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Center for Compressible Multiphase Turbulence

DSE* of CMT-nek using BE**

Sai Prabhakar Rao Chenna

Advisor: Dr. Herman Lam, Dr. Greg Stitt

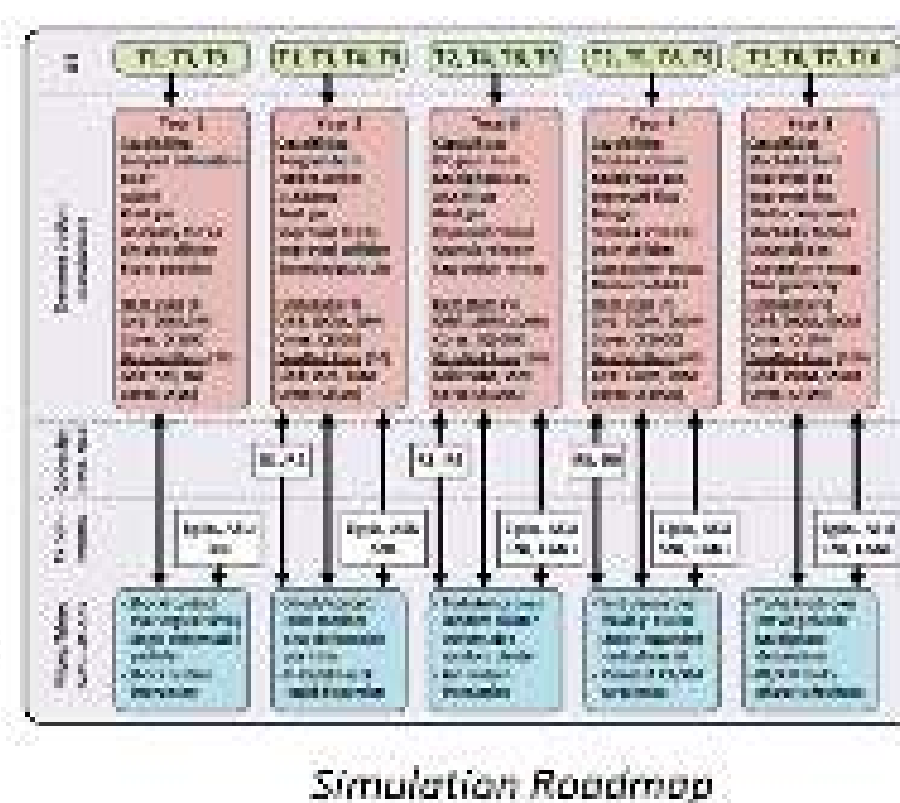
Department: ECE, UF

Goals

- Use BE methods & tools to perform extensive DSE on CMT-nek design space
- Perform trace-driven simulations to optimize CMT-nek performance on HPC systems

Simulation roadmap

- Early DSE to enhance CMT-nek performance on future exascale systems



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

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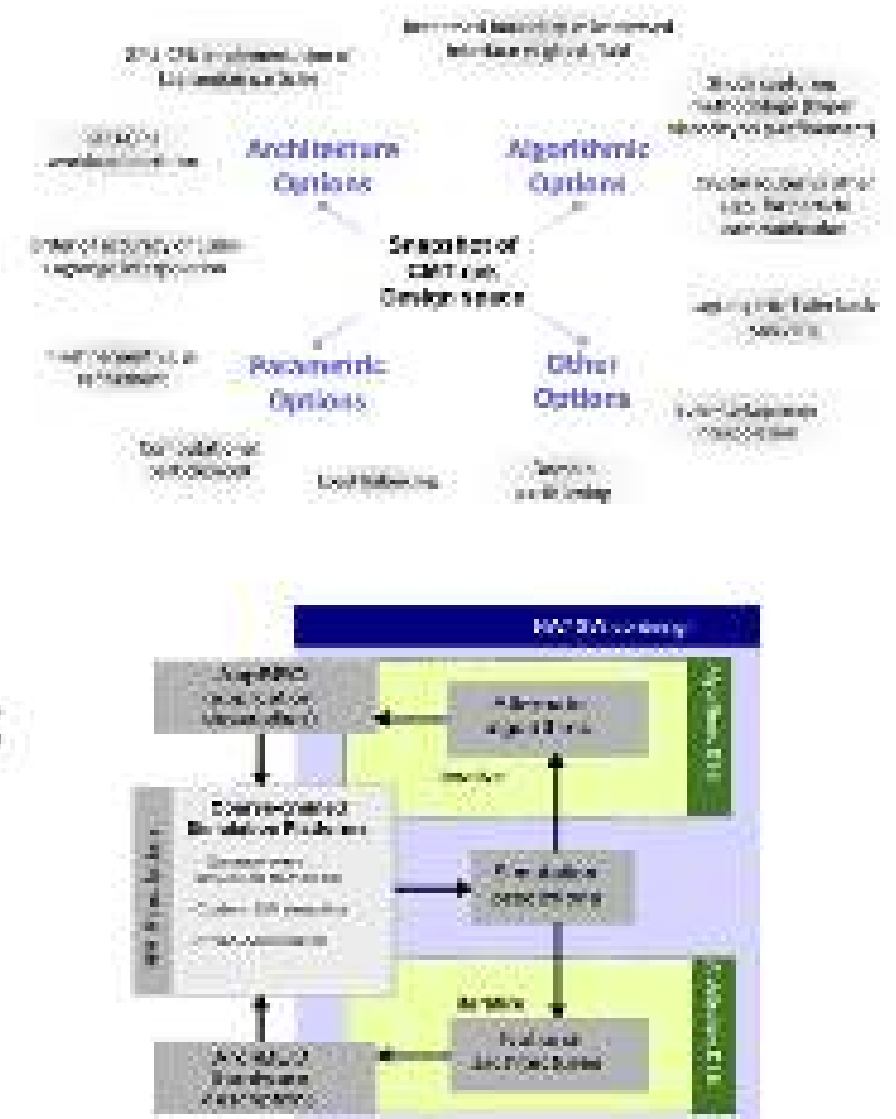
Motivation & Approach: CMT-nek DSE

- Motivation: Very large design space

- CMT-nek provides various algorithmic and parametric options
- DSE helps in rapid performance evaluation of these options on future exascale systems

Iterative DSE steps:

- Identify DSE candidates - most expensive subroutines and promising architectures
- Build BE Models for algorithms and architecture
- Use BE to predict performance



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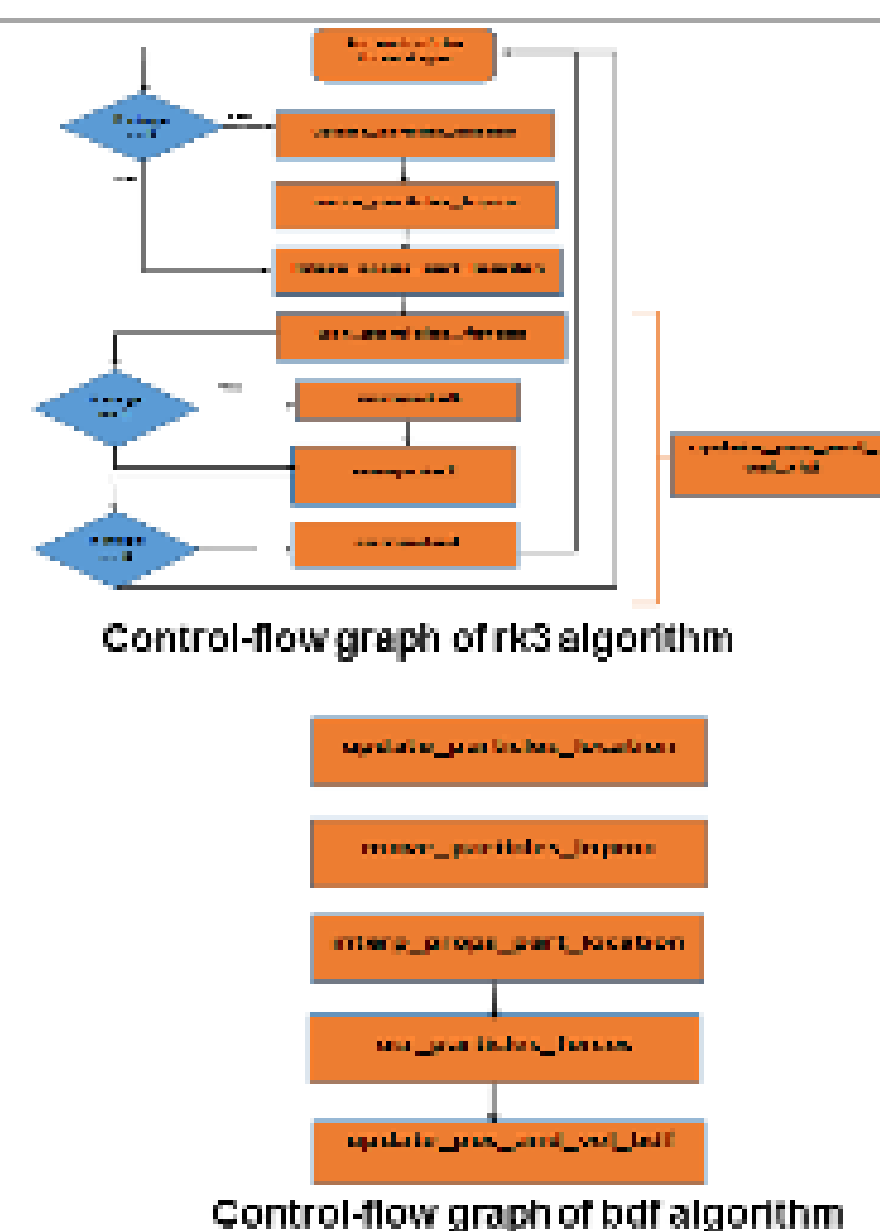
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CMT-nek Alternate Algorithms

- Explore accuracy vs execution time trade-off of alternate algorithms for portions of CMT-nek (particles phase)

- Time Integration - solve differential equations to calculate particle properties
 - Current : Runge Kutta 3 (rk3) - 3 stage time integration
 - Alternate : Backward Differentiation Formula (bdf) - single stage time integration

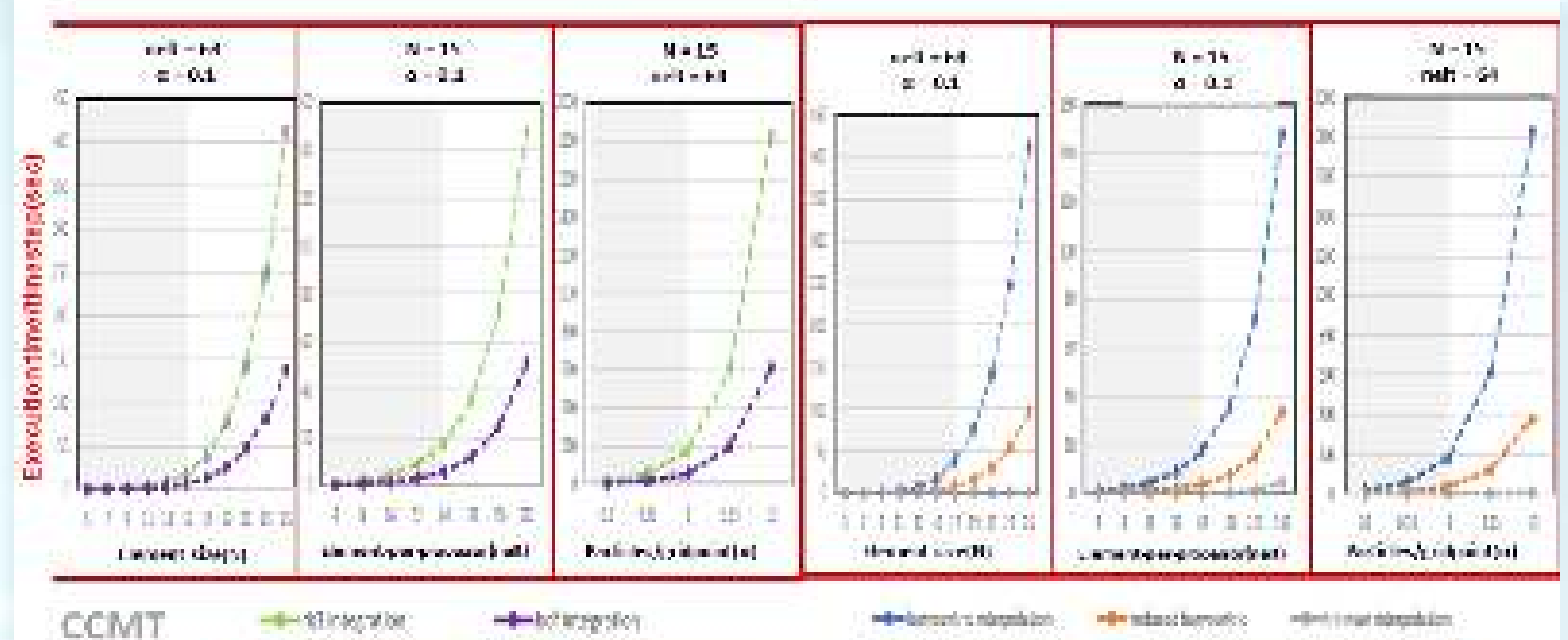
- Particle Interpolation - interpolates fluid properties acting on particles:
 - Current : Barycentric Interpolation
 - Alternate : Reduced Barycentric Interpolation, Tri-linear Interpolation



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BE-SST: Predictions on Vulcan

- Performance of algorithms vary
 - Non-linearly w.r.t. element-size(N) and elements-per-processor(nelt)
 - Linearly w.r.t. particles/gridpoint(n)
- bdf time integration provides 3x speedup over rk3
- Reduced barycentric interpolation provides 5x speedup
- Tri-linear interpolation provides 164x speedup



