133.8%	3.75E-02	7.4%	14.8x

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Outline

- Review & Overview:
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- Research thrusts & achievements
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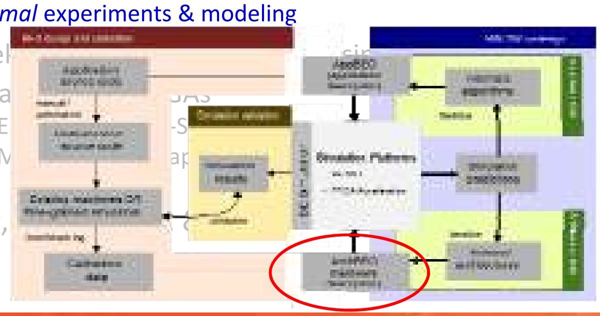
  - BE method enhancements
    - *Multi-fidelity surrogate model* for performance prediction
    - *Symbolic regression* for performance modeling
    - *Thermal* experiments & modeling
  - CMT-ne
  - Accelera
    - Of BE
    - Of CM
- Summary,



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Thermal Benchmarking & Modeling

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

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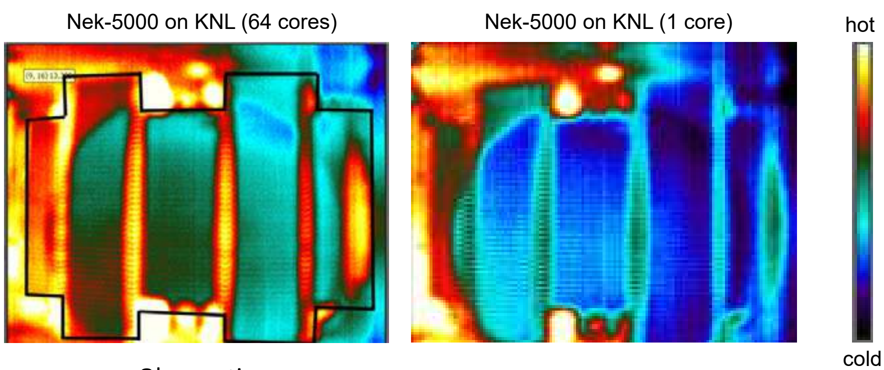
Thermal Benchmarking & Modeling



- Observations:
  - Heat sink “blocks” much of processor
  - Minimizing the maximum temperature may not be most appropriate optimization goal
- Future work: investigate how heat changes for different load balancing optimizations
  - Determine most approach optimization goal

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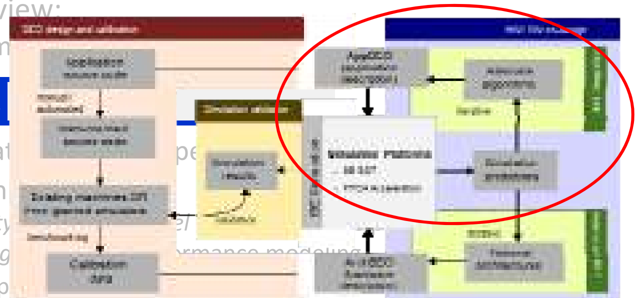
Outline

- Review & Overview:
  - Behavioral Em
- Research thrusts
  - BE-SST simulat
  - BE method en
    - *Multi-fidelity*
    - *Symbolic reg*
    - *Thermal* exp



  - CMT-nek design space exploration using BE simulation
  - Acceleration using FPGAs
    - Of BE: speedup vs BE-SST, scale up on multiple FPGAs
    - Of CMT-nek kernels: approach & preliminary results
- Summary, conclusions, & future work

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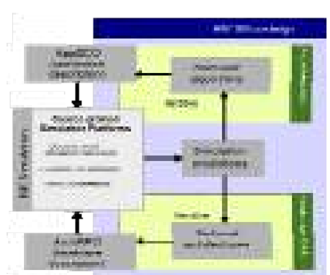
CMT-nek DSE: Motivation & Approach

