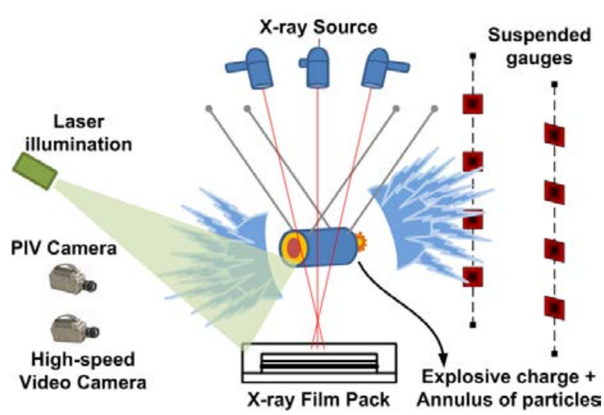
CCMT

CENTER FOR COMPRESSIBLE MULTIPHASE TURBULENCE

TST Meeting

November 5-6, 2015



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Center for Compressible Multi-Phase Turbulence

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

Agenda for TST Site Visit November 5 and 6, 2015

<u>Thursday November 5, 2015</u>

7:45	Van pick up at University Hilton
8:00-9:00	Full Breakfast (site visit team caucus with AST members)
9:00-9:40	CCMT Overview/Highlights
9:40-10:30	Macroscale Team
10:30-10:45	Coffee break
10:45-11:45	Microscale Team
11:45-1:00	Lunch
1:00-1:30	ASU Experiments
1:30-2:00	CMT-nek
2:00-2:50	Exascale – Part 1
2:50-3:00	Coffee break
3:00-3:50	Exascale – Part 2
3:50-4:00	Short Break
4:00-4:30	Internship presentations by Chris Hajas, Chris Neal, Carlo Pascoe and Nalini Kumar
4:30-5:00	Marianne Francois (LANL) and Mark Schraad (LANL)
5:15	Transportation to University Hilton
6:00-7:30	Dinner at the University Hilton, hosted by CCMT Faculty
7:30	TST members transported back to hotel

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Friday November 6, 2015

7:45	Van pickup at University Hilton
8:00-8:30	Continental Breakfast
8:30-9:45	UB Team
9:45-10:30	CS
10:30-11:00	Discussions between TST and CCMT PIs
11:00	Box Lunch; Transportation as need to hotel and/or airport

Center for Compressible Multiphase Turbulence

Attendee List for TST Meeting November 5-6, 2015

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
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Bertrand Rollin	Embry-Riddle	bertrandrollin@gmail.com
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

TST Members

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Sam Schofield	LLNL	schofield5@llnl.gov
Mark Schraad	LANL	schraad@lanl.gov
Justin Wagner	Sandia	jwagner@sandia.gov
Greg Weirs	Sandia	vgweirs@sandia.gov

AST Members

Jim Costa	Sandia	jecosta@sandia.gov
Nels Hoffman	LANL	nmh@lanl.gov
Dan Nikkel	LLNL	nikkel1@llnl.gov

NNSA Visitors

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Students

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Angela Diggs	University of Florida	angela.diggs.1@us.af.mil
Brad Durant	University of Florida	neoncrash@ufl.edu
Giselle Fernandez	University of Florida	gisellefernandez@ufl.edu
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Carlo Pascoe	University of Florida	poppyc@ufl.edu
Na Qiu	Tong-Ji University (China)	nqiu@ufl.edu
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Prashanth Sridharan	University of Florida	shan1130@ufl.edu
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Administration Staff

Hollie Starr	University of Florida	hstarr@ufl.edu

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Overview and Integration

S. Balachandar

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AST Meeting Agenda

Thursday

- Overview and Integration
- Macroscale
- Microscale
- *Lunch*
- ASU Experiments
- CMT-nek
- Exascale
- Internship (4) presentations
- DOE laboratory talks
- *Dinner at University Hilton with CCMT Faculty and Staff*

Friday

- Uncertainty Budget
- CS
- Discussions between TST and CCMT PIs
- *Lunch and transportation to airport*

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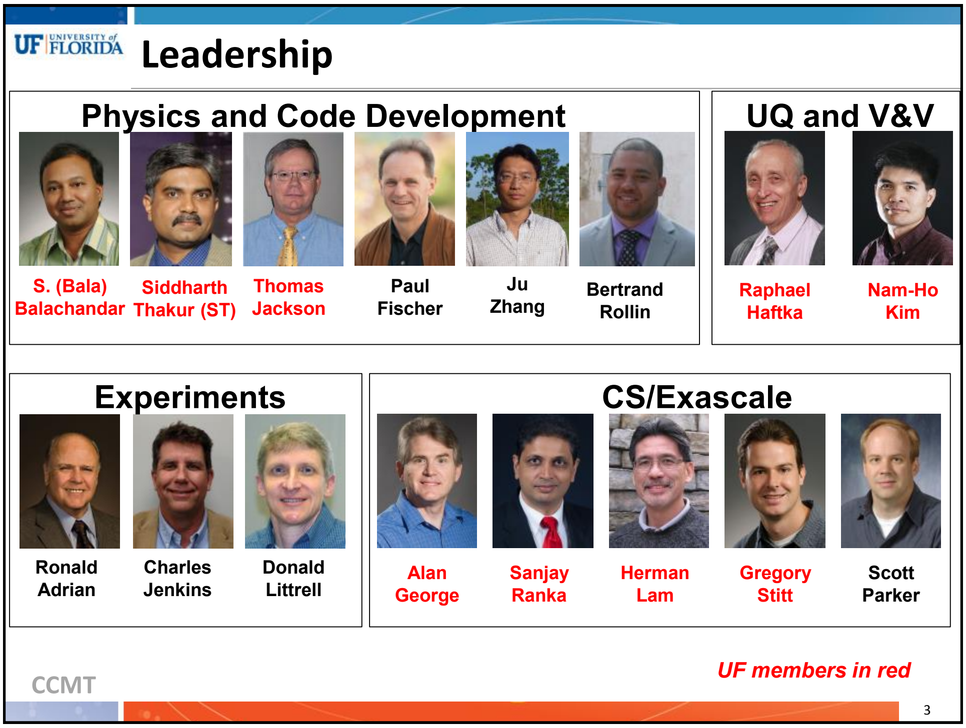
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Leadership
Physics and Code Development
S. (Bala) Balachandar
Siddharth Thakur (ST)
Thomas Jackson
Paul Fischer
Ju Zhang
Bertrand Rollin
UQ and V&V
Raphael Haftka
Nam-Ho Kim
Experiments
Ronald Adrian
Charles Jenkins
Donald Littrell
CS/Exascale
Alan George
Sanjay Ranka
Herman Lam
Gregory Stitt
Scott Parker
UF members in red
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Research Staff & Senior PhD Students
Subramanian Annamalai
Tania Banerjee
Charles Cook
Jason Hackl
Chanyoung Park
Mrugesh Shringarpure
2Lt. Myles Delcambre
Carlo Pascoe
Nalini Kumar
Dylan Rudolph
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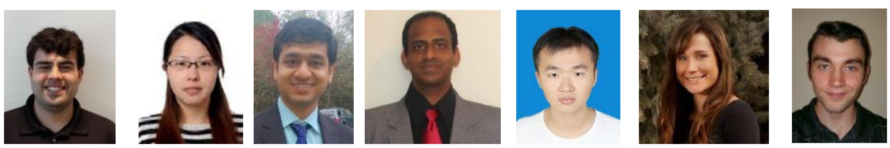
Current Students (Undergraduate & Graduate)

Kasim Alli | *Georges Akiki* | *Saptarshi Biswas* | *Paul Crittenden* | *Angela Diggs* | *Brad Durant* | *Giselle Fernandez* | *Mohamed Gadou*

Chris Hajas | *Rahul Koneru* | *Ting-Hsin Kuo* | *Goran Marjanovic* | *Justin T. Mathew* | *Yash Mehta* | *Christopher Neal* | *Sam Nili*



Frederick Ouellet | *Na Qiu* | *Parth Shah* | *Prashanth Sridharan* | *Yiming Zhang* | *Heather Zunino* | *David Zwick*

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Outline

- Demonstration problem
- Sequence of events and physics models
- Simulation roadmap
- Uncertainty quantification and reduction
- Y1.5 accomplishments
- Goals for next year

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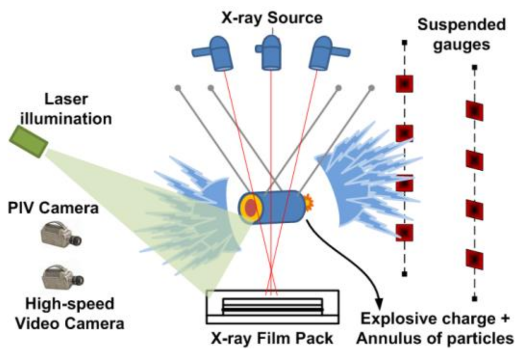
Demonstration Problem

- Explosive-driven cylindrical annulus of particles



- Integrated effort toward predictive simulations
- Experimental measurements for validation

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Demonstration Problem

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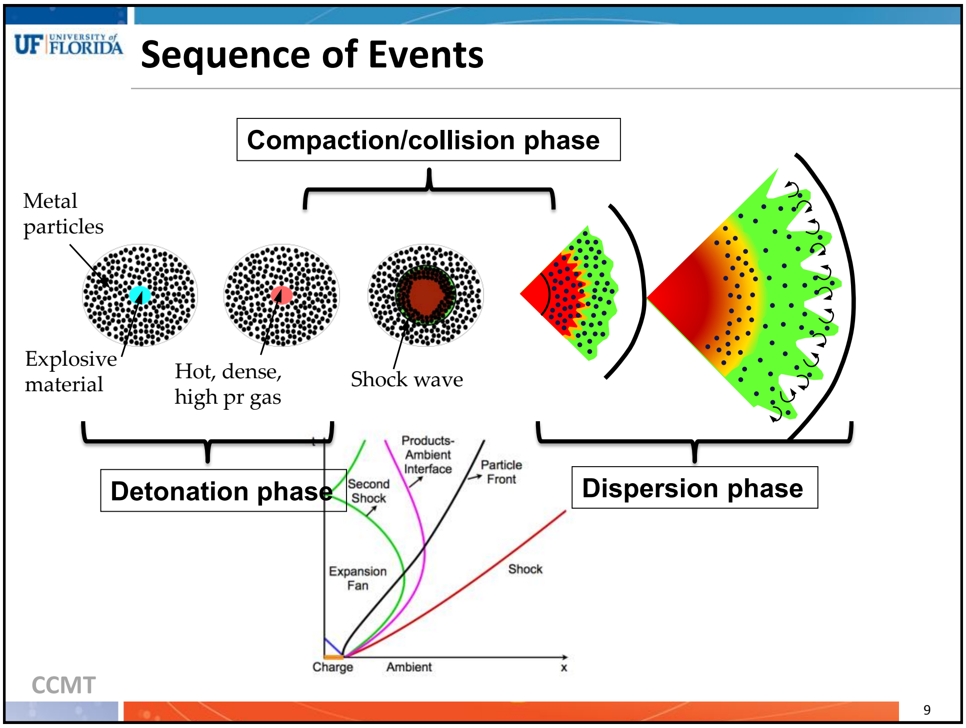
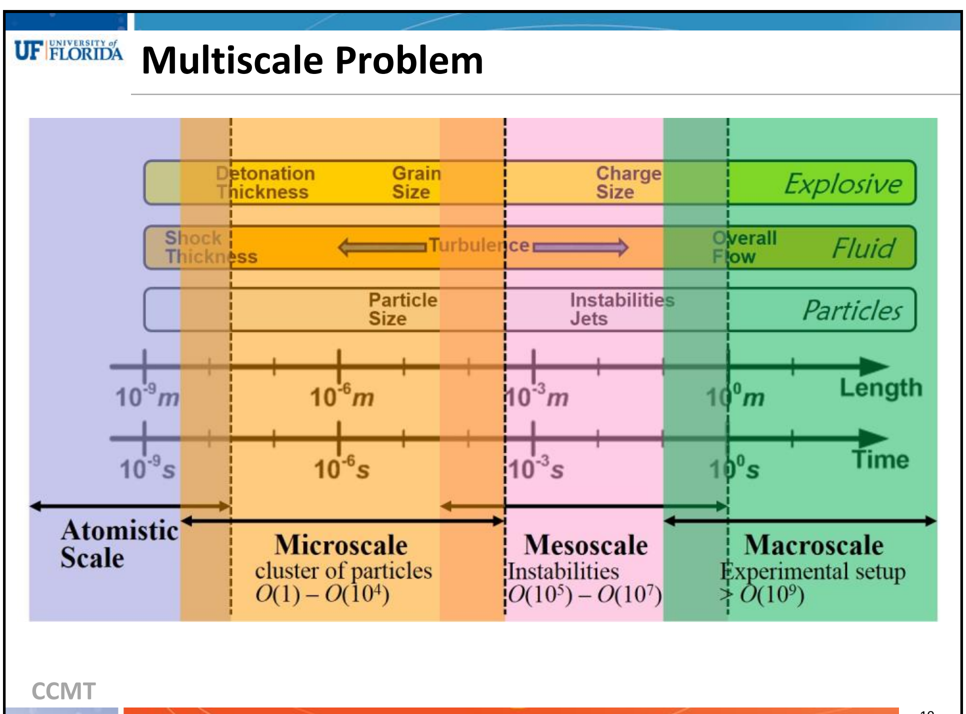
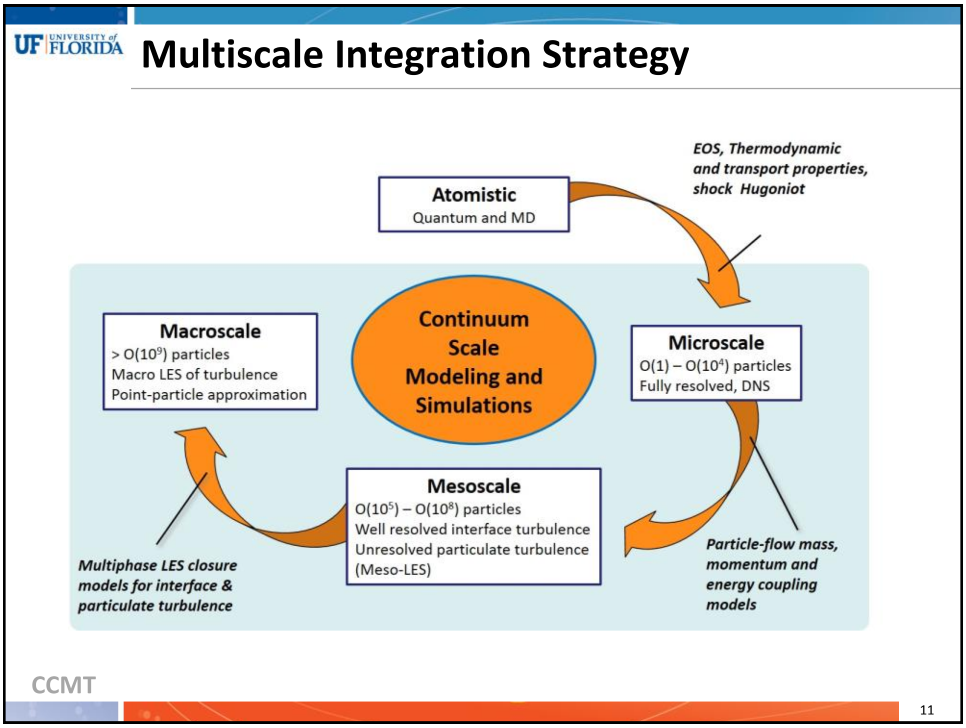
Sequence of Events



Multiscale Problem

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Multiscale Integration Strategy
Atomistic
Quantum and MD
EOS, Thermodynamic and transport properties, shock Hugoniot
Continuum Scale Modeling and Simulations
Macroscale
> $O(10^9)$ particles
Macro LES of turbulence
Point-particle approximation
Microscale
$O(1) – O(10^4)$ particles
Fully resolved, DNS
Mesoscale
$O(10^5) – O(10^8)$ particles
Well resolved interface turbulence
Unresolved particulate turbulence
(Meso-LES)
Multiphase LES closure models for interface & particulate turbulence
Particle-flow mass, momentum and energy coupling models
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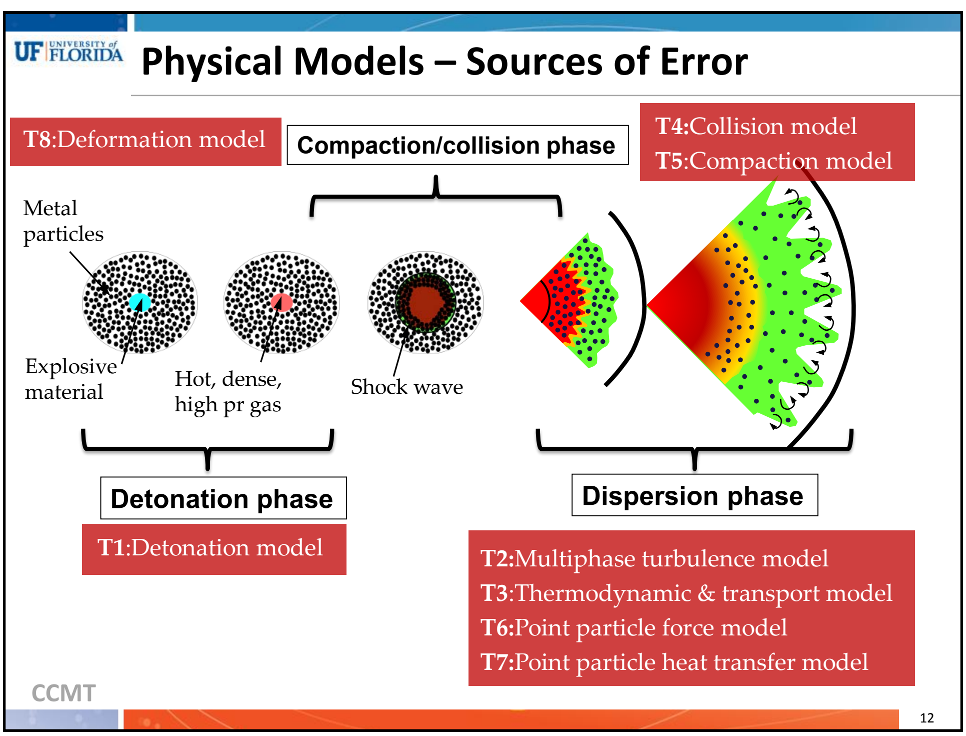
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Physical Models – Sources of Error
T8:Deformation model
Compaction/collision phase
T4:Collision model
T5:Compaction model
Metal particles
Explosive material
Hot, dense, high pr gas
Shock wave
Detonation phase
T1:Detonation model
Dispersion phase
T2:Multiphase turbulence model
T3:Thermodynamic & transport model
T6:Point particle force model
T7:Point particle heat transfer model
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Sources of Errors & Uncertainties

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

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

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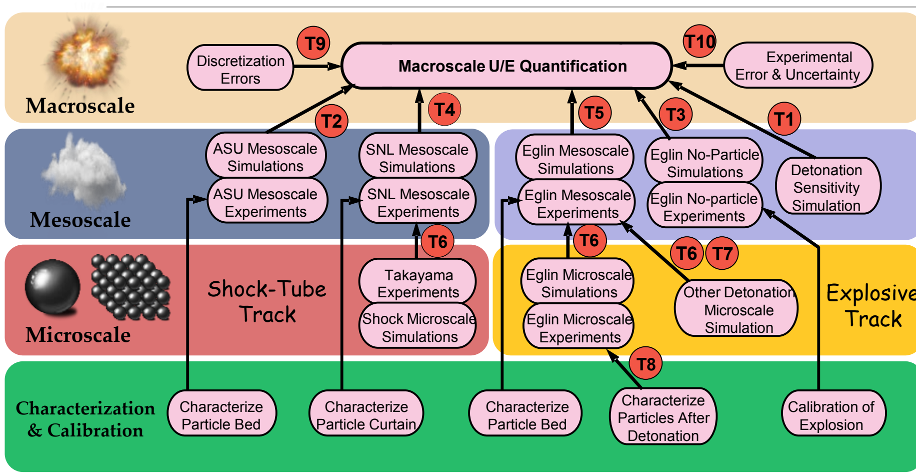
Uncertainty Budget – Overall Plan



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

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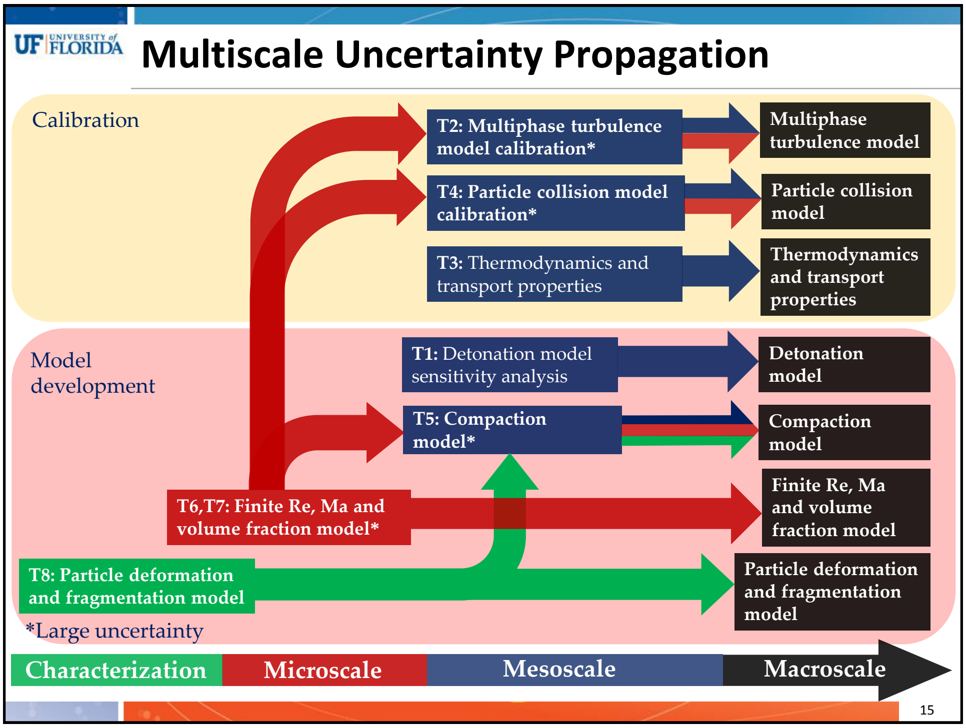
Multiscale Uncertainty Propagation
Calibration
T2: Multiphase turbulence model calibration*
T4: Particle collision model calibration*
T3: Thermodynamics and transport properties
Multiphase turbulence model
Particle collision model
Thermodynamics and transport properties
Model development
T1: Detonation model sensitivity analysis
T5: Compaction model*
T6,T7: Finite Re, Ma and volume fraction model*
T8: Particle deformation and fragmentation model
Detonation model
Compaction model
Finite Re, Ma and volume fraction model
Particle deformation and fragmentation model
*Large uncertainty
Characterization
Microscale
Mesoscale
Macroscale
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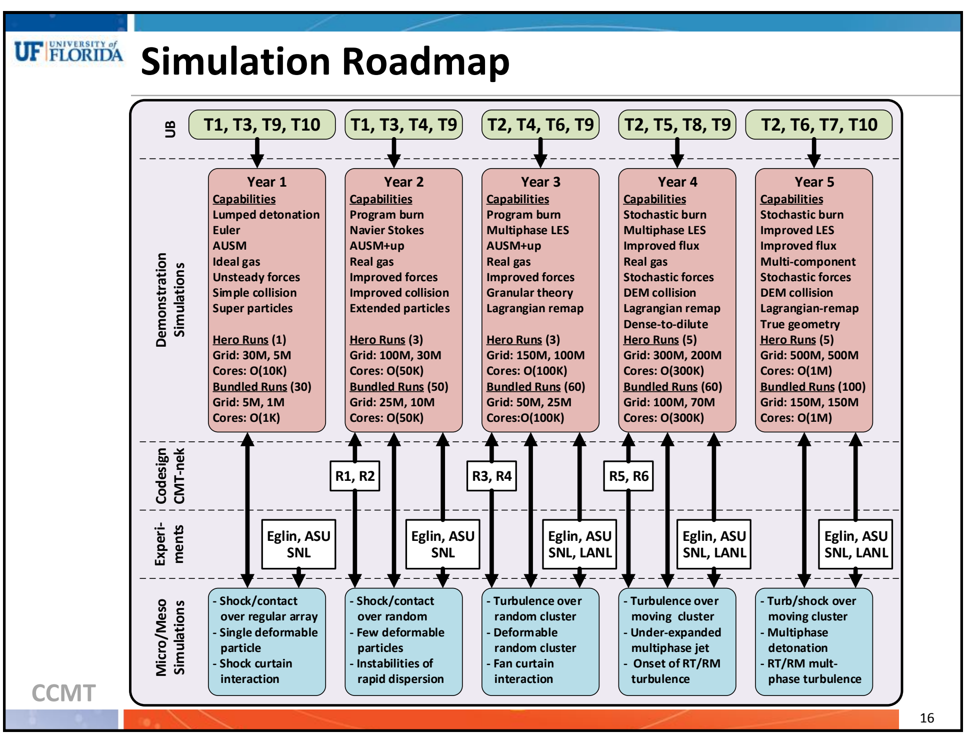
Simulation Roadmap
UB
T1, T3, T9, T10
T1, T3, T4, T9
T2, T4, T6, T9
T2, T5, T8, T9
T2, T6, T7, T10
Demonstration Simulations
Year 1
Capabilities
Lumped detonation
Euler
AUSM
Ideal gas
Unsteady forces
Simple collision
Super particles
Hero Runs (1)
Grid: 30M, 5M
Cores: O(10K)
Bundled Runs (30)
Grid: 5M, 1M
Cores: O(1K)
Year 2
Capabilities
Program burn
Navier Stokes
AUSM+up
Real gas
Improved forces
Improved collision
Extended particles
Hero Runs (3)
Grid: 100M, 30M
Cores: O(50K)
Bundled Runs (50)
Grid: 25M, 10M
Cores: O(50K)
Year 3
Capabilities
Program burn
Multiphase LES
AUSM+up
Real gas
Improved forces
Granular theory
Lagrangian remap
Hero Runs (3)
Grid: 150M, 100M
Cores: O(100K)
Bundled Runs (60)
Grid: 50M, 25M
Cores:O(100K)
Year 4
Capabilities
Stochastic burn
Multiphase LES
Improved flux
Real gas
Stochastic forces
DEM collision
Lagrangian remap
Dense-to-dilute
Hero Runs (5)
Grid: 300M, 200M
Cores: O(300K)
Bundled Runs (60)
Grid: 100M, 70M
Cores: O(300K)
Year 5
Capabilities
Stochastic burn
Improved LES
Improved flux
Multi-component
Stochastic forces
DEM collision
Lagrangian-remap
True geometry
Hero Runs (5)
Grid: 500M, 500M
Cores: O(1M)
Bundled Runs (100)
Grid: 150M, 150M
Cores: O(1M)
Codesign CMT-nek
R1, R2
R3, R4
R5, R6
Experi-ments
Eglin, ASU SNL
Eglin, ASU SNL
Eglin, ASU SNL, LANL
Eglin, ASU SNL, LANL
Eglin, ASU SNL, LANL
Micro/Meso Simulations
- Shock/contact over regular array
- Single deformable particle
- Shock curtain interaction
- Shock/contact over random
- Few deformable particles
- Instabilities of rapid dispersion
- Turbulence over random cluster
- Deformable random cluster
- Fan curtain interaction
- Turbulence over moving cluster
- Under-expanded multiphase jet
- Onset of RT/RM turbulence
- Turb/shock over moving cluster
- Multiphase detonation
- RT/RM mult-phase turbulence
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Demonstration Simulations

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

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

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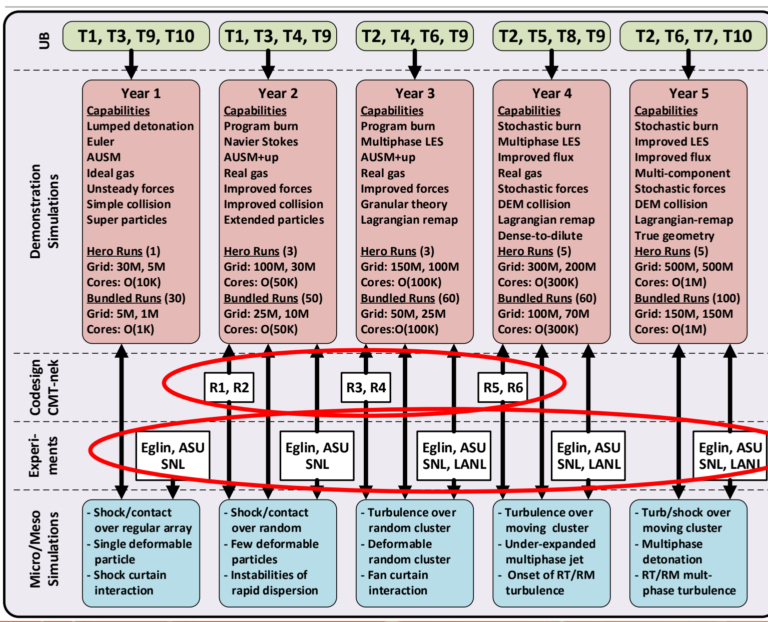
Simulation Roadmap



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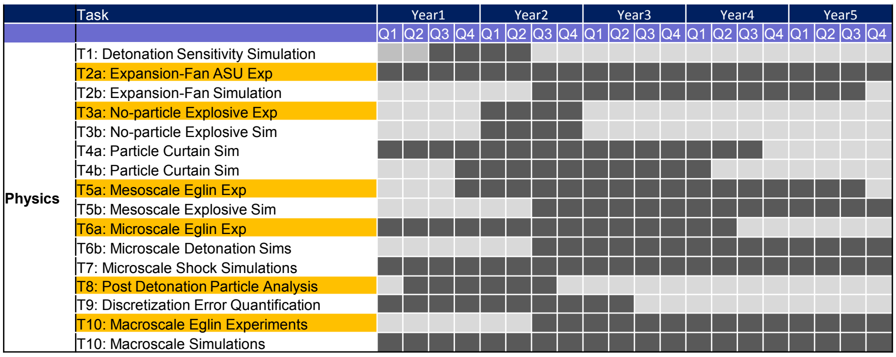
Timeline: T1-T10 Uncertainty Reduction



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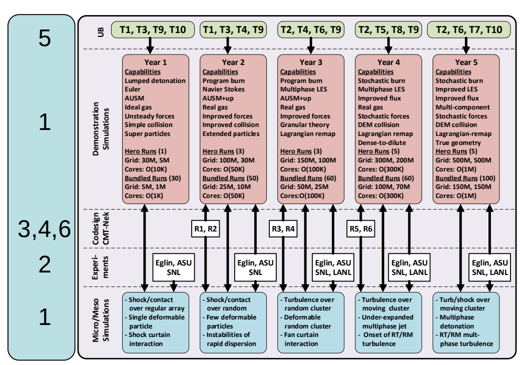
Year 1.5 Key Accomplishments

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



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1: Demonstration Problem (Macroscale)

Goal

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

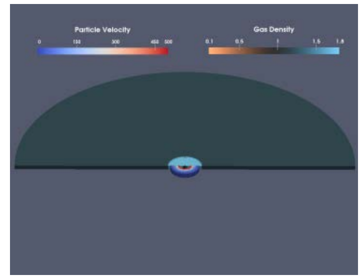
Year 1.5

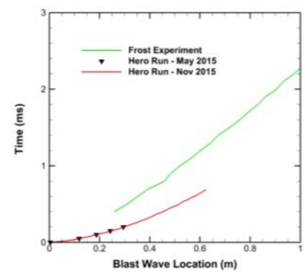
- Use existing code to perform petascale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)
- Develop capabilities for the next hero run: real gas EOS, AUSM+up, collision modeling

Presentation

- Subbu Annamalai

3-D demonstration Simulations





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1: Mesoscale Simulations

Goal

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

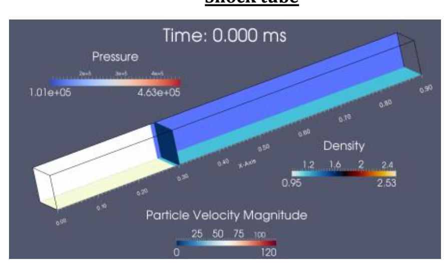
Year 1.5

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

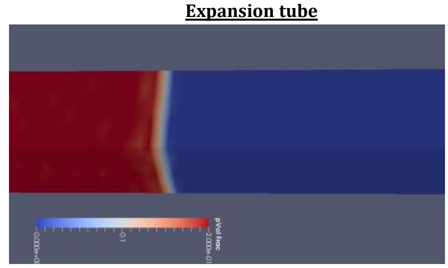
Presentation

- Bertrand Rollin

Shock tube



Expansion tube



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1: Microscale Simulations

Goals

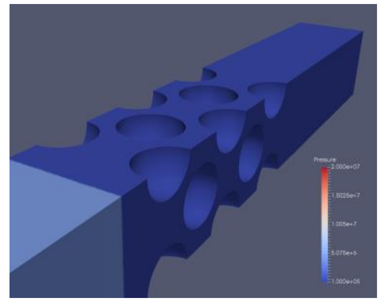
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation to the demonstration problem

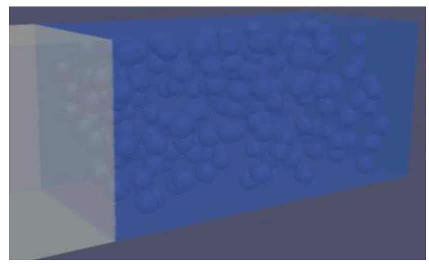
Year 1.5

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

Presentation

- Christopher Neal





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1: Microscale Simulations

Goals

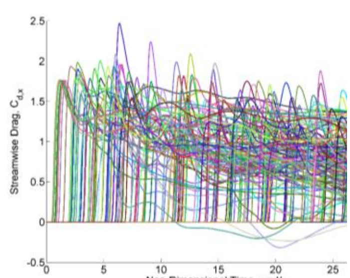
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation to the demonstration problem

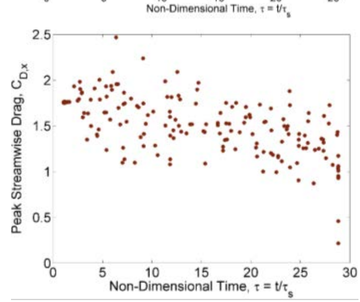
Year 1.5

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

Presentation

- Christopher Neal





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1: New Point-Particle Framework

Goals

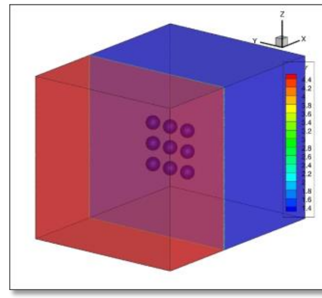
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation to the demonstration problem

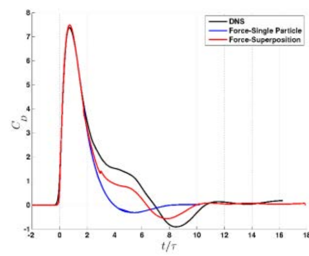
Year 1.5

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

Presentation

- Yash Mehta





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2: Validation Experiments

Goals

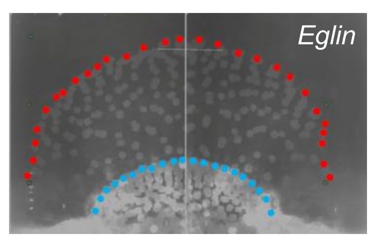
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

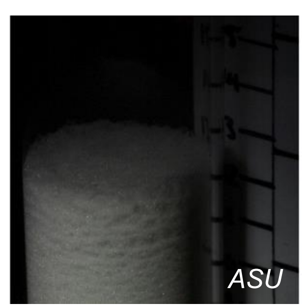
Year 1.5

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

Presentation

- Heather Zunino (ASU)





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3: CMT-nek Development

Goals

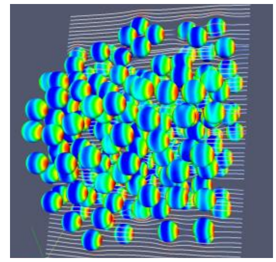
- Co-design an exascale code (CMT-nek) for compressible multiphase turbulence
- Perform micro, meso and demonstration-scale simulations
- Develop & incorporate energy and thermal efficient exascale algorithms

Year 1.5

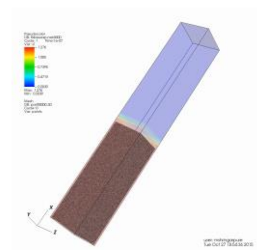
- Develop and release first version of CMT-nek for microscale simulations
- Develop and release first version of CMT-nek for mesoscale simulations
- CMT-bone development
- CMT-nek in nek5000 repository

Presentation

- Mrugesh Shringarpure and Jason Hackl



Micro simulation - 4000 MPI ranks



11520 elements, LX1=15, 1
2 million particles, 7680 MPI ranks

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3: CMT-bone Development

Goals

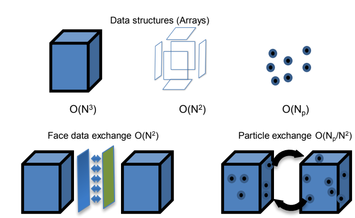
- Co-design an exascale code (CMT-nek) for compressible multiphase turbulence
- Perform micro, meso and demonstration-scale simulations
- Develop & incorporate energy and thermal efficient exascale algorithms

Year 1.5

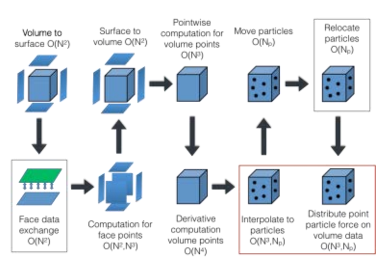
- Develop and release first version of CMT-nek for microscale simulations
- Develop and release first version of CMT-nek for mesoscale simulations
- CMT-bone development
- CMT-nek in nek5000 repository

Presentation

- Mrugesh Shringarpure and Jason Hackl



Data-types, kernels & workflow



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4: Energy & Thermal Aware Computing

Goal

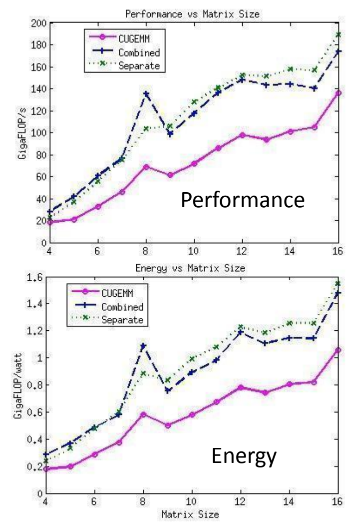
- Derive computationally intensive portions of the CMT-nek code and understand its performance, thermal and energy issues

Year 1.5

- Carried out extensive investigation of performance and energy issues for CMT-bone kernels using CHILL and Genetic algorithm
- Optimization of kernels on CPU-GPU hybrid architecture

Presentation

- Tania Banerjee & Sanjay Ranka



GPU performance and energy of CMT-bone

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5: Uncertainty Budget

Goals

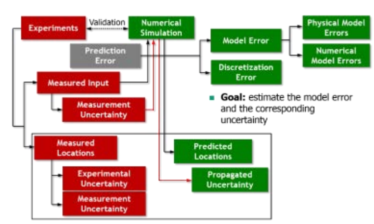
- Develop UB as the backbone of the Center
- Unified application of UB for both physics and exascale emulation

Year 1.5

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

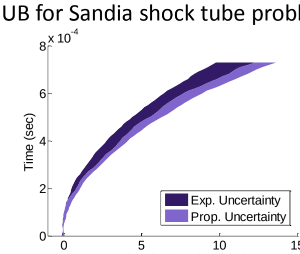
Presentation

- Rafi Haftka, Chanyoung Park, Yiming Zhang



UQ Framework

UB for Sandia shock tube problem



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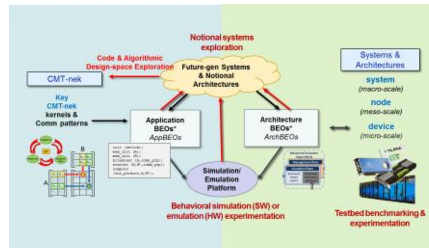
6: Exascale Emulation

Goal

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

Year 1.5

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



Presentation

- Herman Lam, Greg Stitt, Nalini Kumar, Carlo Pascoe, Dylan Rudolph, Kasim Alli

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Major Goals For Next Year

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

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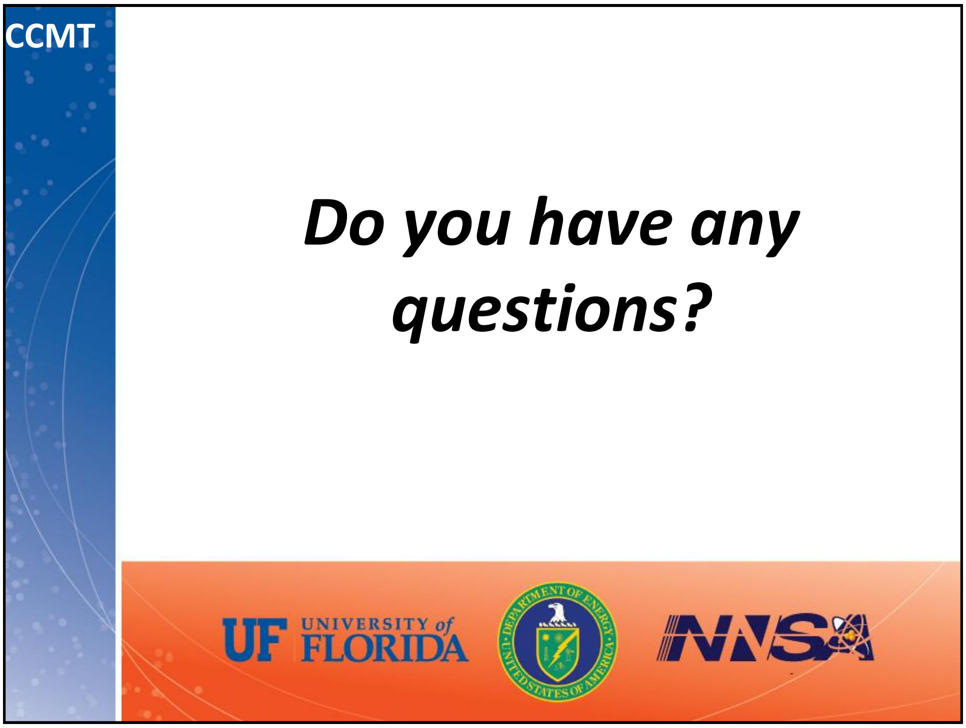
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Do you have any questions?
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NNSA