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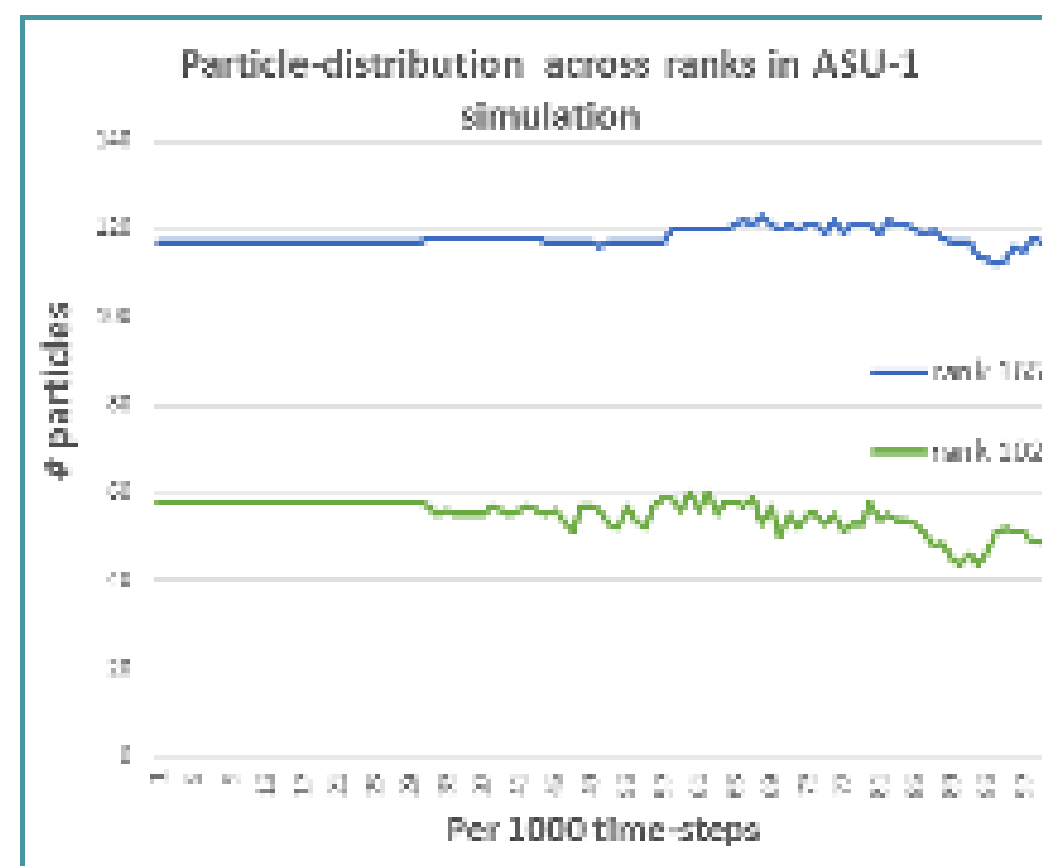
Trace-driven Simulation: Particle-distribution tool

CMT-nek Particle-solver:

- Workload per processor depends on # particles
- # particles/processor is dynamic - varies:
 - among processors
 - at each timestep

Particle-distribution tool:

- Input: trace-data containing particle-to-element mapping @ time-step
- Output:
 - # particles residing in each rank - computational workload
 - # particles moving across each rank - communication workload
- Particle movement is independent on processor count



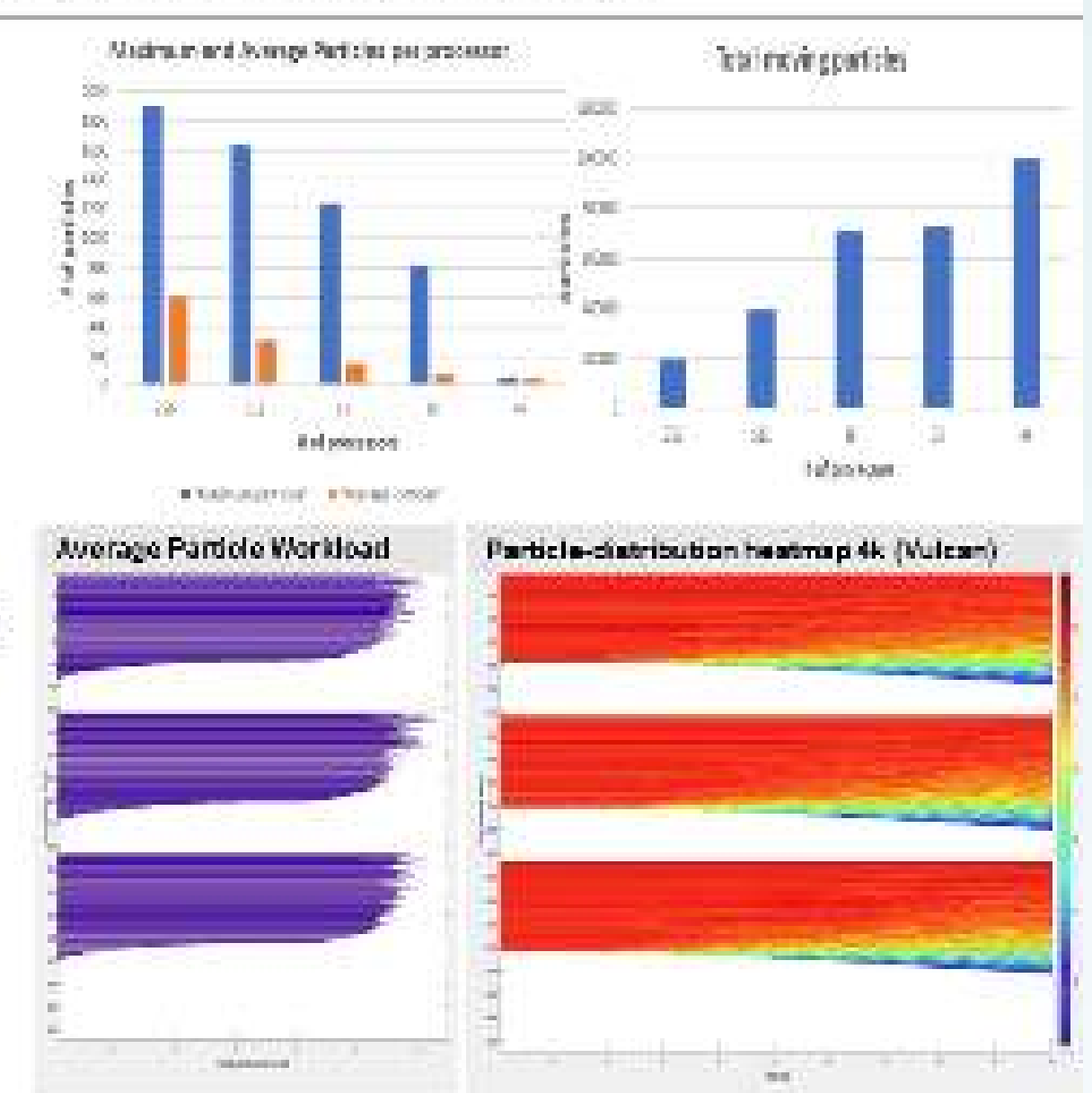
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Particle-distribution tool: Results

- Increase in processor count results in:
 - Reduced average particles per-processor (workload)
 - Poor resource utilization
 - Increase in particle-communication

- Load-balancing algorithm can result in better resource utilization:
 - Particle-distribution tool can be helpful in determining the frequency of load balancing to optimize the overhead

- Trace-driven simulation provides optimal configuration by identifying:
 - Computation cost
 - Communication cost
 - Resource utilization



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Uncertainty Quantification of Shock Tubes

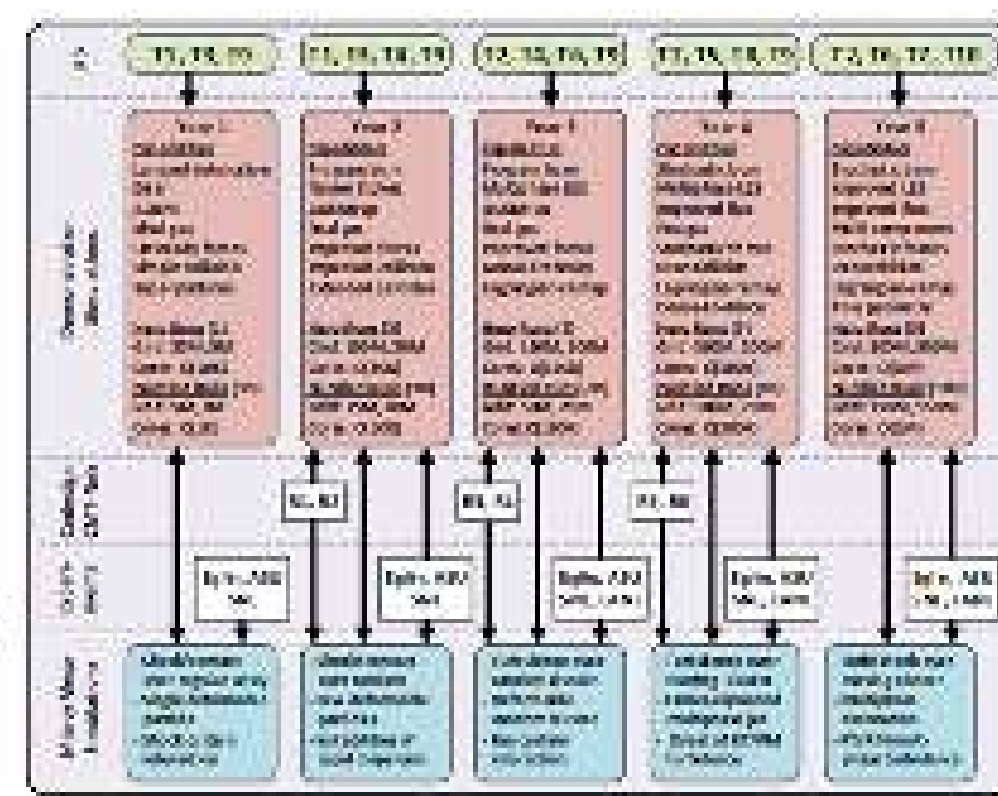
Brad Durant

Advisor: S. Balachandar

Department: Mechanical Engineering, UF

Goals

- Reproduce measurement processing from Sandia shock tube to identify sources of uncertainty
 - Propagate identified sources of uncertainty from experiments into simulations
- #### Simulation roadmap
- T6: Force coupling
 - T4: Particle-particle interaction



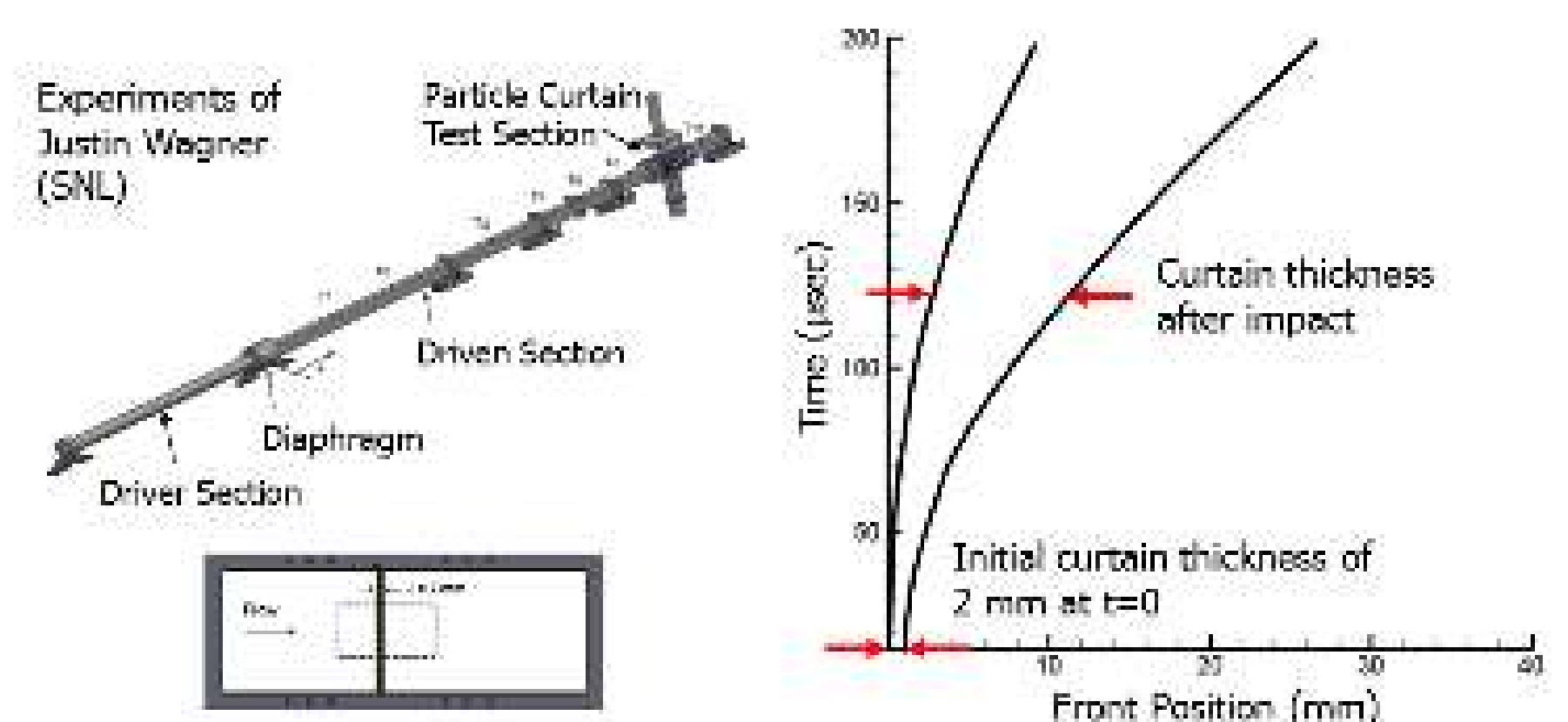
Simulation Roadmap

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Motivation

- To study dynamics of densely packed particles influence explosive process
- To observe shock-particle interactions in dense gas-solid flows
- Upstream and downstream particle front positions are quantities of interest