- Motivation:
  - CMT-nek has huge design space
  - Various architectural options exist for Exascale systems
- Goal:
  - Use BE methods & tools to perform DSE
  - Approach: Iterative DSE steps
    - Perform BE Simulations of CMT-nek (baseline)
    - Identify optimization candidates (i.e. most expensive subroutines)
    - Create and validate models of algorithms for these subroutines
    - Use BE to predict performance



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BE-SST Predictions: Particle solver

- Summary of results
  - Interpolation:
    - scales non-linearly w.r.t element size and elements-per-processor, linearly w.r.t particles/gridpoint
    - Reduced barycentric is 5x faster than barycentric interpolation
    - Trilinear interpolation is on average 164x faster than barycentric interpolation
  - Time integration:
    - scales non-linearly w.r.t element size and elements-per-processor, linearly w.r.t particles/gridpoint
    - Bdf is 3x faster than rk3 time integration
- Refer to Sai Chenna's presentation
  - BE Simulations of CMT-nek

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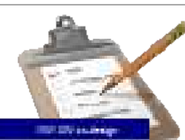
Outline



- Review & Overview:
  - Behavioral Emulation (BE)

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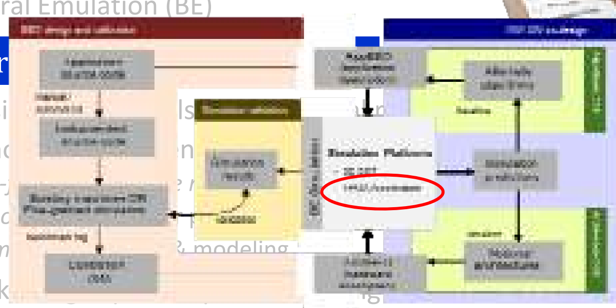
    - Therm
  - CMT-nek



  - Acceleration using FPGAs
    - Of BE: speedup vs BE-SST, scale up on multiple FPGAs
    - Of CMT-nek kernels: approach & preliminary results
- Summary, conclusions, & future work

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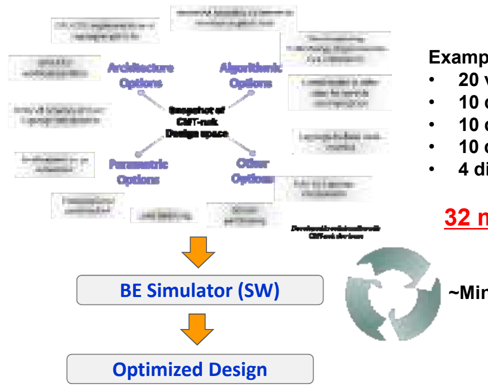
BE Design-Space Exploration



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

32 million options to explore

~Minutes per simulation

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

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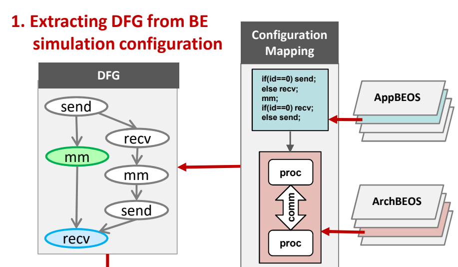
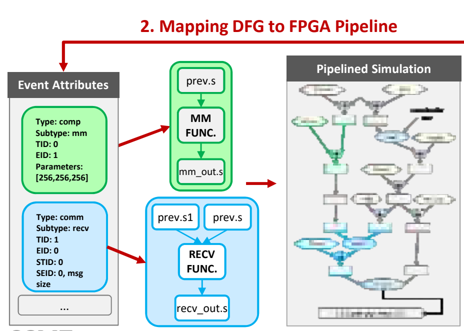
Fully-expanded Pipeline (FEP)