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Macroscale and Mesoscale Simulations of Compressible Multiphase Turbulence (CMT)

Subramanian Annamalai
Bertrand Rollin

CMT in Explosive-Driven Particle-Laden Flows

Sarychev peak (source: wikipedia)

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

- Bring predictive capabilities to particle-laden flow simulations

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Goals

- Hero runs
  - Continue scaling up simulations
- UQ Team – Macro-Meso Team collaboration
  - Perform mesoscale uncertainty quantification
- Macro-Meso integration (multi scale approach)
  - Progressively improve macroscale modeling via mesoscale physics

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Outline

Macroscale:

- Hero run

Mesoscale:

- Real gas equation of state (JWL)
- Exploration of a surrogate model for EoS
- Updated numerical scheme: AUSM+up
- Preliminary mesoscale study:
  - 3D SNL's experiment
  - Wall gap effect SNL's experiment
  - ASU's experiment

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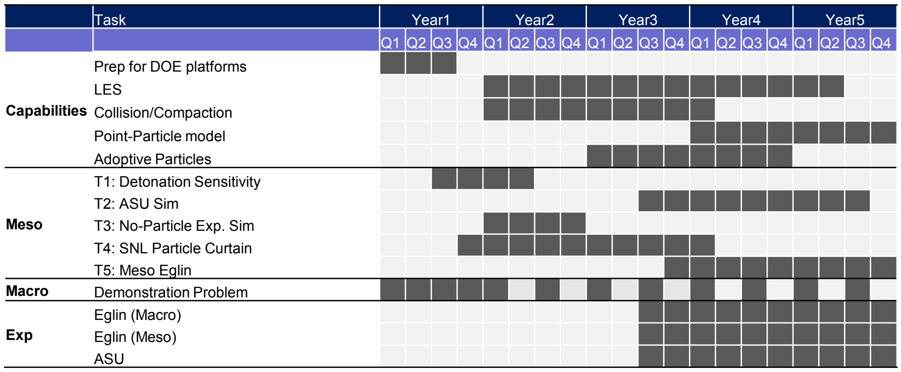
Macro/Mesoscale Gantt Chart



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Outline

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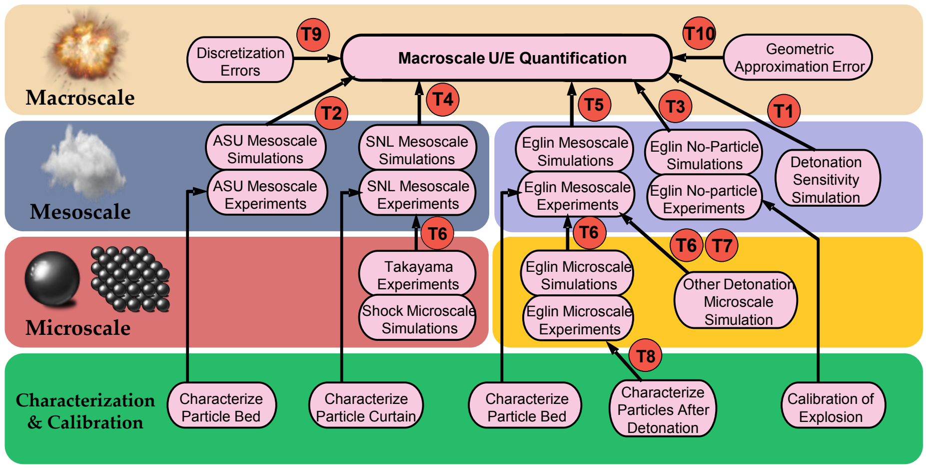
Demonstration Problem



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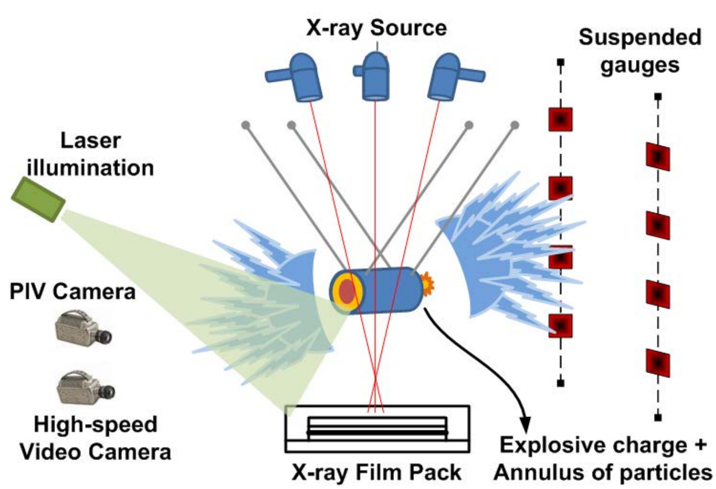
CCMT's Demonstration Problem



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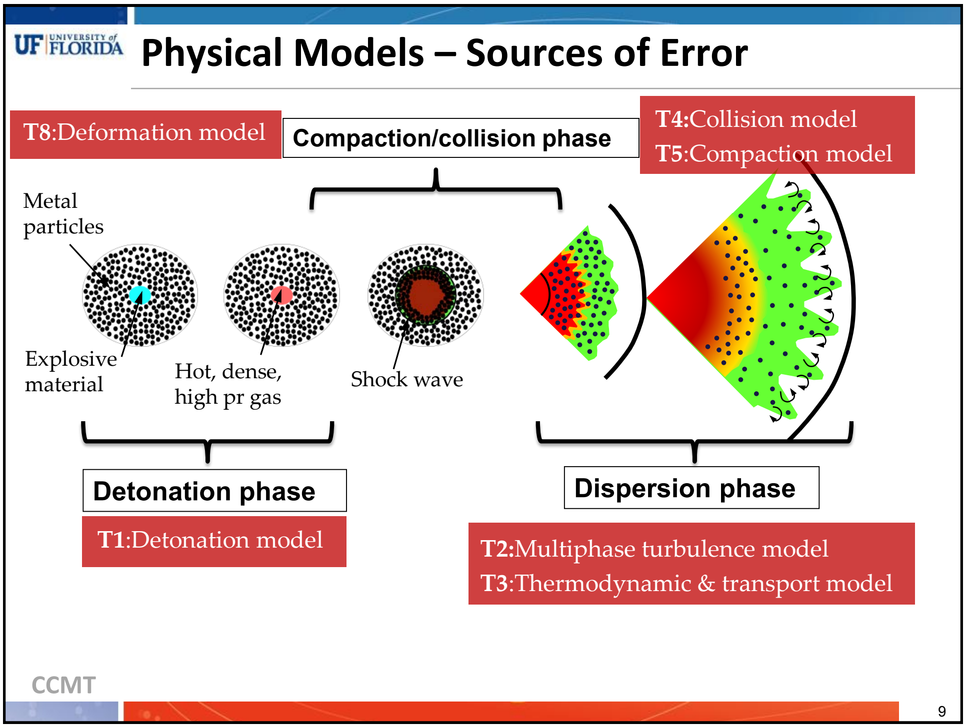
Physical Models – Sources of Error
T8:Deformation model
Compaction/collision phase
T4:Collision model
T5:Compaction model
Metal particles
Explosive material
Hot, dense, high pr gas
Shock wave
Detonation phase
T1:Detonation model
Dispersion phase
T2:Multiphase turbulence model
T3:Thermodynamic & transport model
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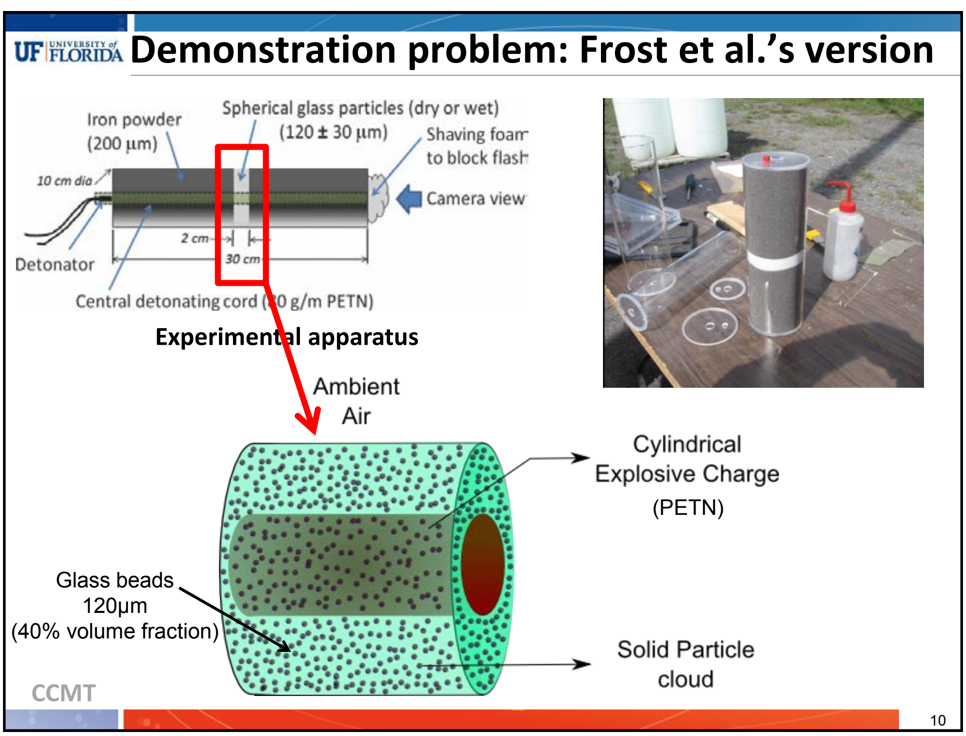
Demonstration problem: Frost et al.'s version
Iron powder (200 μm)
Spherical glass particles (dry or wet) (120 ± 30 μm)
Shaving foam to block flash
10 cm dia
Camera view
2 cm
30 cm
Detonator
Central detonating cord
Experimental apparatus
Ambient Air
Cylindrical Explosive Charge (PETN)
Glass beads 120μm (40% volume fraction)
Solid Particle cloud
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High Speed Video of an Explosive Dispersal of Particles

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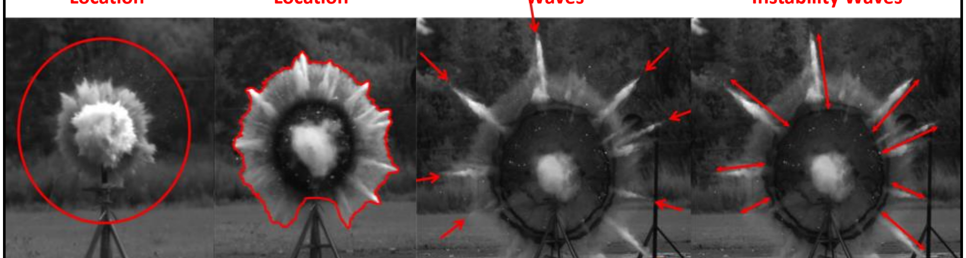
Prediction Metrics

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



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Major Challenges

- "Rigidity" of input for particles ✓
- Rocflu IO incompatible to the size of our cases
- Rocflu memory leak preventing successful run on Vulcan ✓
- Rocflu unadapted post-processing strategy
- Initialization slowness due to bug and extreme memory requirement ✓
- Inability to have a random distribution of particle ✓
- Parallel partitioning
- Limited performance on BG/Q platform

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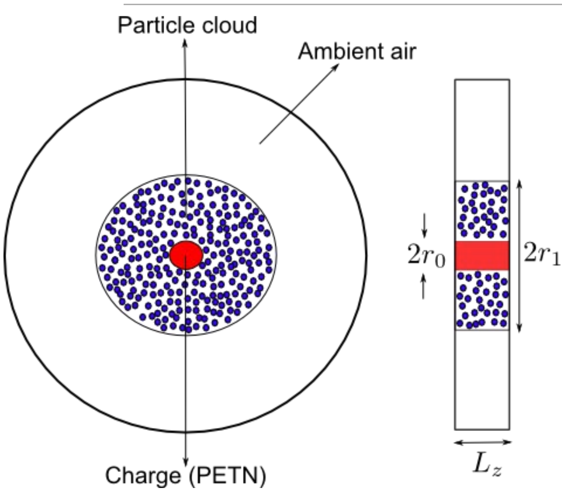
Simulation Description



Parameter	Value
ρ_B^{HE}	1770 kgm^{-3}
ρ_B^{Air}	1.203 kgm^{-3}
ρ^p	2500 kgm^{-3}
ϕ_B^p	5 %
r_0	3.8 mm
r_1	5 cm
L_z	2 cm
N^{cp}	5 x 10^6

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

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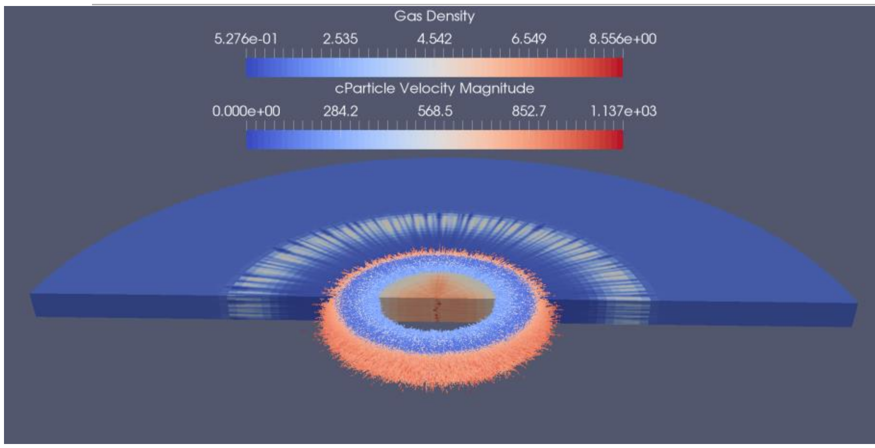
Demonstration Problem: Simulation



- Features:
  - 30 Million computational cells
  - 5 Million computational particles
  - r_{max} = 4.00m
  - t_{max} = 0.80ms
  - 4096 cores

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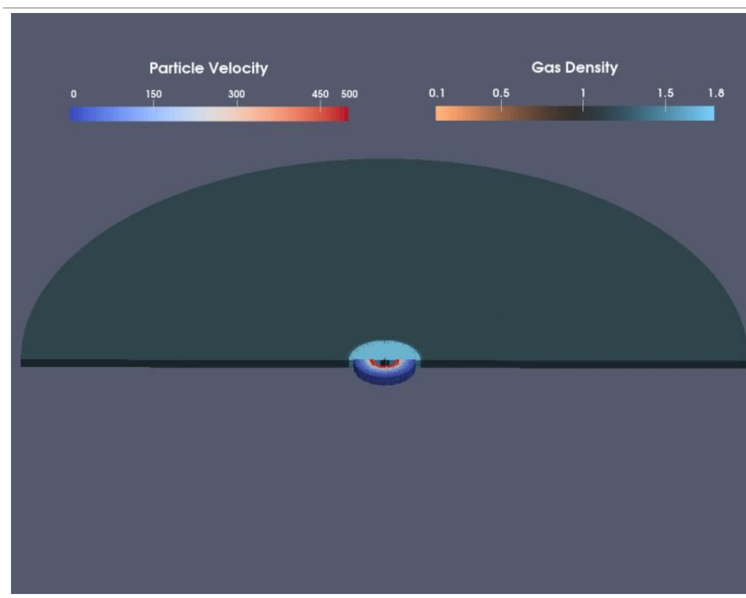
Demonstration Problem: Simulation



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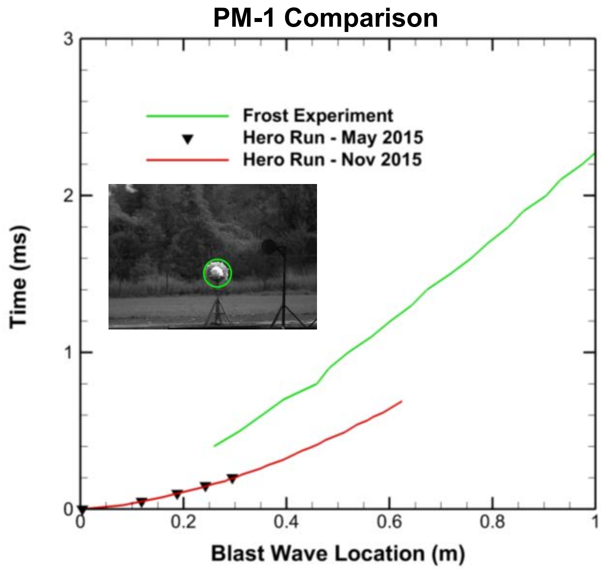
Demonstration Problem: Predictions



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

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

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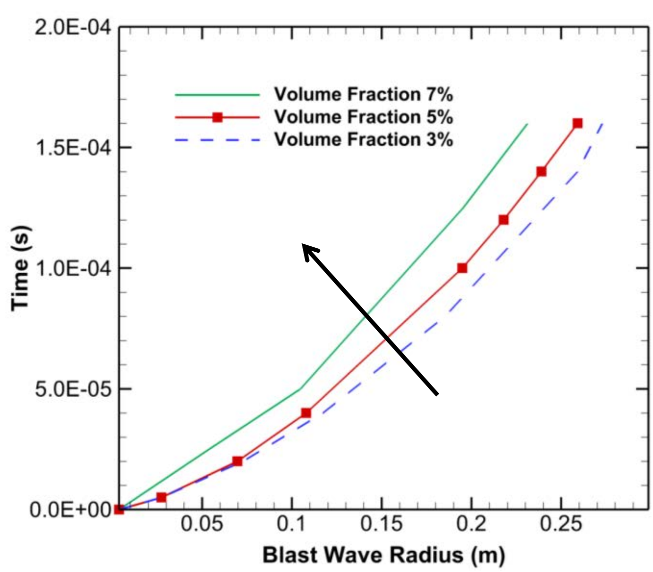
Particle Volume Fraction Effect on Blast Wave



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

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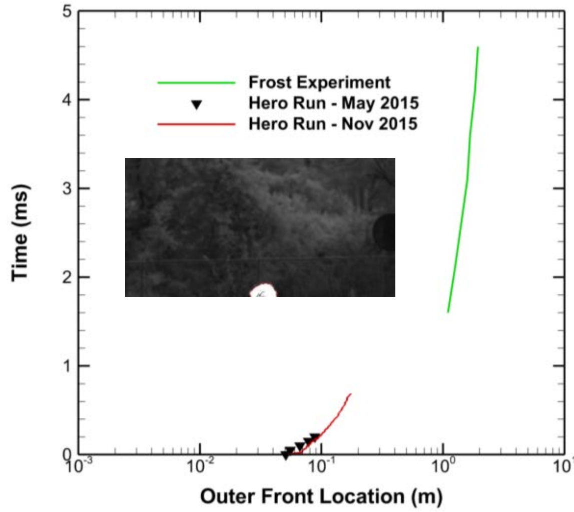
Demonstration Problem: Predictions

PM-2 Comparison



- Data from Frost experiment video starts at 1.500 milliseconds
- Possible sources of discrepancy: EoS, initial particle volume fraction, ...

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

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Outline

Macroscale:

- Hero run

Mesoscale:

- Real gas equation of state (JWL)
- Exploration of a surrogate model for EoS
- Updated numerical scheme: AUSM+up
- Preliminary mesoscale study:
  - 3D SNL's experiment
  - Wall gap effect SNL's experiment
  - ASU's experiment

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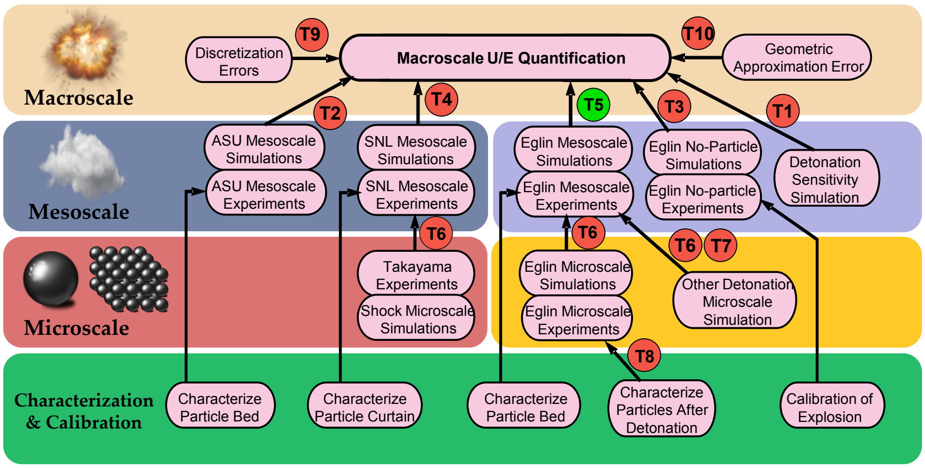
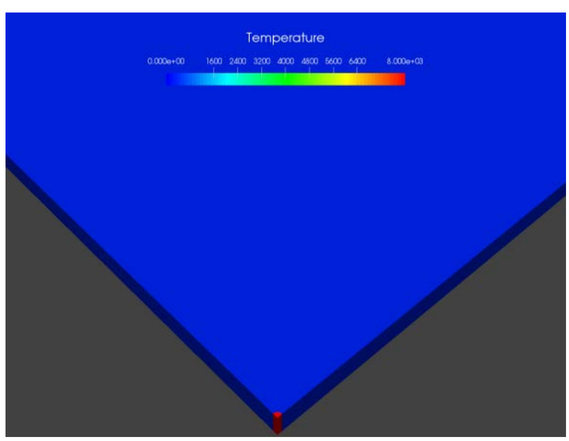
T5: Mesoscale explosive dispersal of particles simulations



Mesoscale Detonation – Ideal Gas



Experimental results show that the detonation temperature of single crystal PETN is approximately 4100 K

A real gas equation of state is needed to improve the simulation

JWL Equation of State

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

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

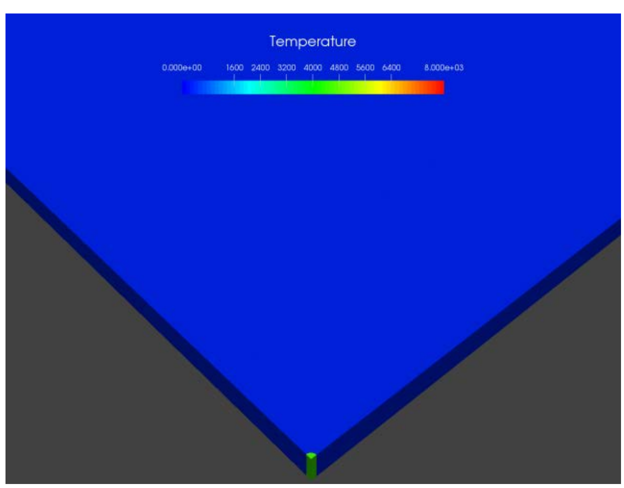
$$T_{JWL}(P, \rho) = \left(\frac{1}{\rho \omega C_v}\right)\left(P - Ae^{-R_1 V} - Be^{-R_2 V}\right)$$

where $V = \frac{\rho_o}{\rho}$, ρ_o, A, B, C, R_1, R_2 and ω are input parameters

- Implementation for mixed cells:
  - Mixed air/product cells need to have pressure and thermal equilibrium
  - This is done by an iterative process between the equations of state
  - Inputs: Mixture density, mixture energy, product mass fraction
  - Outputs: Pressure, Temperature

This implementation is costly in terms of computation time on large grids

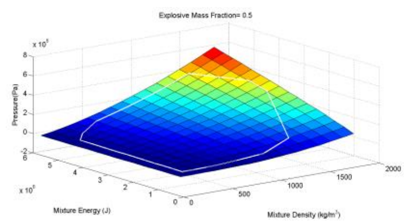
Mesoscale Detonation - JWL

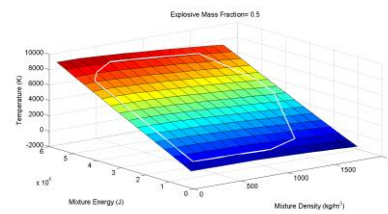


Note that the detonation temperature here is much closer to the experimental results

Surrogate Model for Mixed-Cell JWL

- A surrogate model was developed for use in the pressure/temperature update
- The model was developed by generating a sample solution space from 40 input triplets and then fitting a surrogate to pressure and temperature
  - The initial set of input triplets was found to contain physically unrealizable points
  - Solution was to take the range of pressures and temperatures we believed were possible during the detonation and work in reverse to get the inputs
  - Then, a convex hull of the possible input space was created and placed into the model
- This model removes the need for iterating between the equations of state
  - This approach will save more computational time as the number of species in the problem increases
- More details on this can be found in the UQ team presentation





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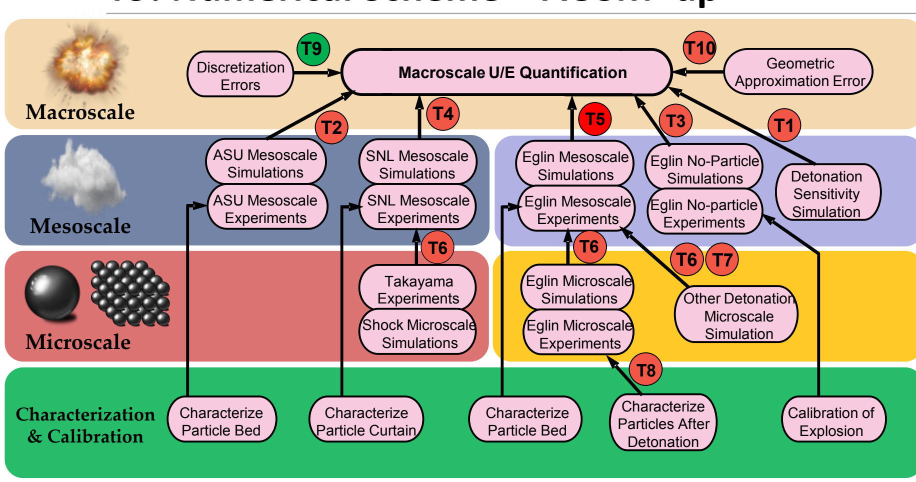
T9: Numerical Scheme – AUSM+up



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AUSM+up Motivation

- Single-phase flux computation scheme introduces oscillations/discontinuities where volume fraction changes
- Multiphase flux scheme should be used for multiphase flow simulations
- Formulated Eulerian-Lagrangian framework of the original Eulerian-Eulerian based multiphase AUSM+up scheme

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AUSM+up for Eulerian-Lagrangian

Eulerian-Lagrangian formulation requires:

- Balanced gas phase pressure flux:
  - Eulerian-Eulerian balances mixture pressure flux
  - Eulerian-Lagrangian requires balance of the gas phase
  - Particle-based volume fraction calculation is key
- Consistent force and heat transfer terms:
  - Particle force and heat transfer must be fed back to gas
  - Hyperbolicity term for gas must be fed forward to particles
- Dependent variable decoding step:
  - Eulerian-Eulerian assumes fluid-fluid, simultaneously solve for pressure and volume fraction
  - Eulerian-Lagrangian finds volume fraction directly from particles
- Interface speed of sound

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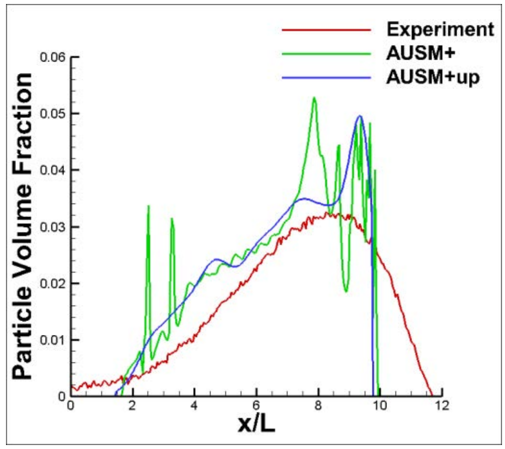
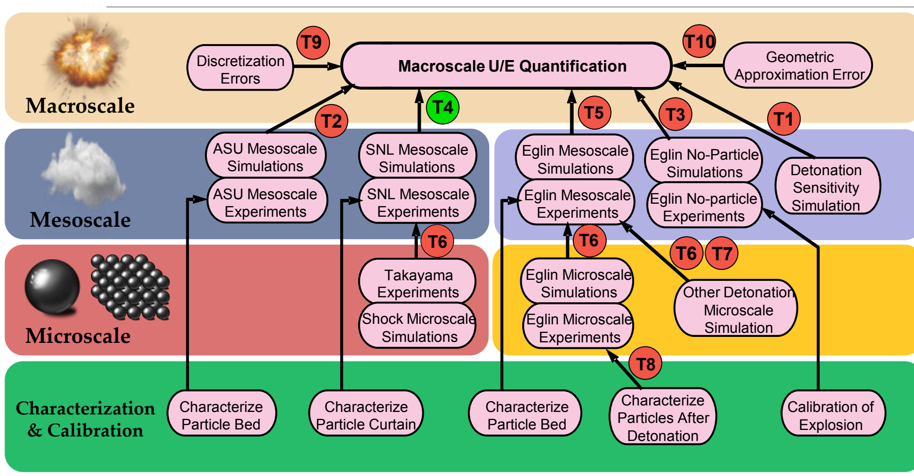
Comparison: AUSM+ vs. AUSM+up

1D simulation of Sandia's Particle Curtain experiment at t=340µs



AUSM+up with improved volume fraction computation is necessary

T4: Shock – particle curtain simulations



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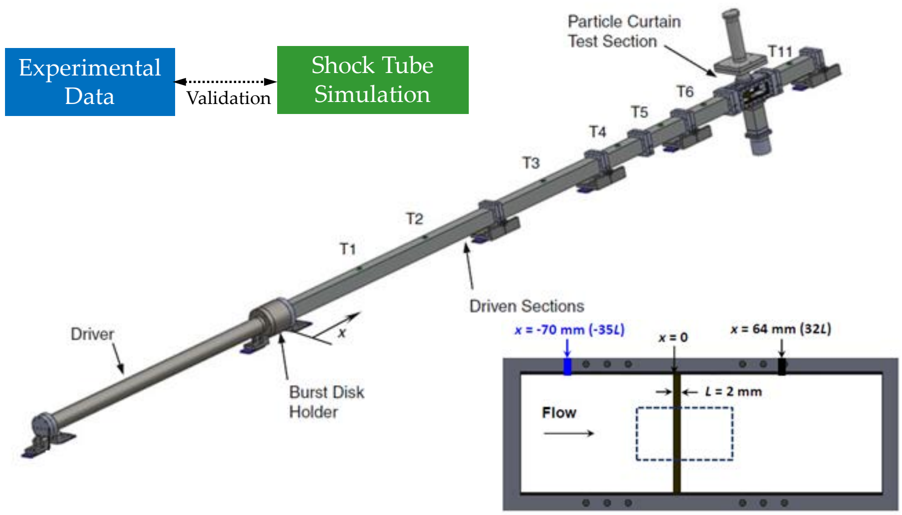
Mesoscale Validation: The Particle Curtain Problem

SNL Shock Tube – Justin Wagner



- Validation of the models for gas and particles interaction

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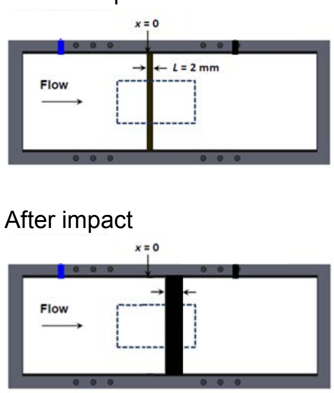
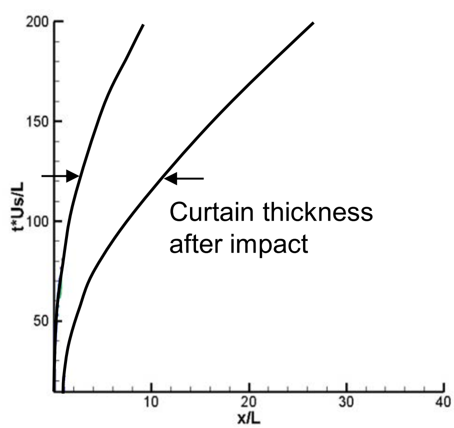
Prediction Metric

Before impact

After impact





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

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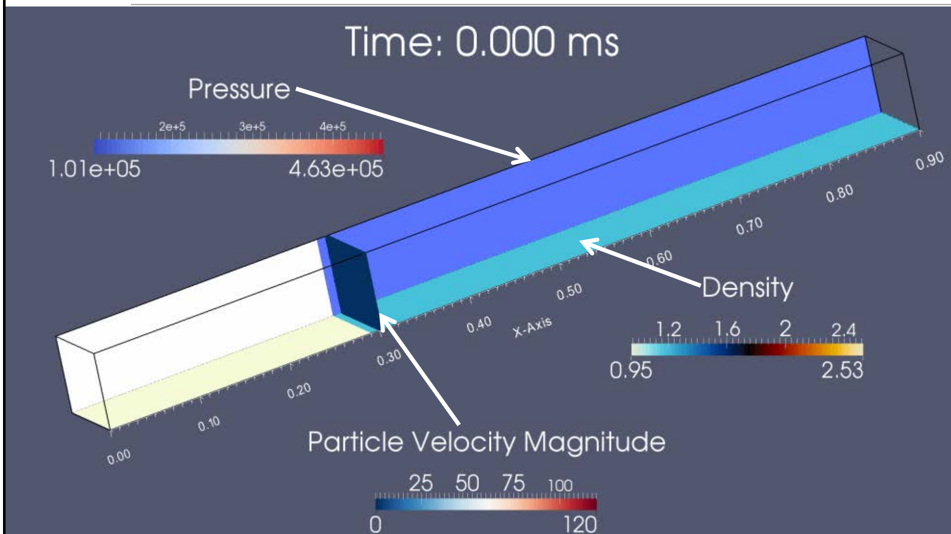
Particle Curtain Simulation



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

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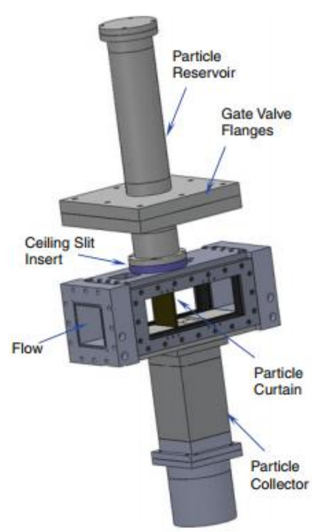
Mesoscale Validation: The Particle Curtain Problem

SNL Shock Tube – Justin Wagner



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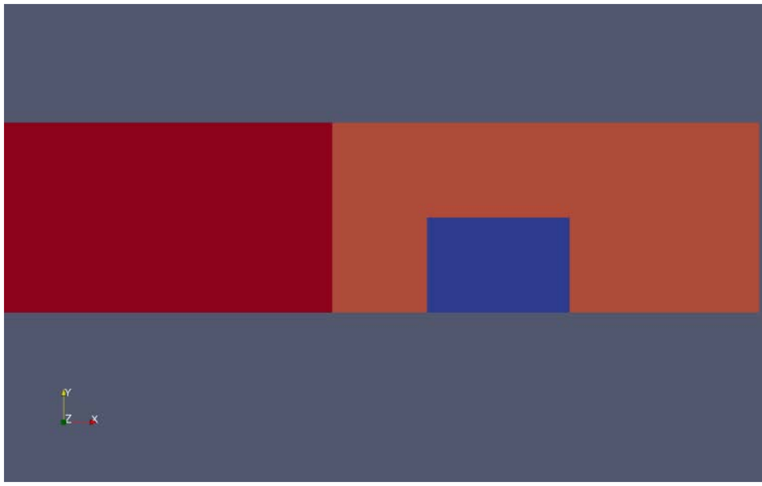
Half Height Gas Curtain problem



Rightmost position of SF6 significantly different between the top and bottom of the shock tube

How does a particle cloud evolve in a similar setting?

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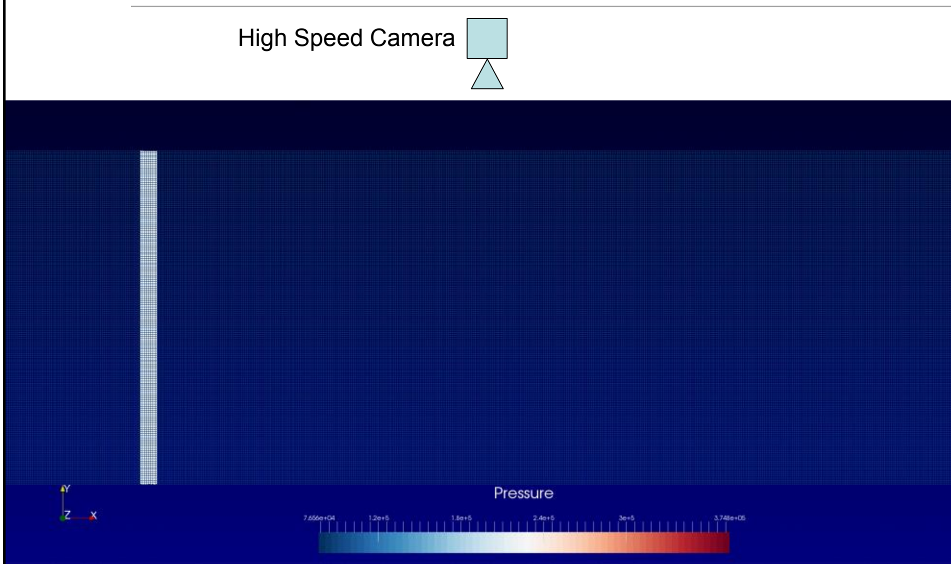
The Particle Curtain Problem Near the Wall



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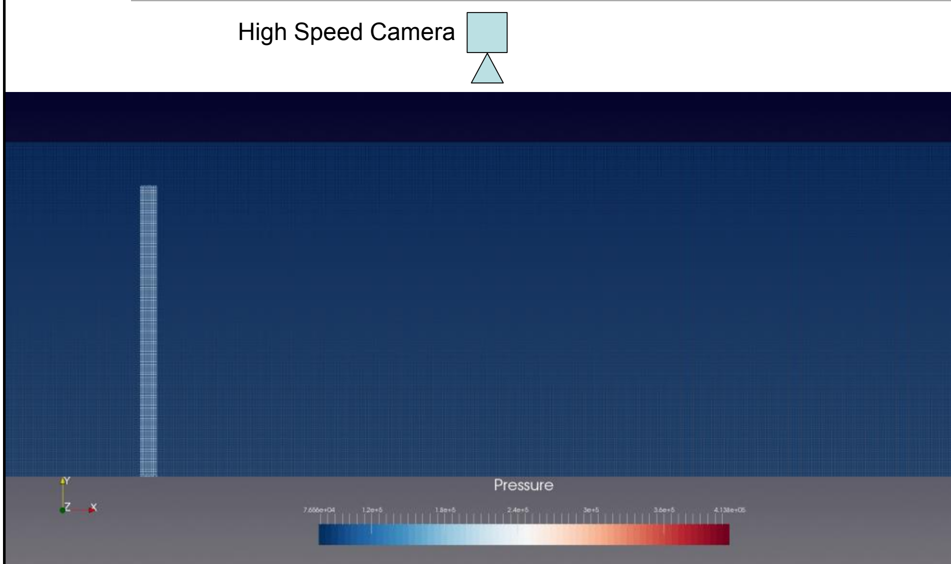
The Particle Curtain Problem Near the Wall



How opaque is the layer of particles near the top wall?