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UB Workflow - Experiment Worksheet

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

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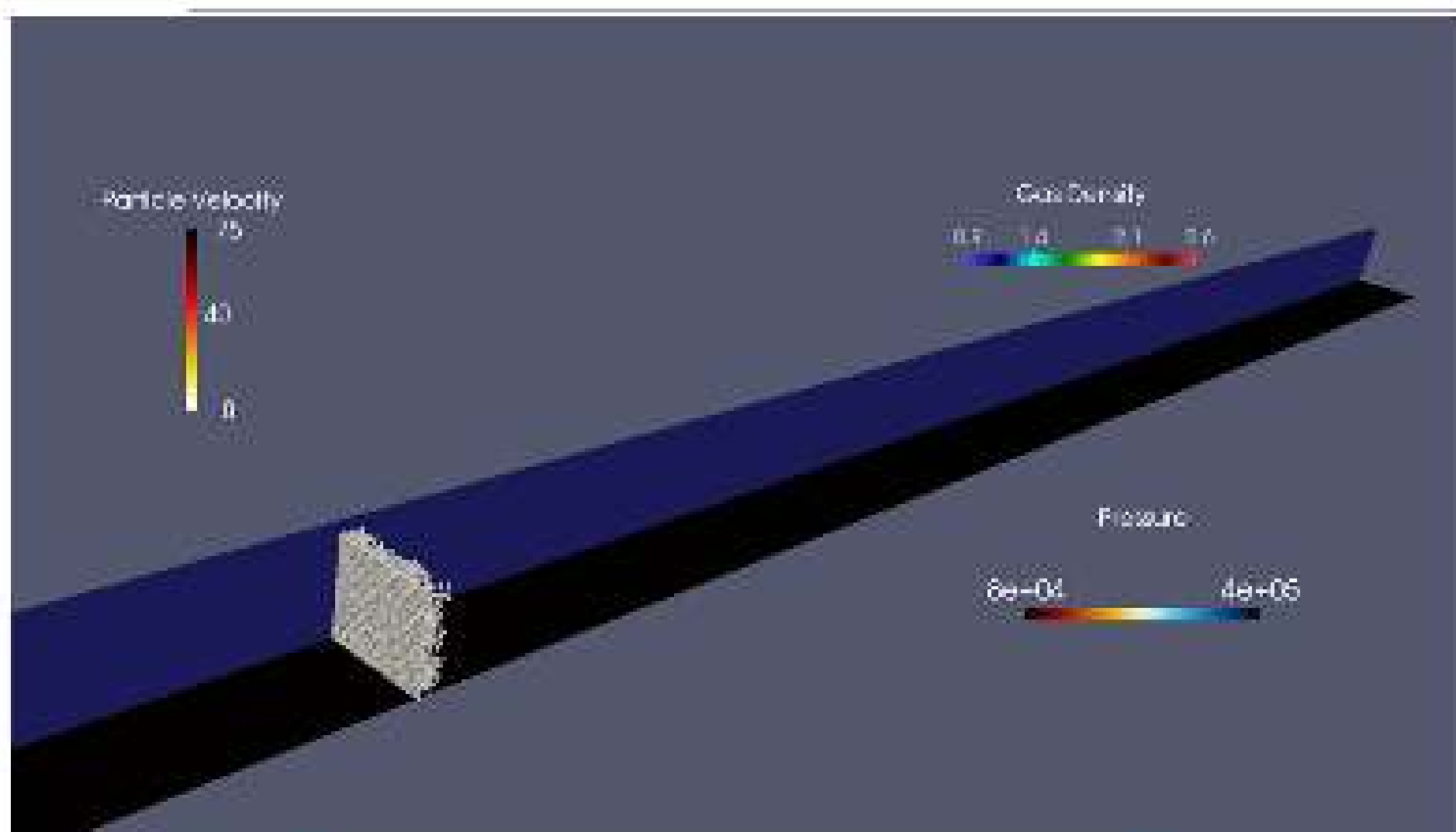
UB Workflow Simulation Worksheet

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

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Typical Particle Curtain Simulation



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

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Summary and Future Work

- Implement Dakota for large production runs of Sandia shock tube
- Additional 1D simulation runs to determine response to identified uncertainties to determine sensitivity of force coupling model
- Carry out model improvement based on sensitivity analysis
- Consideration for 2D simulations by accounting for variation of quantities of interest through the vertical direction
- Carry out limited 3D simulations based on inputs from 1D and 2D simulations and error analysis

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Particles Departure from Axisymmetry

Maria Giselle Fernandez

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

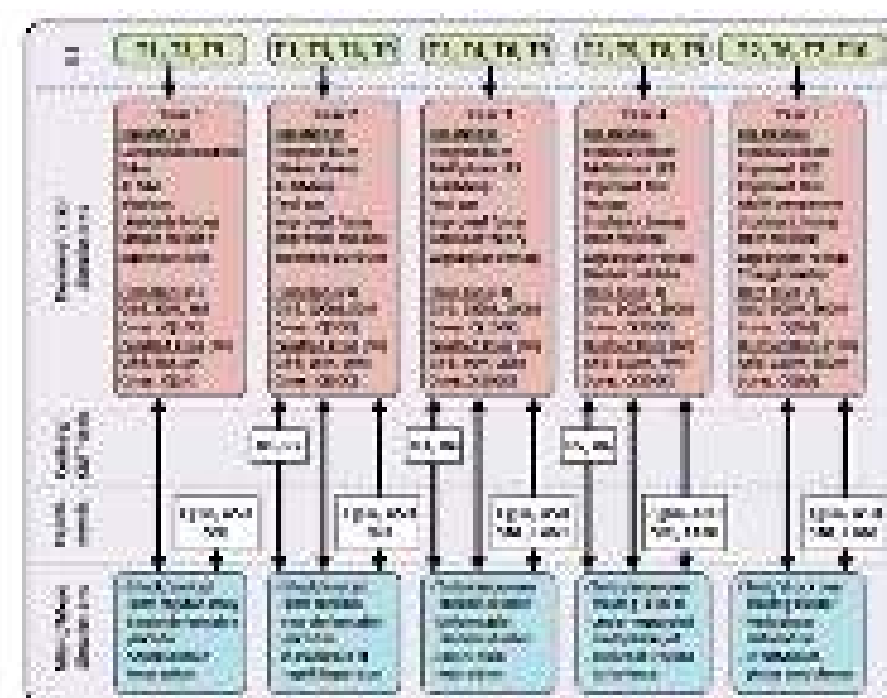
Department: Mechanical and
Aerospace, UF

Goals

- Determine what initial perturbation in particles leads to the maximum departure from axisymmetry

Simulation roadmap

- Collaboration with UB and Macroscale teams studying particles departure from axisymmetry



Simulation Roadmap

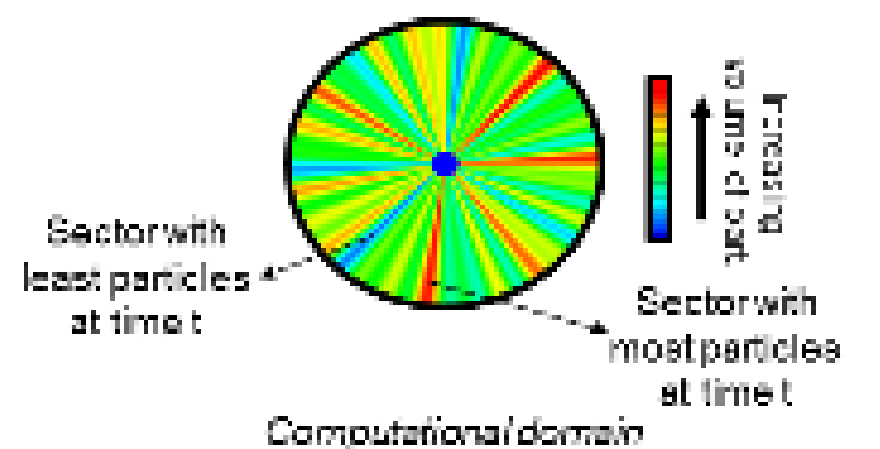
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Questions

- What is a good metric of **departure** from **axisymmetry**?

- Difference between the volume of particles in the sector with most particles and the one with least



- Which **initial disturbances** **amplify most** the departure?

- Multimodal initial perturbations in particle volume
- Surrogate models → more than 2,500 simulation already ran (9,113,600 core hours)
- Optimization

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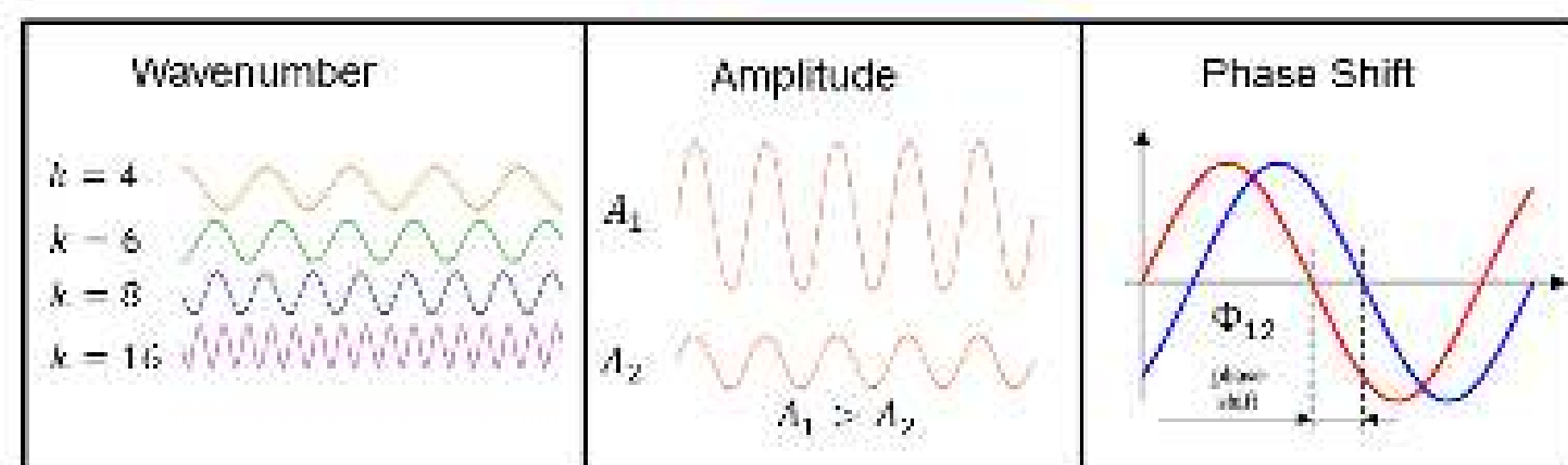
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Parametrization of Initial PVF Perturbation

$$\varphi^p(\theta) = \varphi_0^p [1 + A_1 \cos(k_1 \theta) + A_2 \cos(k_2 \theta + \Phi_{12}) + A_3 \cos(k_3 \theta + \Phi_{13})]$$

Particle Volume Fraction (PVF) Base PVF

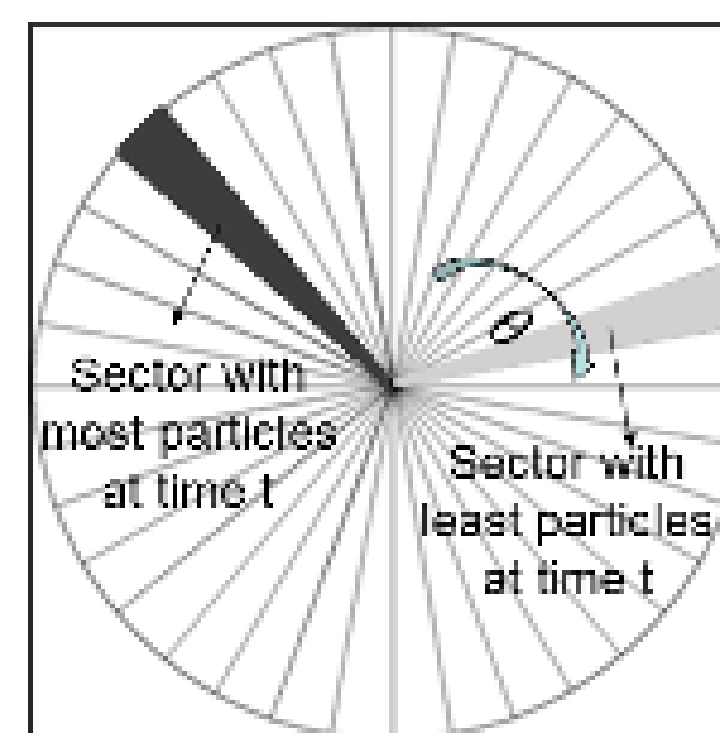
Parameters



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Amplification of Departure from Axisymmetry



Computational domain is divided in as many sectors as cells in θ

The amplification factor ζ is the ratio between the difference of the sector with most particles and the one with least at time t and the same difference at initial time t_0