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





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

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

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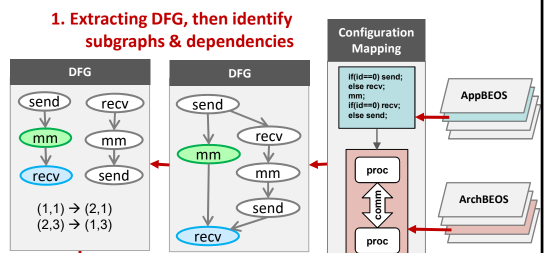
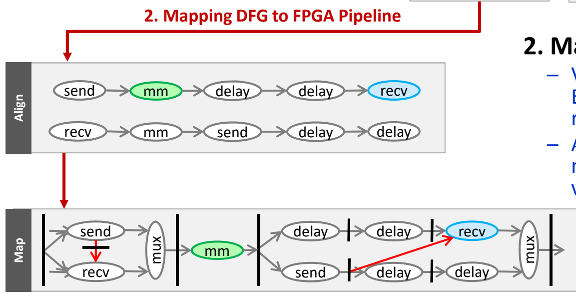
Collapsed Pipeline (CP)

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

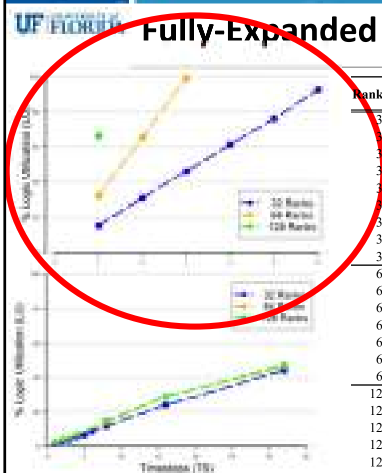




2. Map DFG to pipeline circuit
   - Vertex attributes define operations and Edge attributes instantiate pipeline register between src/dst pairs
   - Align subgraph traces such that cost is minimized and no dependencies are violated

Because each subgraph instruction mapped to independent HW, each vertex able to start next subgraph 1 cycle after current subgraph. *All subgraphs must complete before sim can complete*

Fully-Expanded & Collapsed Pipeline Tradeoffs



Fully-Expanded Pipeline

Ranks	TS	Num. of Events	% LU	Latency (cycles)	Hardware MSPS†	Hardware GEPS‡	BE-SST KEPS‡	Hardware Speedup
32	1	1,344	15 / 2	64 / 278	300 / 10.5	403 / 14.1	4.4	92x10⁶ / 3x10⁶
32	2	2,688	31 / 3	118 / 512	300 / 10.5	806 / 28.2	7.8	103x10⁶ / 4x10⁶
32	3	4,032	46 / 4	172 / 746	300 / 10.5	1,210 / 42.3	10.6	114x10⁶ / 4x10⁶
32	4	5,376	61 / 6	226 / 980	300 / 10.5	1,613 / 56.4	12.9	125x10⁶ / 4x10⁶
32	5	6,720	76 / 7	280 / 1,214	300 / 10.5	2,016 / 70.6	14.8	136x10⁶ / 5x10⁶
32	6	8,064	92 / 9	334 / 1,488	300 / 10.5	2,419 / 84.7	16.5	147x10⁶ / 5x10⁶
32	8	10,752	– / 12	– / 1,916	– / 10.5	– / 113	19.1	– / 6x10⁶
32	16	21,504	– / 24	– / 3,788	– / 10.5	– / 226	24.2	– / 9x10⁶
32	32	43,008	– / 44	– / 7,532	– / 10.5	– / 452	28.9	– / 16x10⁶
64	1	2,880	32 / 2	65 / 394	300 / 5.23	864 / 15.1	7.7	112x10⁶ / 2x10⁶
64	2	5,760	65 / 4	119 / 712	300 / 5.23	1,728 / 30.1	12.6	137x10⁶ / 2x10⁶
64	3	8,640	99 / 5	173 / 1,030	300 / 5.23	2,592 / 45.2	16.2	160x10⁶ / 3x10⁶
64	4	11,520	– / 7	– / 1,348	– / 5.23	– / 60.2	17.9	– / 3x10⁶
64	8	23,040	– / 14	– / 2,620	– / 5.23	– / 121	23.2	– / 5x10⁶
64	16	46,080	– / 29	– / 5,164	– / 5.23	– / 241	26.9	– / 9x10⁶
64	32	92,160	– / 46	– / 10,252	– / 5.23	– / 482	29.1	– / 17x10⁶
128	1	5,952	66 / 2	66 / 458	300 / 2.62	1,786 / 15.6	10.8	165x10⁶ / 1x10⁶
128	2	11,904	– / 4	– / 776	– / 2.62	– / 31.2	14.9	– / 2x10⁶
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128	4	23,808	– / 7	– / 1,412	– / 2.62	– / 62.4	18.4	– / 3x10⁶
128	8	47,616	– / 15	– / 2,684	– / 2.62	– / 125	20.8	– / 6x10⁶
128	16	95,232	– / 30	– / 5,228	– / 2.62	– / 250	22.3	– / 11x10⁶
128	32	190,464	– / 47	– / 10,316	– / 2.62	– / 499	22.8	– / 22x10⁶