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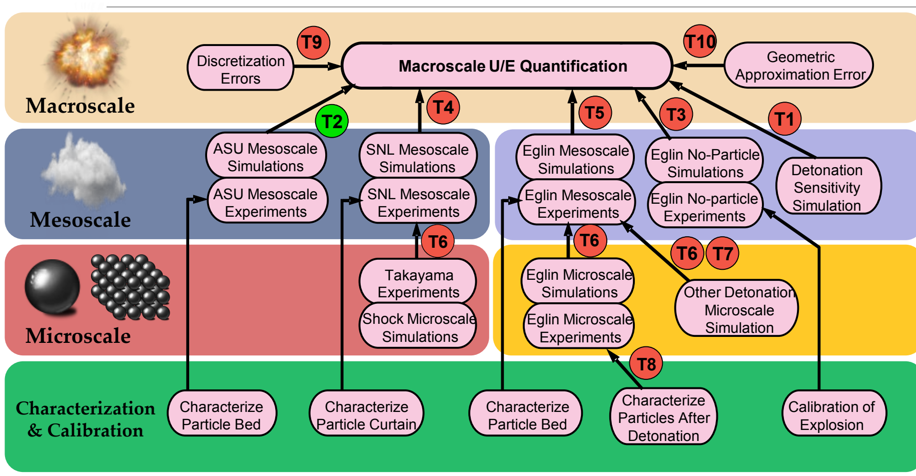
T2: Expansion fan – particles interaction simulations



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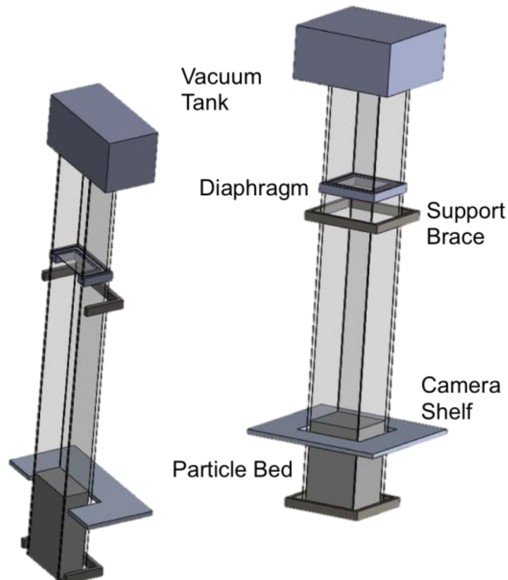
T2: Experimental Setup

ASU Vertical Shock Tube – Heather Zunino



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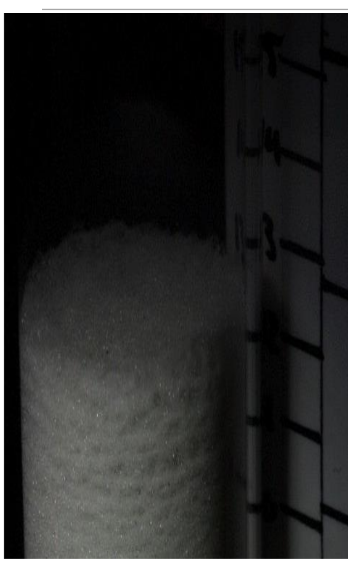
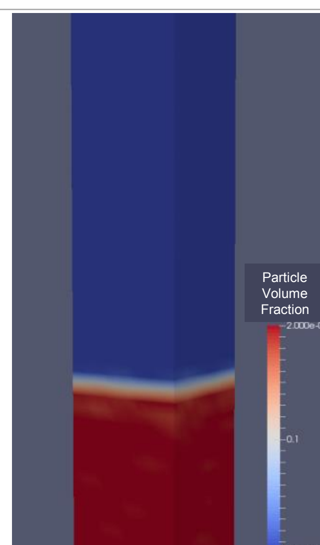
Particle Cloud - Expansion Fan Interaction





- Features: 20% particle volume fraction

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Future Work

- Code optimization on BG/Q
- Co-processing (Catalyst)

- Improved particle collision model
- Particle based volume fraction
- Compaction modeling
- Multiphase compressible LES

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Do you have any questions?

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Microscale Simulations

Siddharth Thakur, Chris Neal, Yash Mehta, Prashanth Shridharan

Microscale Team

Siddharth Thakur (ST)

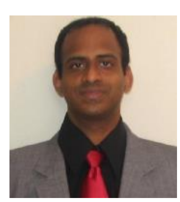
S. (Bala) Balachandar

Thomas Jackson

Ju Zhang

Christopher Neal

Yash Mehta



Prashanth Sridharan

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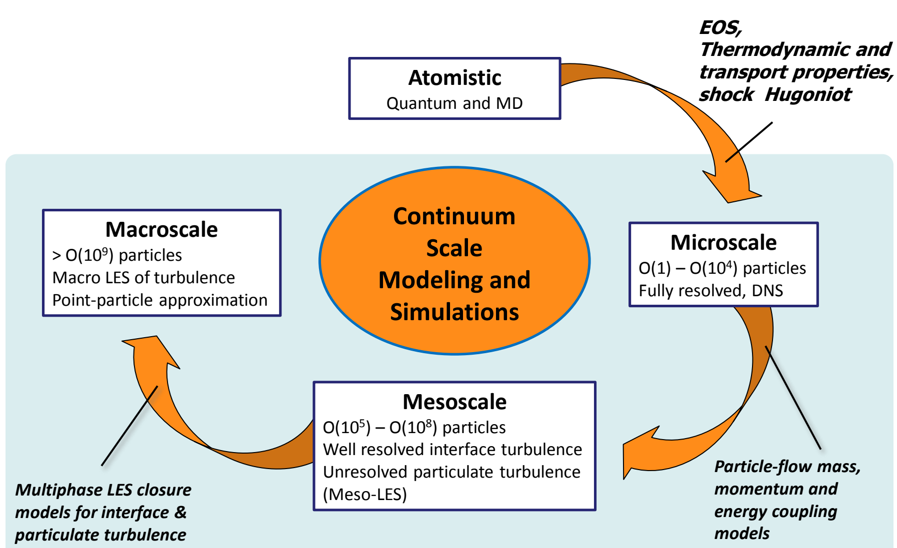
Goal of Microscale Simulations

- Fully Resolved Simulations of
  - Structured arrangements of particles
  - Random arrangements of particles
  - Moving and deforming particles
- Develop state-of-the-art point-particle models to account for the effects of volume fraction, Mach number, Reynolds number on
  - Unsteady forces
  - Heat transfer
  - Velocity fluctuations

Multiscale Coupling



Key Accomplishments

- Studies of shock-particle interaction
  - Arrays
  - FCC
  - Random
- UQ-guided grid resolution studies for single and multiple particle simulations
- Improvements to current point-particle model for shock-particle interaction

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Gantt Organization Chart

	Task	Year1				Year2				Year3				Year4				Year5			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Simulation	Structured Stationary (FCC)																				
	Random Stationary																				
	Random Moving																				
	Deforming Particle																				
Model	Point-Particle Model Development																				
	Model Integration into Demonstration Problem																				
	UQ-Hybrid Surrogate Model																				
Integration	Catalyst integration																				
	Dakota Simulation Bundling																				

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Part 1: Structured Arrays

- Single particle simulations
- Limiting cases of FCC simulations
  - Horizontal array of particles
  - Transverse array of particles
- FCC array of particles
- UQ-guided grid resolution studies

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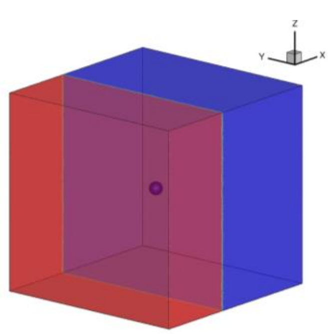
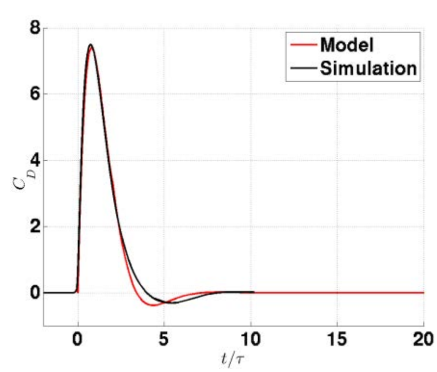
Single Particle Simulation $M_s = 1.22$

- Model comparison with DNS, without bow-shock effects





- Point particle model accurately predicts force on a single particle for sub-critical Mach number

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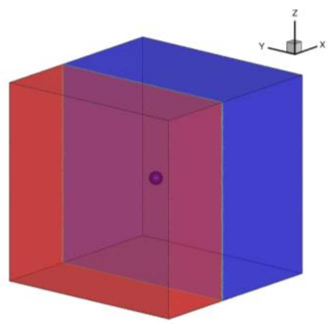
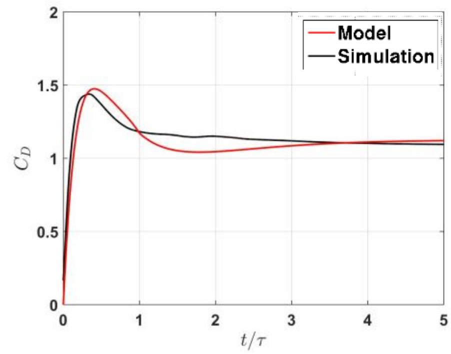
Single Particle Simulation $M_s = 6$

- Model comparison with DNS, with bow-shock effects present





- Model with numerical fit to include the effect of bow shock for supercritical Mach number

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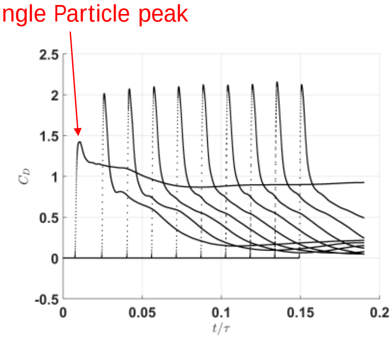
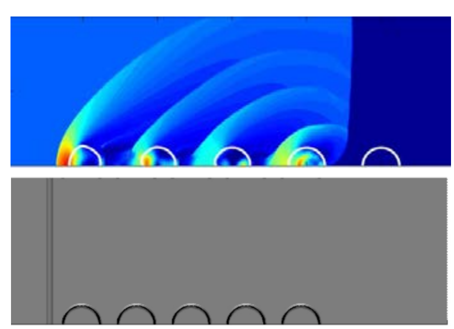
Effect of Particle Spacing: Horizontal Array

- Array of spherical particles aligned with flow direction

Single Particle peak



- Shock Mach number – 6.0



- Similar simulation was done with $M_s = 1.22$

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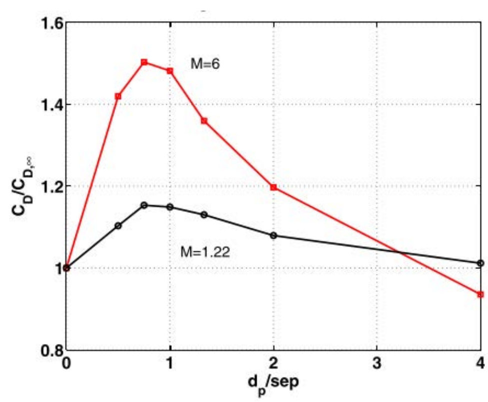
Effect of Particle Spacing: Horizontal Array

- Shock-particle dynamics at various inter-particle spacing
  - Peak drag coefficient increase is influenced by the incident shock Mach number and inter-particle spacing
  - Particles' peak drag coefficient has a maximum
  - Peak drag ratio drops below one as inter-particle spacing goes to zero



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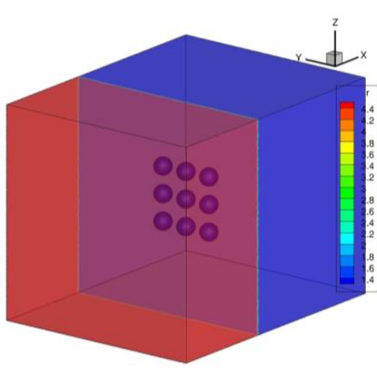
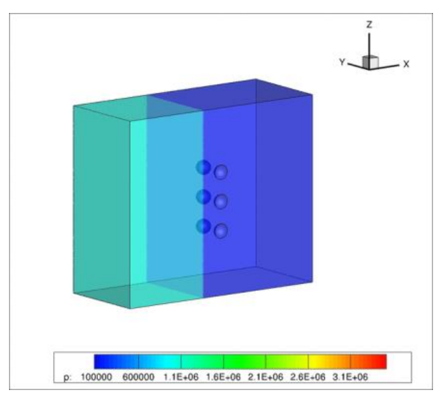
Transverse Array Simulation





Pressure contour along X-Z cut-plane

- Shock Mach numbers $M_s = 3.0$ and 6.0
- Particle spacing L/D = 1.2, 1.5, 2.0, 3.0, and 4.0

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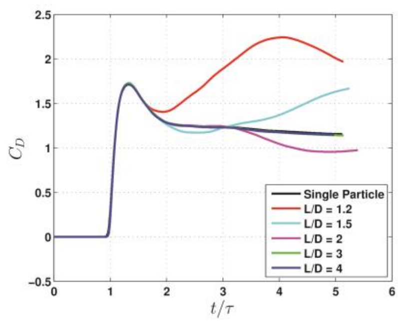
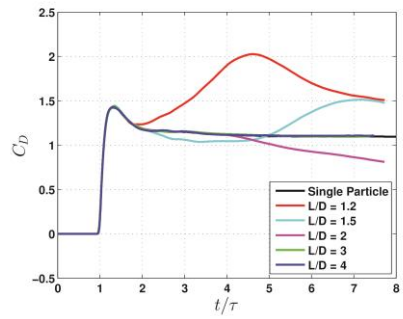
Transverse Array Simulation



Total force on the center particle for $M_s = 3.0$



Total force on the center particle for $M_s = 6.0$

- Effect of Mach number and the particle spacing on the force
- Force comparison against single particle

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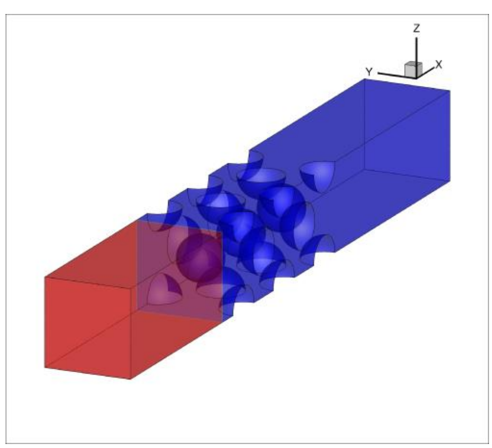
FCC Array (2 unit cells) Simulation



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FCC Array Simulations

- Simulation matrix for studying effects of volume fraction and Mach number on the drag

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

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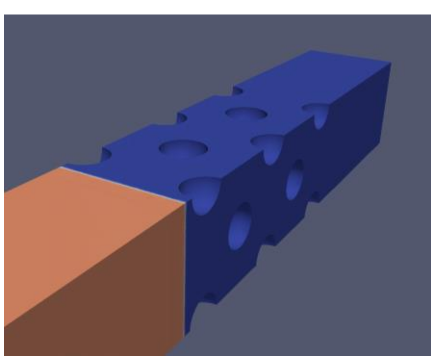
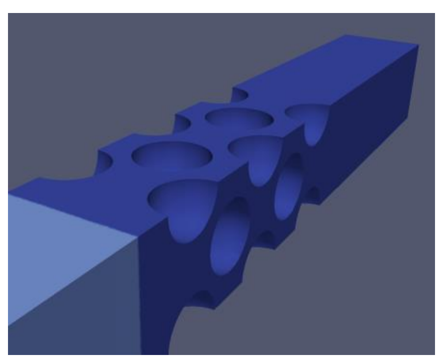
FCC Array Simulation



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



$M_s = 6.0\,;\ \varphi = 40\%$

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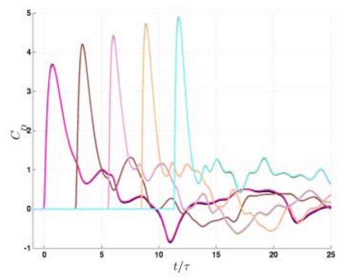
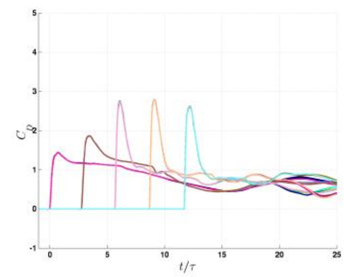
FCC - Effect of Mach number



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



$M_s = 6.0$ and $\varphi = 10\%$

- $M_s = 1.5$ shows same trend as horizontal array simulation
- For $M_s = 6.0$ peak force drops after 3rd particle – this is different form horizontal array simulation

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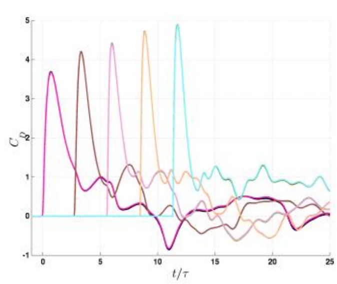
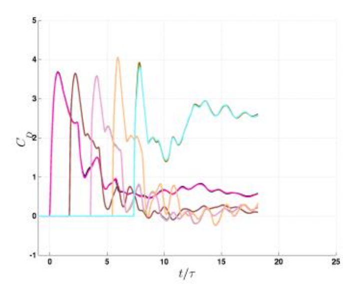
FCC - Effect of Volume-fraction



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



$M_s = 1.5$ and $\varphi = 40\%$

- $\varphi = 10\%$ shows same trend as horizontal array simulation
- $\varphi = 40\%$ does not show any standard trend for the peak force

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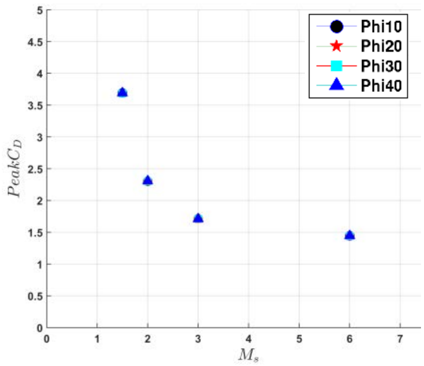
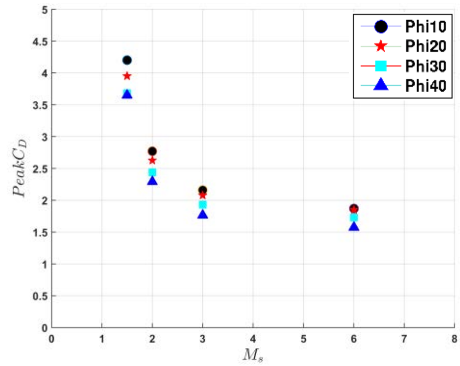
FCC – Peak Force

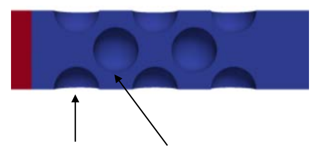


Plane 1



Plane 2

- There is no effect of volume fraction on the peak force for plane 1
- Effect of volume fraction is more prominent for downstream particles



Plane 1 Plane 2

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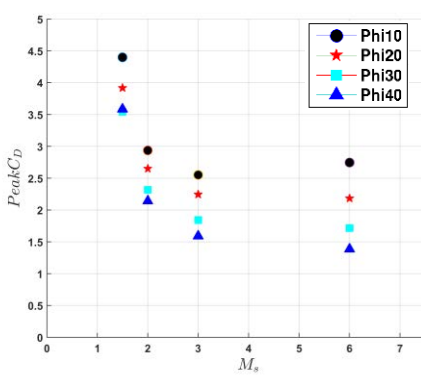
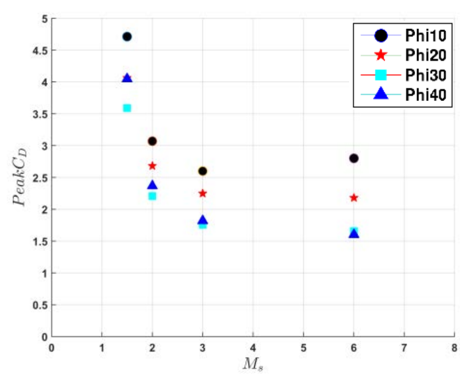
FCC – Peak Force

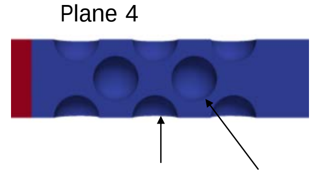


Plane 3



Plane 4

- For supercritical Mach bow shock is formed in front of particles
- Bow shocks causes dissipation of energy for lead shock and subsequent decrease in peak force



Plane 3 Plane 4

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FCC Grid Resolution Studies

- Collaborating with UQ team on this work

Simulation Matrix

Surface Mesh / Volume Mesh	110,000	82,000	70,000	57,000	43,000
30 million	RUN1	RUN6	RUN11	RUN16	RUN21
23 million	RUN2	RUN7	RUN12	RUN17	RUN22
18 million	RUN3	RUN8	RUN13	RUN18	RUN23
14 million	RUN4	RUN9	RUN14	RUN19	RUN24
6 million	RUN5	RUN10	RUN15	RUN20	RUN25

- Results will be presented by UQ team

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Structured Array - Summary

- Structured arrays give very different results compared to single particles
- There is strong effect of φ and Mach number
- These simulations provide an insight on effect of Mach number and ϕ and help in guiding random particle simulations
- Grid resolution studies for structured arrays will serve as benchmark for future simulations

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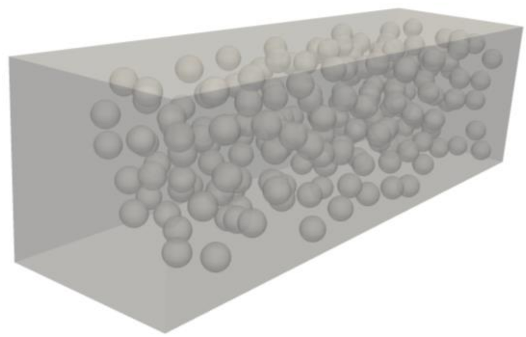
Part 2: Random Particle Packs



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Key Components

- Generate 3D Voronoi tessellations for the particles in the random particle packs to estimate local volume fraction & identify nearest neighbors
- Random particle pack simulations for different volume fraction & Mach number
- Framework for extracting information from the force & flow field data from the random particle pack simulations

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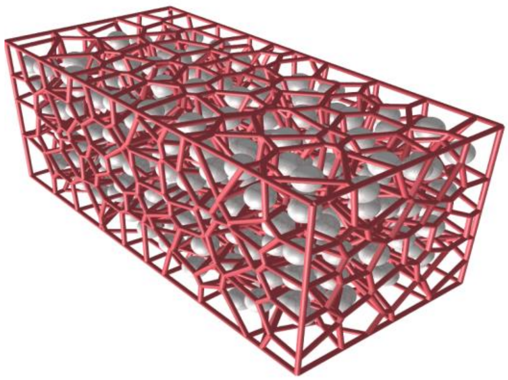
Random Pack Tessellation

- **Task**: Voronoi tessellation of random particle packs
- Commonly used for granular flow simulation analysis
  - Local volume fraction estimate
  - Nearest neighbors identification



Random Pack Tessellation

- Global volume fraction – 20%
- 400 spherical particles

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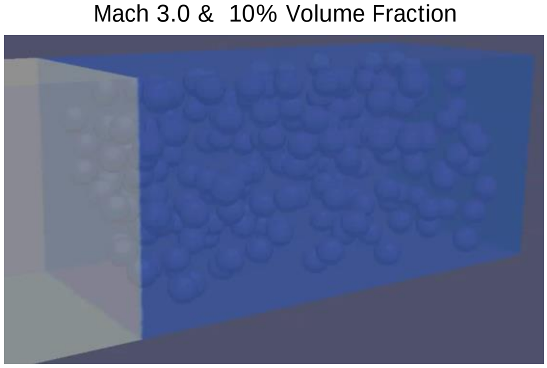
Random Pack Simulations

- **Task**: Perform 3D multi-particle simulations with randomly packed spherical particles

Mach 3.0 & 10% Volume Fraction



Volume Fraction	# Particles
10	200
20	300
30	400
40	500

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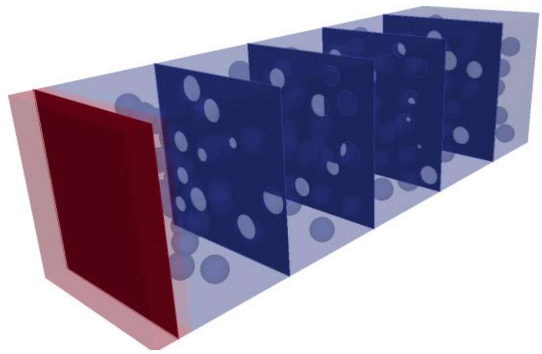
Random Pack Data Analysis

- **Task**: Develop a framework for extracting data from the flow field results of the random particle simulations
- Challenging to extract relevant information from data-rich 3D simulations
- Paraview was used to extract transverse averaged flow field quantities

Transverse Averaging Planes

- Global volume fraction – 10%
- 200 spherical particles



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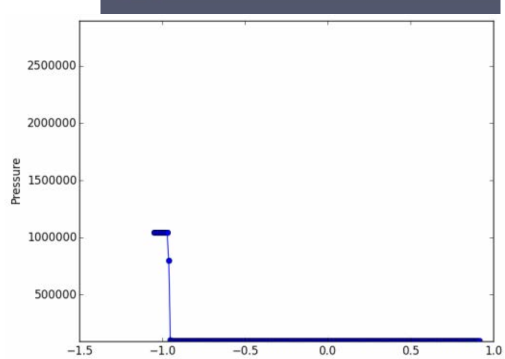
Random Pack Data Analysis

- Transverse averages allow us to see the average streamwise variations during shock interaction
- The shock front can be tracked as it moves through the particle bed using transverse averages
- The pack affects the behavior of the planar shock as it moves through the particle pack



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Random Pack Data

- Mach 3.0 shock traveling through the particle beds

ϕ =10%

ϕ =15%

ϕ = 20%

ϕ =25%

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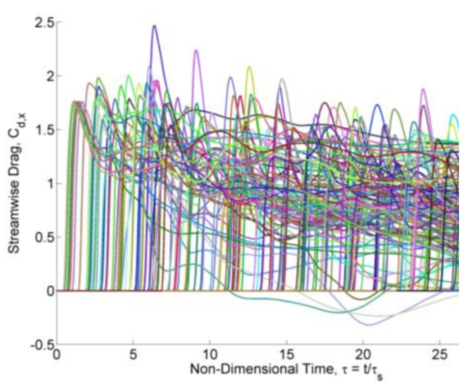
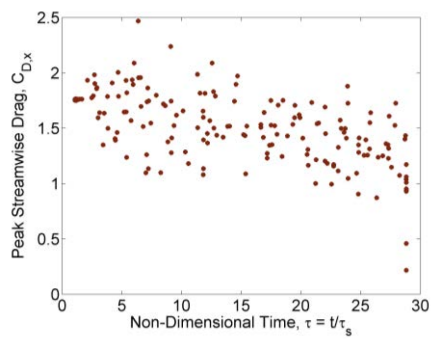
Random Pack Data

- Particle drag coefficients & peak drag coefficients within particle bed





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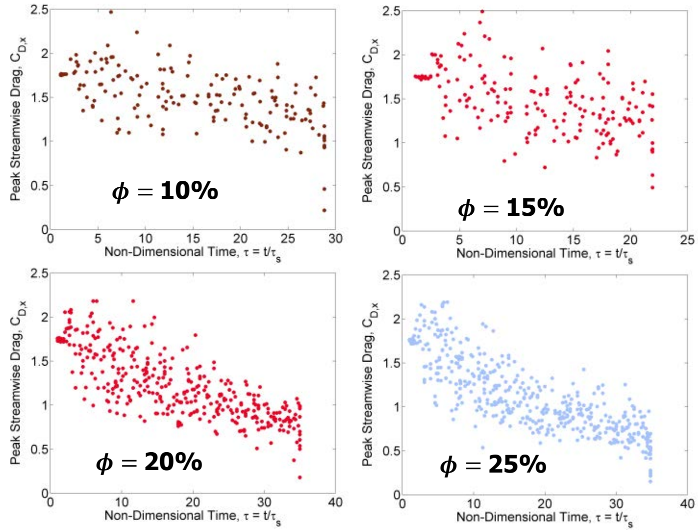
Random Pack Data

- Mach 3.0 shock traveling through particle bed



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Random Particle Packs - Summary

- Forces on particles are chaotic
- Volume fraction of bed does have a noticeable effect on shock
- Methods for descriptive analysis of data are still being produced
- There is an obvious need for information from simpler problems in order to understand the random particle packs

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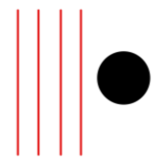
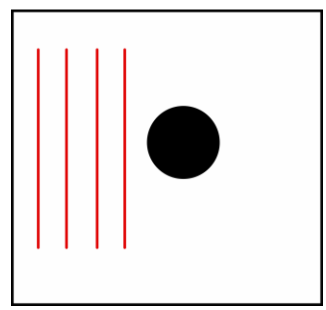
Part 3 : Point Particle Modeling

$$F(t) = ?$$





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

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Point Particle Model

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

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

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

Current Model (Generalized Faxen Theorem)

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

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

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

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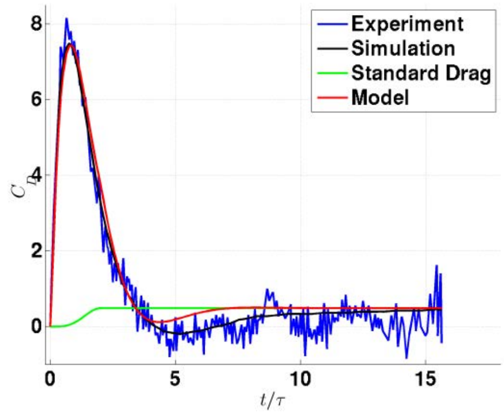
Point Particle Model



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

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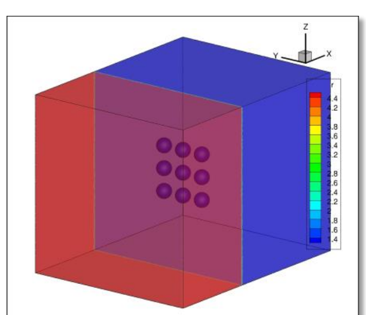
Point Particle Model

- We have state-of-the-art model to predict force on a single particle
- This model takes averaged velocity and density as an input
- How to obtain the force on a particle, when it is surrounded by other particles?
- We have a novel approach – **" Binary Superposition "**



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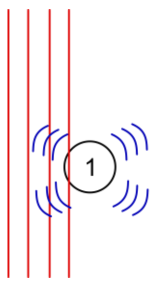
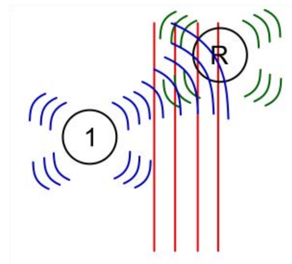
Binary Superposition





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

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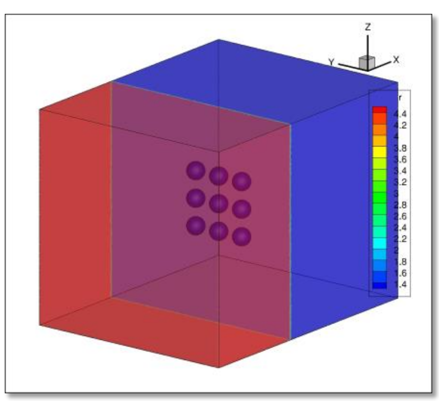
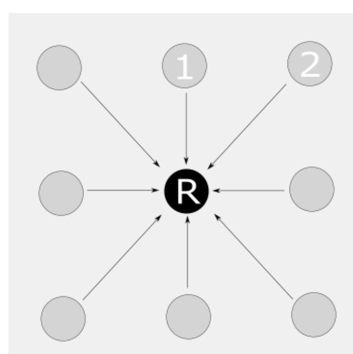
Binary Superposition





- Simulation for $M_s = 1.22$; $L/d_p = 1.5$
- $\mathrm{F_R = F_{shock} + F_{1-R} + F_{2-R}} + \cdots$

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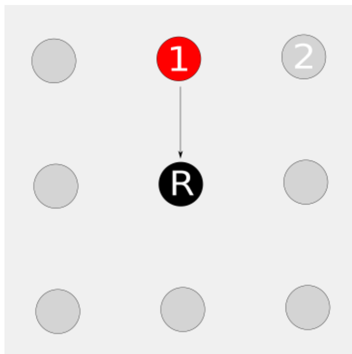
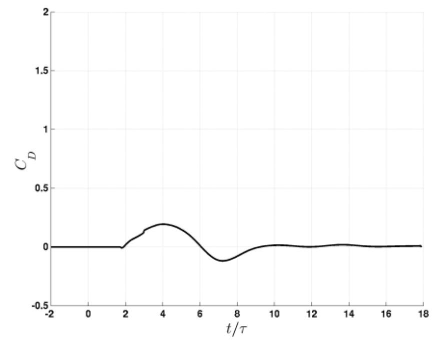
Virtual Particle Simulation





F_{1-R}

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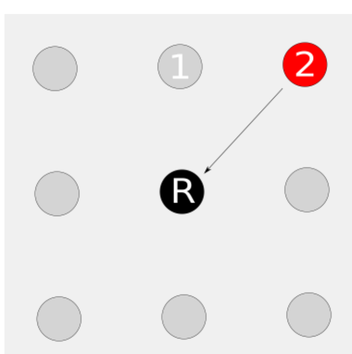
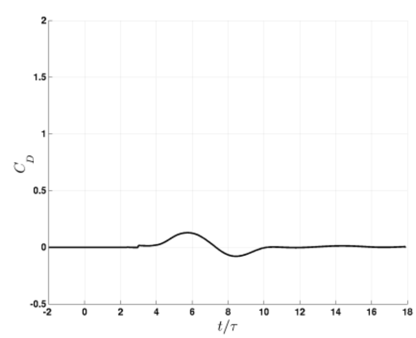
Virtual Particle Simulation





F_{2-R}

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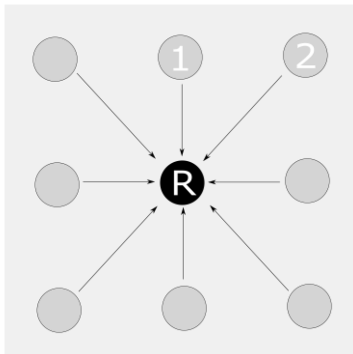
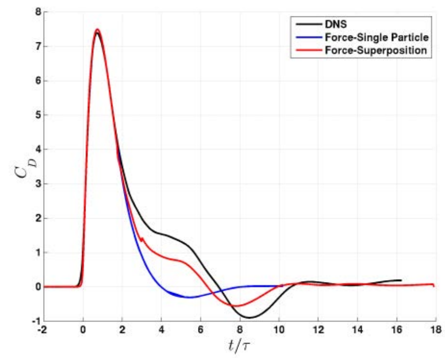
Binary Superposition - Drag





- $F_R = F_{shock} + 4 * F_{1-R} + 4 * F_{2-R}$

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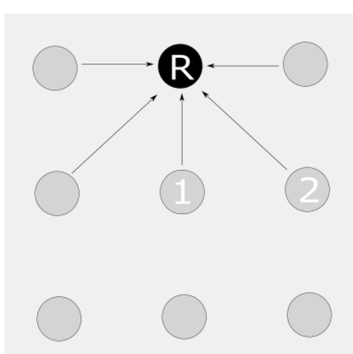
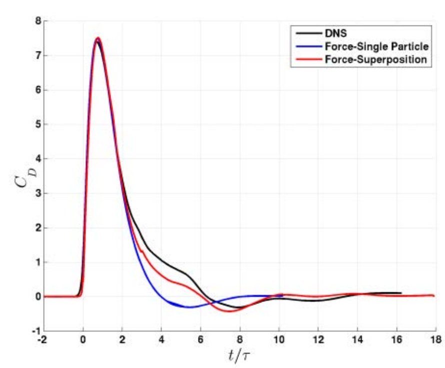
Binary Superposition - Drag





- $F_R = F_{shock} + 3 * F_{1-R} + 2 * F_{2-R}$

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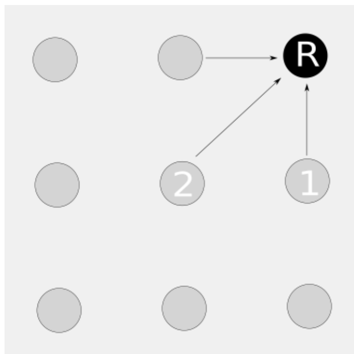
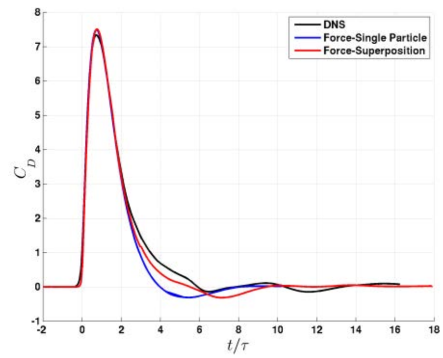
Binary Superposition - Drag





- $F_R = F_{shock} + 2 * F_{1-R} + 1 * F_{2-R}$

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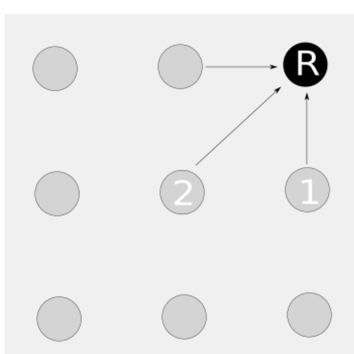
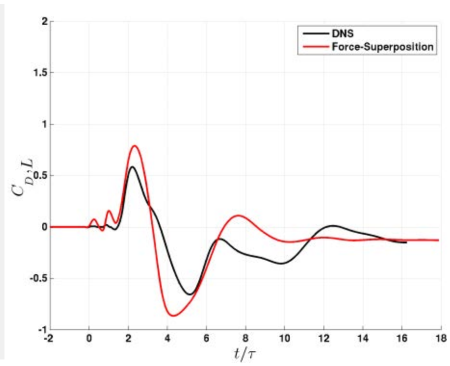
Binary Superposition – Lift(Z)





- $F_R = 2 * F_{1-R} + 1 * F_{2-R}$

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Point Particle Modeling- Summary

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

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Do you have any questions?