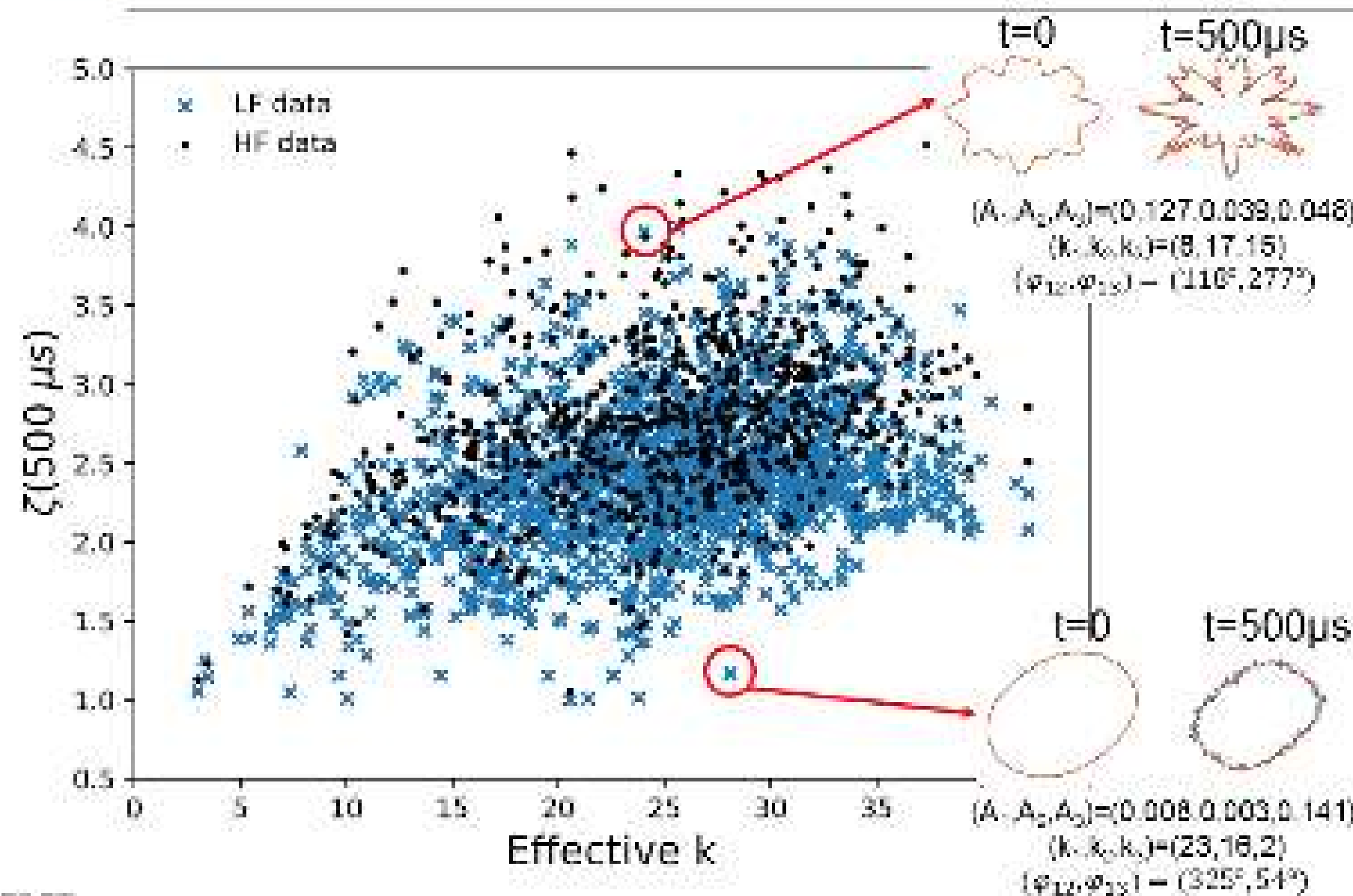
$$\zeta(t) = \frac{\text{Max}(f(\theta, t)) - \text{Min}(f(\theta, t))}{\text{Max}(f(\theta, t_0)) - \text{Min}(f(\theta, t_0))}$$

where f is the volume of particles in the sector θ at time t

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Amplification factors and volume contours



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Summary and Future Work

- Initial 2500 runs show large spread in amplification of departure from axisymmetry
- The future and main goal is **optimization** in 7 variables to find the initial disturbance producing **maximum departure from axisymmetry**
- We have obtained encouraging results using **multi-fidelity surrogate models**. This will allow a reduced cost optimization
- We are finding interesting **interactions between the modes** imposed as a perturbation in the particle volume fraction at initial time

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CMT-bone on KNL and DVFS based Systems

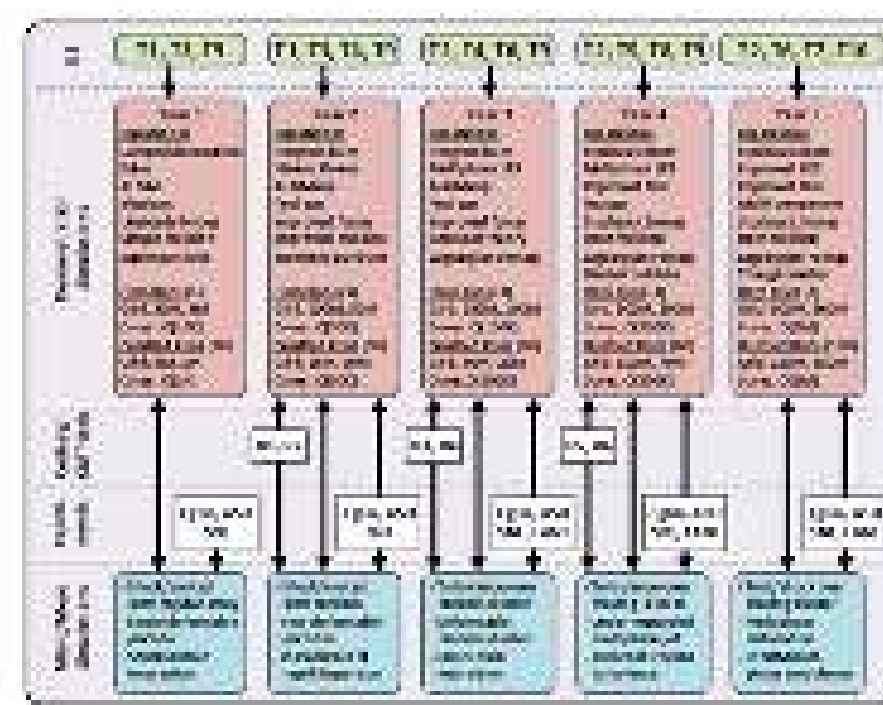
Mohamed Gadou

Advisor: Prof. Sanjay Ranka

Department: CISE, UF

Goals

- Multiobjective Optimization of CMT-bone on DVFS based hybrid Systems
- Performance optimization of CMT-bone on Intel KNL
- Simulation roadmap
 - Our research roadmap is closely tied with CMT-nek development.



Simulation Roadmap

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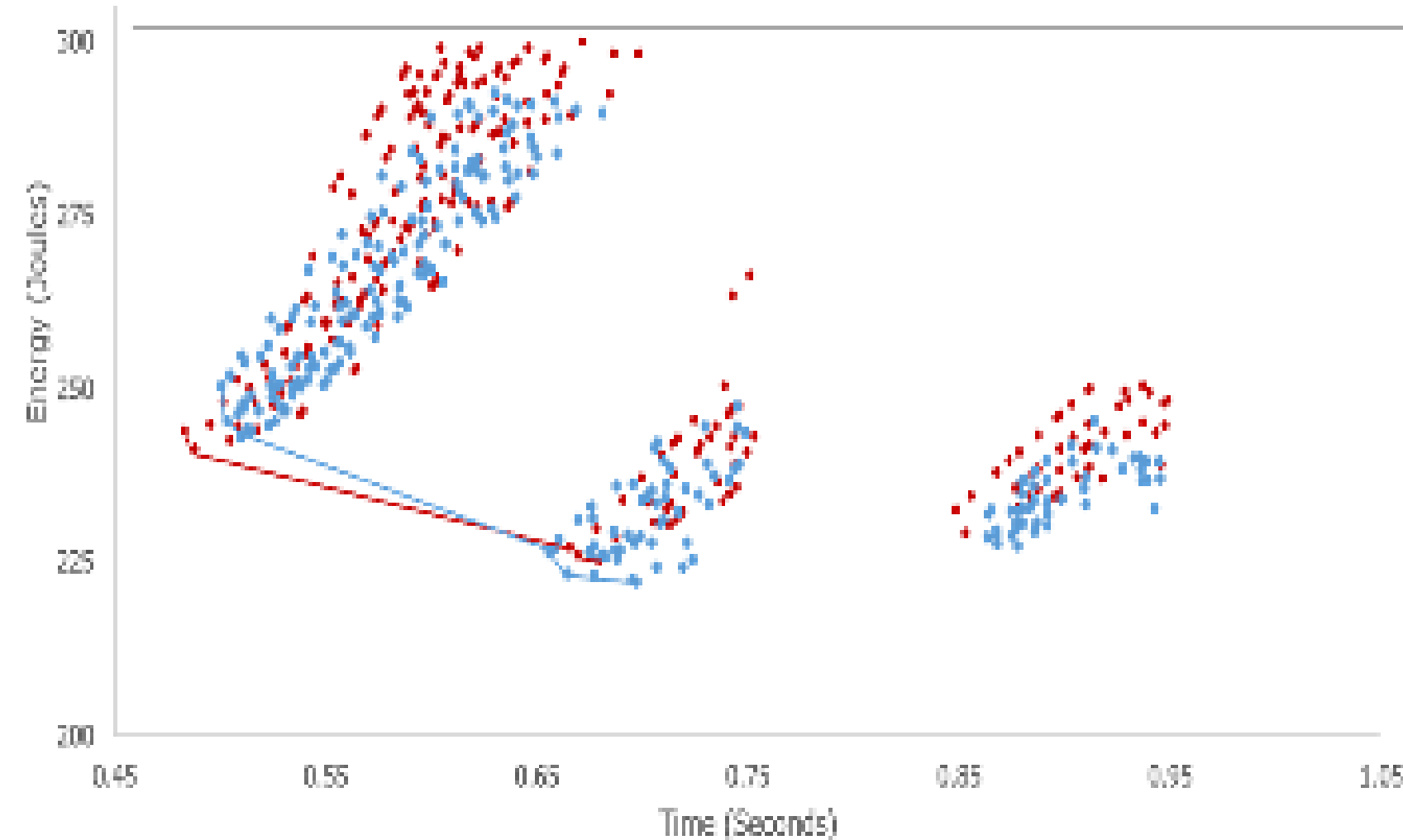
Motivation

- Developing model for Optimizing CMT-bone on DVFS based hybrid systems
- Performance Energy tradeoffs for CMT-bone on hybrid systems
- Exploring a wide variety of architectural configurations consisting of a variable number of GPUs and CPU cores in addition to variable cores frequencies in terms of performance, energy and power requirements
- Optimization of CMT-bone on Intel Knights Landing processors (KNL)