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

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

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

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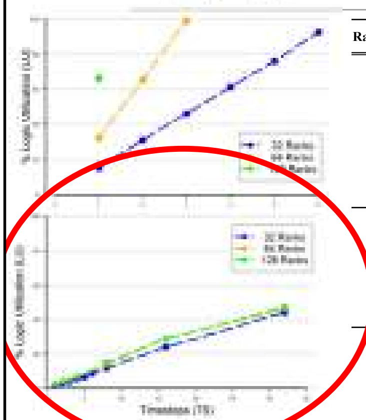
Fully-Expanded & Collapsed Pipeline Tradeoffs



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

Collapsed Pipeline

Advantages:

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

Limitations:

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

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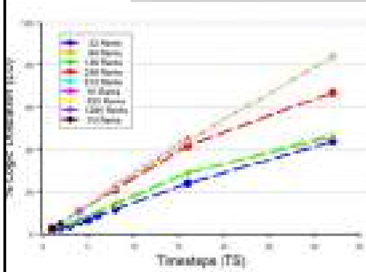
Collapsed Pipeline Single-FPGA Performance/Scalability



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64	32	92,160	46	10,252	5.23	482	24.91	19x10^6
128	32	190,464	47	10,316	2.62	498	24.42	20x10^6
256	32	393,216	67	13,516	1.31	515	23.92	21x10^6
512	32	811,008	84	20,684	0.65	531	21.47	25x10^6
1K	32	1,646,592	84	21,196	0.33	539	18.21	29x10^6
32K	32	55,443,456	84	241,868	1.02×10^{-2}	567	12.96	44x10^6
128K	16	111,673,344	46	333,932	2.56×10^{-3}	285	8.91	32x10^6
1M	2	112,459,776	5	1,148,056	3.19×10^{-4}	36	X	X

As number of ranks increase:

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

Now able to reach million+ rank simulations in hardware

Pipelines scale linearly with length of simulation, however blockram eventually becomes limiting resource

- e.g., only fit 2 TS for 1 million ranks on Stratix V
- Motivation to explore partially-collapsed pipeline approach

Rank limit due to insufficient blockram not logic

Expect greater performance when Stratix 10 becomes available

Increased performance expected with Stratix 10

- Collapsed hardware specifically designed to exploit new Stratix 10 architecture

Throughput > 10Mx higher than BE-SST

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*Collapsed performance of CMT-Bone-BE with varied MPI ranks and simulation timesteps on a single Stratix V 5SGSMD8K1F40C2 @ 335MHz

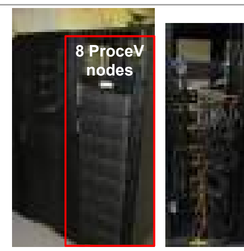
Collapsed Pipeline Multi-FPGA Performance/Scalability

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

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

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

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



Novo-G#
- 64 GiDEL ProceV (Stratix V)
- 4x4x2 3D torus or 5D hypercube
- 6 Rx-Tx links per FPGA
- Measured 32 Gbps per link
- 150 ns latency across links
- Require 64bits/cycle between FPGAs
- 335MHz, 21.4 Gbps, 51 additional lat
- 450MHz, 28.8 Gbps, 68 additional lat
- 500 MHz before link BW saturation

C. Pascoe, S. Chenna, G. Stitt, H. Lam, "A FPGA-Pipelined Approach for Accelerated Discrete-Event Simulation of HPC Systems", accepted to Heterogeneous High-performance Reconfigurable Computing (H2RC), Denver, CO, Nov. 13, 2017.