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Experimental Studies of Gas-Particle Mixtures Under Sudden Expansion

Heather Zunino
Ph.D. Student

Ira A. Fulton Schools of Engineering
ASU

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

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Problem Statement and Goals

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

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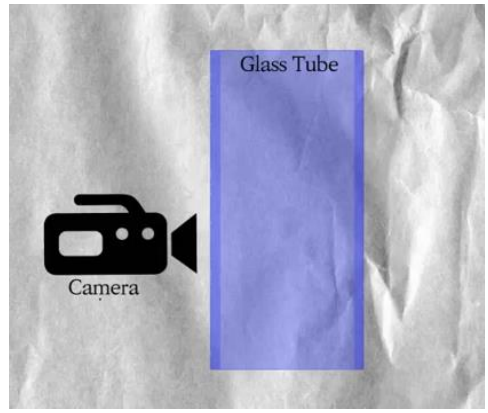
Review Proposed Experiment

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



Simple Test Bed for Early-Stage Code Numerics

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Shock Tube Experimental Structure Setup

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New Shock Tube Alterations

- New location secured to put shock tube
  - Taller
  - May reuse some parts from old shock tube
- Round cross section works well
  - Easier and cheaper to assemble (will allow us to make taller)
- Camera purchase
  - Vision Research v641

Vision Research (Phantom) v641	
Resolution	2560 x 1600
Frame rate (at max resolution)	1450 fps (best for pixel count)
HD resolution (1080p)	1920 x 1080 up to 2,560 fps
HD resolution (720p)	1280 x 720 up to 5,350 fps
Max frame rate	219,000 fps (256 x 8)
Bits	12 bits
Internal memory	16 GB
High G (impact survivability)	Up to 30G
FAST data offload to laptop	10 GB Ethernet (7.68 GB per minute)
Warranty	2 years
Resolution at 10,000 fps	600 x 800
ISO Sat	16,000T; 6,400D

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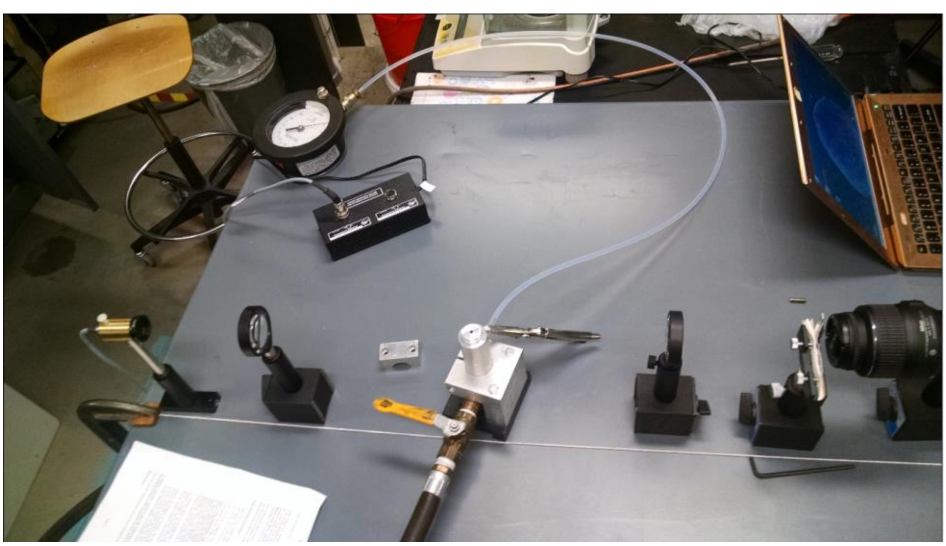
Schlieren



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<Schlieren Video>

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Background Oriented Schlieren

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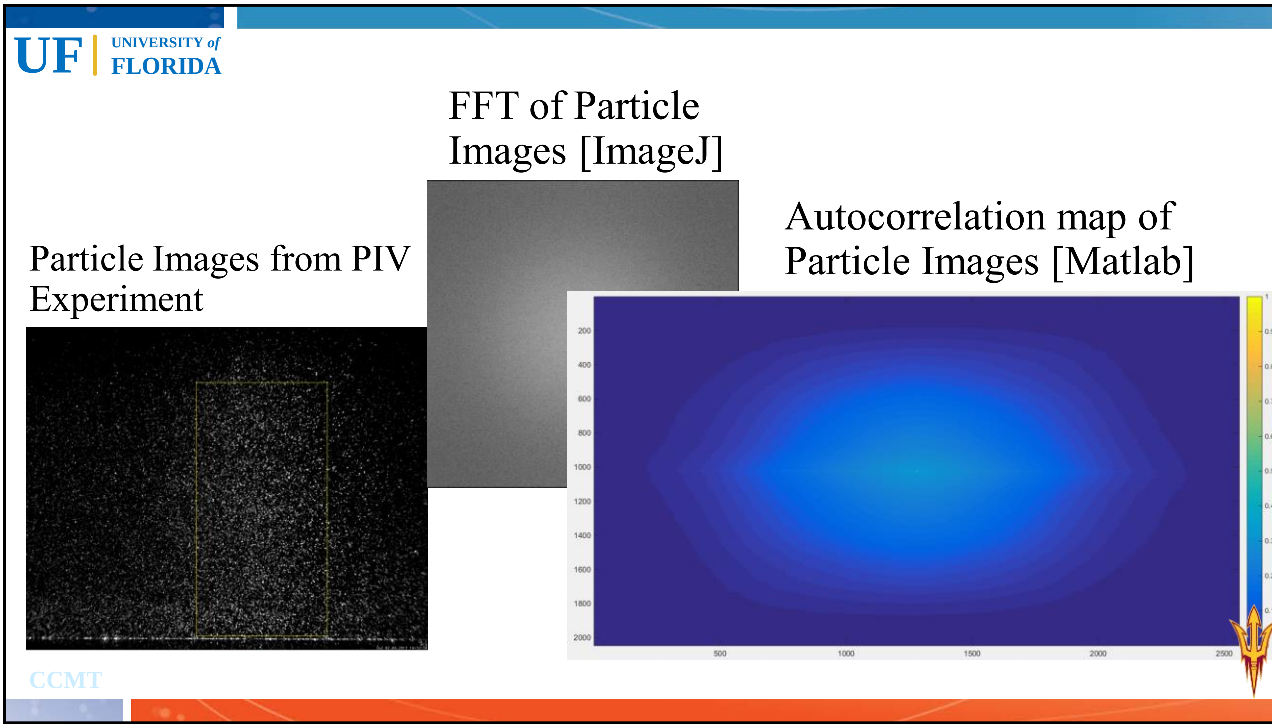
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FFT of Particle Images [ImageJ]
Autocorrelation map of Particle Images [Matlab]
Particle Images from PIV Experiment
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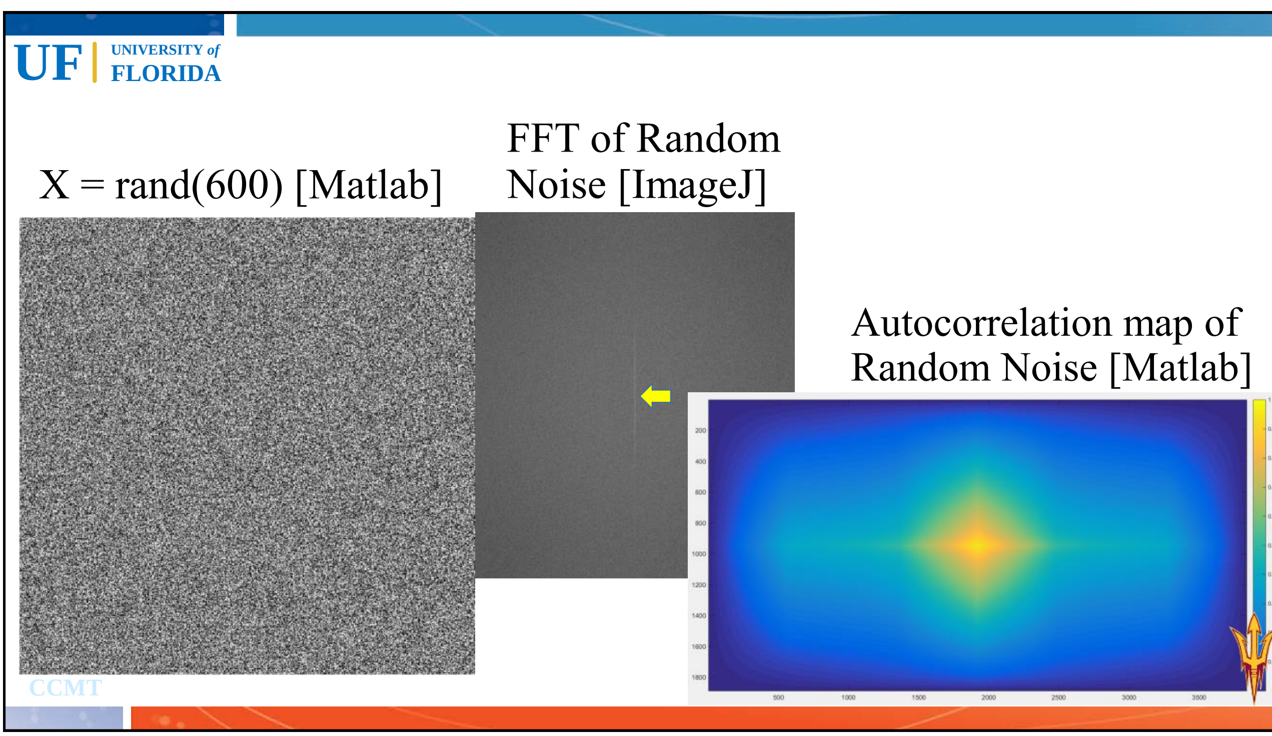
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X = rand(600) [Matlab]
FFT of Random Noise [ImageJ]
Autocorrelation map of Random Noise [Matlab]
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Broad peak for random noise autocorrelation

- Xcorr2 doesn't apply periodic boundary conditions
  - Need to manually code the autocorrelation, to get a narrower peak (which will be more representative of the background)
  - Because the features are very small in the random noise pattern, the autocorrelation yields a very broad peak
    - The peak is more associated with the area used to correlate the images than the actual pattern
    - I need to add periodic extensions, so the peak will be more associated with the patterns (or non-pattern) in the random noise, rather than the fact that the features are small.
- See next slide for example

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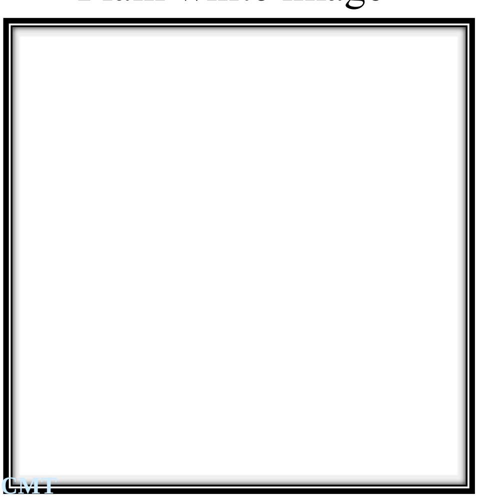
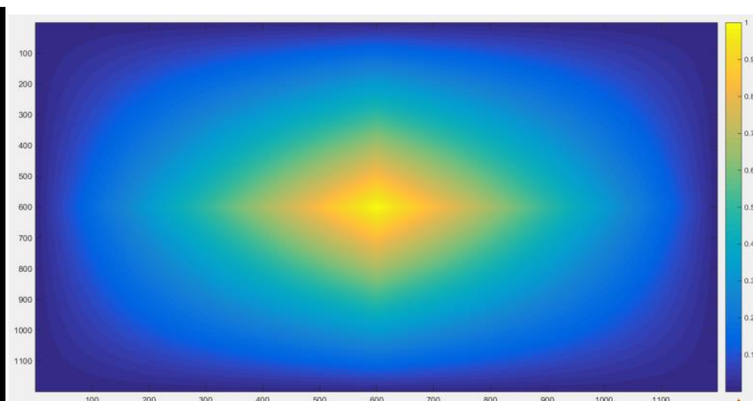
Autocorrelation should be a small peak

Plain white image



Autocorrelation yields broad peak



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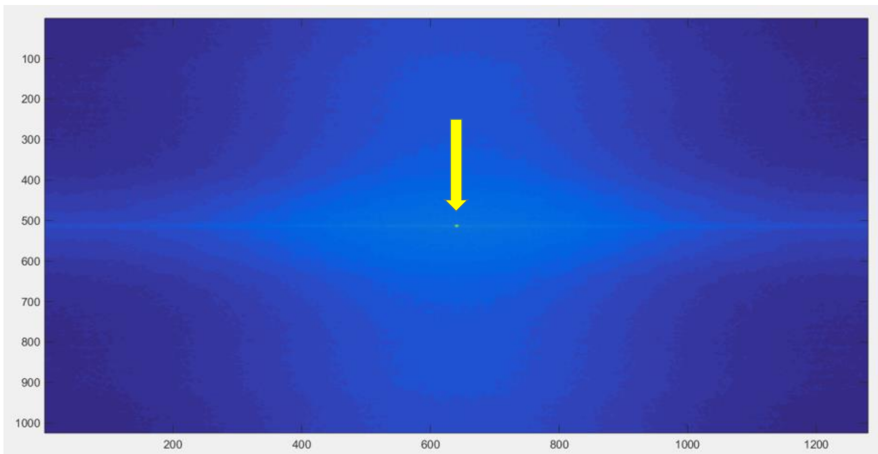
Random Particles FFT with periodic extension



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Random Noise FFT with periodic extension

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<Background Oriented Schlieren Video>
Particles

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<Background Oriented Schlieren Video>
Random Noise

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Theoretical Calculations

Expansion Fan (air only)		
Length of p4 region, L 4	0.1	[m]
gamma	1.4	
p1	1	[kpa]
p2	15.80620265	[kPa]
p3		[kPa]
p4	101	[kPa]
p4/p1	101	
p1/p4	0.00990099	
M shock, table value	3.7001393	
speed of sound, a1	343	[m/s]
speed of sound, a2		[m/s]
speed of sound, a3	146.9252388	[m/s]
speed of sound, a4	343	[m/s]
Contact line velocity, u_p	-980.373806	[m/s]

Reflected Shock Wave (air only)		
M r/(M r^2 - 1)	0.579020077	
M r	y, goal seek to 0	
2.184128312	-0.00098147	
U reflected	320.9035738	[m/s]
U shock	1269.14778	[m/s]
Length of p1 region, L1	3	[m]
Time before reflection	0.011712394	[s]
t = 0 is diaphragm rupture		

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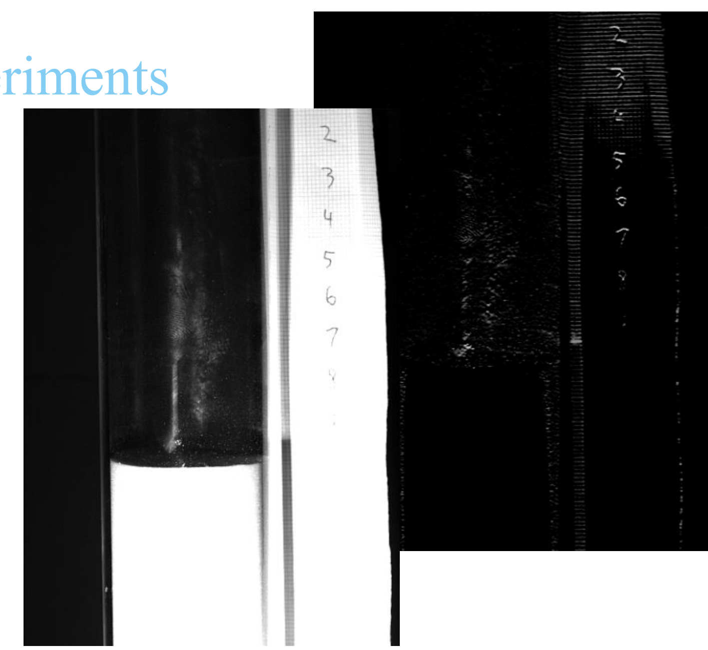
Variability in Experiments

- Particle bed height
  - Measuring at 90% intensity
    - No particles is 0%
    - All particles is 100%



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Conclusions

- New camera purchase
- Secured location for new shock tube
  - Much taller, longer period before re-shock
- Schlieren
- Background Oriented Schlieren
  - Backgrounds
  - Round tube
- Variability in Measurements
  - Height of rising particle bed

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CMT-Nek
Status and Progress

Jason Hackl and Mrugesh Shringarpure

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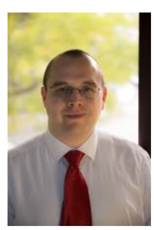
CMT-nek team

Paul Fischer, UIUC

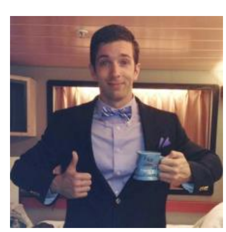


Jason Hackl, UF

Mrugesh Shringarpure, UF

Li Lu, UIUC

David Zwick, UF



Goran Marjanovic, UF

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Goals

- Exascale code for predictive simulations of compressible multiphase flows at
  - Microscale (resolved flow over individual particles)
  - Mesoscale (point particles and DNS)
  - Macroscale (point particles and LES)
- Spectral accuracy, robust multiphysics capability
- Co-design of code and algorithm selection by simulation on uncertain notional architectures

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Y1.5 Accomplishments

- Compressible Navier Stokes solver
- Particle tracking, 1-way coupling
- CMT-nek committed to nek5000 repository
- Mesoscale simulation: Rarefaction through particle bed (ASU experiment)
- Microscale simulation: Force response of a particle in an expansion fan
- CMT-bone development with CS and Exascale team

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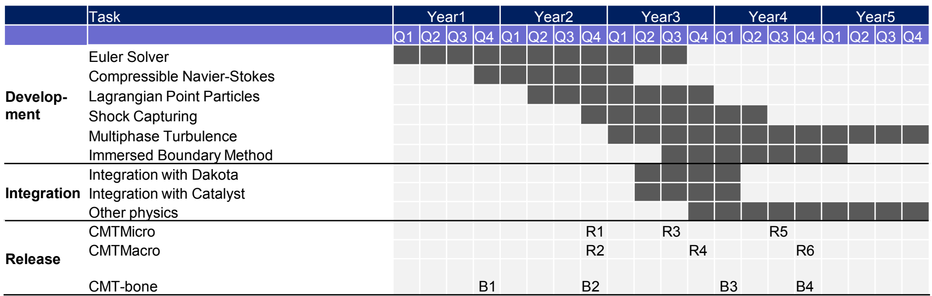
CMT-nek development roadmap



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Outline

1. Brief review of CMT-nek framework
2. Accomplishments
   a. Compressible Navier Stokes solver
   b. Microscale: particle in an expansion fan
   c. Particle tracking, 1-way coupling
      - Mesoscale simulation: rarefaction through particle bed
   d. Refinement, upstream Nek integration
   e. CMT-bone development
3. Current and near-future work

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1. Brief review of CMT-nek framework

$$\boxed{\mathbf{U} \equiv \phi_g \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} \rightarrow \frac{\partial U_i}{\partial t} + \nabla \cdot \mathbf{H}_i\left(\mathbf{U}, \nabla \mathbf{U}\right) = R_i}$$

flux = convective + diffusive

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

Mass

$$\mathbf{H}_i^c = \phi_g \begin{bmatrix} \rho u \\ \rho v \\ \rho w \end{bmatrix}, \mathbf{H}_1^d = 0$$

Momentum

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

$$H_{i+1,j}^d = -\phi_g \tau_{ij} \quad \boxed{H_{ij}^d = G_{ijkl} \frac{\partial U_k}{\partial x_l}}$$ Viscous flux Jacobian

Energy

$$\mathbf{H}_5^c = \phi_g \left(\rho E + p\right) \begin{bmatrix} u \\ v \\ w \end{bmatrix}, H_{5j}^d = -\phi_g \left(u_k \tau_{kj} + q_j\right)$$

Gas-particle coupling

$$\boxed{\mathbf{R} = -\begin{bmatrix} \mathcal{C}_{gp} \\ p \nabla \phi_g + \mathcal{M}_{gp} \\ p u_j \left(\partial \phi_g / \partial x_j\right) + \mathcal{E}_{gp} \end{bmatrix}}$$

Powers, Joseph M. "Two-phase viscous modeling of compaction of granular materials." *Physics of Fluids*,16.8 (2004).

Lv, Y. and Ihme, M. "Discontinuous Galerkin method for multicomponent chemically reacting flows and combustion." *J. Comp. Phys.* **270** pp. 105-137 (2014)

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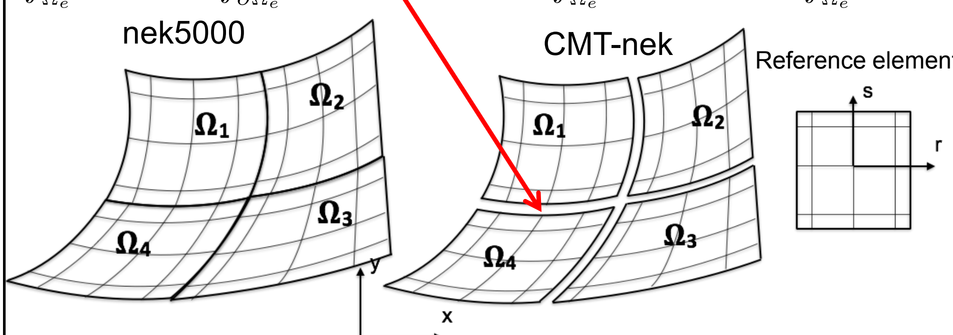
1. Review of CMT-nek: nodal DG

$$\int_{\Omega_e} v \frac{\partial U}{\partial t} \, dV = \int_{\partial \Omega_e} v \left(\mathbf{H} - \mathbf{H}^*\right) \cdot \mathbf{n} \, dA - \int_{\Omega_e} v \left(\nabla \cdot \mathbf{H}\right) \, dV + \int_{\Omega_e} v R \, dV$$



$$\forall v \in \chi_h^N,$$

$$U_m,\ v,\ H_{mj}(\mathbf{U}, \nabla \mathbf{U}),\ R_m \in \chi_h^N = \left\{ U_h : U_h \approx \bigoplus_{e=1}^{nel} U_e^N, U_e^N \in \mathbb{P}^N \right\}$$ Piecewise polynomials

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

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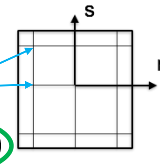
1. Review of CMT-nek: nodal DG

$$\int_{\Omega_e} v \frac{\partial U}{\partial t}\, dV = \int_{\partial\Omega_e} v\,(\mathbf{H}-\mathbf{H}^*)\cdot\mathbf{n}\, dA - \int_{\Omega_e} v\,(\nabla\cdot\mathbf{H})\, dV + \int_{\Omega_e} vR\, dV$$

- Approximate all functions (*f=U,v,x* and flux functions) by
  - Lagrange polynomials *L(r)* of degree *N*=nx1-1
  - evaluated at Gauss-Legendre-Lobatto quadrature nodes



$$f(\mathbf{x}) \to^{\Omega_e} f(\mathbf{r}) \approx \sum_{l,m,n=1}^{\mathtt{nx1}} f\left((r_l,s_m,t_n)^\mathsf{T}, e\right) L_l(r)L_m(s)L_n(t)$$

- Integrals become matrix-vector products
  - between vectors of nodal values
  - and the **Mass Matrix M**

$$\int_{\Omega_e} vf\, dV \approx v_i\,[M_{ij}]\, f_j$$

$$M_{ij} \equiv \int_{\Omega_e} \phi_i\phi_j\, dV$$

- Further approximate all integrals by
  - Gaussian quadrature on the GLL points

$$\int_{\Omega_e} vf\, dV \to \sum_{l,m,n=1}^{\mathtt{nx1}} \omega_l\,\omega_m\omega_n\,[v(\mathbf{r})f(\mathbf{r})J(\mathbf{r})]|_{\mathbf{r}=(r_l,s_m,t_n)^\mathsf{T}}$$

Diagonal **M** !

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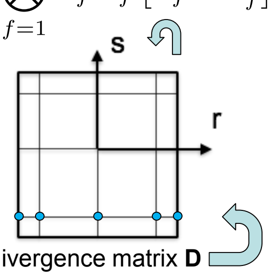
1. Review of CMT-nek: nodal DG

$$\mathbf{v}^\mathsf{T}\left[\frac{\partial}{\partial t}(JU)\right] = \mathbf{v}^\mathsf{T}\left[\mathbf{M}^{-1}\bigotimes_{f=1}^{6}\mathbf{E}_f\mathbf{A}_f\left[\mathbf{h}_f-\mathbf{h}_f^*\right] - \mathbf{D}\mathbf{h} + [JR]\right]$$

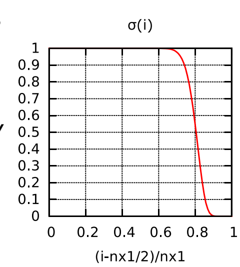
Fully explicit TVDRK3 of Gottlieb & Shu (1998)



$\mathbf{h}_f^*$ numerical flux normal to face *f* (face data exchange, AUSM+)

- The quadrature choice
  - tensor-nests finite-difference divergence matrix **D**
    - even for deformed elements with curved faces, edges
  - is **not exact**
- This "variational crime" must be stabilized
  - Implement variational dealising (fixing a mistake)
  - For now, filter Legendre modes via Vandermonde matrix *V*

$$\mathcal{V}\,\mathrm{diag}(\sigma)\mathcal{V}^{-1}\,\mathbf{u}_m$$



Liou (1996) *J. Comp. Phys.* **129**, pp. 362-382
Gottlieb & Shu (1998) *Math. Comp.* **67**(221), pp.73-85
Hesthaven & Warburton (2008) *Nodal discontinuous Galerkin methods* Springer

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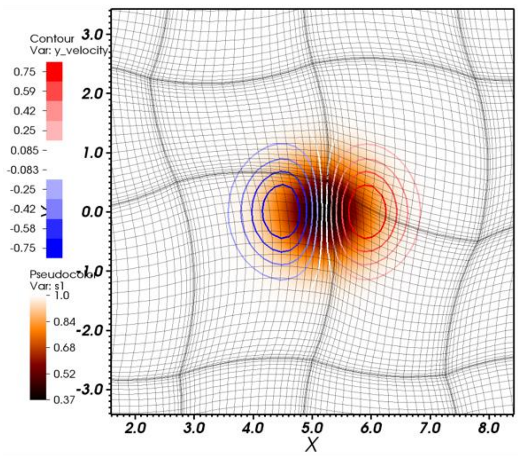
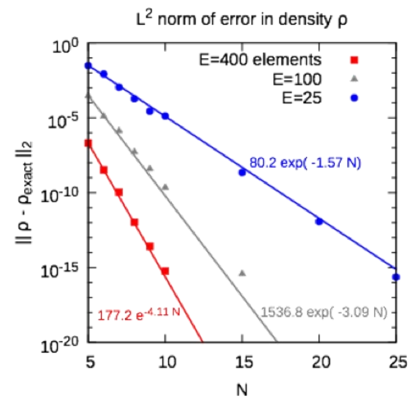
1. Review of CMT-nek: validation

2D compressible vortex flows validated without viscosity



Spectral convergence



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Yee, Vinukor & Djomehri (2000) J. Comp. Phys. 162

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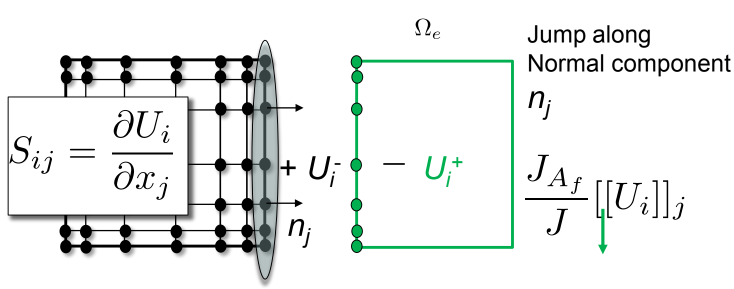
2.a Compressible Navier Stokes solver

$$\int_{\Omega_e} \frac{\partial}{\partial x_j} \mathbf{H}^d(\mathbf{x}) v(\mathbf{x}) dV = \int_{\partial\Omega_e} \left(G_{ijkl} S_{lk} - \mathbf{H}^{S*}\right) v(\mathbf{x}) n_j dA - \int_{\Omega_e} \frac{\partial}{\partial x_j} \left(G_{ijkl} S_{lk}\right) v(\mathbf{x}) dV,$$

Viscous flux of the m^th conserved variable in terms of auxiliary variable S_{ij} satisfying

$$S_{ij} - \frac{\partial U_i}{\partial x_j} = 0 \qquad \int_{\Omega_e} v S_{ij}\, dV = \int_{\Omega_e} v \frac{\partial U_i}{\partial x_j}\, dV + \int_{\partial\Omega_e} v \left(U_i - S^*\right) n_j\, dA$$

Central flux $S^*=(U_i^+ + U_i^-)/2$ ("+" from neighbor, "-" from)



$$\mathbf{H}^{S*} = \frac{1}{2}\left((G_{ijkl} S_{lk})^+ + (G_{ijkl} S_{lk})^- \right)$$

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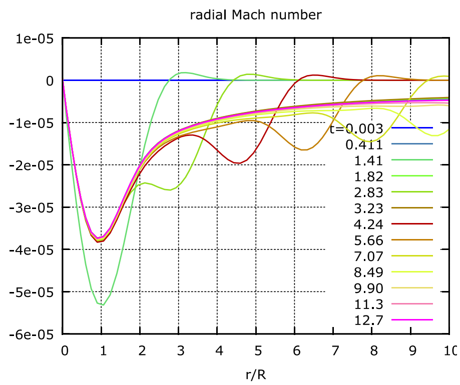
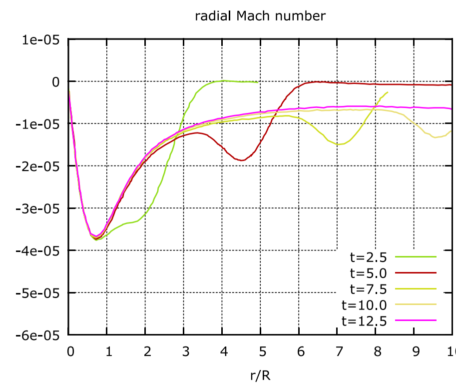
2.a Compressible Navier Stokes solver

2D compressible vortex flows validated **with viscosity**

- Homentropic initialization, viscosity turned on, decay
  - but first, a low-Mach number radial-velocity pulse





CMT-nek, 2D, periodic
nx1=31, max Mach 0.5

Colonius, Lele, Moin (1991) *JFM* **230**
dedicated axisym CFD code

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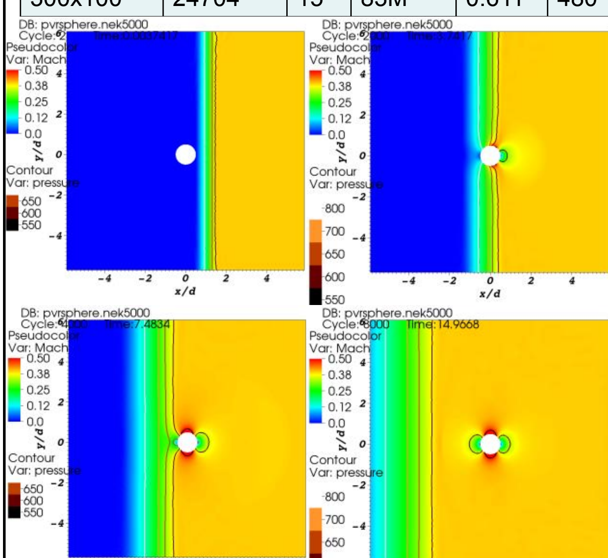
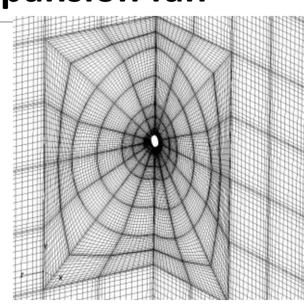
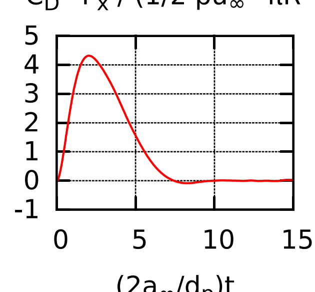
2.b Microscale: particle in expansion fan

$L_xL_yL_z$ (d_p)	elements	nx1	points	CFL	cores
300×100^2	24704	15	83M	0.611	480





$C_D = F_x / (1/2\ \rho u_\infty^2\ \pi R^2)$



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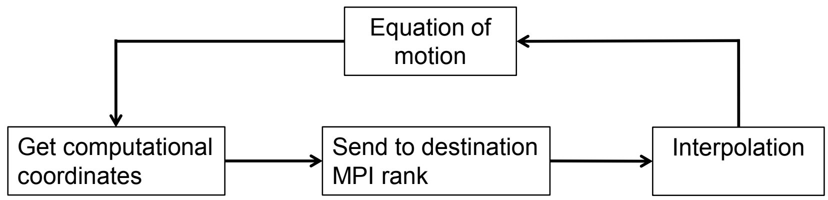
2.c Particle tracking, 1-way coupling



Old
- Get computational coordinates
- Interpolation

New
- Get computational coordinates
- Send to destination MPI rank
- Interpolation
  - Barycentric Lagrange interpolation

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2.c Particle tracking, 1-way coupling

Particle tracking performance
- 1000 elements, 14th order polynomial representation inside the element
- 3,375,000 Degrees of Freedom
- Particles with small response time being swept by u = (0.15,0,0)
- Run on Mustang using 960 MPI ranks

Average execution time per time step per MPI rank. All values are in milliseconds

Particles	125,000		1,000,000		3,375,000	
	Old	New	Old	New	Old	New
Flow solver	32.37	32.08	32.41	32.24	32.57	32.48
Particle tracking time	45.54	21.46	207.91	34.82	641.29	77.58
Get computational coordinates	39.36	18.93	173.17	20.27	533.40	28.06
Send to destination MPI rank	-	0.30	-	1.83	-	7.71
Interpolation	5.17	1.49	33.49	11.85	105.57	39.97

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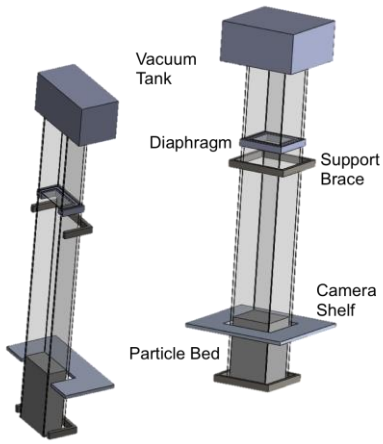
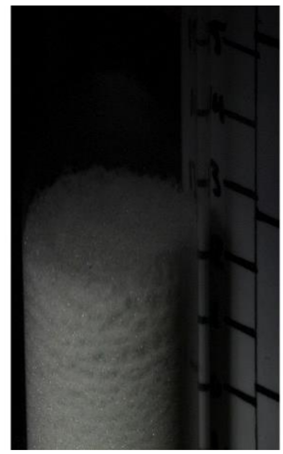
2.c Particle tracking, 1-way coupling

Mesoscale simulation: rarefaction through particle bed





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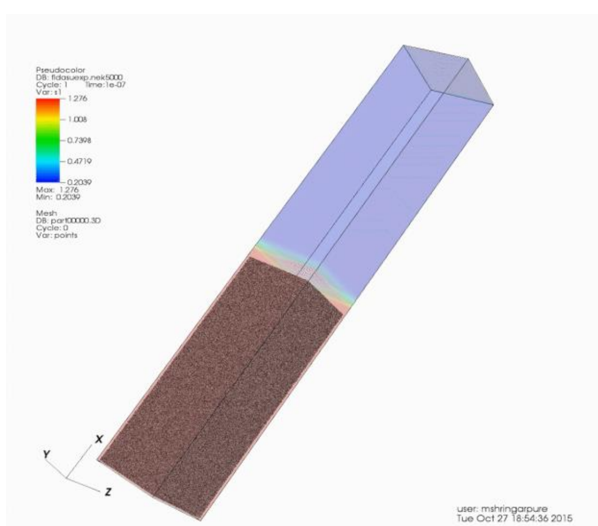
2.c Particle tracking, 1-way coupling

11520 elements, LX1=15, 12 million particles, 7680 MPI ranks



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2.d Refinement, upstream Nek integration

- CMT-nek framework refined
  - Adheres to the core design principles of nek5000
  - Consistent design choices makes it easier for existing nek users to start using CMT-nek
- Upstream Nek integration
  - CMT-nek has been folded into nek5000 repo
  - Available for all users to checkout and run CMT-nek
  - Sample CMT-nek cases also added
- Mrugesh and Jason enrolled as developers to ANL's nek5000 repo
  - CCMT commits CMT-nek updates directly to nek repo

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2.e CMT-bone development

- Work with CS team
  - Performance improvement of derivative operation through loop unrolling methods
  - Performance of CMT-nek derivative kernels on GPUs
- Work with Exascale team
  - Development of CMT-bone a representative mini-app
  - Modeling communication in CMT-nek/nek5000
  - Nalini Kumar, Mrugesh Sringarpure, Tania Banerjee, Jason Hackl, S. Balachandar, Herman Lam, Alan George and Sanjay Ranka. "CMT-bone: A mini-app for Compressible Multiphase Turbulence Simulation Software ", Workshop on Representative Applications (WRAp 2015), IEEE Cluster 2015, Chicago Sep 8th (2015)

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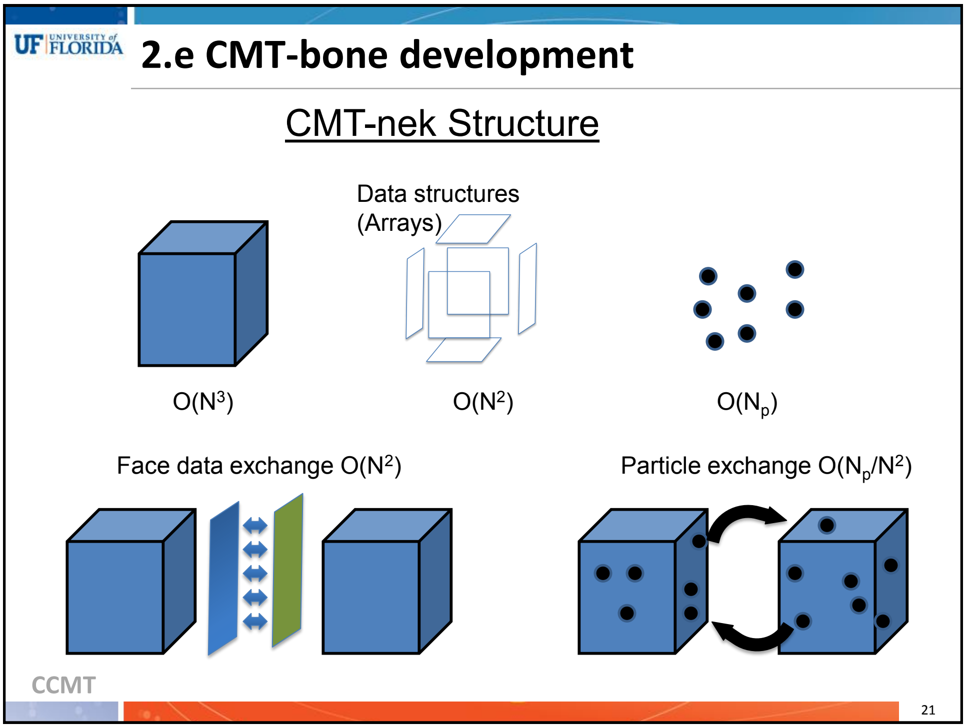
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2.e CMT-bone development
CMT-nek Structure
Data structures
(Arrays)
O(N³)
O(N²)
O(N_p)
Face data exchange O(N²)
Particle exchange O(N_p/N²)
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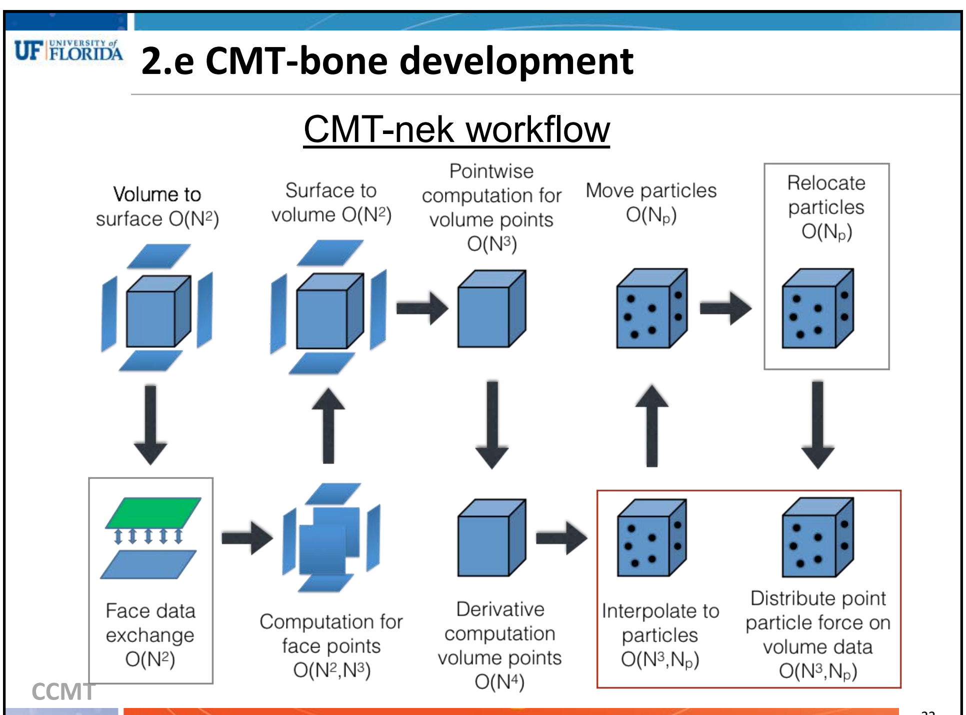
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2.e CMT-bone development
CMT-nek workflow
Volume to surface O(N²)
Surface to volume O(N²)
Pointwise computation for volume points O(N³)
Move particles O(Nₚ)
Relocate particles O(Nₚ)
Face data exchange O(N²)
Computation for face points O(N²,N³)
Derivative computation volume points O(N⁴)
Interpolate to particles O(N³,Nₚ)
Distribute point particle force on volume data O(N³,Nₚ)
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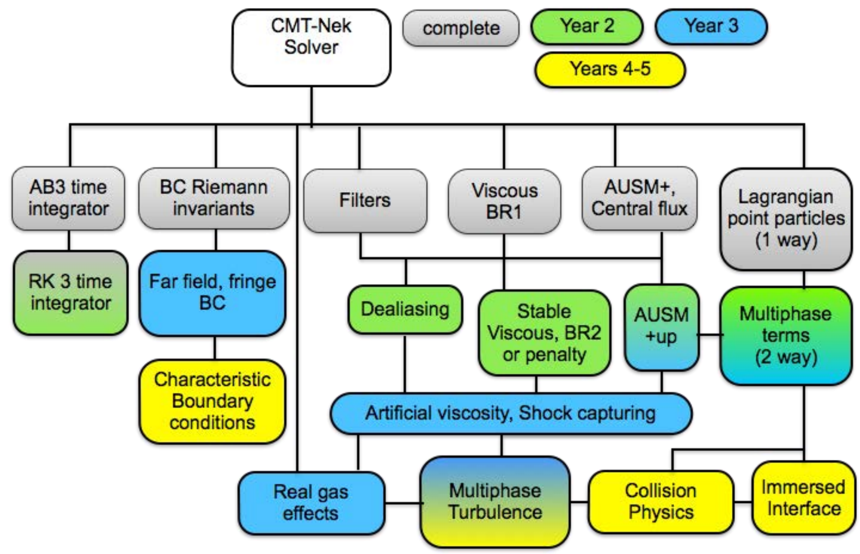
3. Current and near-future work



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Do you have any questions?