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Results

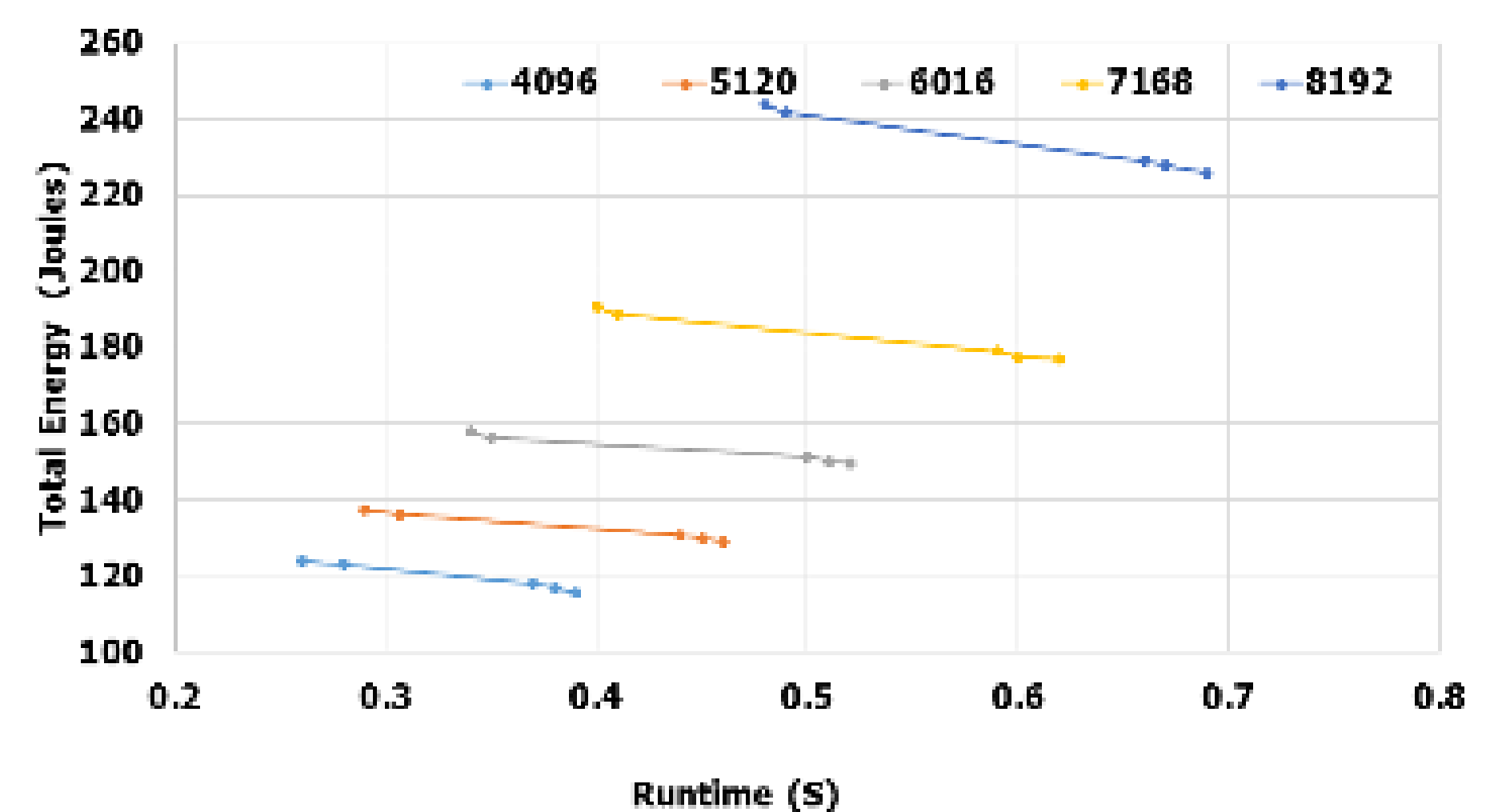


- Estimated and Actual Pareto Optimal curves matches

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3

Results

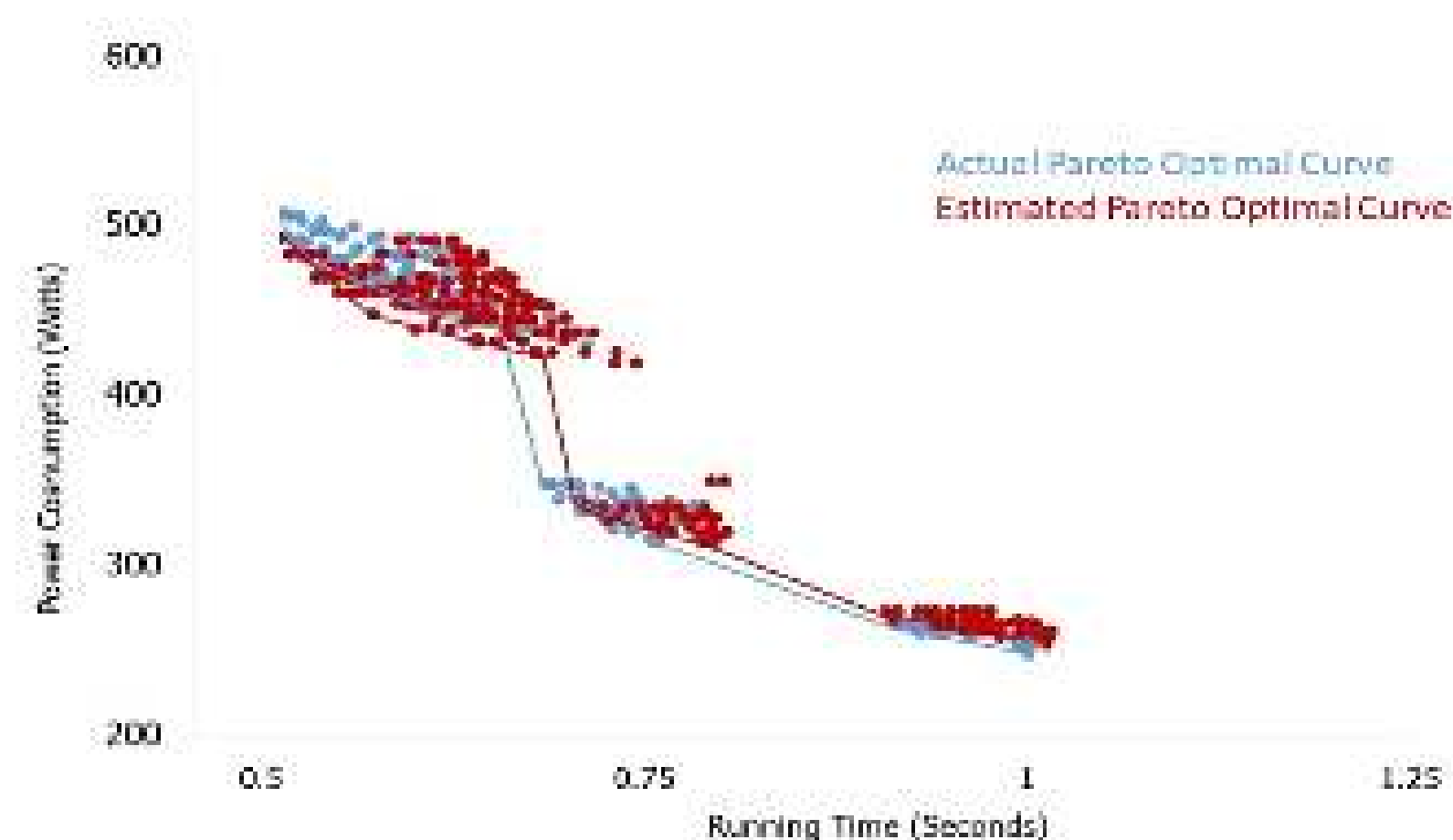


- Estimated Pareto Optimal Curves for different problems sizes

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Results

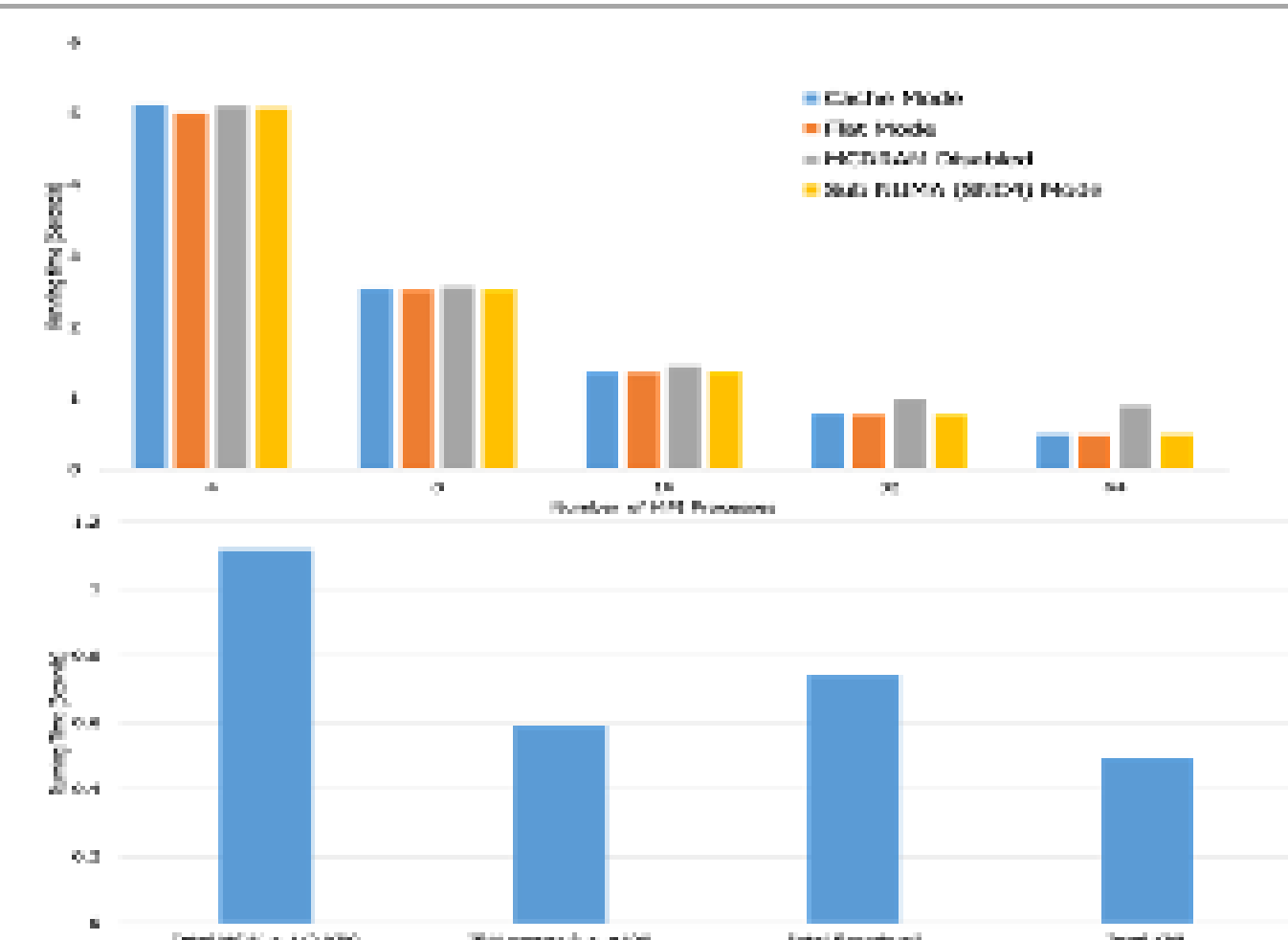


- Pareto Optimal Curve for Power Versus Time

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Results



- Intel KNL performance is comparable to GPU performance and better than regular multicore processors

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Eglin Explosive Barrel Ejection Simulations

Joshua Garno

Advisor: Dr. S. Balachandrar

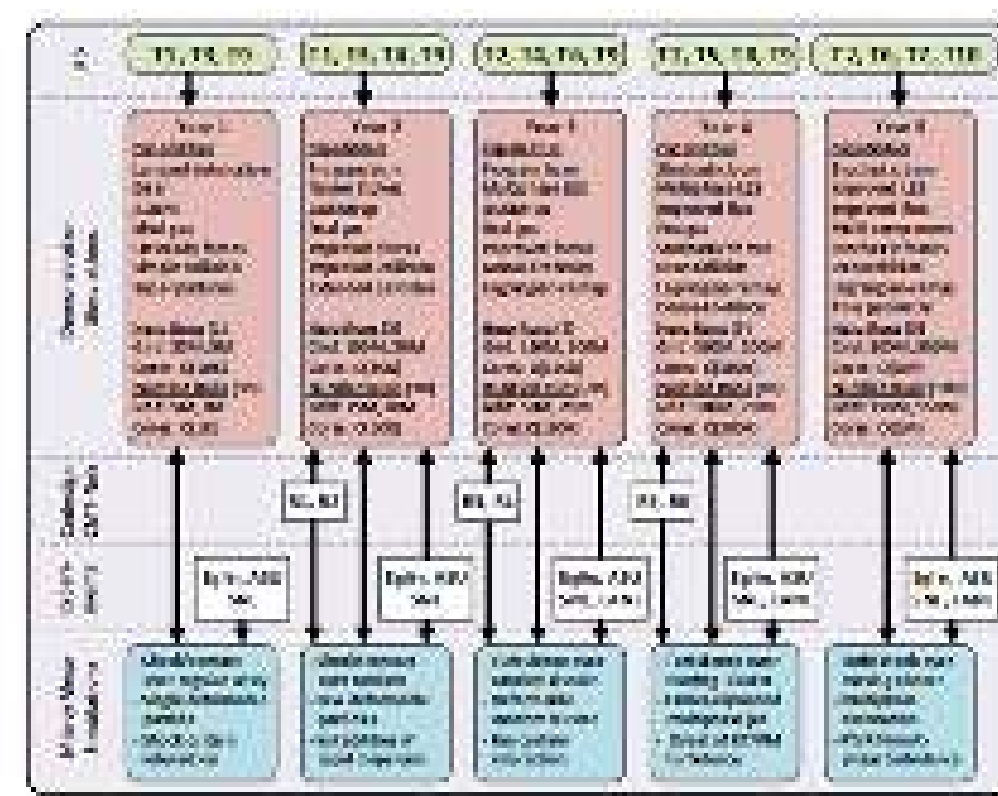
Department: MAE, UF

Goals

- Simulate trajectory of 1, 9 and many particle configurations
- Simulate dispersal of 0.5g packet of particles
- Validate Rocfluo models governing particle motion

Simulation Roadmap

- Real Gas
- EL-AUSM+UP
- Improved Forces
- Reactive Burn



Simulation Roadmap

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1

Motivation – Eglin Microscale Experiments

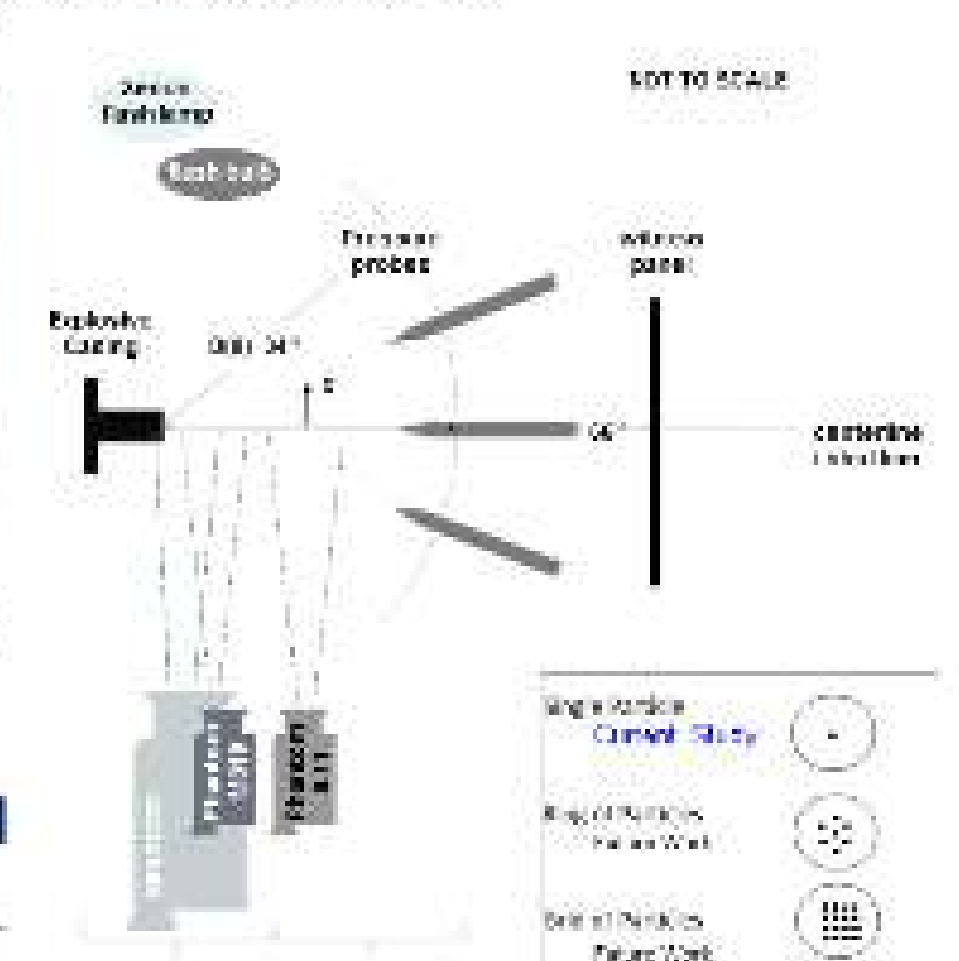
Source: Black, Litrell, and Delcambre, internal written report, 3/1/2015