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

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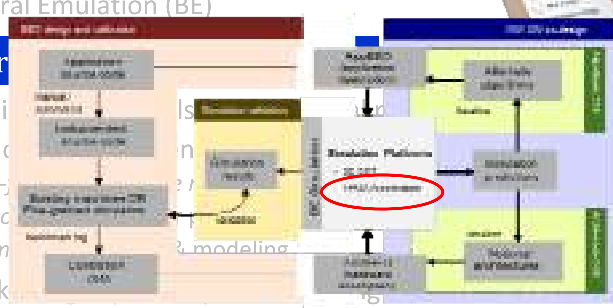
Outline

- Review & Overview:
  - Behavioral Emulation (BE)

Research thr

  - BE-SST si
  - BE meth
    - Multi-
    - Symbc
    - Therm
  - CMT-nek



  - Acceleration using FPGAs
    - Of BE: speedup vs BE-SST, scale up on multiple FPGAs
    - Of CMT-nek kernels: approach & preliminary results
- Summary, conclusions, & future work

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FPGA Acceleration Trends

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

Energy Comparison of BDW+A10 vs. Broadwell

Precision	*Kernel Size*	*Image Size* 256x256	512x512	1024x1024	2048x2048	*Avg*
16-bit Fixed	3x3	35×	47×	67×	68×	54×
	5x5	68×	116×	171×	179×	133×
	7x7	58×	135×	153×	164×	128×
	9x9	44×	98×	135×	148×	106×
	Avg	51×	99×	131×	140×	
32-bit Float	3x3	33×	46×	65×	66×	53×
	5x5	64×	111×	162×	169×	127×
	7x7	55×	113×	131×	139×	109×
	9x9	32×	58×	71×	75×	59×
	Avg	46×	82×	108×	112×	

Energy Comparison of BDW+A10 vs. P6000 GPU

Precision	*Kernel Size*	*Image Size* 256x256	512x512	1024x1024	2048x2048	*Avg*
16-bit Fixed	3x3	15.5×	19.8×	19.4×	19.0×	18.4×
	5x5	12.9×	18.6×	19.5×	19.8×	17.7×
	7x7	10.5×	18.2×	19.7×	20.5×	17.2×
	9x9	8.1×	15.3×	16.9×	18.6×	14.7×
	Avg	11.8×	18.0×	18.9×	19.5×	
32-bit Float	3x3	14.6×	19.4×	19.0×	18.6×	17.9×
	5x5	12.2×	17.8×	18.6×	18.7×	16.8×
	7x7	9.9×	15.2×	16.9×	17.3×	14.8×
	9x9	5.8×	9.0×	8.9×	9.4×	8.3×
	Avg	10.6×	15.4×	15.8×	16.0×	

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Summary & Conclusions

- BE methods & tools
  - BE method enhancements: network models, interpolation & symbolic regression schemes, energy & thermal modeling
  - BE-SST enhancements: functionality, tools, & scaling
- Large-scale experiments
  - Validation (100k+ MPI ranks) on Titan & Vulcan
  - Predictive simulations to million+ MPI ranks; on notional archs
- CMT-nek DSE using BE simulation
  - Profiling of key CMT-nek particle solver routines
  - Accuracy/performance tradeoffs using BE simulation
- FPGA acceleration of BE simulation
  - Validation of dataflow, pipelined approaches (FEP, CP)
  - multi-FPGA scalability prediction & validation

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Do you have any questions?
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NNSA