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Exascale Behavioral Emulation

Principal Investigators:
Alan George, Herman Lam, Greg Stitt

Supported Students:
Doctoral: Kasim Alli, Nalini Kumar, Carlo Pascoe, Dylan Rudolph
Masters: Chris Hajas, Parth Shah
Undergrad: Ting-Hsin Kuo

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

Goal*

Develop ***behavioral emulation (BE)*** methods & tools to support:

- Co-design for algorithmic DSE (design-space exploration)
- Optimization of key CMT-nek kernels & applications

On future architectures, up to Exascale

* Goal stated at AST review May 2015

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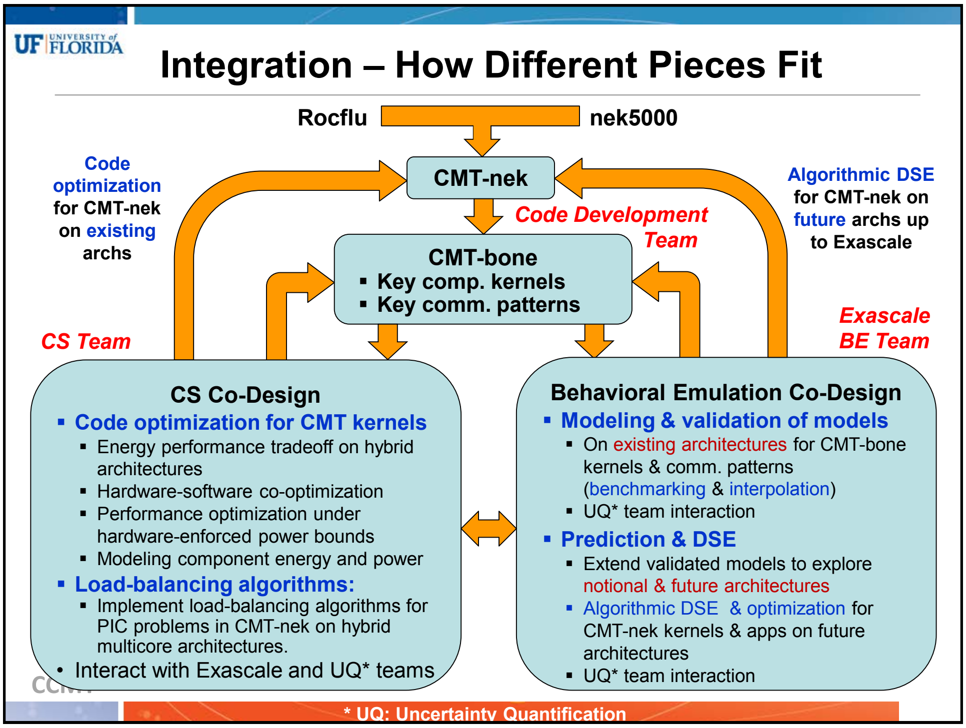
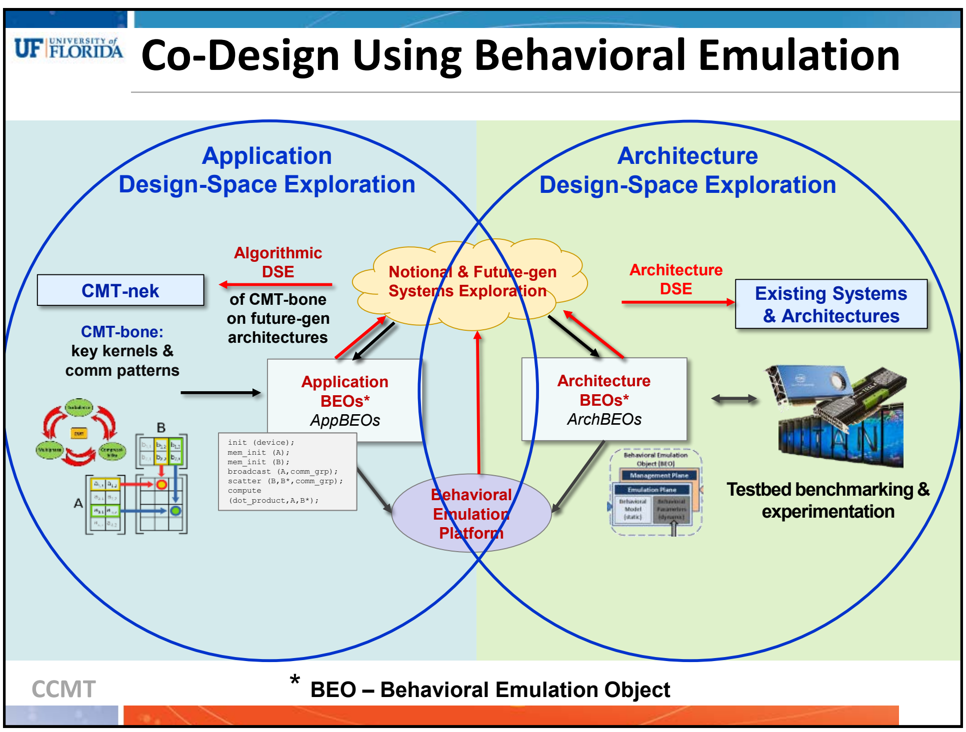

Integration – How Different Pieces Fit
Rocflu
nek5000
CMT-nek
Code optimization for CMT-nek on existing archs
Algorithmic DSE for CMT-nek on future archs up to Exascale
Code Development Team
CMT-bone
▪ Key comp. kernels
▪ Key comm. patterns
CS Team
Exascale BE Team
CS Co-Design
▪ Code optimization for CMT kernels
▪ Energy performance tradeoff on hybrid architectures
▪ Hardware-software co-optimization
▪ Performance optimization under hardware-enforced power bounds
▪ Modeling component energy and power
▪ Load-balancing algorithms:
▪ Implement load-balancing algorithms for PIC problems in CMT-nek on hybrid multicore architectures.
• Interact with Exascale and UQ* teams
Behavioral Emulation Co-Design
▪ Modeling & validation of models
▪ On existing architectures for CMT-bone kernels & comm. patterns (benchmarking & interpolation)
▪ UQ* team interaction
▪ Prediction & DSE
▪ Extend validated models to explore notional & future architectures
▪ Algorithmic DSE & optimization for CMT-nek kernels & apps on future architectures
▪ UQ* team interaction
* UQ: Uncertainty Quantification


Co-Design Using Behavioral Emulation
Application Design-Space Exploration
Architecture Design-Space Exploration
Algorithmic DSE
of CMT-bone on future-gen architectures
Notional & Future-gen Systems Exploration
Architecture DSE
CMT-nek
Existing Systems & Architectures
CMT-bone: key kernels & comm patterns
Application BEOs* AppBEOs
Architecture BEOs* ArchBEOs
init (device);
mem_init (A);
mem_init (B);
broadcast (A,comm_grp);
scatter (B,B*,comm_grp);
compute (dot_product,A,B*);
Behavioral Emulation Platform
Testbed benchmarking & experimentation
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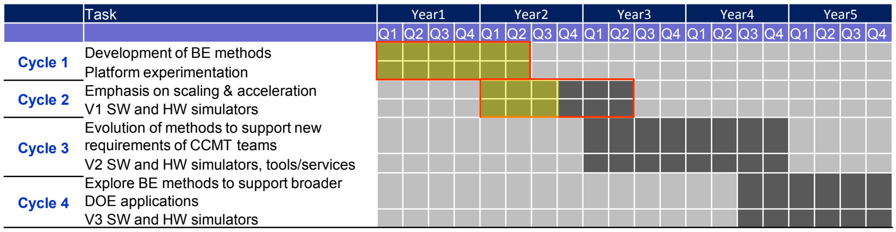
* BEO – Behavioral Emulation Object

Exascale Behavioral Emulation



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

Cycle 2:
- **BE concepts and methods:** Emphasis on scaling, communication (synchronization, congestion), and acceleration; focus on CMT-Bone
- **Tools:** V1 SW simulator (leverage production simulators) & V1 HW simulator (scalable design); enable early use of simulators for design-space exploration for CCMT researchers

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

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

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* Gannt chart presented at AST review May 2015

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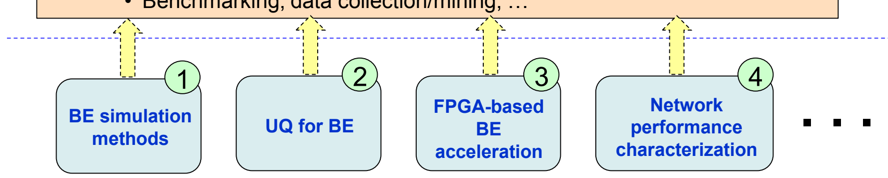
Experimental Testbed: Beyond Cycle 1

Experimental Testbed will:
- Support algorithmic design-space exploration for CCMT researchers
- Provide behavioral emulation within SST ecosystem

CCMT Exascale Behavioral Emulator: Released Version

- SST-based coarse-grained simulator
- Growing libraries of arch & app BEOs
- Services and tools:
  - Management, monitoring, reporting, visualization, …
  - Benchmarking, data collection/mining, …

1 BE simulation platform



Evaluation Platforms
- Used to perform R&D and experiments on various aspects of BE
- Promising and stable methods and tools migrate into next platform release

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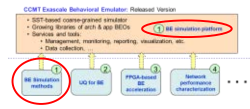
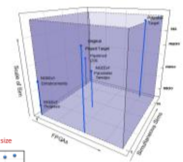
Outline: remainder of presentations

Session 1

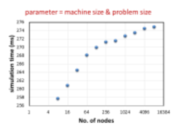
1. BE simulation methods & platform
   - BE methods at scale
   - Progress on SST-based BE simulator
2. UQ for BE
   - Introduction of UQ method for BE
   - Progress & walk-through example





Session 2

3. FPGA-based BE acceleration
   - Review of first-year FPGA studies
   - NGEEv1* design enhancements
   - Accelerating DSE** using BE
4. Network performance characterization
   - Use existing tools (SST) to analyze performance of key CMT-nek communication routines
   - Lessons learned to guide development of network models in BE simulation platform



*NGEE: Novo-G Exascale Emulator
**DSE: Design-Space Exploration

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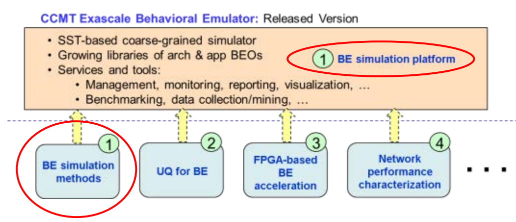

BE Simulation Methods & Platform

Dylan Rudolph (PhD Student)

UF UNIVERSITY of FLORIDA

NNSA

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Overview

Driving Goals:

Develop BE methods at scale

Find a long-term simulation framework to pair with BE

Term Motivation:

We need to determine the **accuracy** of BE at scale.

We need to estimate the **performance** (simulation speed; by extension: maximum simulated size) of BE methods (with SST).

Outline:

- Simulator advancements (new capabilities, refinements)
- Overview of full-scale experiment (application, hardware)
- Comparison of simulated and measured execution times
- Our efforts to integrate BE into SST (progress, methods)
- Speed comparison of BE-infused SST and SST alone
- Conclusions and future work

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Simulator Advancements

We have added new simulation capability to allow for a greater variety of simulations and results.

New Capabilities:

1) Probabilistic simulation (results now shown as distributions); details in next section
2) Greater software modeling capability (can model more types of applications)

Refinements:

1) Input / output formalization
2) Run-time analysis capability (largely for debugging)
3) Separated front-end (compilation, structure generation) from back-end (simulation) to reduce duplication across evaluation platforms

Note: results shown are executed on single-threaded evaluation platform, but should be identical to production version.

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Full-Scale Experiment (overview)

In order to evaluate the speed and accuracy of BE simulations, we need to pick a full-scale test application and architecture.

Application Requirements:

1) Must be fairly representative of CMT or NEK-like applications
2) Must be easy to instrument and do performance evaluation
3) Should be fairly portable and easy to implement in simulation
4) Must run on any reasonable architecture without modification

Architecture Requirements:

1) Must be accessible (reasonable node and time allocations)
2) Must have a known and available network/node configuration
3) Should be sufficiently big for a meaningful ‘full-scale’ test

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Full-Scale Experiment: Application

We are using a mini-app which is **coarsely representative** of CMT or NEK-like applications.

Specifics:

- Uses MPI-level parallelism
- Process count driven by Cartesian grid parameters
- Blocking communication with Cartesian, but not necessarily physical, neighboring processes

Pseudo-Code:

```
1) initialize
2) make a Cartesian virtual topology
3) main phase:
     perform some surrogate computation
     talk to my Cartesian neighbors
4) finalize
```

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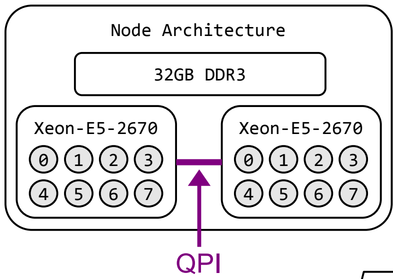
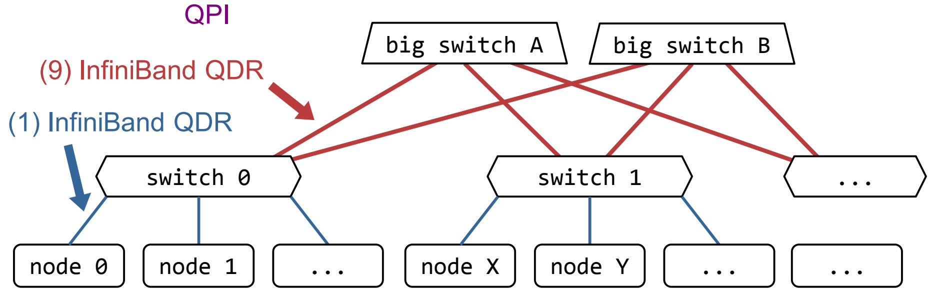
Full-Scale Experiment: Architecture



Cab: Computing cluster at LLNL

- 1296 nodes, 40 TB memory, 2.6Ghz Cores
- Two-level switch InfiniBand QDR network
- Fat-tree-like layout
- Microsecond latencies



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Full-Scale Experiment: Setup

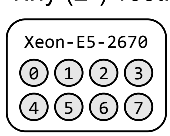
We simulate the test application on three different subsets of Cab.

The sizes of the modeled subsets are driven by 3D Cartesian mesh sizes:

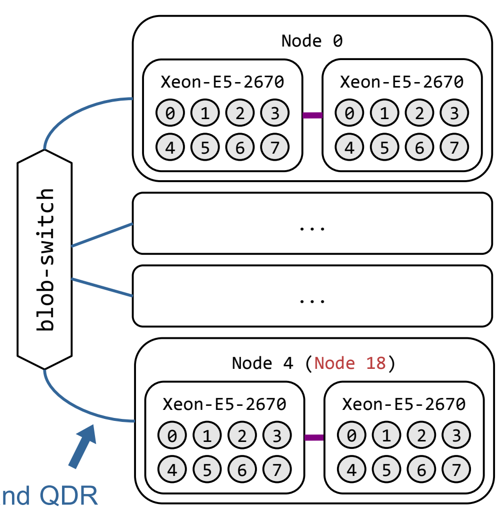
- Tiny: 2^3 mesh (8 processes)
- Small: 4^3 mesh (64 processes)
- Medium: 6^3 mesh (216 processes)

We then run the test application on the real Cab machine, and compare simulated versus real execution time.

Tiny (2^3) Test:



Small (4^3), Medium (6^3) Tests:



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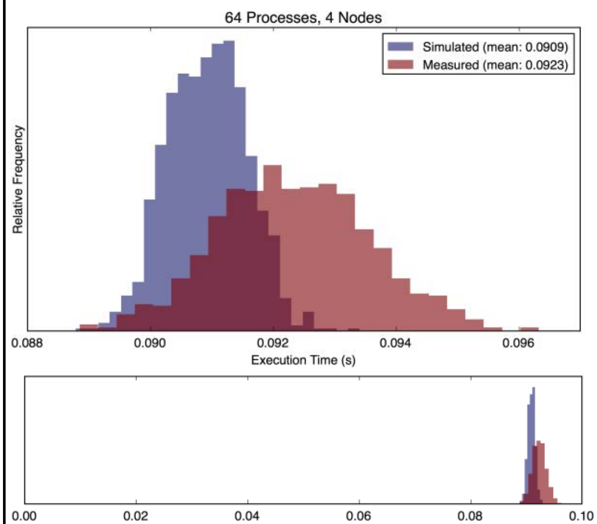
Experiment Results: Accuracy (4^3)

Small Example: Comparison of simulated and real execution time (histogram of 1000 runs of each)

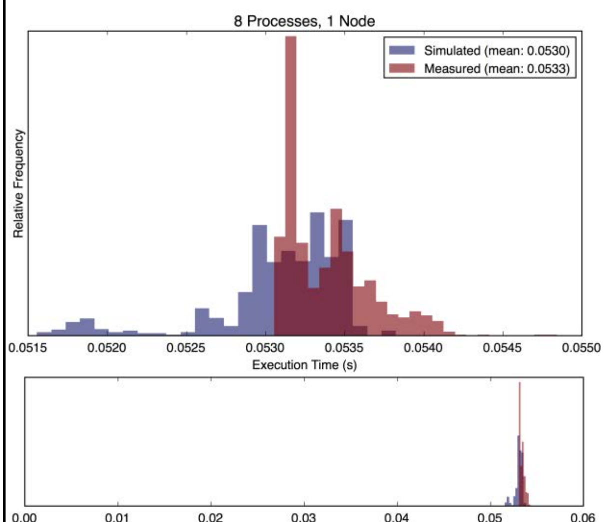


Observations:

- Mean error of roughly 1%
- Measured distribution is comparatively wide due to unrelated system load
- Measured distribution has higher mean due to unrelated system load
- Cab network appears to be well-characterized by a single-switch model

Experiment Results: Accuracy (2^3)

Tiny Example: Comparison of simulated and real execution time (histogram of 1000 runs of each)

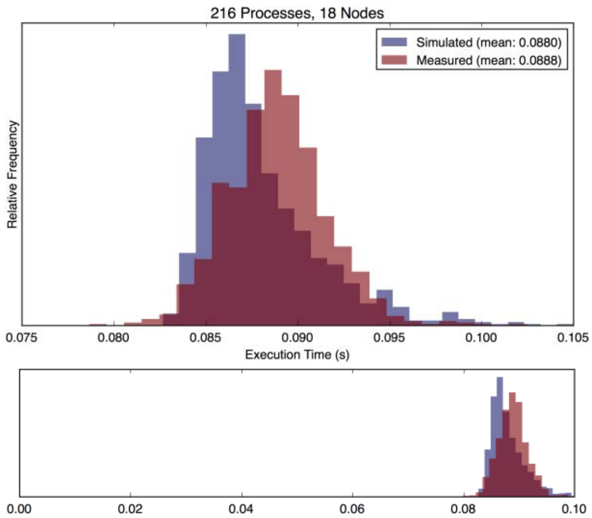


Observations:

- Mean error of roughly 1%
- Measured distribution has higher mean due to unrelated system load
- Assorted software and hardware state parameters affect result distributions
- Distribution is not well simulated, but we are not targeting network-less simulations

Experiment Results: Accuracy (6^3)

Medium Example: Comparison of simulated and real execution time (histogram of 1000 runs of each)



Observations:

- Mean error of roughly 1%
- Measured distribution is comparatively wide due to unrelated system load
- Measured distribution has higher mean due to unrelated system load
- Network (compared to small example) is faster and less consistent

SST Integration

We've been integrating BE into SST, this is how:

SST Capabilities:

Framework (core)
Network Models
Component Models

BE Influences:

Abstract Network Definitions
Abstract Hardware Definitions
Software Definitions
Probabilistic Simulation

Final Capability:

Framework (Simulation Environment)
Software Definitions
Probabilistic Simulation
Abstract Network Models
Abstract Component Models

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SST Integration: Progress / Performance

We are slightly shy of half-way done mapping BE-style simulation on top of SST, but can still estimate performance.

Napkin-Math Methodology:

1) Benchmark things that we've completed in the BE-SST integration
2) Compare how long those things take to how long they take in the single-threaded evaluation platform
3) Extrapolate and estimate for a few test-case simulator inputs

- Expected accuracy: within an order of magnitude, no better
- Proper estimates will be expected on actual benchmark numbers on BE-SST

How big of a simulation (part count) can we run in under an hour?
100-ULoC*-App (1000-ULoC-App)

1) BE single-threaded platform: 10^6 (10^5) processes and parts
2) BE on SST (single-threaded): 10^7 (10^6) processes and parts
3) BE on SST (multi-threaded): 10^8 (10^7) processes and parts
(This could certainly be Exascale, depending on modeling granularity)

*ULoC: Unrolled (no loops) Lines of Code

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Conclusions and Future Work

Conclusions:

- For **small-subset** Cab prediction, BE is sufficiently accurate (1% error)
- **Initial estimates** show that we should be able to perform Exascale simulations with BE in a parallel SST environment

Future Work:

- Find a machine which permits us to do **larger experiments** (tens, hundreds, thousands of nodes)
- Ensure that BE methods still hold at those **scales (accuracy-wise)**
- Complete the development and integration of **BE into SST**

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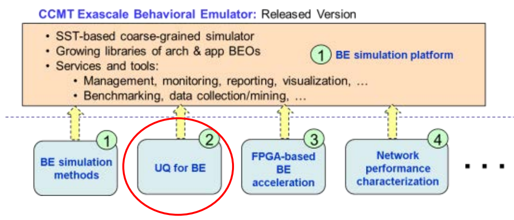
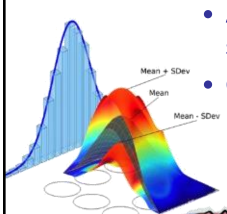


UQ for BE

Carlo Pascoe (PhD Candidate)

Overview

- Motivation
  - Quantification of errors and uncertainties is required to establish reliable predictive capabilities
- Goal
  - Go beyond our previous V&V efforts to quantify effect that uncertain inputs & model imperfection have on BE
    - Determine variance and confidence intervals for simulation output
    - Analyze output sensitivity to variance in simulation inputs
    - Quantify uncertainty when using calibrated BE models for prediction



Outline of Presentation

- Sources of Uncertainty in BE
- BE as a Stochastic Processes Chain
- Probabilistic Uncertainty Propagation via Monte Carlo Simulation
  - Model BE simulation as non-Markov stochastic process
- Walk-through Example
  - Results
- Conclusions

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Sources of Uncertainty in BE (1/2)

- BE: thread-level discrete-event simulation of coarse-grained compute and communication events
  - Comp: modeling time for a collection of local operations to execute on a specified target architecture
  - Comm: modeling time for message of specific size to travel through a target network from one point to another
- Implicit wait and queue "events" used as slack variables to reconcile clocks after comm events
  - Wait: thread is ready to receive before message arrives
  - Queue: message arrives before thread is ready to receive

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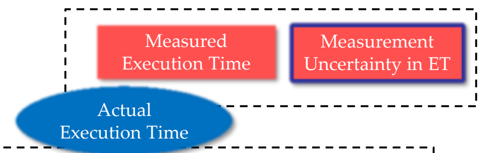
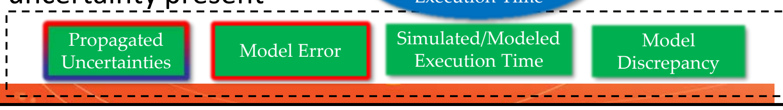
Sources of Uncertainty in BE (2/2)

- Uncertainty & error introduced due to BE’s coarse-grained abstraction of system details
  - **Comm uncertainties:** network congestion, nondeterministic arbitration or scheduling, …
  - **Comp uncertainties:** kernel overhead, locality of operands, contention for shared resources, …
  - **Measurement uncertainties:** sensor noise/resolution, randomization, …
  - **Model uncertainties:** model inadequacy, surrogate error, …
  - **Statistical uncertainties:** limited number of test/measurements, experiment variability,…
- Many sources of both *aleatory* and *epistemic* uncertainty present





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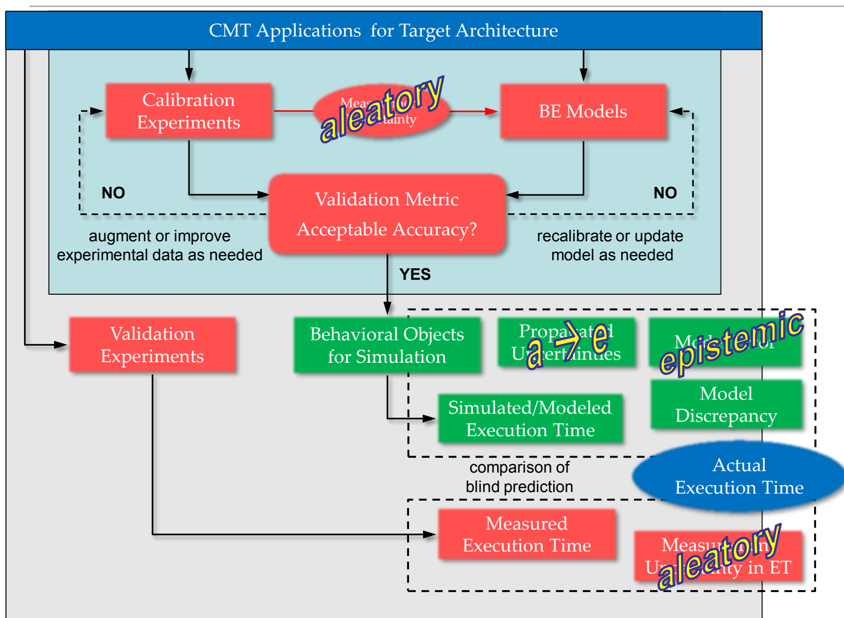
Behavior Emulation V&V Process



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BE as a Stochastic Processes Chain

- BE simulations comprise multiple thread level simulations executing in parallel
  - $\{t_1, t_2, \ldots t_n\}$
- Thread simulation is ordered sum *(i.e., not commutative)* of its simulated comp & comm events
  - $t_i = e_{i1} + e_{i2} + \cdots + e_{im}$
  - Comp events function of surrogate inputs and previous local events
  - Comm events function of surrogate inputs, previous local events, and previous events of other sending/receiving thread
  - Wait/queue timings added to reconcile mismatched send/recv clocks
- Simulated system time is largest simulated thread time
  - $S_{time} = max(t_1, t_2, \ldots t_n)$

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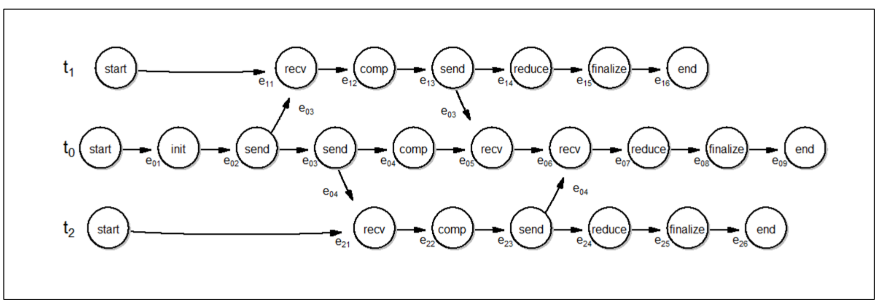
Simple 3-Thread Example

- Example:
  - Thread 0 initializes an array and sends chunks to threads 1 & 2
  - Threads 0-2 perform work on their respective chunks
  - Threads 1-2 communicate modified chunks back to thread 0
  - Threads 0-2 reduce, finalize, and exit



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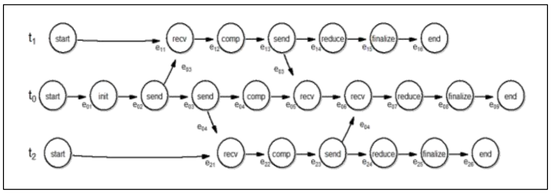
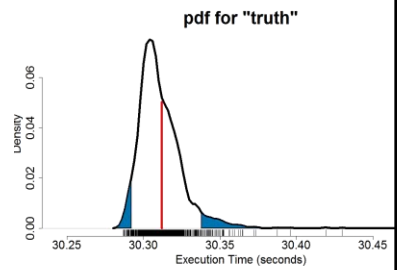
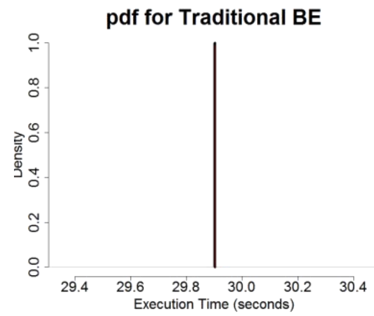
“Truth” vs. Traditional BE Simulation Method





- Example code executed on 3 nodes of LLNL Cab system (1,000 runs)
  - **Considered “truth” for our experiment**
  - **mean: 30.31, sd: 0.23, 90%CI: [30.14, 30.49]**
- Traditional BE simulation of example targeted at CAB architecture
  - **mean: 29.90**
  - **relative error between means: -1.35%**



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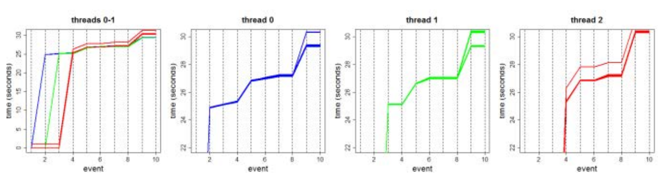
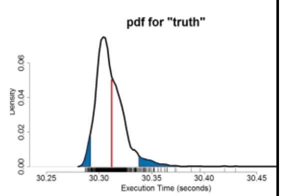
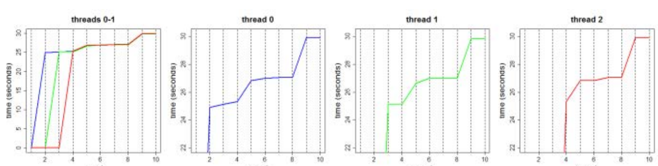
Breakdown of Event Timing: 1,000 Runs

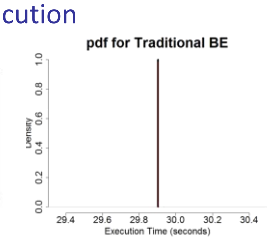
Recorded “walks” for example code execution





Traditional BE simulated “walk” of example code execution





Traditional BE Simulation method only takes one of many possible paths

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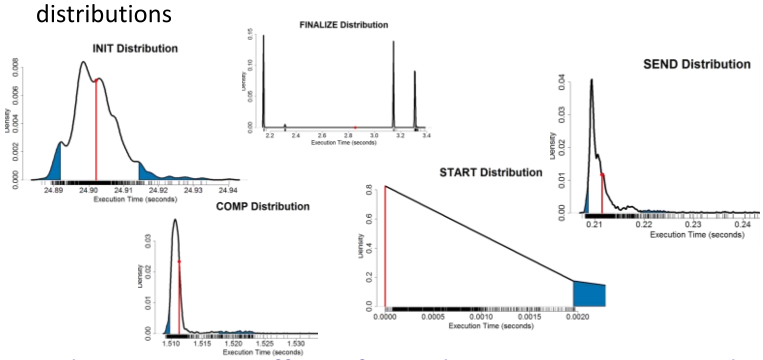
Monte Carlo (MC) Approach to BE

- Traditional BE event timing deterministic
  - i.e., single interpolated value generated from microbenchmark distributions



- How do we capture effect of non-deterministic event ordering
  - Use these distributions as input to MC simulation
  - Generate random walks by sampling from distributions with replacement
  - Analyze resulting output **distribution**

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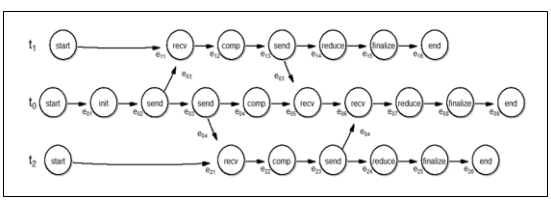
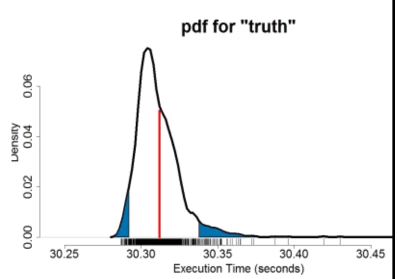
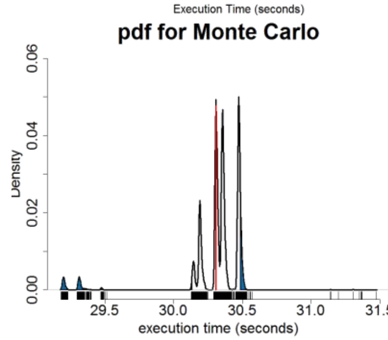
"Truth" vs. Monte Carlo BE Simulation





- MC-based approach (10,000 walks)

Predicted execution:		**Compare to actual execution:**	
mean	30.31	mean	30.31
median	30.35	median	30.31
standard dev	0.2365	standard dev	0.0344
range	[29.18 to 31.38]	range	[30.29 to 31.30]
90% CI	[30.14 to 30.49]	90% CI	[30.29 to 30.34]



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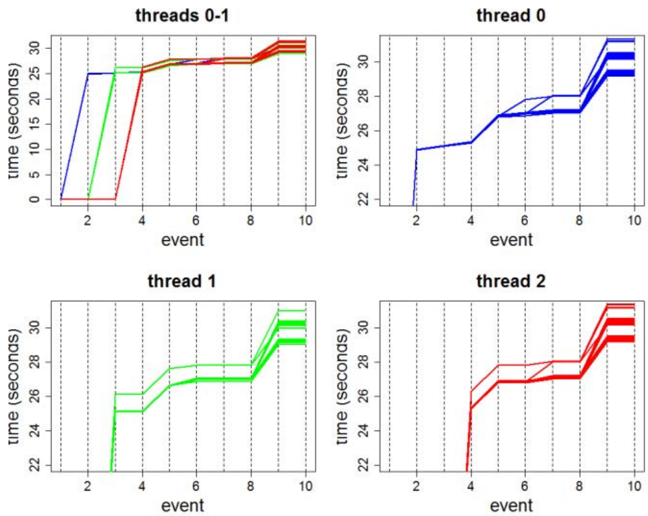
Breakdown of Event Timing: 10,000 Runs

Monte Carlo-based BE Simulated walks of example code execution



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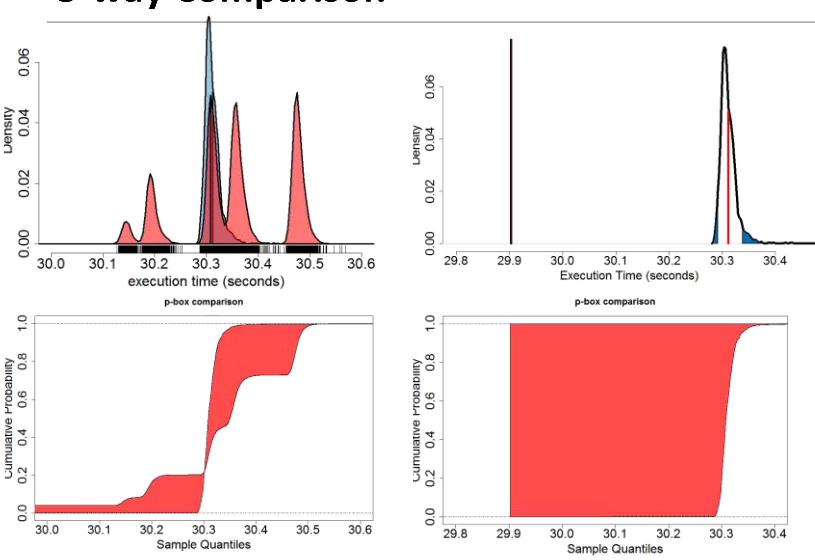
3-way Comparison



Analysis of MC simulation output may help reduce
“area discrepancy” of Traditional BE Simulation method

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Conclusions

- Developed framework for inserting UQ directly into BE simulator
- Presented results for single set of parameters (e.g., # of nodes, size of messages, …)
  - Further experiments required
  - UQ with CMT-bone
- Future work:
  - Explore possible improvements to BE models
  - Exploring FPGA-accelerated BE Monte Carlo simulations

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Do you have any questions?

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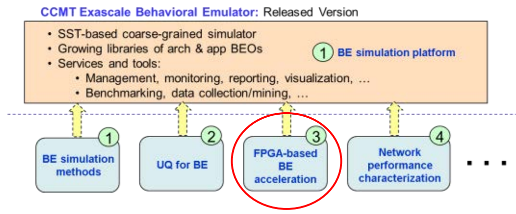
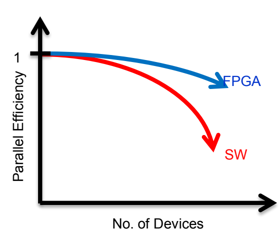


FPGA-based BE Acceleration

Carlo Pascoe (PhD Candidate)
Kasim Alli (PhD Student)

Overview

- Motivation
  - Behavioral Emulation (BE): coarse-grained, multi-scale simulation approach to balance accuracy, speed, and scalability
  - Is it enough as we approach Exascale?
- Goal
  - Complement and accelerate BE approach via FPGA-based reconfigurable computing



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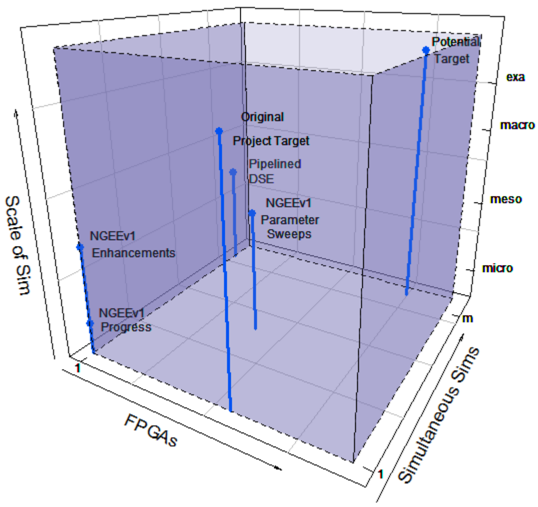
Landscape of FPGA-acceleration Studies



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

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

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

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

Pipelined Design-Space Exploration

Potential Target
- *Several large, Exascale sims distributed over many FPGAs*

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

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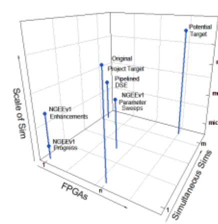
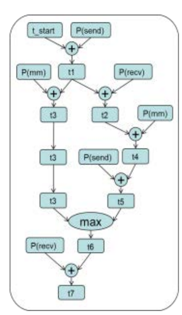
Outline of Presentation

- Review of first-year FPGA studies
- NGEEv1 design enhancements
  - Simulation scaling
  - Increased functionality
- Accelerating DSE using BE
  - Pipelining simulations for higher simulation throughput
- Conclusions





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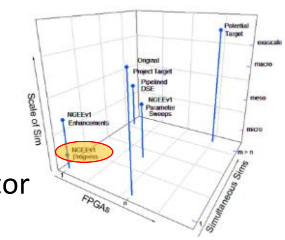
Review of First-Year FPGA Studies

NGEEv1: Current experimental platform for BE-FPGA studies

- Functioning prototype running on single FPGA of Novo-G
- Current core density of 90 for Stratix IV, 256 for Stratix V
  - Each core contains one each of appBEO, procBEO, and commBEO
- Limited optimization (i.e., max-resource implementation)
- Isolated experiments showed **~100x** speedup over Year-1 SMP simulator



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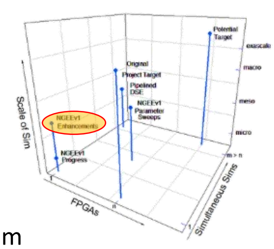
NGEEv1 Enhancement: Simulation Scaling (1)

Issue 1: appBEO scripts stored as thread-level instruction traces in on-chip block RAMs

- Thread-level instruction traces limit simulation size
  - Finite BRAM per FPGA



Short-term solution: FPGA checkpointing

- Checkpointing instruction added to NGEEv1 ISA*
- Store/load BEO states from within instruction stream
- Reassemble (not resynthesize!) between FPGA checkpoints
- Initial tests look promising

Long-term solution: Shared appBEO streaming

- Reduce total appBEO resources per simulation
- Runtime instruction stream from host

**ISA: Instruction Set Architecture*

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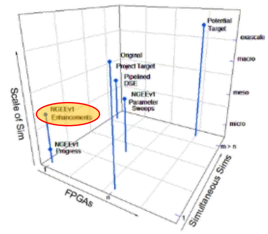
NGEEv1 Enhancement: Simulation Scaling (2)

Issue 2: Current NGEEv1 ISA limiting
- Necessitates verbose representations of simple code
- Inconsistent with recent developments in BE methodology/functionalities



Solution: Augment existing ISA with spanning subset of new BE control-flow instructions
- Allows for more succinct representation of thread traces
- Increases effectiveness/desirability of previously discussed checkpointing method
- Negatively impacts FPGA BEO density
  - Ongoing experiments to explore this area-functionality tradeoff

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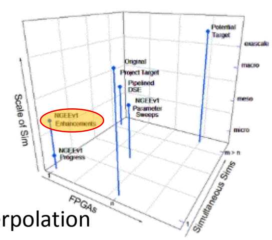
NGEEv1 Enhancement: Simulation Scaling (3)

Issue 3: Explicit emulation of target communication fabric
- Necessitates resynthesis of new circuit when simulating "new" network configuration
- Undesirable for fast DSE



Possible short-term solution: utilize analytical models for communication
- Explicit routing of messages replaced with models or interpolation
- Single optimized FPGA network for all simulated networks, but …
  - Possible reduction in simulation accuracy & deviation from software results
  - Experimentation required to assess extent of reduction & deviation

Long-term solution: virtual routing overlaid on explicit routing fabric
- Single optimized FPGA network to handle all simulated networks, but …
  - Much more difficult to implement efficiently than analytical models
- Existing network reconfigured when simulating "new" network configuration

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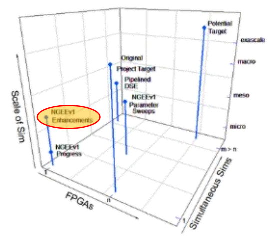
NGEEv1 Enhancement: Functionality (1)

Issue 4: HW utilization < 100%

– app & proc BEOs idle while waiting for comm instruction processing



Possible short-term solution: introduce concept of "BEO hyperthreading"

– Add ability for procBEOs to read from multiple instruction streams
– Switch thread context when stalled for comm events
– Added functionality at expense of added resources
– Experiments to determine if benefits outweigh costs

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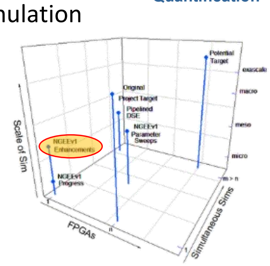
NGEEv1 Enhancement: Functionality (2)

MC* for probabilistic simulation & UQ⁺ analysis

*MC: Monte Carlo
⁺UQ: Uncertainty Quantification

– Earlier session discussed benefits of MC-based simulation
– Disadvantage: greatly increased simulation time
– Lessen impact with FPGAs



Potential solution(1): Implemented at simulation-level

– Sequentially run same simulation configuration
– Random sampling of distributions implemented with memory initialization file preprocessing & FPGA checkpointing

Potential solution(2): Implemented at event-level

– Random number generators used to sample distributions on FPGA
– Each event executed multiple times per simulation
– Reduces overhead associated with starting/stopping multiple sims
– Greatly increase per BEO resource requirements

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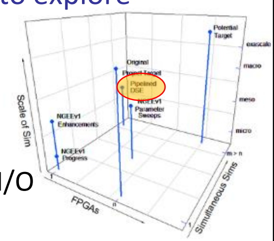
Accelerating DSE using BE

Pipelined Simulations

- Investigate acceleration of DSE to complement NGEEv1 efforts, which focused on single-simulation speed up
  - DSE is critical due to need to optimize CMT for different potential Exascale architectures
- Goal is to pipeline more than one simulation to explore a different configuration every cycle
  - After some initial latency, can explore large number of different configurations – fast DSE
- Ideal for an FPGA
  - Pipeline is bounded by resources rather than I/O
  - Multiple FPGAs can be used to explore a vast input space – almost embarrassingly parallel



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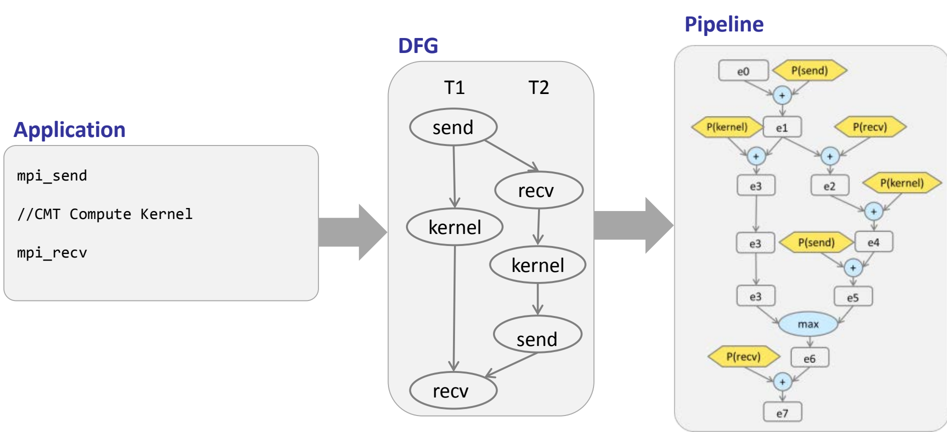
Pipelined Simulations : Approach