Side view photograph showing the concave pressure probe array

Summary of test shots performed in February 2015

Test#	Driver	Particle(s)
Feb15-1	10 + 10 + 10 kg	Single (2mm dia) Tungsten sphere
Feb15-2	10 + 10 + 10 kg	Single (2mm dia) Tungsten sphere
Feb15-3	RP 33 + 3 kg	112 mm dia) Tungsten spheres (diamond pattern)

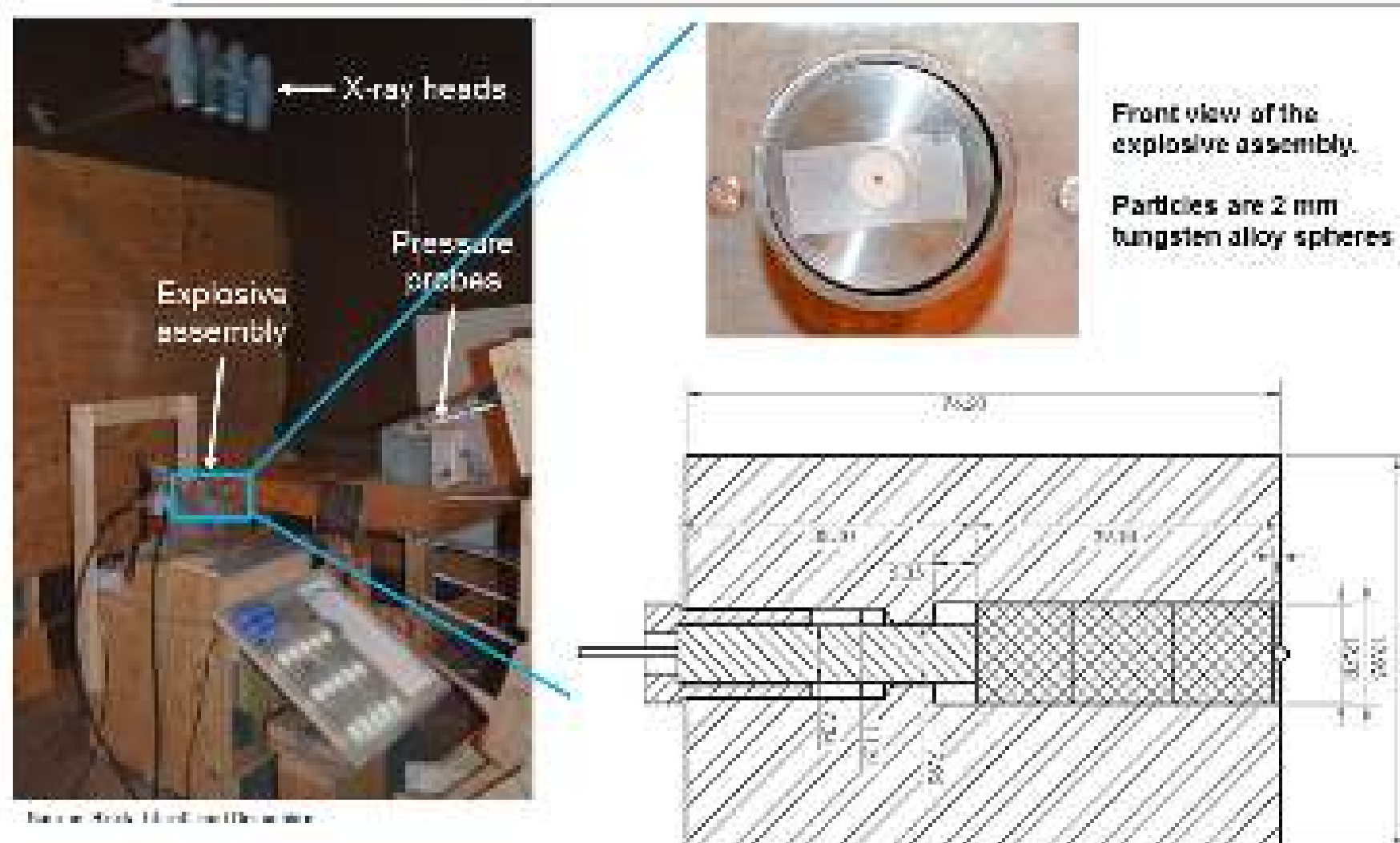


Overhead schematic of the test set up

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Motivation – Eglin Microscale Experiments



Three repeated single particle shots performed at Eglin AFB.

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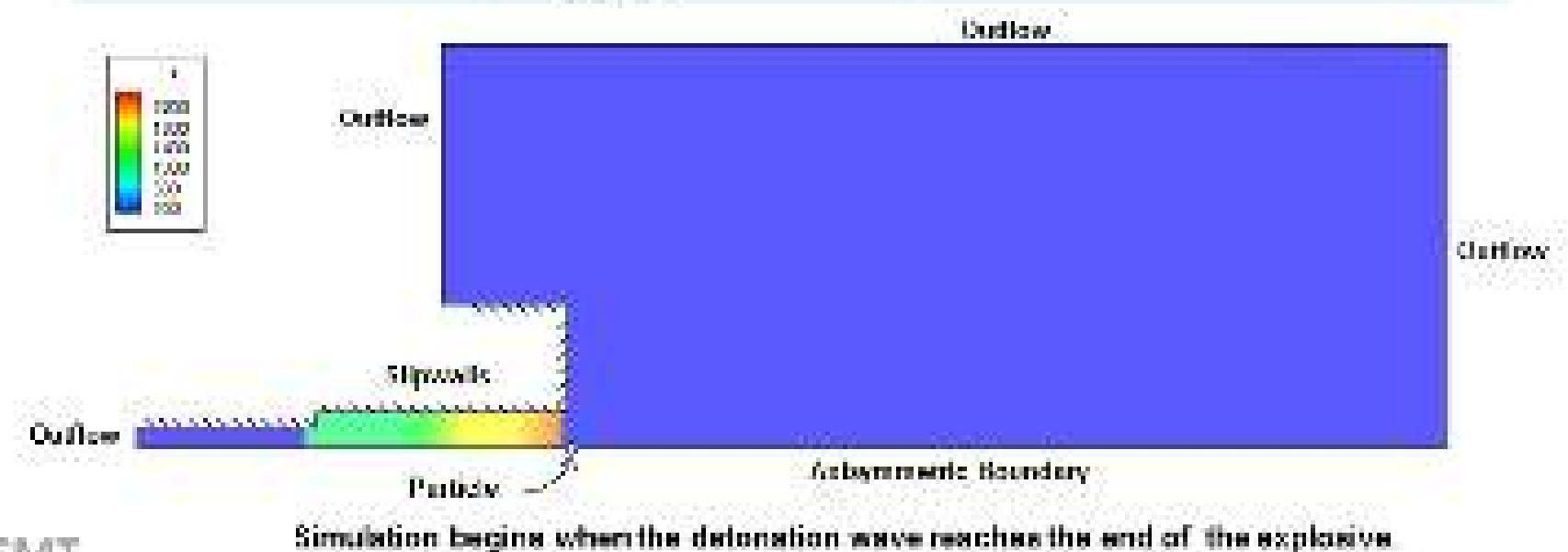
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Results

- Experimental uncertainties are analyzed to obtain a Design of Simulations
 - Uncertain inputs include particle diameter, particle density, and explosive density
 - Suite of $5 \times 5 \times 5 = 125$ simulations
- Simulation Setup

Code/Gov'n. Eqns	Initial Condition	EOS	Particle
------------------	-------------------	-----	----------

• Euler-Lagrange • Euler Equations	• Explosive LX-10-1 • Reactive Burn (RB) profile	• JWL	• MRG • One-way coupled
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Simulation begins when the detonation wave reaches the end of the explosive

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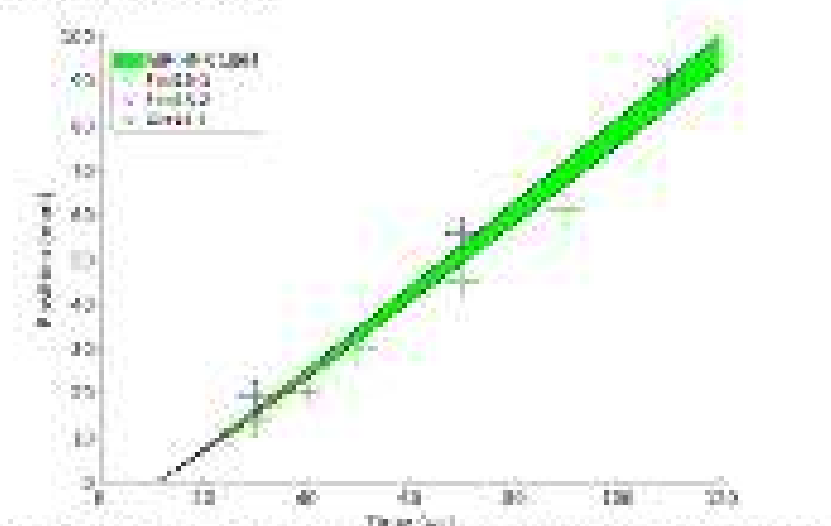
Results



Simulation Schlieren rendering at $t = 22.5$ microseconds

Validation Data Details:

- Crosshairs show experimental data points, with uncertainty
- Simulation results are time shifted based on Reactive Burn detonation times
- The filled band outlines the max and min trajectories of the 25 particles
- Simulation unreacted explosive density, $\rho_{exp} = 1804 \text{ kg/m}^3$



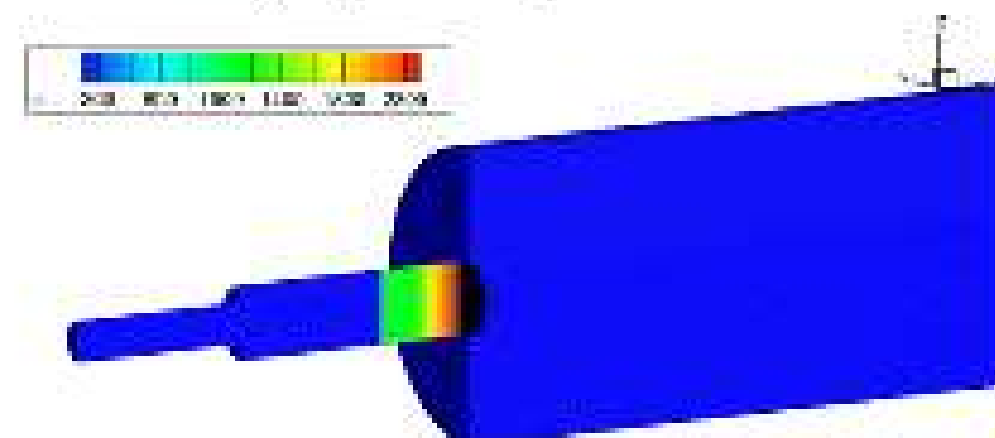
Experimental particle trajectories compared with simulation output

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Summary

- Summary - Eglin Microscale Experiments
 - Compile data from suite of 125 simulations for Uncertainty Quantification Analysis
 - Simulate ring and grid of particles
- Future work – Eglin Mesoscale Experiments
 - Simulate dispersal of 0.5 g packet of tungsten particles
 - Particle diameter, $d_p = 112.5 \mu\text{m}$



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Macroscopic Explosive Dispersal of Particles

Kyle Hughes

Advisor: Prof. Kim, Balachandar, and Haftka

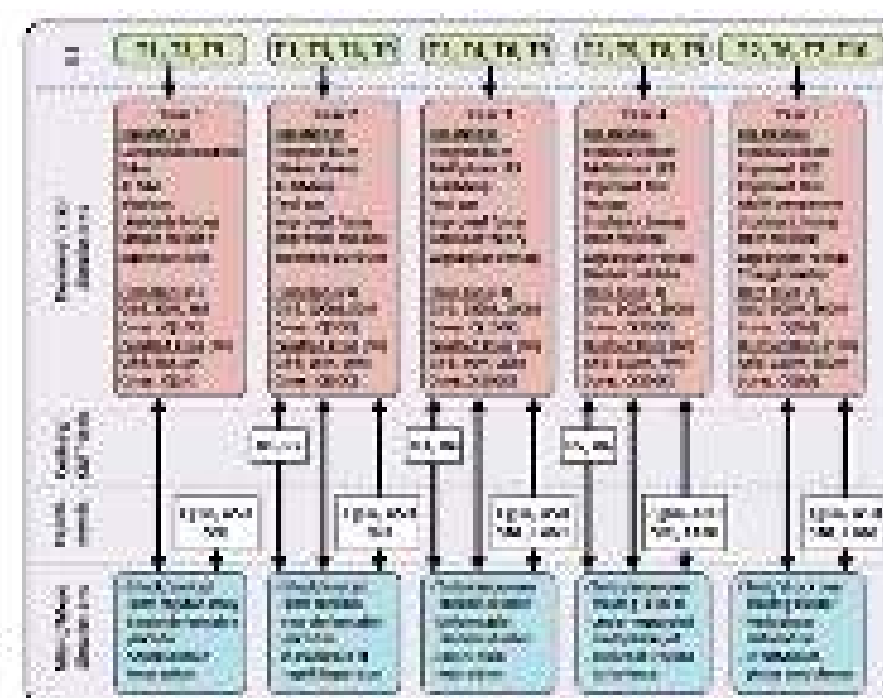
Department: Mechanical and Aerospace Engineering, UF

Goals

- Perform forensic uncertainty quantification of past experiments to inform future experiments
- Design validation experiments to meet simulation assumptions and capabilities
- Perform uncertainty quantification of validation experiments

Simulation roadmap

- Tie experiments performed at LANL and Eglin AFB to simulations using CCMT uncertainty quantification

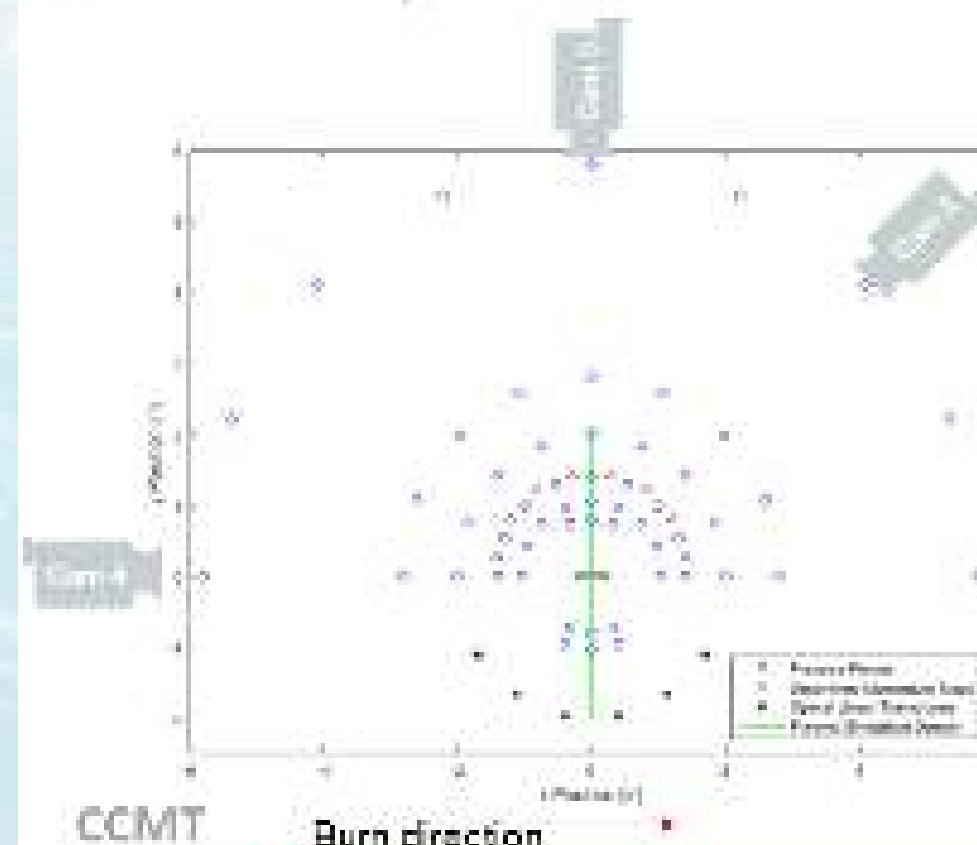


Simulation Roadmap

Experimental Setup - AFRL Blastpad

- Instrumentation suite at Eglin AFB consisting of 54 in-ground pressure transducers, 6 optical linear encoders, 8 unconfined momentum traps, and 4 high-speed cameras
- Phantom v1212 sampled at 12000 fps (Camera 1/4) and Phantom v711 sampled at 7500 fps (Camera 2/3)
- Six tests total performed

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



Test Article Casing and Geometry

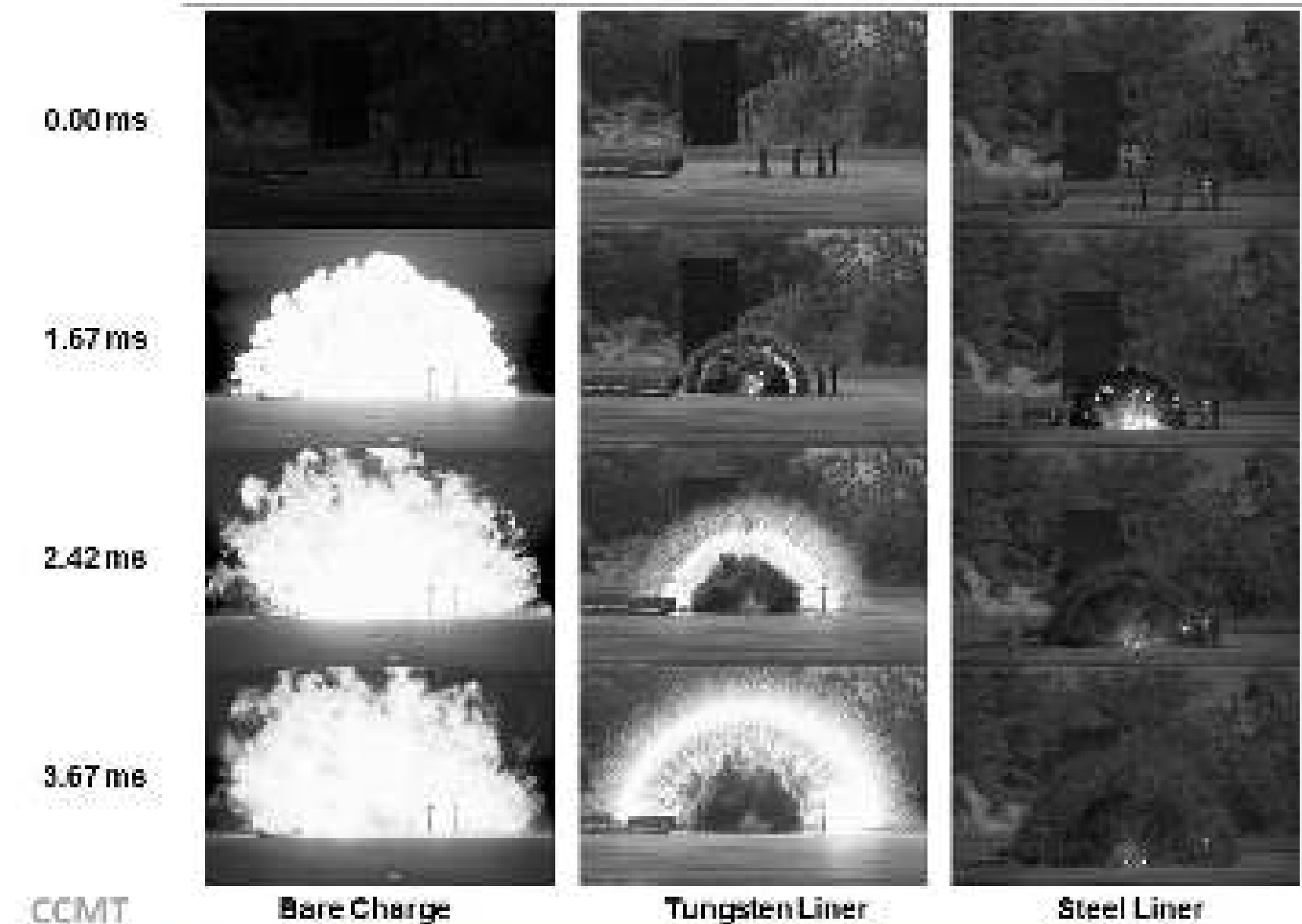
- Case fracture may be a possible mechanism for jetting instability [Zhang et al. 2001, Xu et al. 2013]
- Case influence was minimized by using thin phenolic tubing and notches to attempt to control the casing failure
- The ratio of the mass of the particles to the mass of the charge (M/C) is critical to formation of instabilities. Literature review (Frost, Zhang) suggests $M/C \geq 10$ is reasonable
- Bare charge geometry is chosen to match legacy blastpad data (increases sample size by two for bare charge)



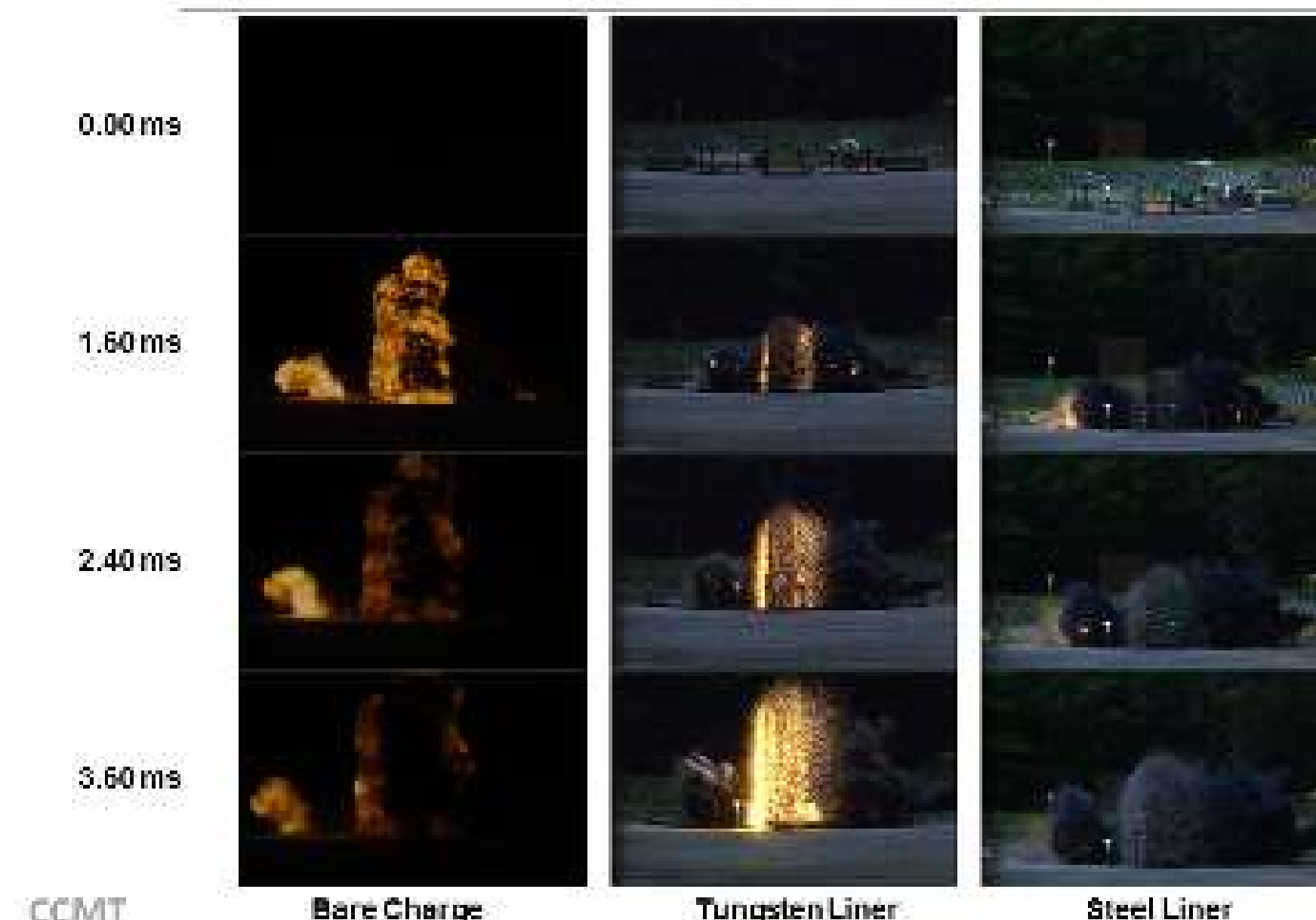
Top view of notched casing (steel liner)



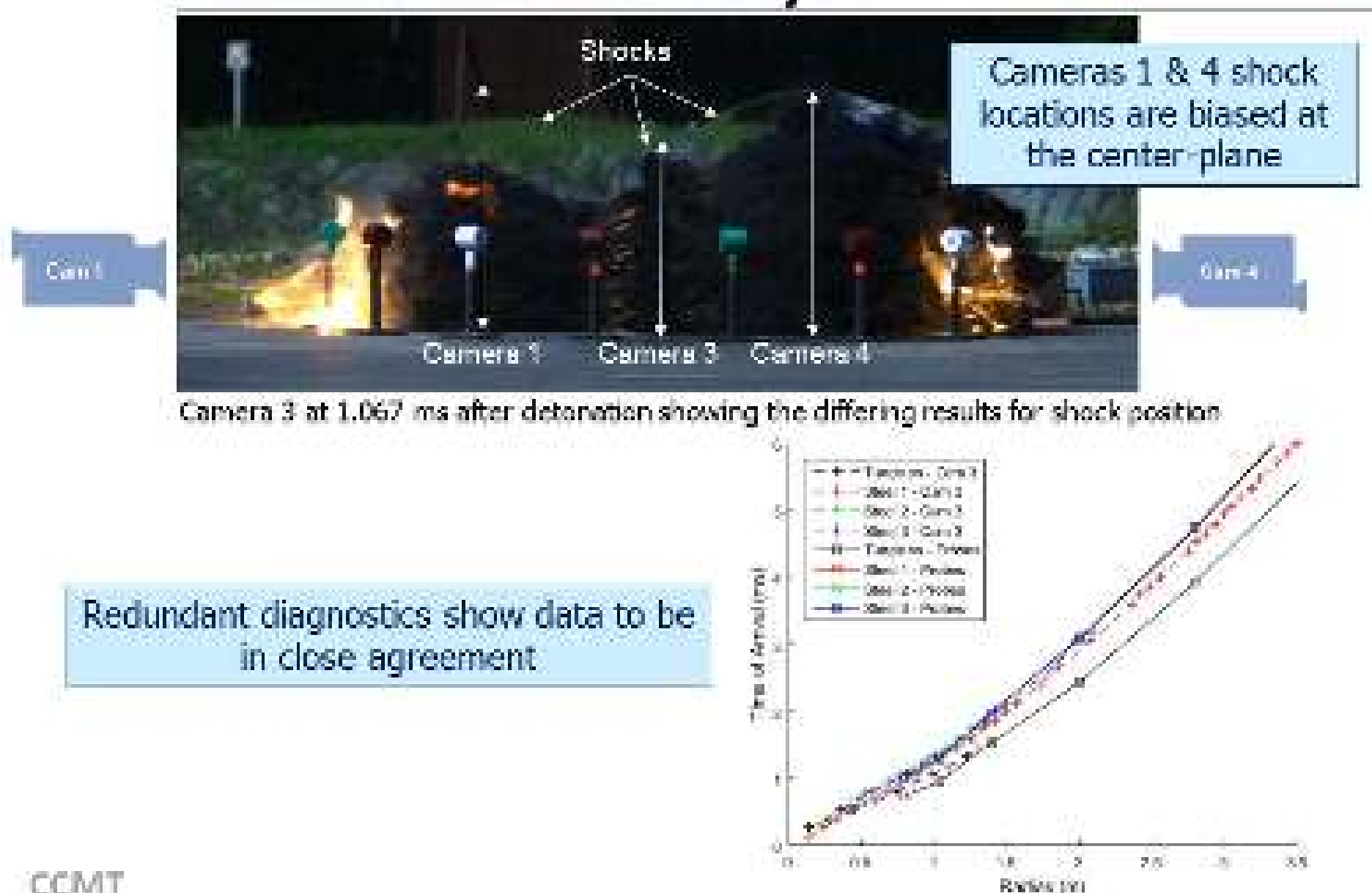
High Speed Imagery – Camera 1



High Speed Imagery – Camera 3



Shock Location Analysis



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Macroscopic Explosive Dispersal of Particles