- For a given application (left) extract DFG (middle)
- Construct a pipeline (right) from DFG and implement on FPGA



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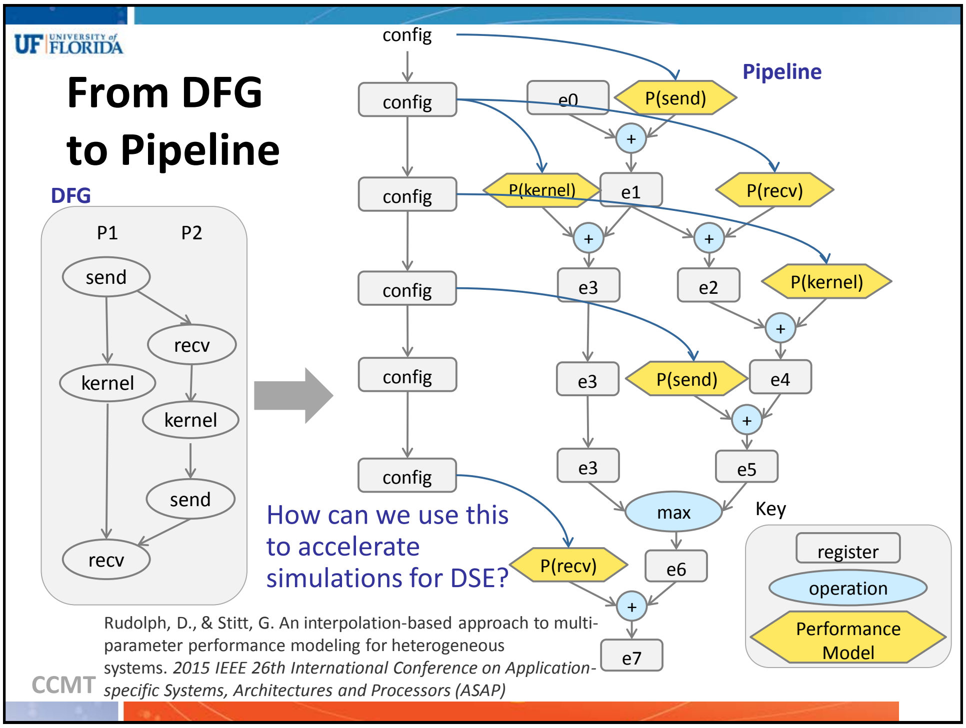
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From DFG to Pipeline
DFG
P1
P2
send
recv
kernel
kernel
send
recv
Pipeline
config
config
config
config
config
config
e0
P(send)
+
P(kernel)
e1
P(recv)
+
+
e3
e2
P(kernel)
+
e3
P(send)
e4
+
e3
e5
max
e6
P(recv)
+
e7
Key
register
operation
Performance Model
How can we use this to accelerate simulations for DSE?
Rudolph, D., & Stitt, G. An interpolation-based approach to multi-parameter performance modeling for heterogeneous systems. 2015 IEEE 26th International Conference on Application-specific Systems, Architectures and Processors (ASAP)
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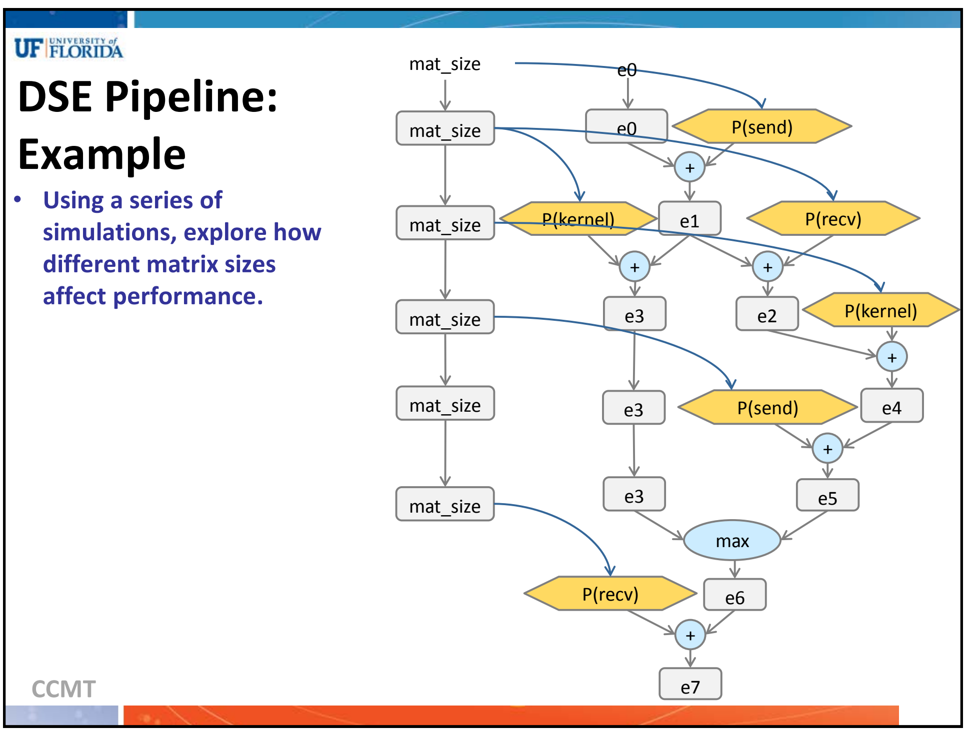
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DSE Pipeline: Example
• Using a series of simulations, explore how different matrix sizes affect performance.
mat_size
mat_size
mat_size
mat_size
mat_size
mat_size
e0
e0
P(send)
+
P(kernel)
e1
P(recv)
+
+
e3
e2
P(kernel)
+
e3
P(send)
e4
+
e3
e5
max
P(recv)
e6
+
e7
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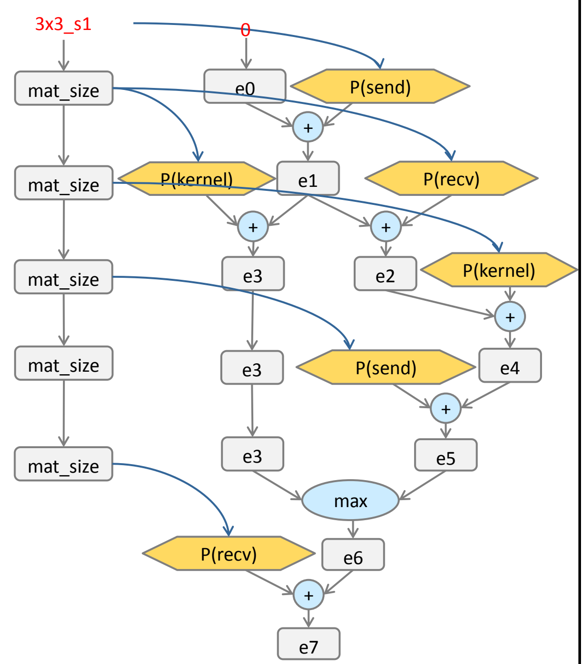
DSE Pipeline: Example

- We start by loading simulation configuration (mat_size) and start time (e0) on each cycle

Sim#	mat_size	e0
sim1	3x3_s1	0



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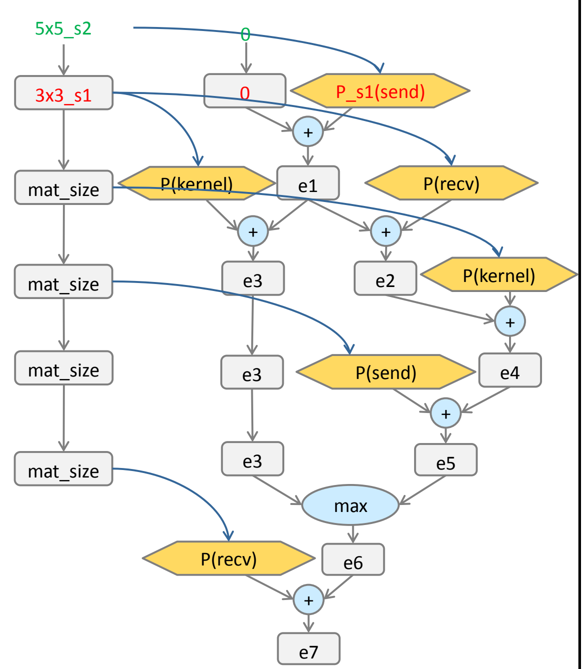
DSE Pipeline: Example

Sim#	mat_size	e0
sim2	5x5_s2	0
sim1	3x3_s1	0



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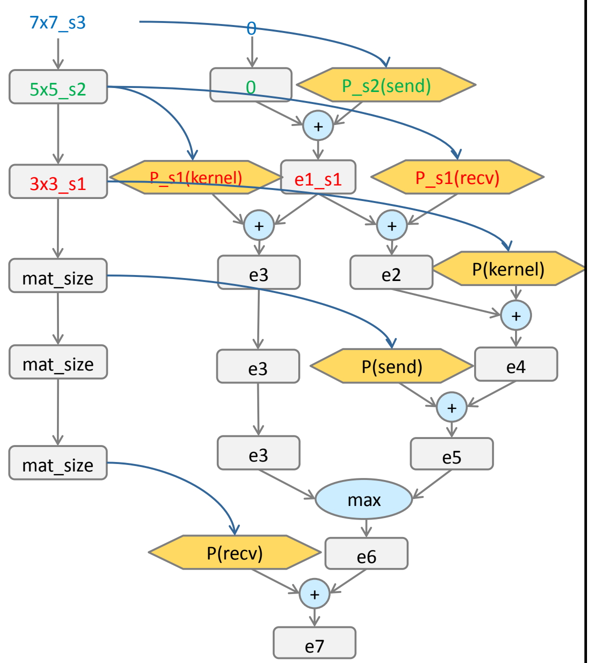
DSE Pipeline: Example

Sim#	mat_size	e0
sim3	7x7_s3	0
sim2	5x5_s2	0
sim1	3x3_s1	0



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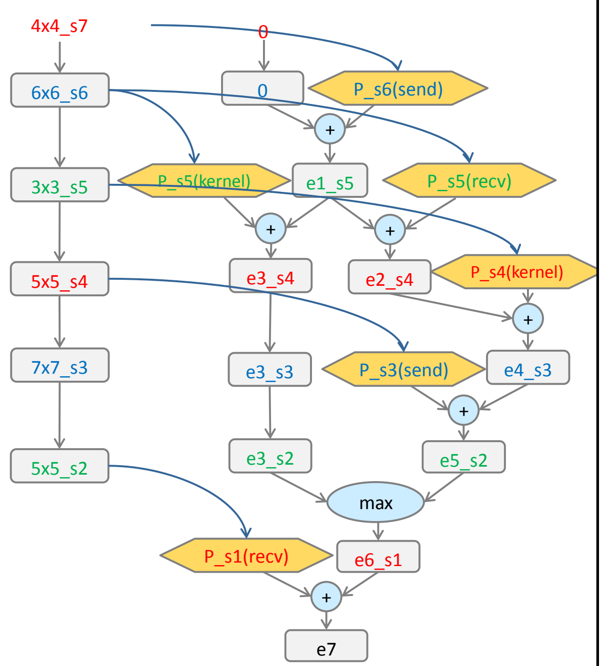
DSE Pipeline: Example

Sim#	mat_size	e0
sim7	4x4_s7	0
sim6	6x6_s6	0
sim5	3x3_s5	0
sim4	5x5_s4	0
sim3	7x7_s3	0
sim2	5x5_s2	0
sim1	3x3_s1	0



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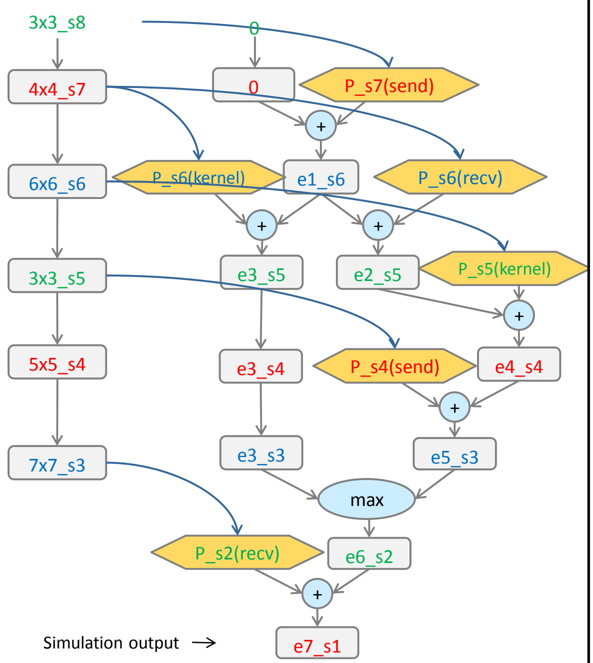
DSE Pipeline: Example

Sim#	mat_size	e0
sim8	3x3_s8	0
sim7	4x4_s7	0
sim6	6x6_s6	0
sim5	3x3_s5	0
sim4	5x5_s4	0
sim3	7x7_s3	0
sim2	5x5_s2	0



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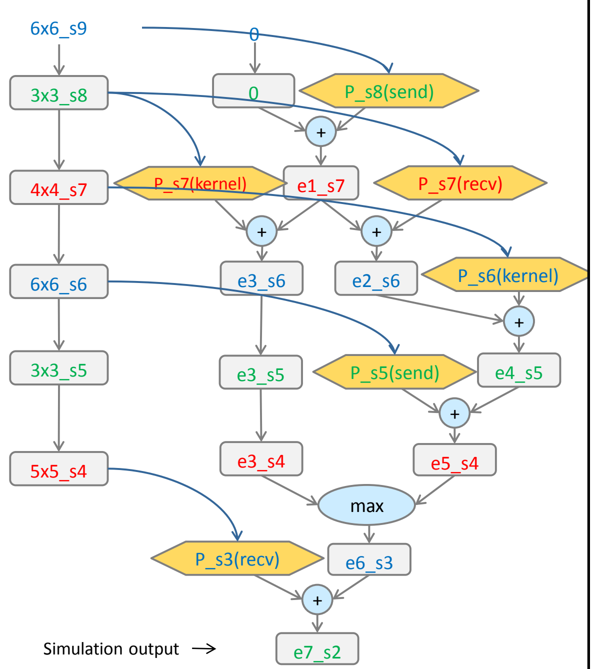
DSE Pipeline: Example

Sim#	mat_size	e0
sim9	6x6_s9	0
sim8	3x3_s8	0
sim7	4x4_s7	0
sim6	6x6_s6	0
sim5	3x3_s5	0
sim4	5x5_s4	0
sim3	7x7_s3	0



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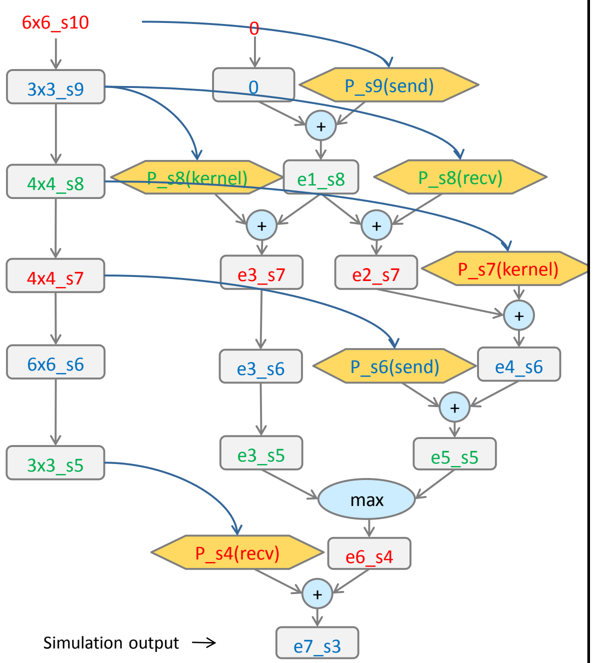
DSE Pipeline: Example

Sim#	mat_size	e0
sim10	5x5_s10	0
sim9	6x6_s9	0
sim8	3x3_s8	0
sim7	4x4_s7	0
sim6	6x6_s6	0
sim5	3x3_s5	0
sim4	5x5_s4	0



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DSE Pipelining Challenges

- Implicit dependency of communication might prevent pipelining
  - Use analytical models
- Pipeline max operation may be inaccurate
  - Use a more sophisticated operation
- Cases where code cannot be pipelined
  - Model at higher level of abstraction
- Simulations may be too large for a single FPGA
  - Implement resource sharing
- Configuration parameters causing changes in FPGA circuit, requires long compile times
  - Leverage virtualization research

Coole, J., & Stitt, G. Fast, Flexible High-Level Synthesis from OpenCL using Reconfiguration Contexts. *IEEE Micro,* 42-53

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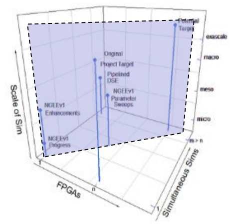
Conclusions

- Analysis of Exascale systems will require FPGA-acceleration of BE
- First-year focus on techniques to speedup individual simulations across multiple FPGAs
- Current focus:
  - Techniques to parallelize simulations across multiple FPGAs (parameter sweeping) & within single FPGA (DSE pipelining)
  - Enables rapid DSE exploration to help answer questions about how to optimize CMT apps on potential Exascale architectures



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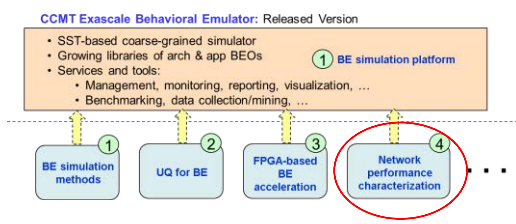

Network Performance Characterization

Nalini Kumar (PhD Candidate)

UF UNIVERSITY of FLORIDA NNSA

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Overview

- Motivation
  - Use existing tools to analyze performance of CMT-nek communication routines
    - In parallel with R&D of BE methods and tools
  - Lessons learned to guide development of network models in BE simulation platform
- Goal
  - Explore performance of CMT-bone comm. routines using SST while BE tools mature
  - Evaluate impact of model granularity on speed and accuracy of simulations

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Outline of Presentation

- SST Network Modeling Libraries
- Application Modeling in SST
- CMT-bone Simulations using SST
  - Application & machine models
- Results
  - Sensitivity to model parameters
  - SST simulation scalability
  - Design-space exploration
- Conclusions

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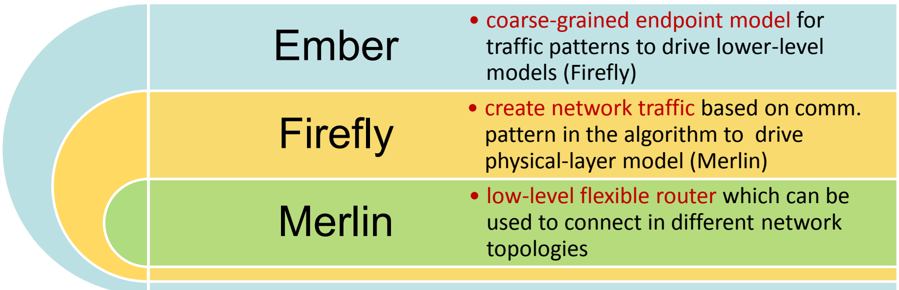
SST Network Modeling Libraries

- SST has various built-in network models



- Ember is very suitable for our purposes
  - Supports MPI and SHMEM functions
  - Supports abstraction of low-level details

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Application Modeling in SST (Motifs)

- Motifs are coarse-grained representations of app behavior, similar to AppBEOs, that capture interactions between network endpoints
  - Look very much like an MPI program (serial flow)
  - Network endpoints can be cores, devices, nodes, etc.
  - Compute blocks or local operations are delay blocks used to pace the simulation similar to our ProcBEOs
- Ember contains motifs for several commonly used comm. patterns
  - e.g., halo exchanges, MPI collectives, sweeps, etc.
  - We extended motifs library by adding models for CMT-nek comm routines

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CMT-bone Simulations using SST (1 of 5)

- For simulations we need:
  1. Motif/abstract application description for CMT-bone
  2. Modeling parameters to describe system
  3. SST configuration file specifying motif parameters

```
// User parameters - application
        uint32_t iterations;            // Total no. of timesteps being simulated
        uint32_t eltSize;               // Size of element (5-20)
        uint32_t variables;             // No. of physical quantities

// User parameters - machine
        int32_t px;                     // Machine size (no. of nodes in 3d dimensions)
        int32_t py;
        int32_t pz;
        int32_t threads;

// User parameters - mpi rank
        uint32_t mx;                    // Local distribution of the elements on a MPI rank
        uint32_t my;
        uint32_t mz;
        uint32_t nelt;                  // Total no. of elements per process (100-10,000)

// User parameters - processor
        uint64_t procFlops;             // no. of FLOPS/cycle for the processor
        uint64_t procFreq;              // operating frequency of the processor
        double m_mean;
        double m_stddev;
```

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CMT-bone Simulations using SST (2 of 5)

- For simulations we need:
  1. Motif/abstract application description for CMT-bone

```
        double nsCompute = m_random->getNextDouble();
        enQ_compute( evQ, nsCompute );          // Delay block for compute

        // +x/-x transfers
        // If even: recv +x, send +x, recv -x, send -x
        // If odd: send +x, recv +x, send -x, recv -x
        if ( myX % 2 == 0){
                if (sendx_pos) {
                        enQ_recv( evQ, x_pos, x_xferSize, 0, GroupWorld );
                        enQ_send( evQ, x_pos, x_xferSize, 0, GroupWorld );
                }
                if (sendx_neg) {
                        enQ_recv( evQ, x_neg, x_xferSize, 0, GroupWorld );
                        enQ_send( evQ, x_neg, x_xferSize, 0, GroupWorld );
                }
        }
        else {
                if (sendx_pos) {
                        enQ_send( evQ, x_pos, x_xferSize, 0, GroupWorld );
                        enQ_recv( evQ, x_pos, x_xferSize, 0, GroupWorld );
                }
                if (sendx_neg) {
                        enQ_send( evQ, x_neg, x_xferSize, 0, GroupWorld );
                        enQ_recv( evQ, x_neg, x_xferSize, 0, GroupWorld );
                }
        }

        // +y/-y transfers
```

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CMT-bone Simulations using SST (3 of 5)

- For simulations we need:
  1. Motif/abstract application description for CMT-bone
  2. Modeling parameters to describe network
  3. SST configuration file specifying motif parameters

```
networkParams = {
    "packetSize" : "2048B",
    "link_bw" : "4GB/s",
    "link_lat" : "40ns",
    "input_latency" : "50ns",
    "output_latency" : "50ns",
    "flitSize" : "8B",
    "buffer_size" : "14KB",
}

nicParams = {
    "module" : "merlin.linkcontrol",
    "packetSize" : networkParams['packetSize'],
    "link_bw" : networkParams['link_bw'],
    "buffer_size" : networkParams['buffer_size'],
    "rxMatchDelay_ns" : 100,
    "txDelay_ns" : 50,
    "nic2host_lat" : "150ns",
}
```

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CMT-bone Simulations using SST (4 of 5)

- For simulations we need:
  1. Motif/abstract application description for CMT-bone
  2. Modeling parameters to describe network
  3. SST configuration file specifying motif parameters

```
    numNodes = 0 # numNodes = 0 implies use all nodes on network
    numCores = 1

    return workFlow, numNodes, numCores

def getNetwork():

        platform = 'default'

        topo = 'torus'
        shape = '2x2x2'

        return platform, topo, shape
```

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CMT-bone Simulations using SST (5 of 5)

- For simulations we need:
  1. Motif/abstract application description for CMT-bone
  2. Modeling parameters to describe network
  3. Ember configuration file specifying motif parameters

```
def getWorkFlow( defaults ):
    workFlow = []
    motif = dict.copy( defaults )
    motif['cmd'] = "Init"
    workFlow.append( motif )

    motif = dict.copy( defaults )
    motif['cmd'] = "CMT3D iterations=10000 elementsize=10 variables=5 px=16 py=16 pz=32"
    workFlow.append( motif )

    motif = dict.copy( defaults )
    motif['cmd'] = "Fini"
    workFlow.append( motif )
```

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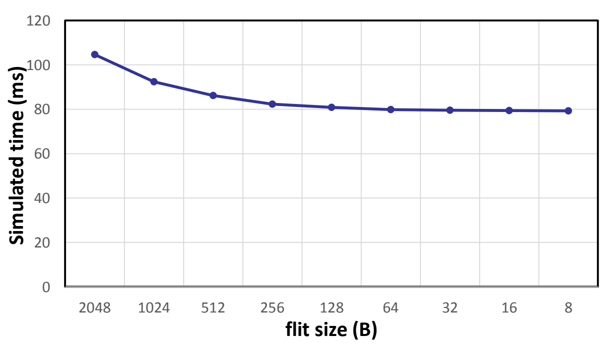
Sensitivity to Model Parameters

- Estimating effect of granularity on simulation accuracy

Simulation accuracy w.r.t. simulation granularity



- **Application setup**: element size=10, iterations=1000
- **Machine setup**: 8x8x8 3D torus, pkt size=2048 B
- **Observations:** As flit size approaches pkt size, simulation estimations become increasingly more inaccurate (~30%)

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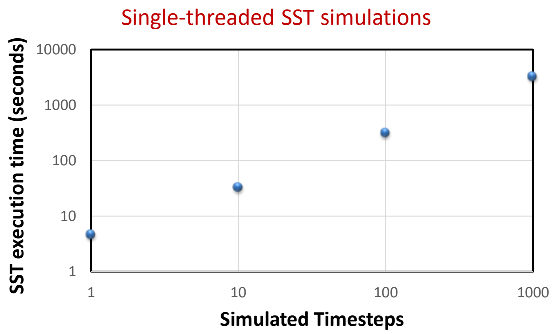
Scaling SST Simulations

- Speed of SST simulations as size of application grows



- **Application setup:** 1000 elements/processor, element size=10
- **Machine setup:** 512 nodes (8x8x8 torus), bw= 4GB/s ,pkt size= 2048B, flit size = 8B
- **Observations:** SST execution time increases linearly with an increase in problem size

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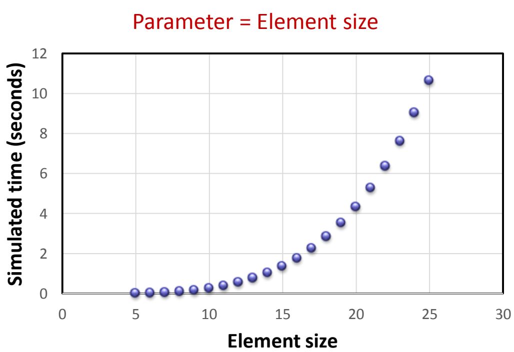
Design-Space Exploration (1 of 3)

- Effect of varying element size on application execution time



- **Application setup:** 1000 elements/process, 1000 timesteps (iterations)
- **System setup:** 4x4x4 torus with 1 process per node, bw=4GB/s, pkt size=2048B, flit size=8B
- **Observations:** As expected, app execution time (estimated) increases exponentially with increase in element size

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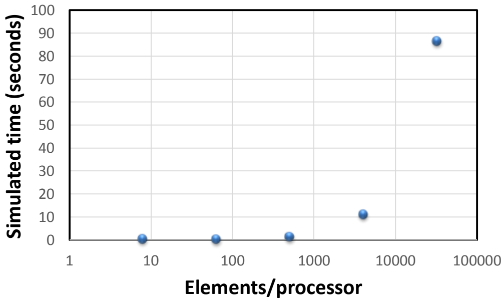
Design-Space Exploration (2 of 3)

- Effect of varying elements on application execution time

Parameter = Elements/processor



- **Application setup:** element size=10, 1000 timesteps (iterations)
- **System setup:** 4x4x4 torus with 1 process per node, bw=4GB/s, pkt size=2048B, flit size=8B
- **Observation:** Execution time increases almost linearly with an increase in processor load. Computation is the major contributor to this increase.

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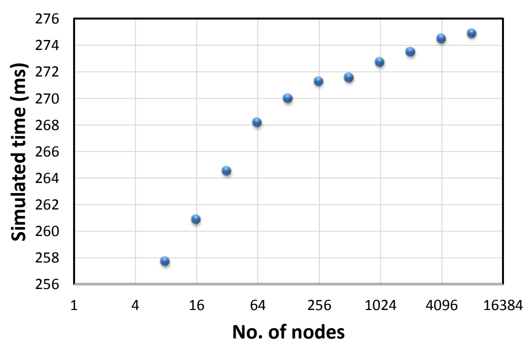
Design-Space Exploration (3 of 3)

- Weak scaling

parameter = machine size & problem size



- **Application setup:** element size=10, 100 timesteps (iterations)
- **System setup:** 3d torus with 1 process per node, bw=4GB/s, pkt size=2048B, flit size=8B
- **Observation:** As problem size and system size increase, the amount of computation per processor remains the same. Communication time grows fast in the beginning before stabilizing.

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Conclusions

- SST, with its built-in network models, is a useful simulation tool
  - Easy to modify granularity
  - Relatively simple software description
- SST execution time scales linearly with size of application being simulated
- In-depth analysis is needed to answer critical load-balancing questions
  - Increasing number of elements processed by a processor has lesser impact on execution time than increasing element size
- Future Work
  - Improve application analysis by improving network and processor calibration
  - Compare scalability and accuracy of SST and BE network models to improve BE models

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Do you have any questions?

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Student Internships

Chris Hajas (MS)
Chris Neal (PhD)
Carlo Pascoe (PhD)
Nalini Kumar (PhD)

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LLNL Internship

Chris Hajas

Mentors: Dr. Scott Lloyd and Dr. Maya Gokhale

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Overview

- Project:
  - "Emulating In-Memory Data Reorganization for HPC Applications"
  - Accelerate SpMV using emulation framework
  - Explore methods to quickly determine future apps to explore
- Highlights:
  - Tours of NIF and Sequoia
  - Many seminars and interactions with different groups in lab
  - Poster session to showcase work
  - Outside events such as rafting, hiking, and exploring the bay area

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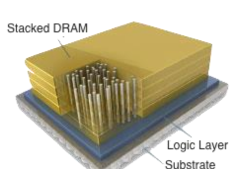
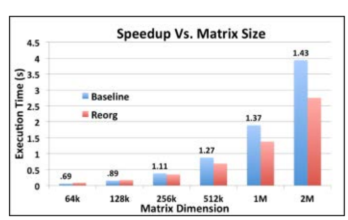
SpMV Acceleration

- Motivation:
  - Emerging memory architectures (e.g. HMC) have logic layer allowing for near memory logic/computation
  - Many apps of interest to DOE exhibit irregular, non-cache friendly memory accesses
- Goal:
  - Use custom framework on Zynq FPGA + ARM SoC to emulate Data Reorganization Engine (DRE) logic and integrate with apps using custom API
  - Show that SpMV, a key kernel in many scientific apps, is amenable to data reorganization and provides speed and power improvements when used with our (DRE)





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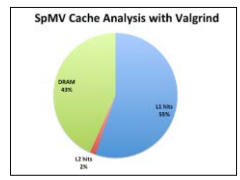
App Amenability Studies

- Motivation:
  - Only apps with specific characteristics will benefit from our DRE and modifying these apps can be time consuming in some cases
  - DOE apps are large and complex-- determining whether they would benefit is non-trivial and time consuming
- Goal:
  - Develop methods to provide quick insight into whether we should further explore a particular app to use in our emulation framework



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Conclusion

- Contributions
  - Accelerated SpMV by 1.4x and explored architectural design tradeoffs
  - Analyzed and instrumented various DOE apps/kernels to determine amenability to DRE
  - Researched architectural performance counters and wrote wrapper to help determine amenability to DRE
  - Contributed to paper presented at MEMSYS in October
  - Presenting poster of work at SC15 in Austin in November

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National Lab Internship

Christopher Neal
Ph.D. Student

S. Balachandar, Ph.D.
William F. Powers Professor of Mechanical & Aerospace Engineering

Kambiz Salari, Ph.D.
Lawrence Livermore National Laboratory

Lawrence Livermore National Laboratory

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NNSA

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Overview

- Mentor: Dr. Kambiz Salari
- Internship Highlights
  - Summer seminars
  - NIF & computing facility tours
- Projects CASC
  - Random particle beds
  - Particle wake study

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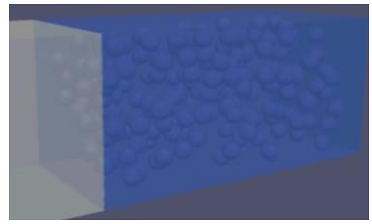
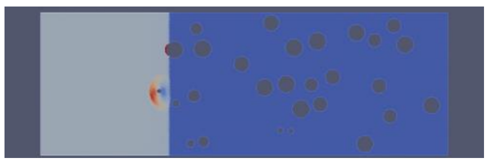
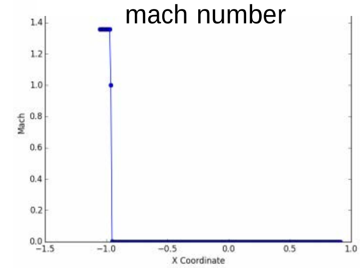
Random Particle Beds

- Motivation – Study the interaction of shockwaves with particle beds
- Random particle bed research aligned with Kambiz's interests
- Ran simulations for 10%, 15%, 20%, 25% bed volume fractions
- Developed analysis script for estimating shock front location





Streamwise average mach number



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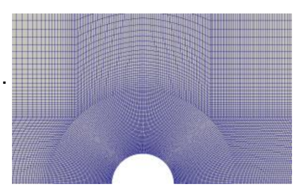
Particle Wake

- Grid generation assistance - David Dawson, Ph.D.
- Discussions about simulation setup - Fady Najjar, Ph.D.
- What error is committed when ignoring viscous effects in compressible multi-particle simulations?



- Work is on-going – Looking into multiple particle effect

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Summary

- LLNL's intern program was excellent
- It was great to see the work that LLNL does to advance the mission of stockpile stewardship
- I look forward to returning to the lab next summer

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LLNL Internship

Carlo Pascoe

"Enabling CCMT Exploration of Future HPC Architectures with Gem5"

Mentor: Dr. Maya Gokhale

Carlo Pascoe

Motivation

- Behavioral Emulation (BE) framework has mainly targeted
  - Micro-level simulations
  - Simple CMT kernels
  - Existing architectures
- Specifics of model/framework to purely notional architectures remain undetermined
- Determination required before BE exploration of future architectures can progress

Goal

- Evaluate feasibility of leveraging gem5 simulator purposed at generating reliable training data for BE notional architecture models

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Carlo Pascoe

Approach

- Learn the tool
- Experiment with CCMT kernels on various architecture configurations
- Evaluate performance with several quantitative (e.g., accuracy, speed) and qualitative (e.g., ease of use) metrics

Contributions

- In depth analysis of gem5 and CCMT-nek source code
- Extensive research into AMD piledriver microarchitecture
- Development of custom gem5 cpu/memory models
- Modification of gem5 source for increased functionality
- Integration with model for Micron's Hybrid Memory Cube
- Setup/execution/evaluation of simulation experiments

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Carlo Pascoe

Conclusion

- gem5 may be useful for generating training data for BE notional architecture models in select situations with a few caveats:
  - Simulations are slow limiting the number of training points that can be productively captured
  - For our purposes, stock gem5 X86 models are not very good representations of contemporary architectures – some internal modification would be needed
  - Workloads taking advantage of advanced processor features (e.g., complicated branch predictors & prefetchers) will not be modeled well
  - Memory behavior is reasonably accurate assuming correct input and setup, but current models only use a few basic write back cache coherency models with the limit of a single read/write port to cache per cpu core
- For training data generation, if components most necessary for capturing dominant workload behavior are modeled well then simulation runtime error should be acceptable

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Internship Talk

Nalini Kumar

Sandia National Laboratories, Albuquerque, NM

March – August, 2015

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NNSA

Overview

- Lab: Computer Science Research Institute (CSRI), SNL
- Mentors: Dr. Simon Hammond, Dr. Arun Rodriguez
- Manager: Dr. Jim Ang
- Buddy: Dr. Gwen Voskuilen,

- Project:
  Simulating CMT-bone communication routines using high-level network endpoint models

- Internship highlights:
  - Presented a poster and gave a random access talk at Salishan conference on High-speed computing in Oregon in April.
  - Submitted abstract and presented poster at the ModSim workshop in Seattle in August.
  - Attended the Center for Computing Research (CCR), summer seminar series
  - Project report submitted to the CCR Summer Proceedings 2015

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Scalable Network Simulation using SST *

We are looking at SST* for supporting scalable network simulation

1. Develop abstract end-point models **'motifs'** for the various communication routines used in CMT-Nek
   - Identified routines: Nearest-neighbor communication using pairwise exchange, all-to-all using crystal routing, allreduce, bcast etc.
2. Of course we need to validate the simulation results:
   - Full application is too complex and cumbersome to do targeted study, so we developed a mini-app 'CMTBone' for in-house use
3. Understand the sensitivity of simulations to the various model parameters
   - Our hope is to reduce the number of component models, parameters, and events being simulated
   - It has to be good enough to provide a first-order approximation of performance which can enable application developers to do some early design space exploration

* Structural Simulation Toolkit

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Summary

- Worked with the SST team to understand and evaluate its potential use as a BE platform
- Collaborated with CMT-nek development team to analyze the network behavior of our app
- Created application models for SST that have been used for research in our center
- Several opportunities to discuss and present my research (done at Sandia and UF) to the community

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Uncertainty Budget

Validation and Uncertainty Reduction

Chanyoung Park, Yiming Zhang
and Raphael (Rafi) T. Haftka
Department of Mechanical & Aerospace Engineering,
University of Florida

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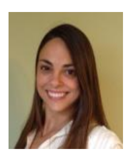
NNSA

Uncertainty Budget Team

Raphael T. Haftka, PhD

Nam-Ho Kim, PhD

Chanyoung Park, PhD



Giselle Fernandez

Yiming Zhang

Sam Nili

- PI: Raphael T. Haftka and Nam-Ho Kim
- Postdoc: Chanyoung Park
- Graduate students
  - Giselle Fernandez (Mesoscale 1-D simulation)
  - Yiming Zhang (Extrapolation)
  - Sam Nili (Mesoscale 1-D and 2-D simulation)
- Visiting PhD student
  - Na Qiu (TBD)
- Undergraduate student
  - Justin T. Mathew (Mesoscale ASU experiment)

Na Qiu

Justin T. Mathew

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Objectives

- In order to validate the prediction capability of the demonstration problem
  - Define measurable quantities of interest as metrics
  - Validate the prediction capability with these metrics
  - Establish appropriate uncertainty quantification and reduction frameworks
- Interactions with the other teams in different disciplines

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Accomplishments

- Mesoscale validation
  - Validated 1D/2D mesoscale simulations
  - Estimated the error and the corresponding uncertainty in the predictions of the simulations
  - Quantified uncertainties and calculated uncertainty budget
- Interactions
  - Modeling the feasible region of JWL-EOS
  - Studying the possibility of using surrogate model in JWL-EOS code for efficient computing
  - Defining matrix multiplication computation time measurement considering its variability
  - UQ study of the ASU expansion fan experiment
- Extrapolation

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UB Team

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

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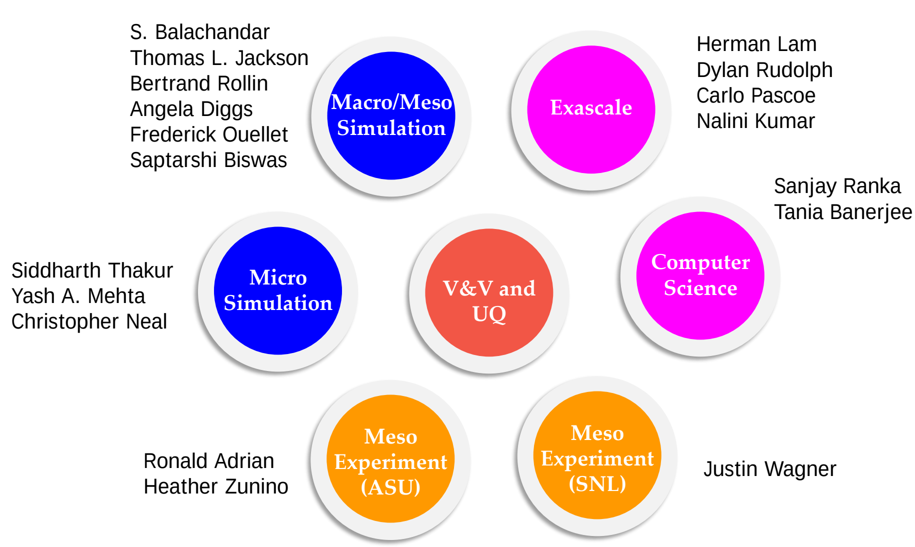
Interactions



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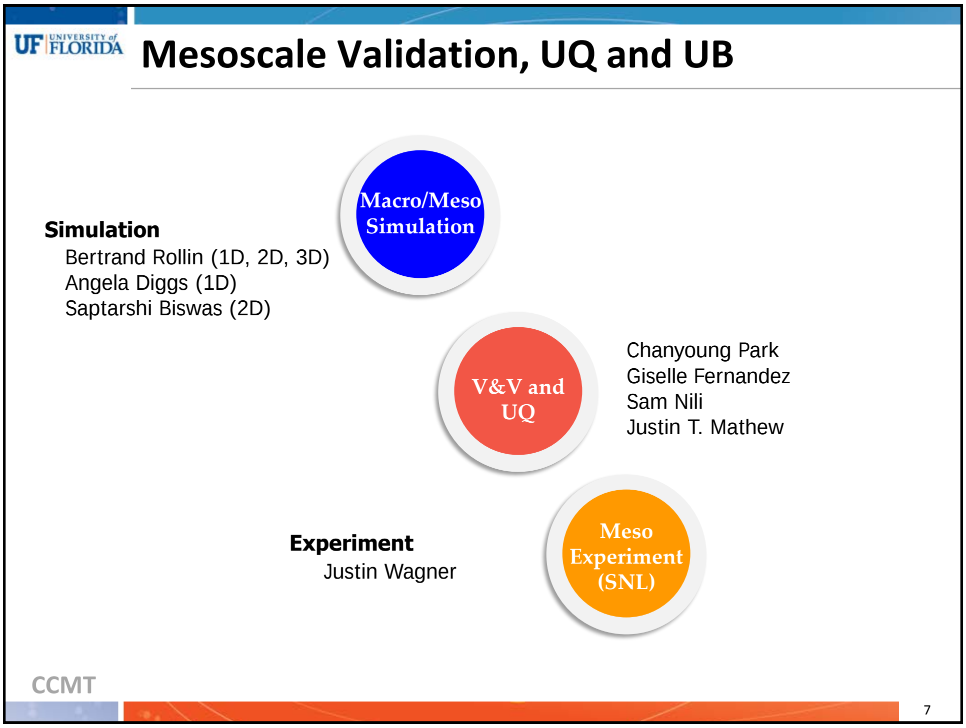
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Mesoscale Validation, UQ and UB
Macro/Meso Simulation
Simulation
Bertrand Rollin (1D, 2D, 3D)
Angela Diggs (1D)
Saptarshi Biswas (2D)
V&V and UQ
Chanyoung Park
Giselle Fernandez
Sam Nili
Justin T. Mathew
Experiment
Justin Wagner
Meso Experiment (SNL)
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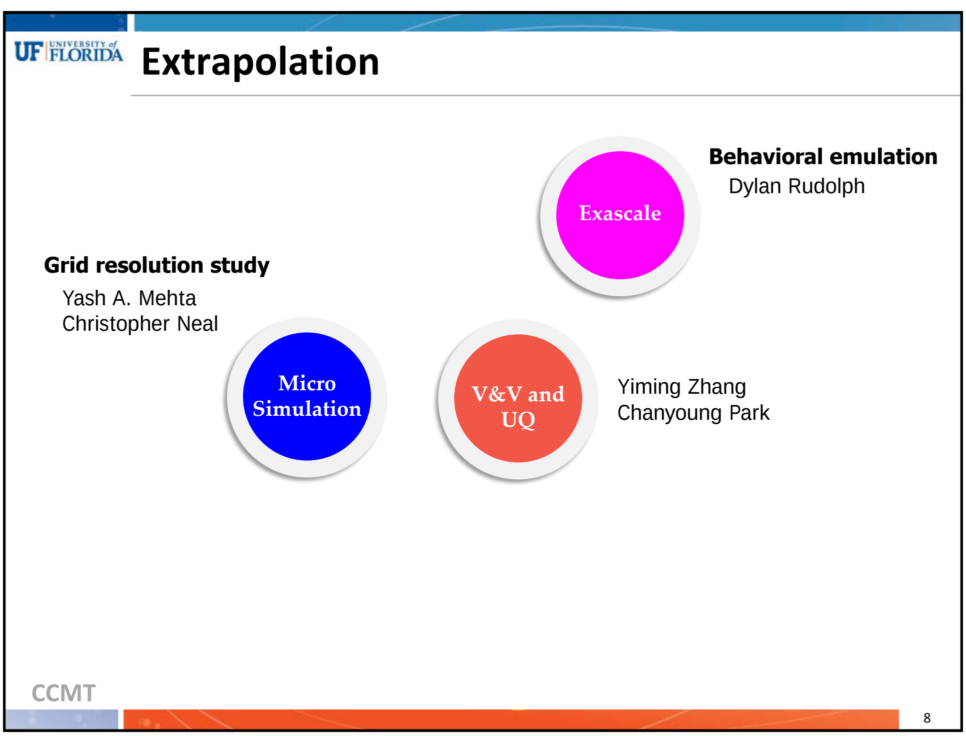
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Extrapolation
Behavioral emulation
Dylan Rudolph
Exascale
Grid resolution study
Yash A. Mehta
Christopher Neal
Micro Simulation
V&V and UQ
Yiming Zhang
Chanyoung Park
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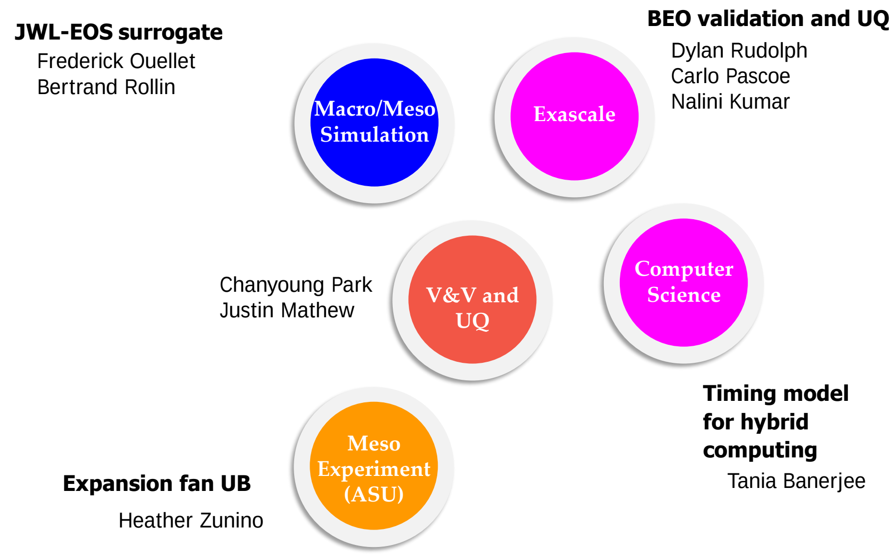
Other Interactions



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Presentation Highlights

- Mesoscale validation, UQ and UB
  - Compensating errors resulted in deceivingly small prediction error
  - Model error masqueraded as numerical noise
- Extrapolation
  - Extrapolation worked with reasonable accuracy for several applications (e.g. convergence of simulation, matrix multiplication)
  - Applying knowledge (such as on monotonicity) improved extrapolation accuracy
- Other interactions
  - The feasible region of JWL-EOS solver needs to be identified and modeled
  - Surrogates can help to improve computation speed of JWL-EOS solver

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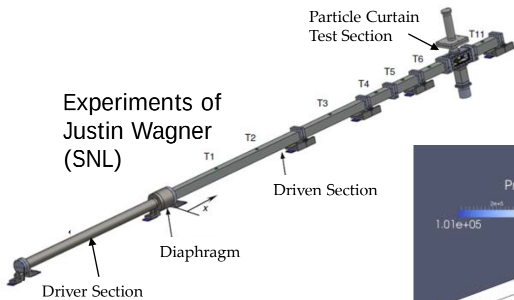
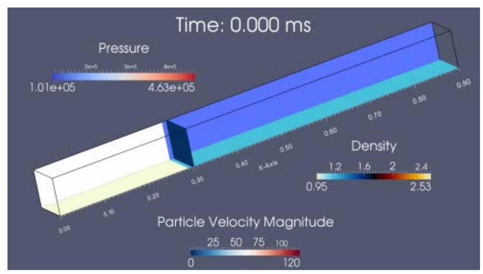
Mesoscale Validation, UQ and UB

- **Goals**
  - Validation of the collision and particle force models
  - Estimating errors in the physics models and the corresponding uncertainties using 1D/2D/3D simulations
  - Quantifying cost for reducing uncertainty (UB)

Experiments of Justin Wagner (SNL)



3D Simulation (Rocflu)



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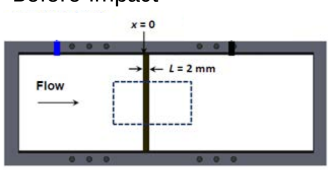
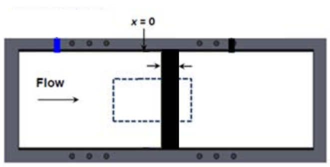
Prediction Metrics

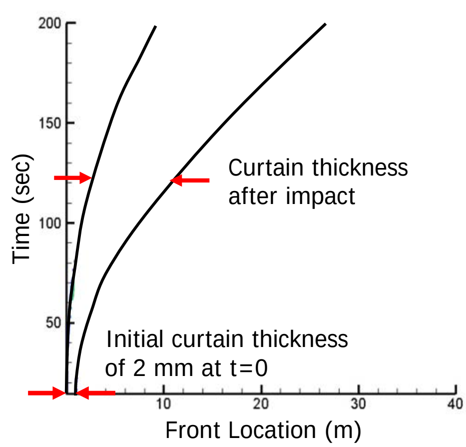
- **Prediction Metrics** are upstream and downstream particle front positions **averaged** over initial particle position and diameter variations

- Before impact



- After impact





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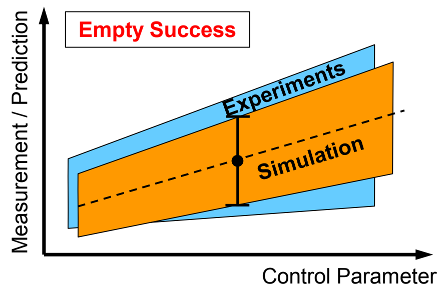
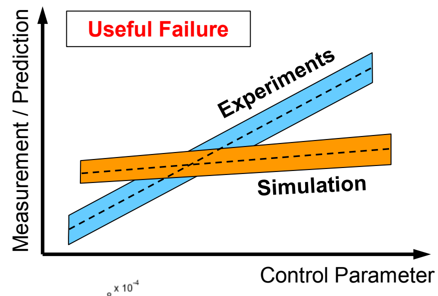
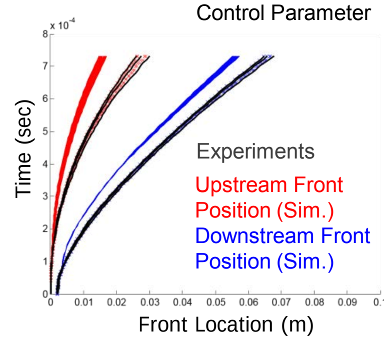
UB: Uncertainty Reduction Budget





- UR requires to make validation meaningful (i.e. Useful Failure) for further model improvements in the future
- Uncertainty reduction budget (UB) provides a guideline for finding the most efficient uncertainty reduction approach
- Further uncertainty reduction (UR) is not immediate requirement for the mesoscale simulation



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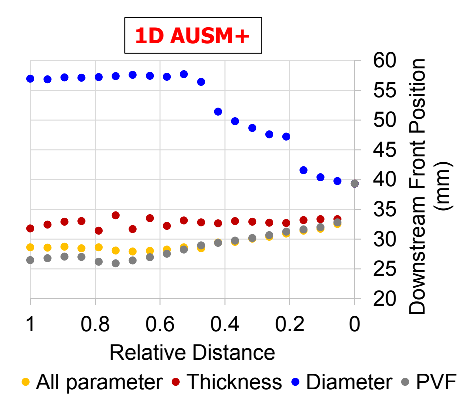
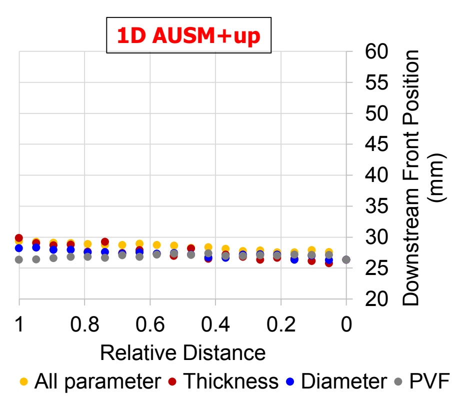
Numerical Model Error Reduction

- The behavior of the diameter line is very different from those of the other groups
- Angela Diggs upgraded the code to a newer version using the scheme AUSM+up
- Improved model substantially reduces error and noise





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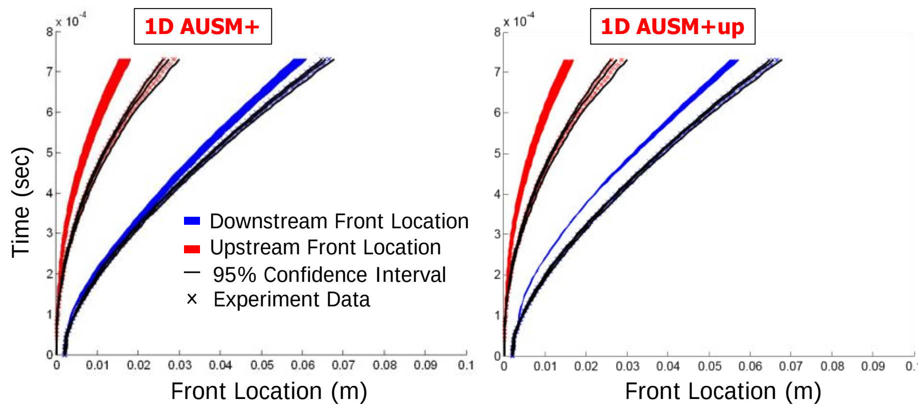
Sim. Improvement Increased Prediction Error



- AUSM+ of Rocflu was improved to AUSM+up
- Numerical model error reduction revealed the physical errors (i.e. collision and particle force models)
- Apparently small prediction error but possibly large compensating errors

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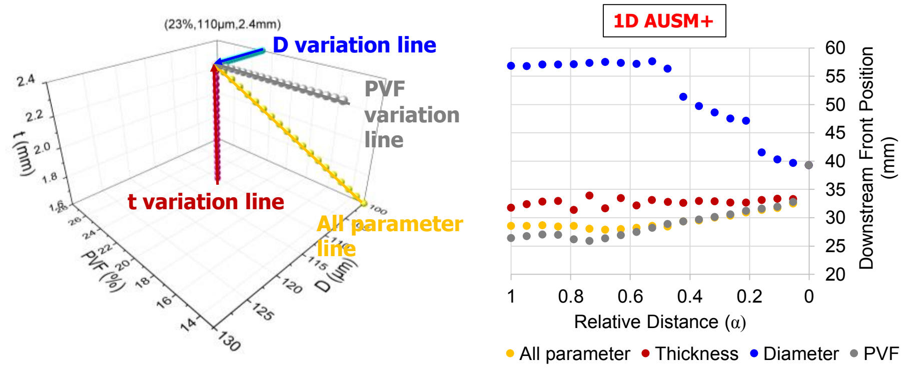
Groups of Runs for Detecting Model Error



- Groups of runs on 4 lines with varying one parameter and varying all parameters
- Curtain thickness (t), particle diameter (D), particle volume fraction (PVF) were considered
- The lines converge to one point (PVF=23%, t=2.4mm, D=110μm)

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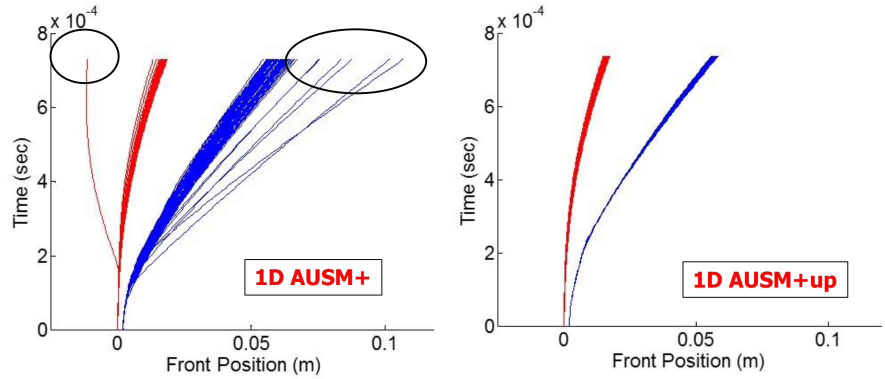
Model Error and Uncertainty Reduction



- The numerical noise looking model error and noise looking uncertainty were reduced by upgrading AUSM+ to AUSM+up
- **Groups of runs** detected the numerical uncertainty in the 1D simulation was huge

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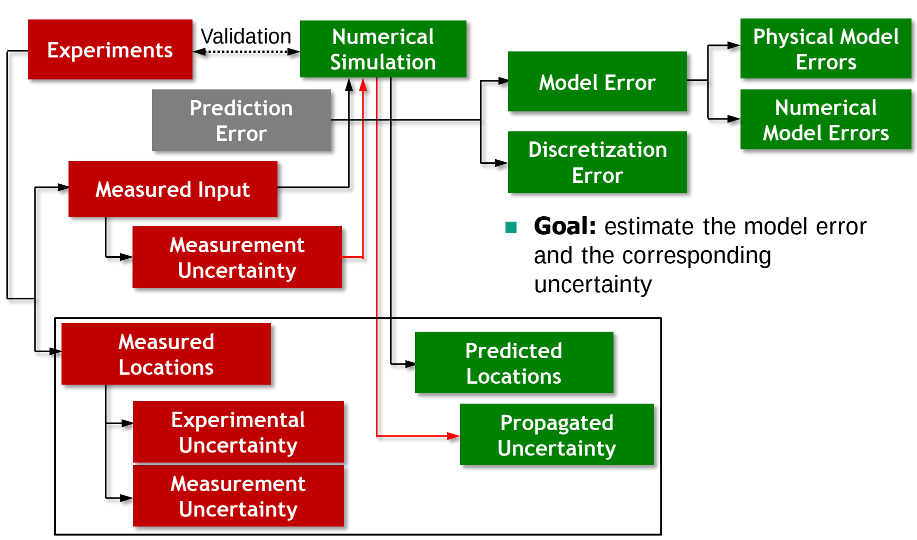
Validation and UQ Framework



- **Goal:** estimate the model error and the corresponding uncertainty

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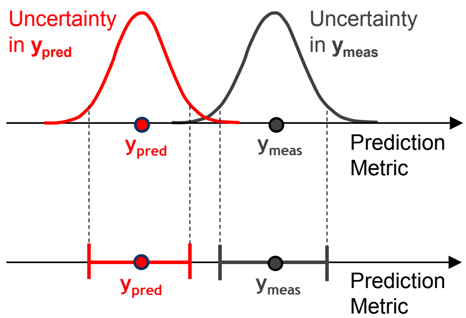
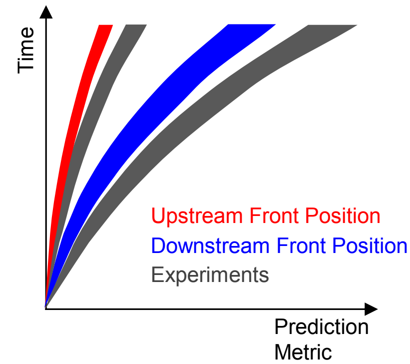
Particle Front Position (PM) with Uncertainty

- Distributions modeling uncertainties



- 95% confidence intervals representing uncertainties

- Particle front positions with 95% confidence intervals



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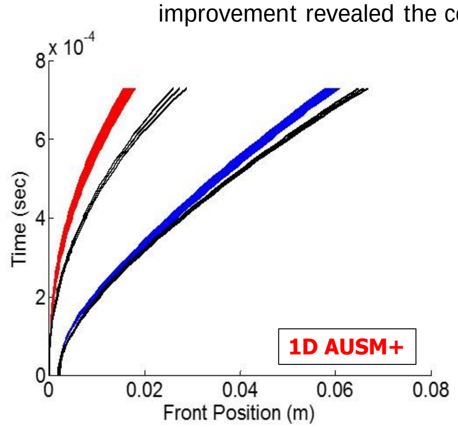
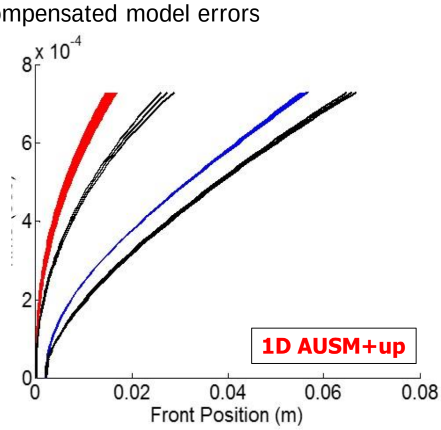
PMs and Uncertainties of 1D Simulations

- 1D simulations with AUSM+ and AUSM+up
- Error reduction in AUSM+ scheme increased the prediction error (discrepancy between the UFP prediction and measurement)
- The error in AUSM+ compensated the errors in physics models (e.g. collision model, particle force model, etc.) and the improvement revealed the compensated model errors





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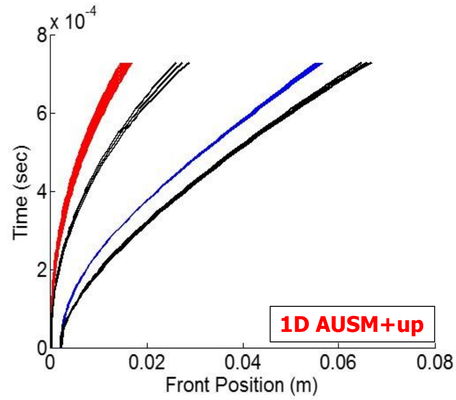
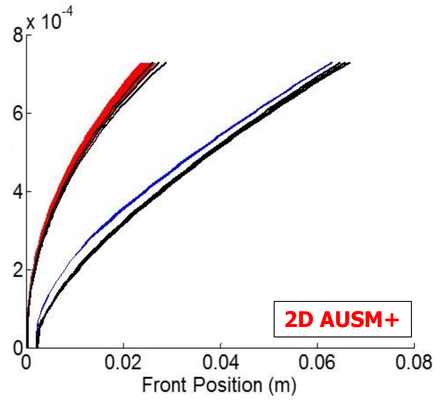
PMs and Uncertainties of 1D/2D Simulations

- 1D (AUSM+up) and 2D (AUSM+)
- The discrepancy of 2D is apparently smaller than that of 1D but it should be justified by applying AUSM+up on 2D





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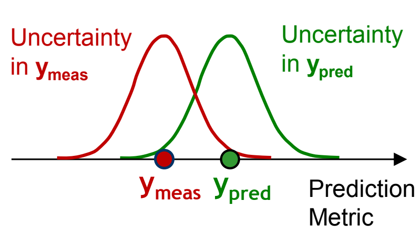
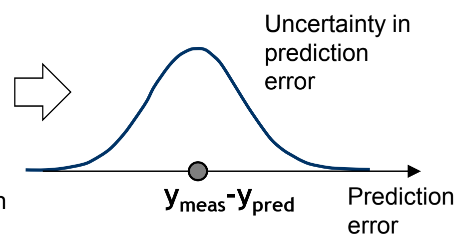
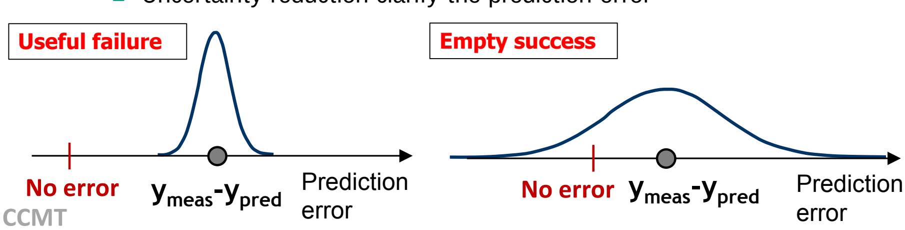
Prediction Error and Uncertainty

- Prediction error and the corresponding uncertainty tells us the prediction capability of a simulation and the uncertainty in the evaluation





- Uncertainty reduction clarify the prediction error



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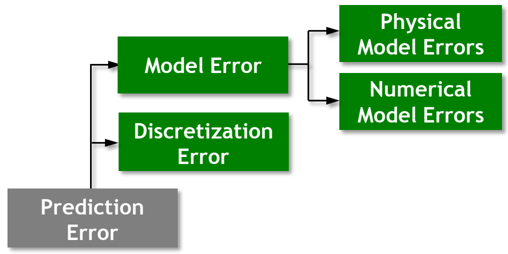
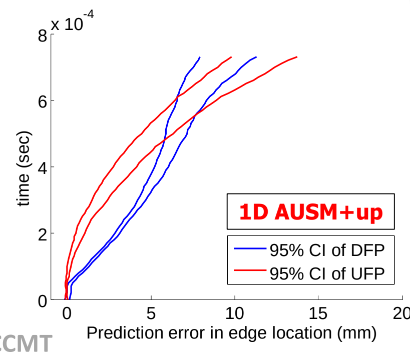
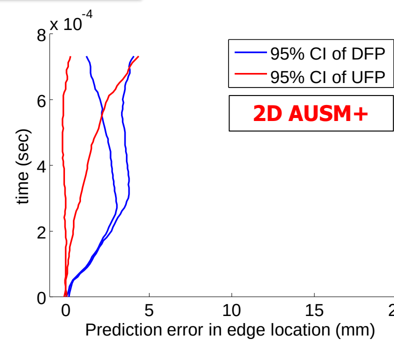
Prediction Errors and Uncertainties of 1D/2D

- Prediction errors of 1D/2D simulations and 95% CI of the uncertainty
- Note that prediction error is the result of model errors and discretization error

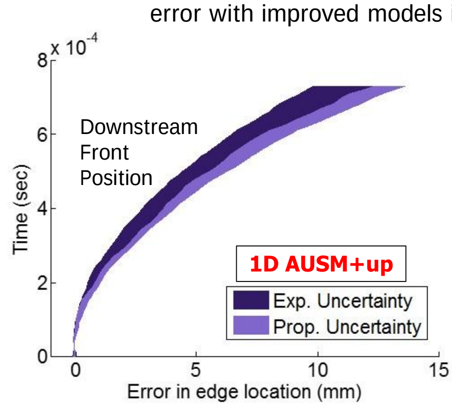


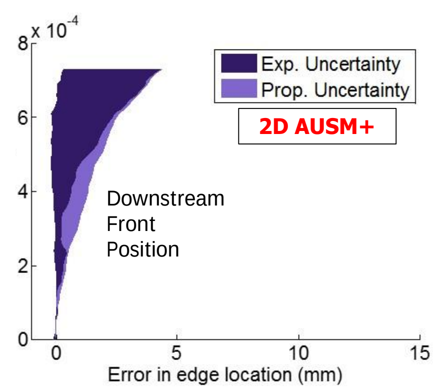




UB and Uncertainty Source Contributions

- Decompose the uncertainty in the prediction error into uncertainty sources and will calculate the cost for reducing the uncertainty sources (UB)
- The uncertainty does not cloud the prediction error for 1D simulation
- However, the uncertainty needs to be reduced for small prediction error with improved models in the future



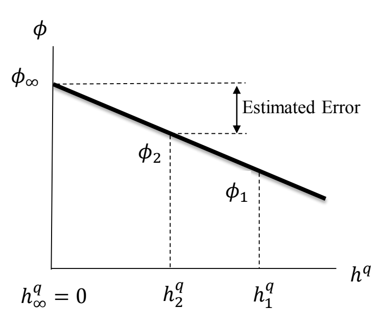


Extrapolation Overview

- Estimating Convergence of Simulation with Multiple Grid Variables
  - Estimating optimum grid resolution and simulation error of shock simulations
- Method of Converging Lines
  - Estimating performance of future simulation platforms for allocating current resource
  - A benchmark function for behavioral emulation: Matrix Multiplication function

Estimating Discretization Error

- Discretization-based simulations
  - Accuracy depends on grid size
  - Extrapolation allows us to estimate simulation error
- Richardson extrapolation
  - Let ϕ be a quantity of interest with the order of error O(h^q)
  - With two different meshes h_1 and h_2, extrapolate at infinity (h = 0)



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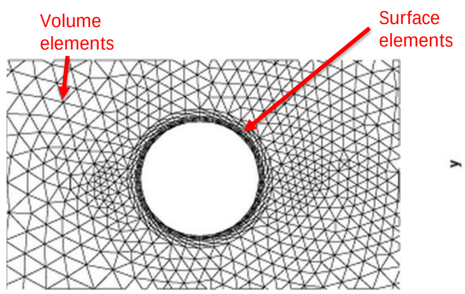
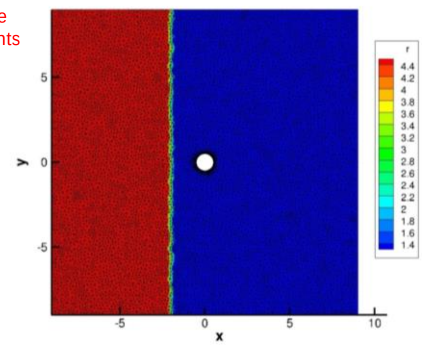
Simulations with Multiple Grid Variables

- 3-D shock simulation with multiple grid variables
  - Volume grid (N_v elements) and surface grid (N_s elements) variables
  - Drag coefficient, C_D, on spherical particle
  - Multiple grid variables may have coupled effect on simulation accuracy
  - Simulations were generated by Yash Mehta from Microscale team





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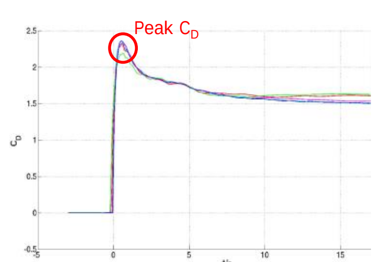
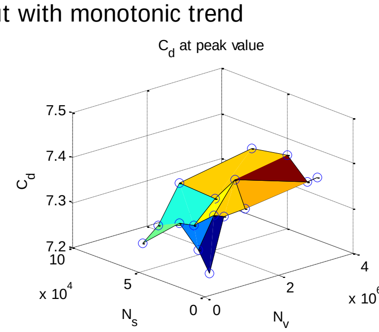
3-D Shock Simulations with One Particle

- **Goals**
  - Optimum set of grid variables
  - Error estimation for single simulation
  - Convergence of simulation while refining grid

- 4x4 design of experiments
  - Number of surface elements didn't affect simulation accuracy noticeably
  - Simulation results look noisy but with monotonic trend





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Extrapolation using Constrained Surrogates

- Surrogate maybe an alternative to estimate convergence of simulation
  - Richardson extrapolation may generate meaningless results (e.g. noisy data)
  - Polynomials may be accurate for estimating convergence of simulation based on Taylor series expansion and more robust with noisy data
  - Cubic polynomial was tailored to satisfy the properties of unimodality and monotonicity by controlling the derivatives

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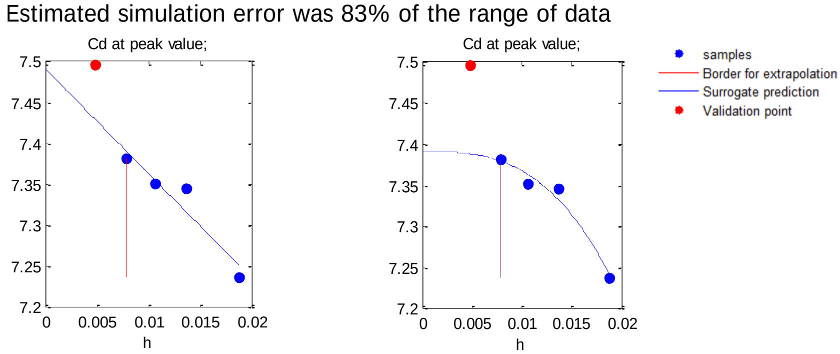
Convergence while Refining Volume Grid

- Estimating convergence of simulation using constrained polynomials and Richardson
  - Transformation for number of volume elements: $h = 1/\sqrt[3]{N_v}$
  - Relative error of extrapolation vary from 0.9%~1.4%
  - Richardson generated suspicious decrease
  - Estimated simulation error was 83% of the range of data



(a) Extrapolation using polynomials
$f = \beta_1 h^3 + \beta_2 h^2 + \beta_3 h + \beta_4$

(b) Extrapolation using Richardson
$f = \beta_1 h^{\beta_1} + \beta_3$

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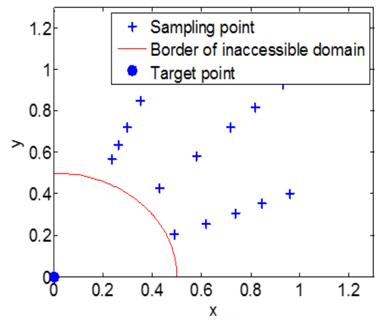
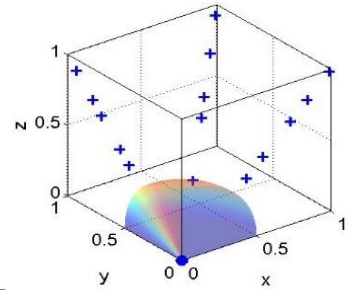
Method of Converging Lines

- Transform multi-dimensional extrapolation into series of 1-D extrapolations
  - Select lines towards extrapolation point
  - One-dimensional modeling
  - Consistence check between lines
  - Combining lines using Bayesian theory
- Potential benefits
  - Number of samples doesn't depend on dimensionality
  - Validation between lines
  - Obtain physical understanding





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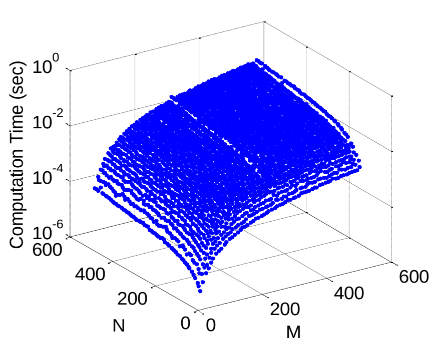
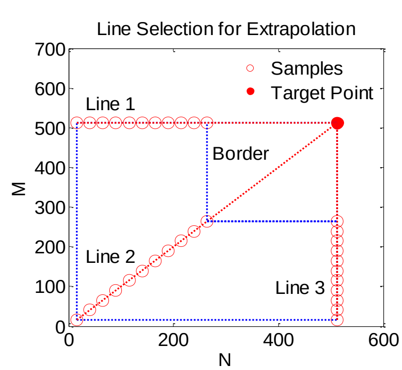
Extrapolation for Behavioral Emulation

- Previous Progress
  - Examining Matrix Multiplication function (MMF)
    $Time$ of $A_{M\times N} \times B_{N\times M}$ generated by Dylan Rudolph from Exascale team
  - Data should be modeled based on quality of data (noise and density)
  - Ridge regression was found to be effective to avoid disastrous error





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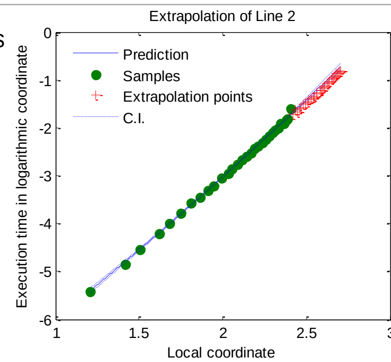
Long-range Extrapolation of Noisy Data

- Extrapolation using method of converging lines
  - Transformation may reveal data pattern: Logarithmic transformation for MMF
  - Line 1 is identified to be outlier mathematically which was verified physically
    Discrepancy d_{ij}=(p_i-p_j)/max(std),
    $d_{12} = 2.75$, $d_{13} = 3.25$, $d_{23} = 0.25$



	Line 1	Line 2	Line 3
Prediction p_i	-0.62	-0.73	-0.75
Prediction variance	0.04^2	0.04^2	0.03^2

- Combined extrapolation has 18% difference with extrapolation point

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Summary and Ongoing Work

- Summary
  - Proposed constrained polynomials for estimating convergence of simulations especially for which are noisy and complicated
  - Extrapolated a two-dimensional benchmark function of behavioral emulation using the method of converging lines
- Ongoing work
  - Evaluating performance of proposed methods
  - Examining more simulations to study grid resolution and error estimation (e.g. shock tube simulation)
  - Testing more benchmark functions of behavioral emulation

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Outline for Other Interactions

- JWL-EOS surrogate
- Timing model for hybrid computing
- Preparation for expansion fan UB study

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JWL-EOS surrogate

- **Goals:**
  - Modeling the feasible region for the JWL-EOS solver
  - Using surrogates for saving computation time
- Determining the feasible region of JWL-EOS within
  - Mass fraction of explosive [0, 1]
  - Mixture density [1.23, 1770] (kg/m^3)
  - Mixture energy [125000, 5700000] (J)
- Fitting surrogates to predict
  - Temperature (K)
  - Pressure (kg/m^3)

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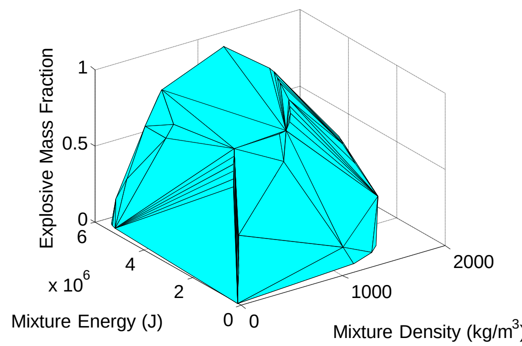
Methodology of Detecting Feasible Region



- JWL-EOS gives non-physical solutions out of its feasible region (e.g. negative pressure)
- A convex hull of the feasible region was obtained using physical meaningful samples

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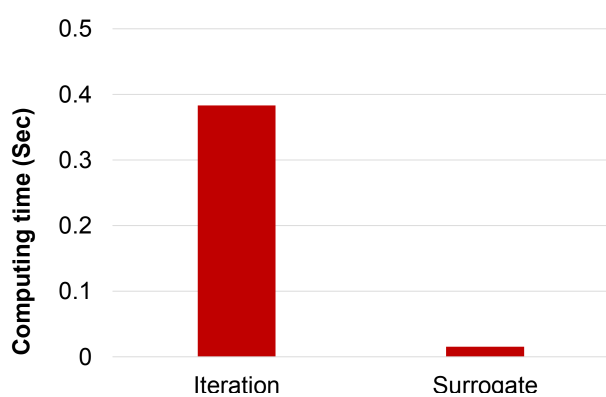
Surrogate vs. Iteration Solver

- Compared the JWL-EOS iteration solver to the JWL-EOS surrogates
- Both are written by MATLAB
- Computing time for 1000 points
- Ratio of 25 (0.383/0.015)



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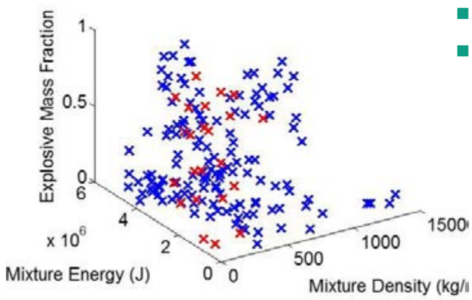
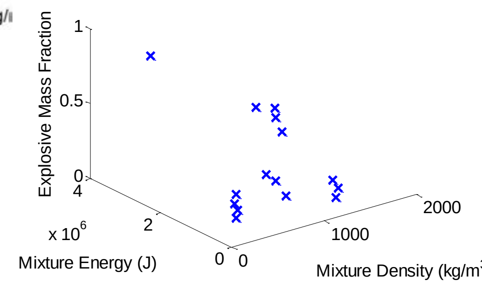
Surrogate Accuracy

- Relative error: $|(y_{iter}-y_{surr})/y_{iter}|$
- Pressure (out of 1000 test points)
  - Rel. error is larger than 1% for small mixture energy and density
  - Red points have more than 10% rel. error





- Temperature (out of 1000 test points)
  - Rel. error is larger than 1% for small mixture density
  - Max abs rel. error is 3%

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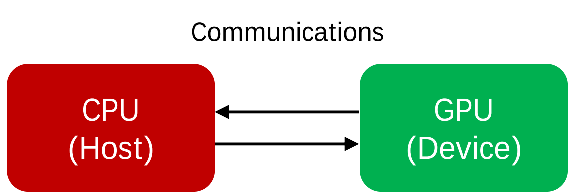
Timing Model for Hybrid Computing

- **Goal**: Finding computing time evaluation measurement
- Matrix multiplication using GPU is much faster than using CPU
- Communications between CPU and GPU cause variability in total computing time



- Computation time for **m** matrix multiplication operations of matrix size **n**
  - $T_{total} = T_{comm} + T_{Comp}$
  - $C_{ijk}=B_{ljk}A_{il}$

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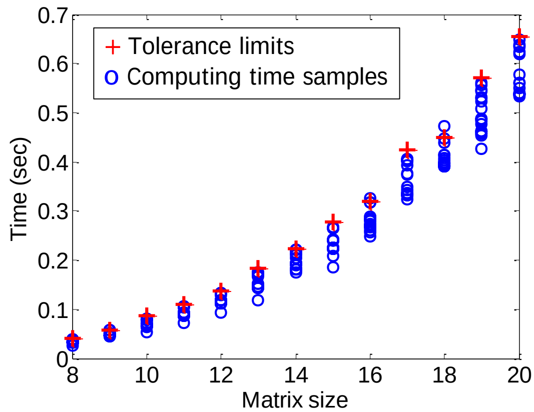
Computing Time with Variability

- 10000 matrix multiplications (10000 elements)



- Tolerance limit for each matrix size: At least 90% of the population of computation time is expected to equal or less than this computation time with 95%

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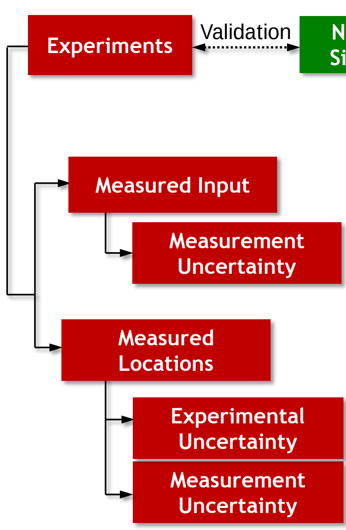
Do you have any questions?

Backup Slides

Key Uncertainty Sources



#	Parameters	Descriptions
1	Volume fraction	Measurement uncertainty
2	Particle location	Variability in particle location
3	Diameter of particle	Variability in diameter
4	Pressure at driver section P	Very small measurement noise
	⋮	⋮

- Particle location and diameter are not measurable
- Average location for random particle locations

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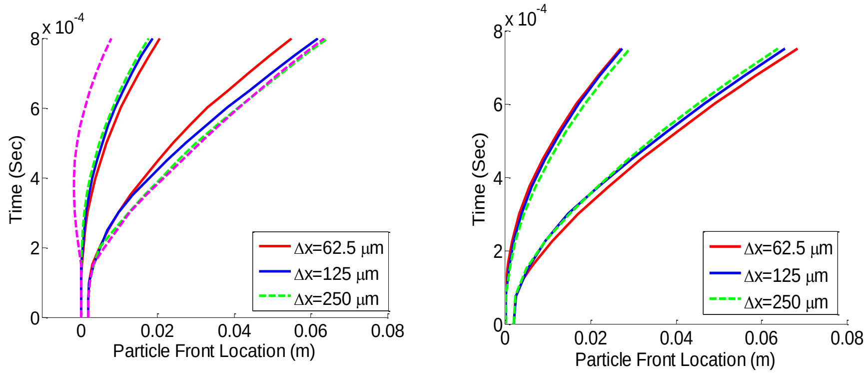
Estimating Discretization Error

- Need to estimate predictions with
- Three key parameters: (1) grid resolution, (2) temporal resolution and (3) the number of particles per cell
- The effects of (2) and (3) are limited
- Refining grid resolution provokes numerical instability



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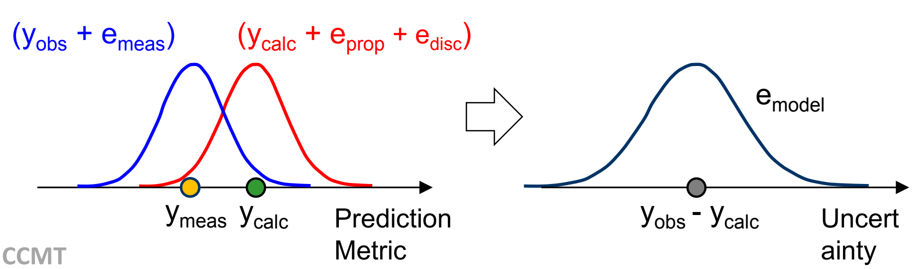
Estimating Model Uncertainty

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

- Goal is to quantify model uncertainty
- Measurement uncertainty is little

$$e_{model} = (y_{meas} + e_{exp}) - (y_{calc} + e_{prop} + e_{disc})$$



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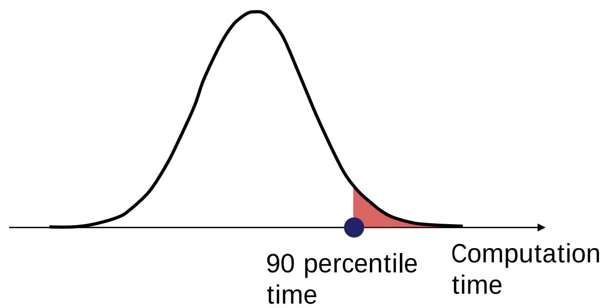
Conservative Estimate using UQ

- Conservative prediction of computation time considering variability
  - At least 90% of the population of computation time is expected to equal or less than this computation time



- Tolerance limit = sample mean + k*sample standard deviation

$$k = t^{-1}\left(\Phi^{-1}(0.9)\sqrt{n}, n-1\right)(0.95)\Big/\sqrt{n}$$

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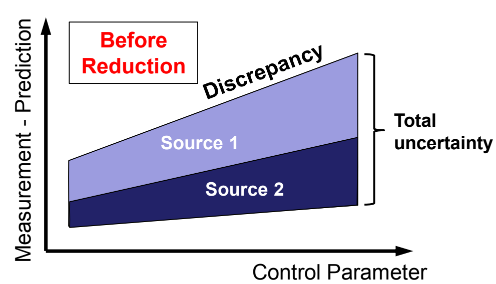
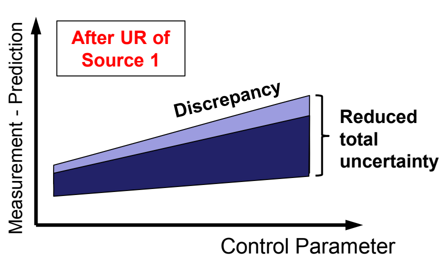
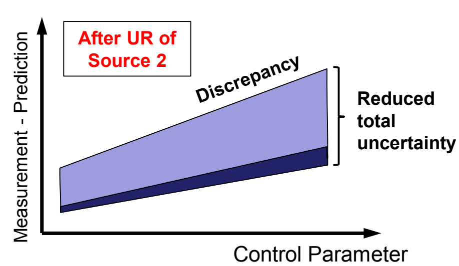
Why UB?

- How much uncertainty can be reduced for given budget?
- The effect of an uncertainty reduction strategy on total uncertainty in discrepancy







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UQ Study of ASU Experiments

- **Goal:** To study the expansion pan shocktube experiment in order to identify uncertainty sources while quantifying their magnitudes
- Preparing a white paper describing the experiment procedure and uncertainty sources and the corresponding magnitudes
- Justin T. Matthew has been communicating with Heather Zunino (ASU) in order to learn the experimental set-up and procedure of the shocktube experiments
- Communications allow us to understand the experimental process as well as contribute to a new shocktube design for better UQ

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Hardware Software Co-design of CMT-nek Codes

Performance, Energy and Thermal Issues

Tania Banerjee, Mohamed Gadou and Sanjay Ranka

Computer and Information Science and Engineering

Long Term Goals

- Parallelization and UQ of Rocflu and CMT-nek beyond a million cores
- Parallel performance and load balancing
- Single processor (hybrid) performance
- Energy management and thermal issues

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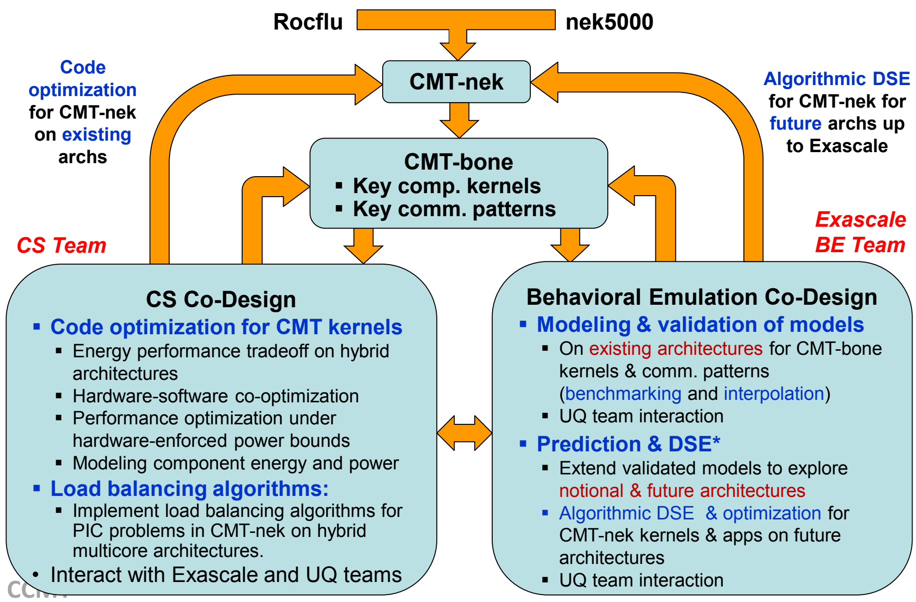
Integration



* DSE: Design Space Exploration

3

Outline of Talk

- CMT-bone development
- Optimizing CMT kernels on hybrid processors
- Hardware software co-optimization of CMT kernels
- Modeling energy requirements
- Future work

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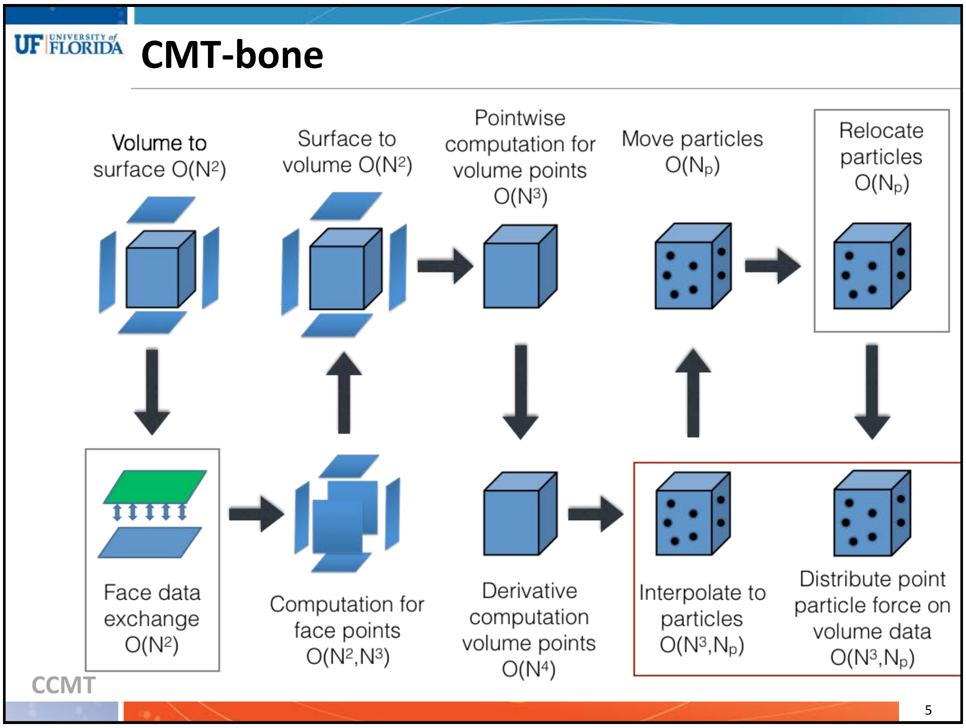
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CMT-bone
Volume to surface $O(N^2)$
Surface to volume $O(N^2)$
Pointwise computation for volume points $O(N^3)$
Move particles $O(N_p)$
Relocate particles $O(N_p)$
Face data exchange $O(N^2)$
Computation for face points $O(N^2,N^3)$
Derivative computation volume points $O(N^4)$
Interpolate to particles $O(N^3,N_p)$
Distribute point particle force on volume data $O(N^3,N_p)$
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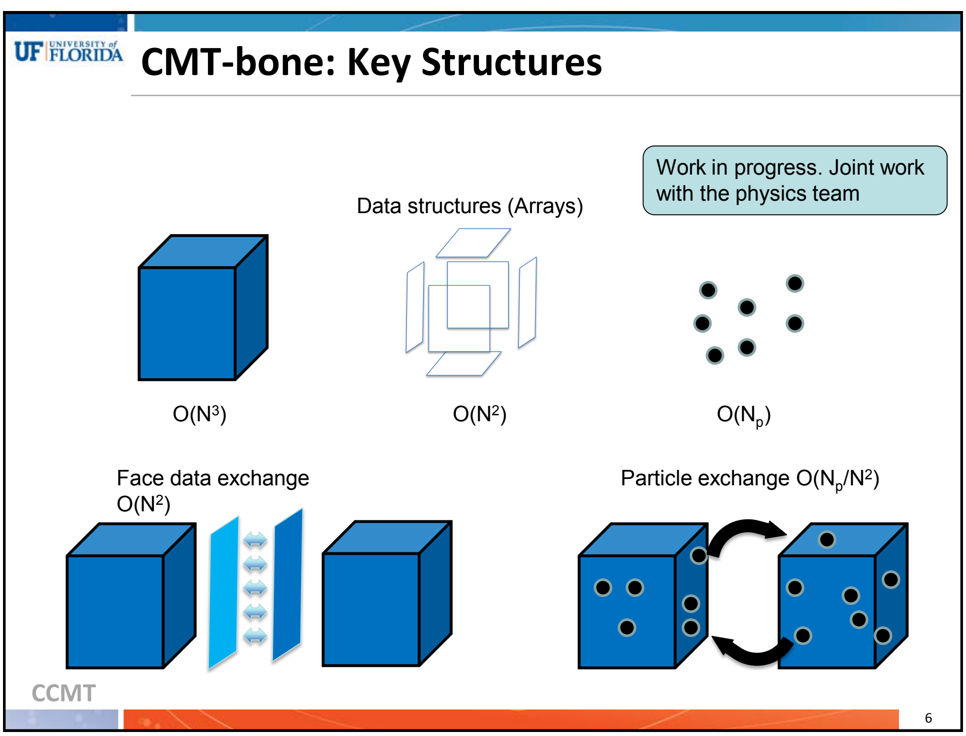
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CMT-bone: Key Structures
Work in progress. Joint work with the physics team
Data structures (Arrays)
$O(N^3)$
$O(N^2)$
$O(N_p)$
Face data exchange $O(N^2)$
Particle exchange $O(N_p/N^2)$
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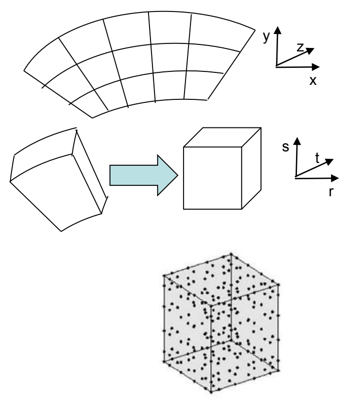
Optimizing CMT kernel on Hybrid Processors



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

The derivative computing kernel requires 25-50% of the total solver time of CMT-nek.

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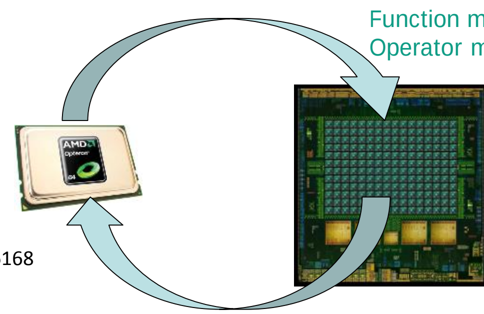
CPU-GPU interaction model

- Master-slave
- CPU sends function and operator matrices to GPU, GPU computes derivatives and sends back to CPU



Idle cores utilized to compute derivatives.

Host:
AMD Opteron 6168
12 cores
1.9GHz clock frequency

Tesla K20c:
13 Processors
192 Cores
48k shared memory
64k registers
1170 GFLOP/s Peak
706MHz clock frequency

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Optimization strategy

- On GPU:
  - The derivative operator matrices are only brought in once per block from the device memory to the shared memory. This reduces the number of memory transactions required.
  - The derivative operator matrices are stored in registers instead of shared memory. This reduces the number of accesses to the shared memory.
- On CPU:
  - Using code transformation with proper loop unroll factor and permutation using CHiLL
- Load balancing strategies on CPU and GPU
  - Performance optimal and energy optimal strategies

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Possible Code Combinations

Algorithm: *dudr-4loop*

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

Number of implementations for N_x=N_y=N_z=10

= 4! * 4 ^ 4

= 24 * 256 = 6144 variants

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

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

Question: Can we use a less expensive search technique?

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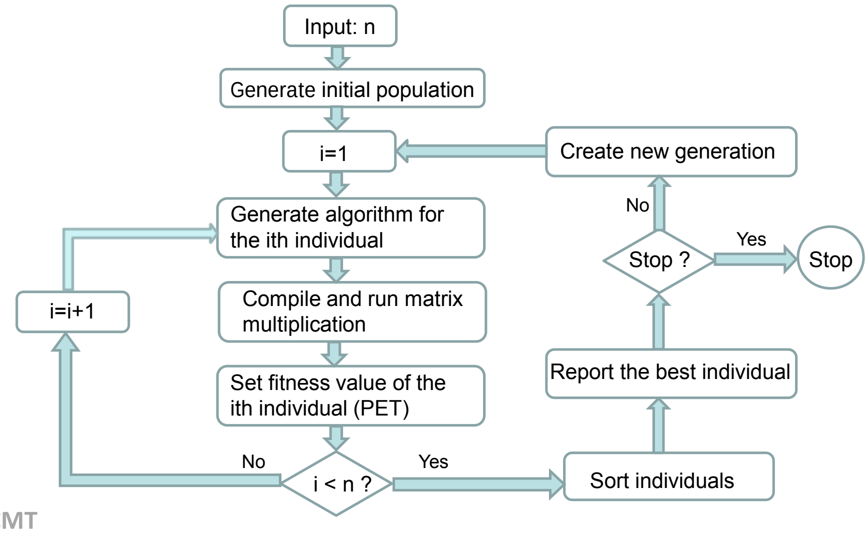
Genetic Algorithm

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



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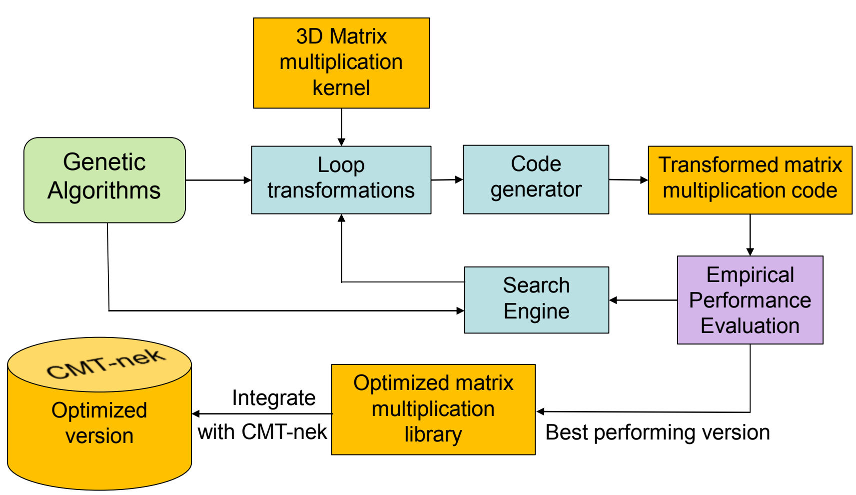
Autotuning Framework



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Comparison of GA with Exhaustive Approach

- Comparison of performance by platform

Platforms	CMT-bone time (seconds)	Exhaustive Autotuning			GA based Autotuning			
		Time	Variants	%improve(cmt)	Time	Variants	%improve(cmt)	%lowerPerf
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-bone energy (Joules)	Exhaustive Autotuning			GA based Autotuning			
		Energy	Variants	%improve(cmt)	Energy	Variants	%improve(cmt)	%lowerEnergy
IBM BG/Q	292.1	131.7	96 top	54.9	135	96 top	53.7	2.5
AMD Fusion	17.6	11.98	32652	32	12.11	485	31	1.1

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Modeling CPU/GPU characteristics

- Modeling helps us gain insight into CPU-GPU characteristics
  - Matrix size N
  - Number of elements, Y
- Helps us balance load using only few runs
  - Alternatives: binary search or autotuning takes large number of experimental runs
- Helps us analyze characteristics of CPU-GPU configurations that are not available to us for direct experimentation

These models will be used as input for simulation by the exascale team.

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Modeling Runtime, Power and Energy

GPU	CPU
Runtime Tgpu = Tcomp + Tcomm Tcomp = $7.17 \times 10^{-11} \times N^{3.76} \times Y$ Tcomm = $6.14 \times 10^{-9} \times N^{3} \times Y$	Runtime Tcpu = $1.02 \times 10^{-9} \times N^{4.4} \times Y$
Power $P_{GPU} = 162.24 \times N^{-0.1}$ Nearly a constant, decreasing very slightly with increasing N. Number of memory transactions per unit of data use decreases with N.	Power P = Pmemory + Pcore $= 5.95 + 12.21 \times N^{0.3}$
Energy $E_{GPU} = 9.28 \times 10^{-7} \times N^{3} \times Y$	Energy $E_{GPU} = 2.51 \times 10^{-8} \times N^{4.5} \times Y$
Runtime on *g* GPUs Tggpu = 1/g * T gpu	Runtime on *p* CPU cores Tpgpu = 1/p * Tcpu

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Load Balancing Results

- Optimal Energy: Given a deadline, the GPU should process most of the load with the remaining load being processed by the CPU

Deadline(s)	Time(s)	Power(W)	Energy(J)	GPU(%)
0.210	0.210	213	38.6	94.46
0.190	0.189	279	48.37	85.47
0.126	0.126	741	93.22	44.56

- Optimal Performance: CPU and GPU finish processing at about the same time

Deadline(s)	Time(s)	Power(W)	Energy(J)	GPU(%)
0.210	0.2072	213	43.5	91.25
0.190	0.185	279	51.8	82.83
0.126	0.1189	807	95.17	43.75

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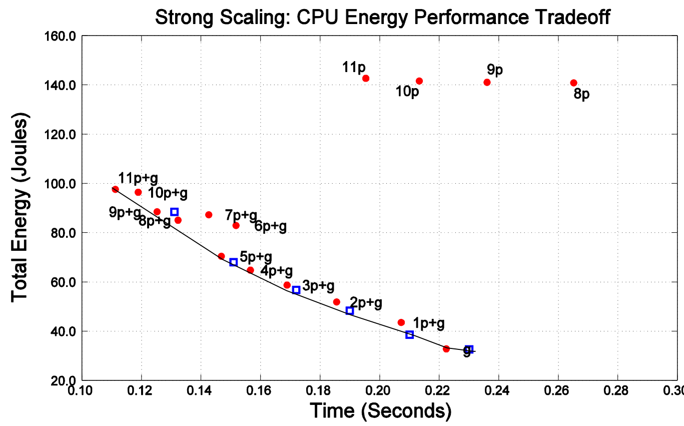
Energy Performance Tradeoff



- Circles represent performance and power for a performance optimal implementation
- Squares represent performance and power for an energy optimal implementation
- Pareto optimal front for hybrid architectures

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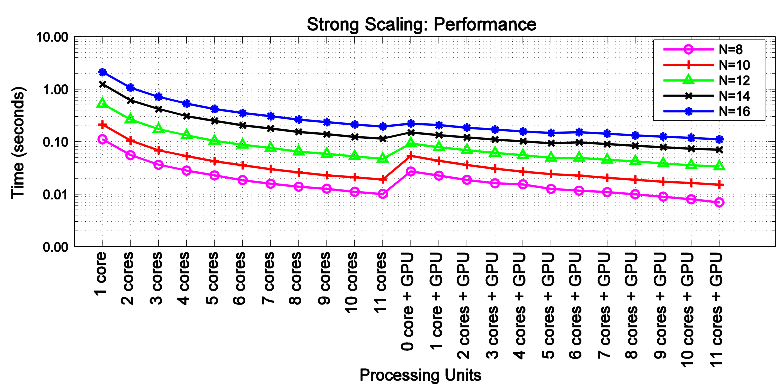
CPU + GPU Performance



- Load = 10000 spectral elements
- For CPU-only configurations, runtime drops by a factor of the number of cores
- For CPU-GPU configurations, runtime does not drop as profoundly

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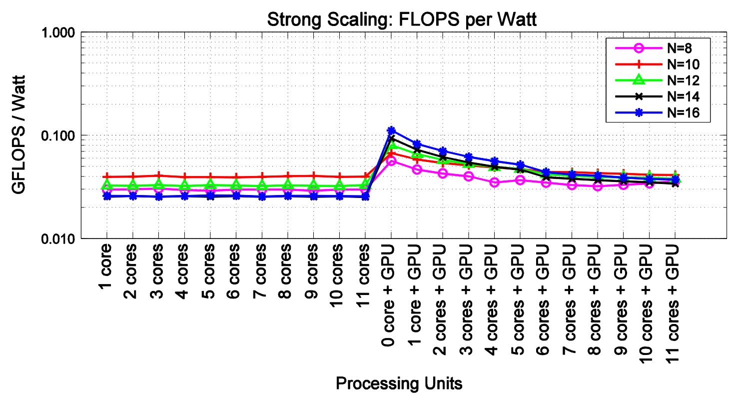
CPU + GPU Power Performance



- CPUs are efficient for smaller matrices
- GPUs are efficient for larger matrices
- CPU+GPU efficiency tend to be independent of matrix size as more CPU cores are added

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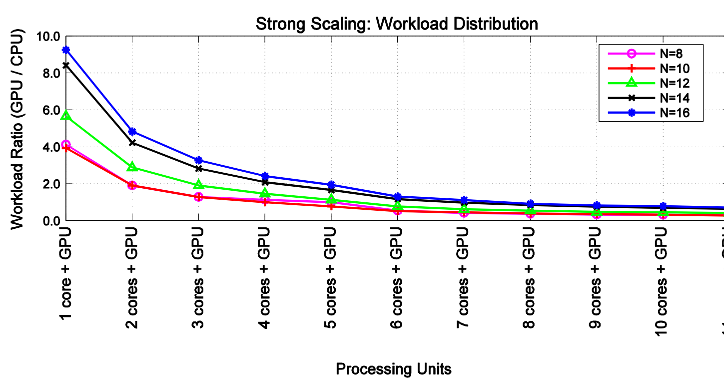
Workload ratio



- With a single CPU core, GPU processes about 4-9 times more load

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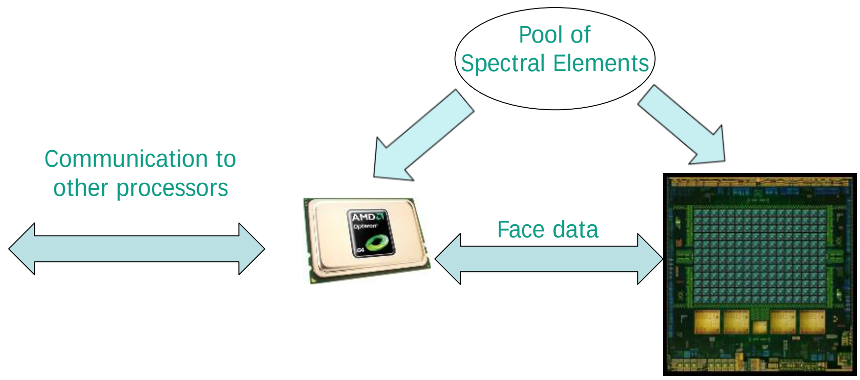
Hybrid processing of CMT-bone



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Summary of work on HMP

- Benchmarked power performance characteristics of the derivative computation kernel on hybrid multi-processors
- Developed empirical models of performance, power and energy consumption of this CMT kernel
- Demonstrated load balancing using performance and energy objectives
- Working on applying these techniques to CMT-bone

Genetic Algorithm based Autotuning Approach for Performance and Energy Optimization, Tania Banerjee and Sanjay Ranka, IGSC, 2015.

Multiobjective Optimization of Spectral Solvers of Hybrid Multicore Platforms, Tania Banerjee, Jacob Rabb and Sanjay Ranka, submitted to IPDPS 2016.

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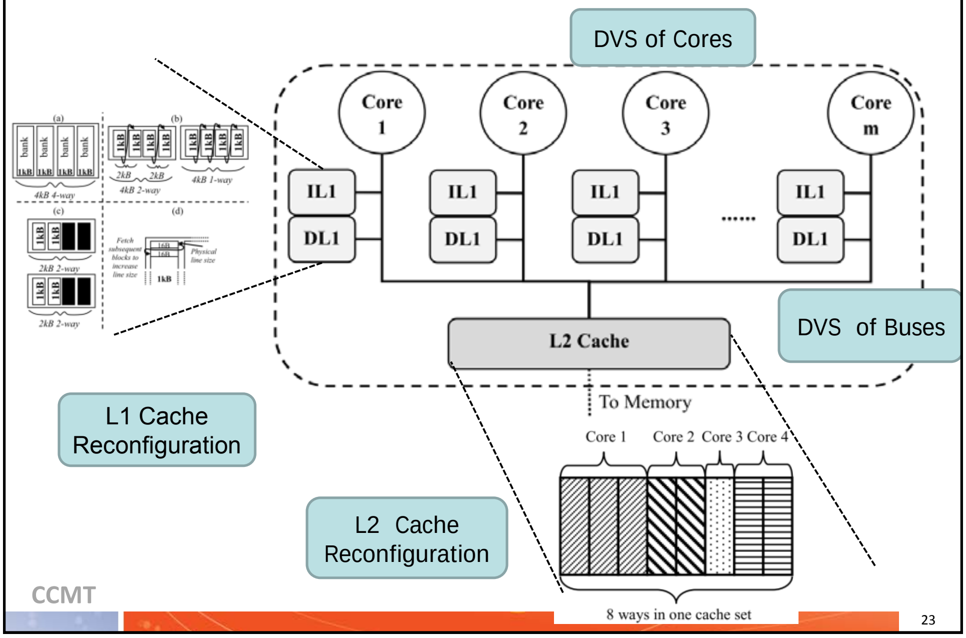
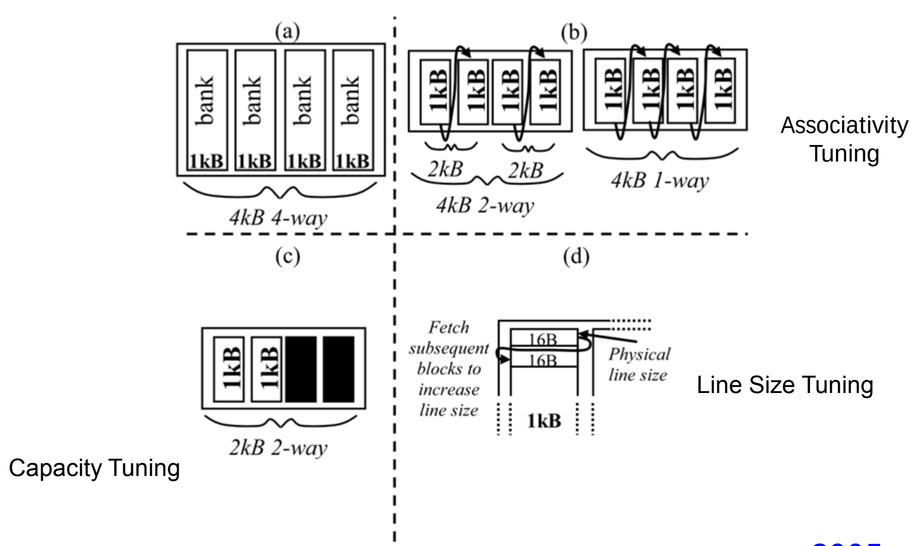
Optimizing Hardware Configurations



Reconfigurable Cache



Zhang et al., ACM TECS 2005

Hardware Software Co-optimization

- Hardware parameters
  - L1 cache size – 2K, 4K, 8K
  - L1 line size – 64, 128, 256
  - L1 associativity – 2, 4, 8
- Code Information
  - Partial derivative computation along direction r
- Software parameters
  - Loop permutation
  - Loop unroll factors
- Problem Size (N) – 16
- Number of Code Variations – 4500
- Details of the GEM5 environment
  - Instruction set architecture: X86
  - CPU model: Out-of-order CPU
  - Memory model: Classic, DDR3
  - Clock frequency: 1GHz

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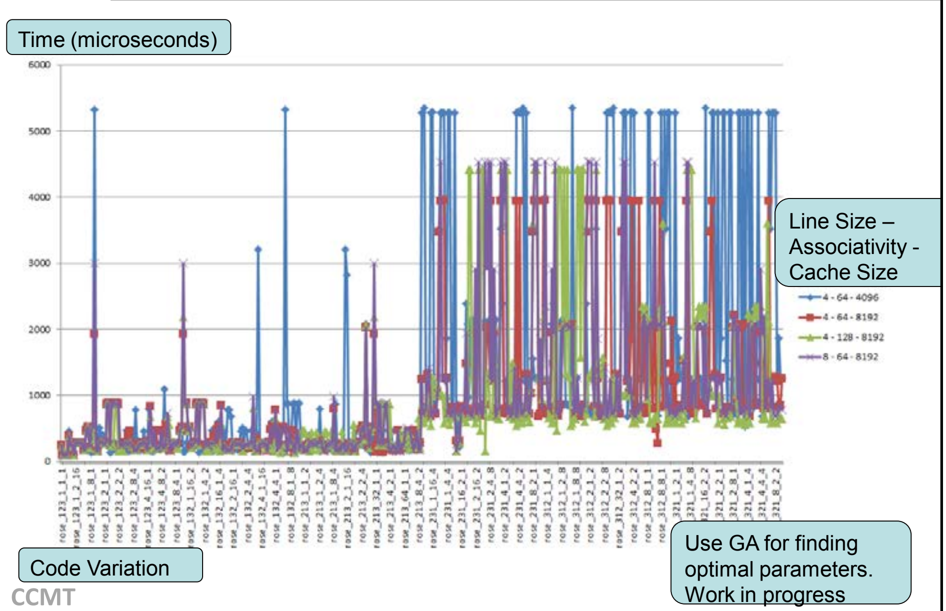
Variation in Time



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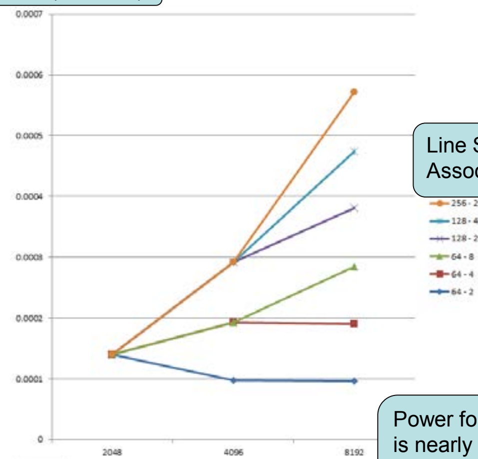
Performance (varying hardware parameters)

Best Time (seconds)



Line Size - Associativity

Cache size

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

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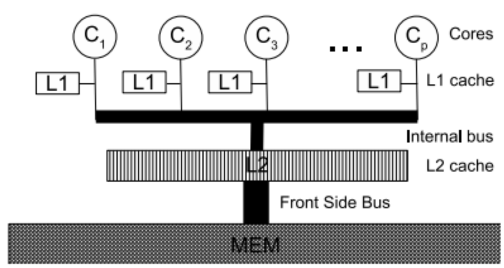
Modeling Energy Requirements



Challenge: Model the power and energy profiles of the different components

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Approach

- We have developed a systematic approach of representing the key components as piecewise linear functions
- This can be developed into an overall linear model that represents the energy requirements
- Such a linear model has a well defined theory for
  - Modeling the component behavior
  - Developing Uncertainty in the model input and output
  - Design of Experiments for minimizing the number of execution runs

Work in progress. Joint work with UQ team

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Piecewise linear approximation

- Let $f_i\,(x_i)$ represent the energy requirements of component i
- The range of x_i is evenly split into k intervals
- Interval h denoted by $[I_{h,} I_{h+1}]$
- Within interval i, f_i is linearly approximated by

$$f_{ih} = a_{ij}.x_i + b_{ij}$$

- If each component energy only depends on one parameter, the total power consumption P can be approximated by

$$P = \sum_{i=1}^{n} \sum_{h=1}^{k} (a_{ih}.x_i + b_{ih}) + P_0$$

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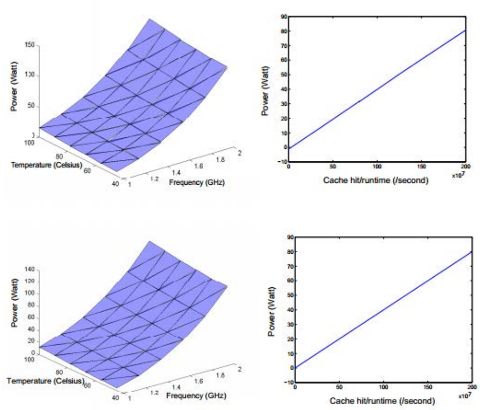
Preliminary Experimental Results

- Multiple parameter modeling



(a) (b)

$$P = \sum_{i=1}^{4} f_i(V_i, T_i) + \sum_{i=1}^{4} g_i(H_i)$$

V_i, T_i is the supply voltage and current temperature of core i

H_i is $\frac{cache\ hit}{runtime}$ of core i

Comparison of reconstructed function and actual function.

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Preliminary Experimental Results

- Synthetic data

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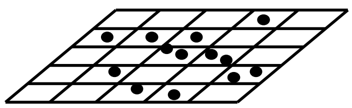
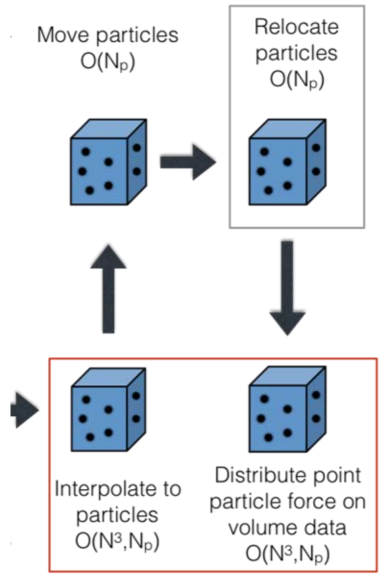
Future Work: CMT-bone Particle Movement



Preferential particle clustering
Lagrangian remap



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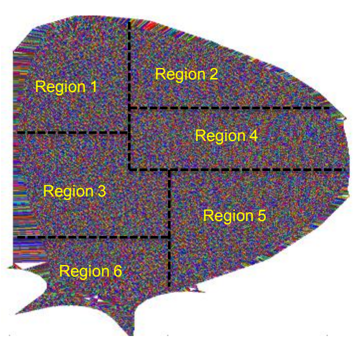
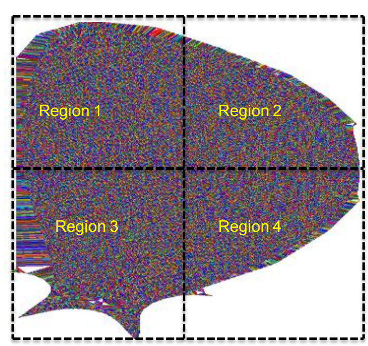
Different Partitioning Approaches (XGC1)





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

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

Experimental Results

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

Non-uniform partitioning

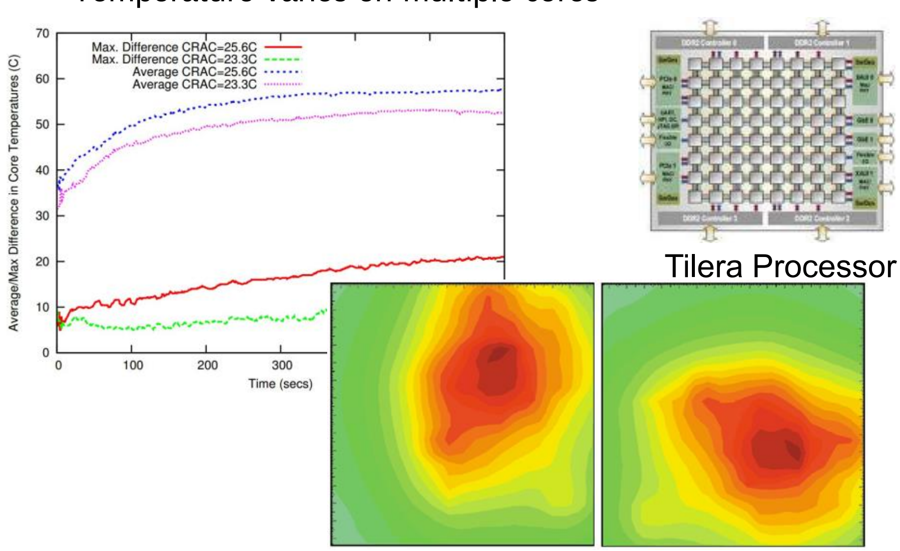
GPU blocks	Time (ms)
1024	12561.06
2779	7235.16
22471	989.88
33464	428.51

Uniform partitioning

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

Future Work: Managing Temperature

Temperature varies on multiple cores



Tilera Processor

[Sarood2011]

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Thermal models

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

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

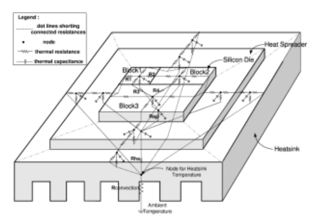
- Transient-state thermal model
  - If the average power of core is *P* over a time period *t*, then the temperature at the end of this period *T(t)* is given by:
  - $T(t) = T_A + e^{-G^{-1}Ct}(T_i - T_A) + G^{-1}(I - e^{-G^{-1}Ct})P$

  G is the thermal conductance matrix

  C is the thermal capacitance matrix

  T_A is the ambient temperature

  T_i is the initial temperature



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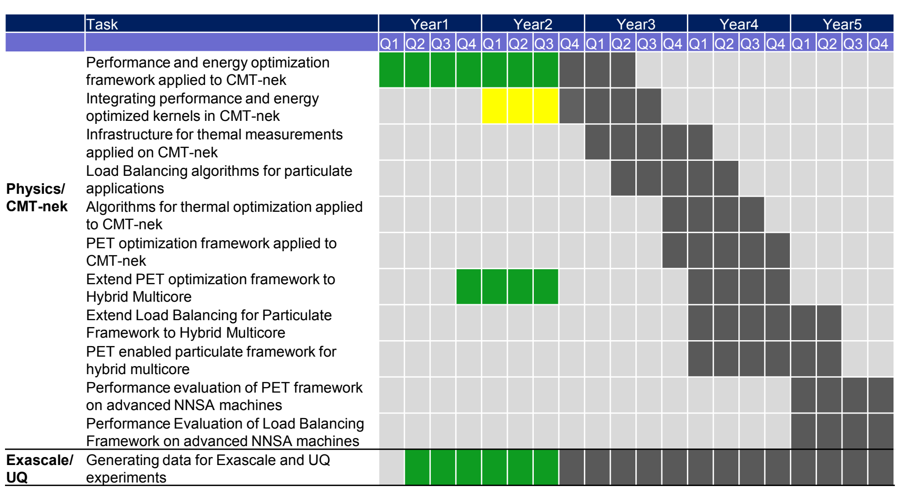
CS Gantt Chart



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Conclusions

- Developed blueprint for CMT-bone development
- Developed novel methods for optimizing CMT kernels on hybrid processors
- Developed hardware software co-optimization approaches for CMT kernels
- Developed methods for modeling energy requirements
- Work in progress on thermal optimization and load balancing for particle in a cell approaches

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Do you have any questions?