Kyle Hughes

Advisor: Prof. Kim, Balachandar, and Haftka

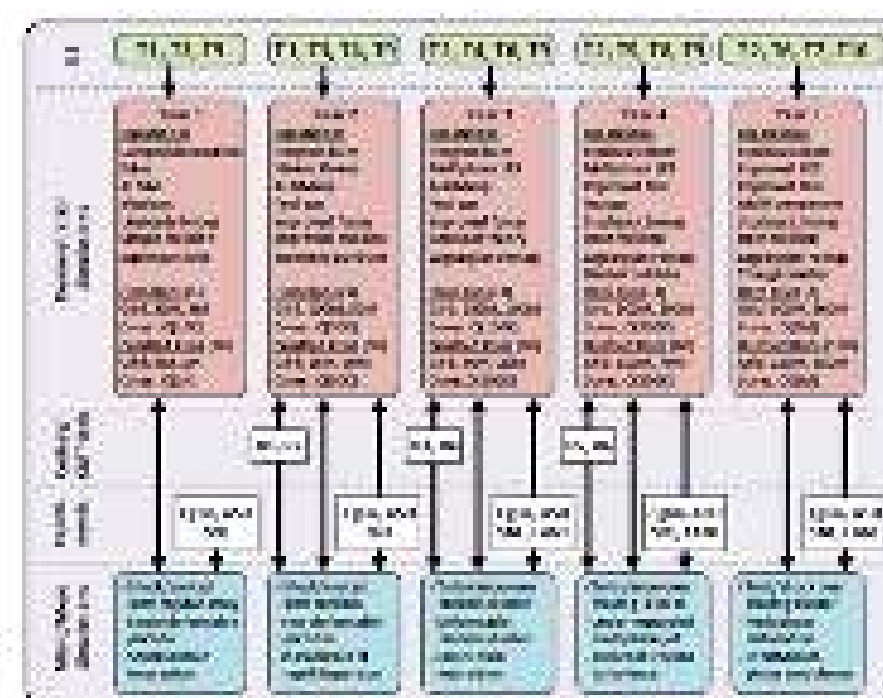
Department: Mechanical and Aerospace Engineering, UF

Goals

- Perform forensic uncertainty quantification of past experiments to inform future experiments
- Design validation experiments to meet simulation assumptions and capabilities
- Perform uncertainty quantification of validation experiments

Simulation roadmap

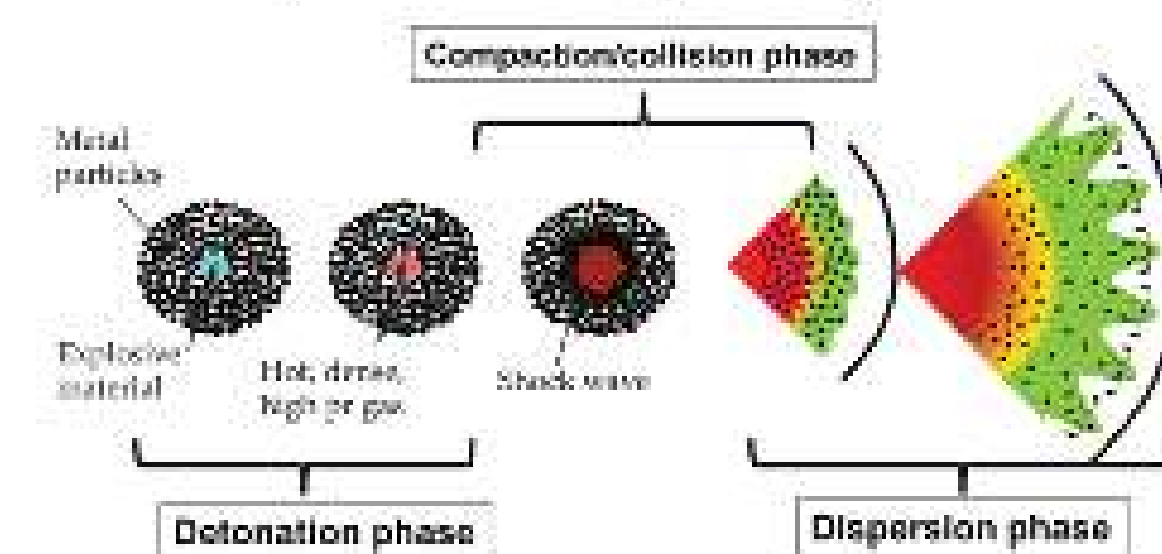
- Tie experiments performed at LANL and Eglin AFB to simulations using CCMT uncertainty quantification



Simulation Roadmap

Motivation

- Goal:** Investigate the physics of particle-particle interactions as the bed of particles goes from compaction/collision to dispersal while providing validation-quality data
- Unique contribution:** Perform an experiment such that the particle bed is subjected to a detonation wave without the complexities of ambient fluid while artificially lowering the volume fraction to "simulatable levels"
- Proton radiography (P-rad) facility enables this investigation because:
 - The 22 time resolved images allow examination of the time evolving particle cloud within the explosive products
 - Test section is kept under vacuum, removing ambient fluid

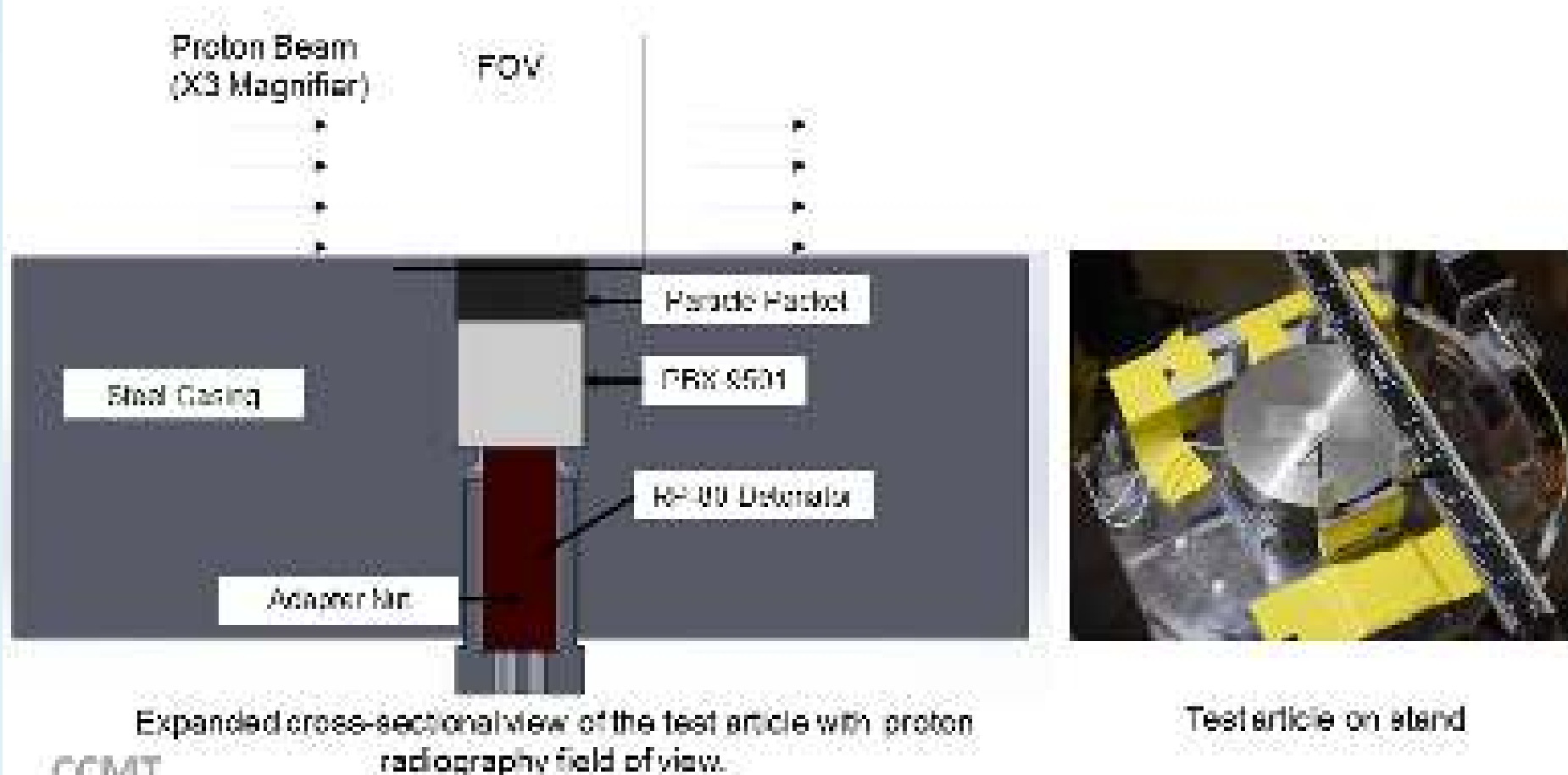


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Experimental Setup

- Eglin AFB mesoscale experiments formed basis for experimental design
- Minimal changes between previous mesoscale experiments and proton radiography experiments to decrease simulation workload



Expanded cross-sectional view of the test article with proton radiography field of view.

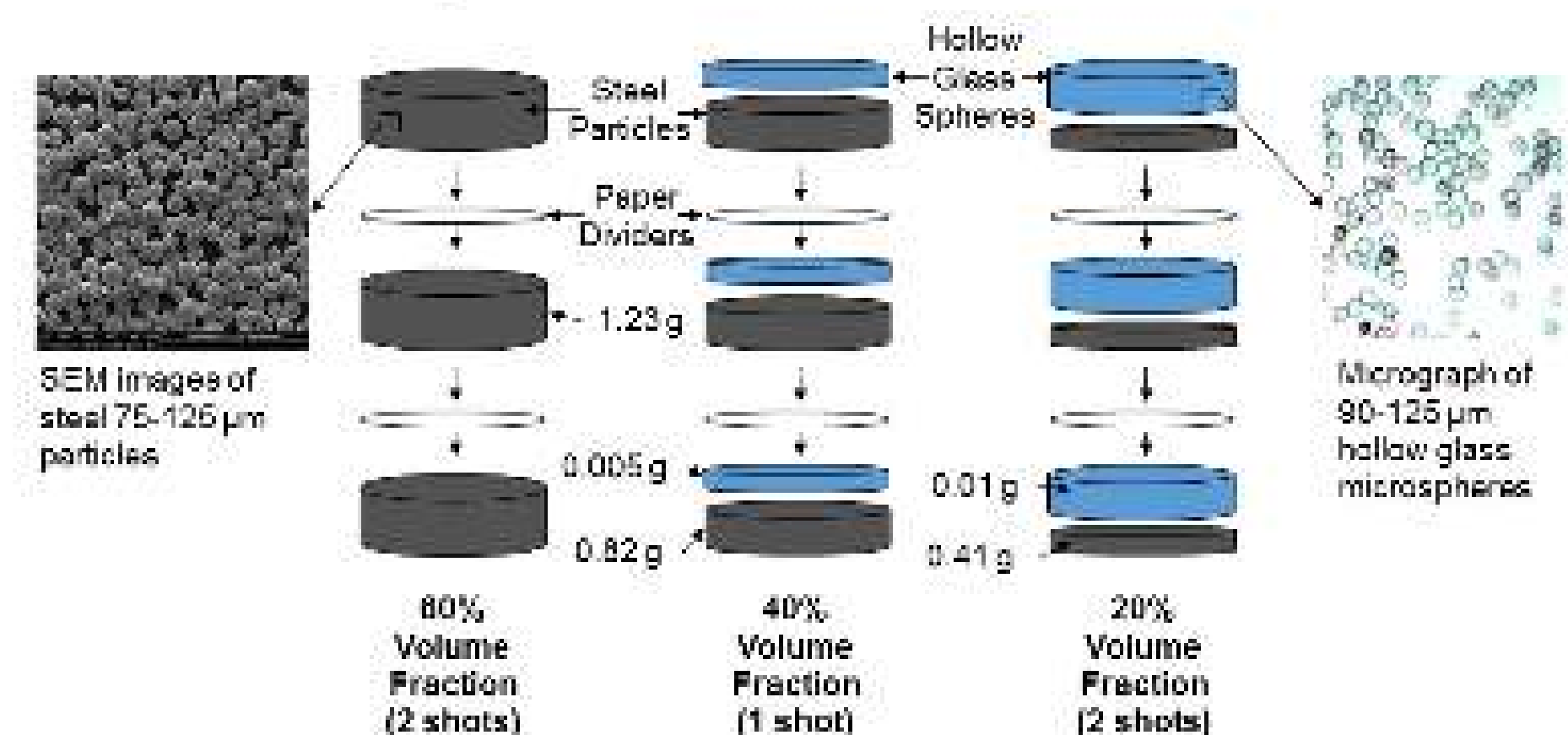
Test article on stand

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Experimental Setup – Particle Packet

Particle packet utilized layering of steel and hollow glass spheres to vary the over-all volume fraction of the particle bed

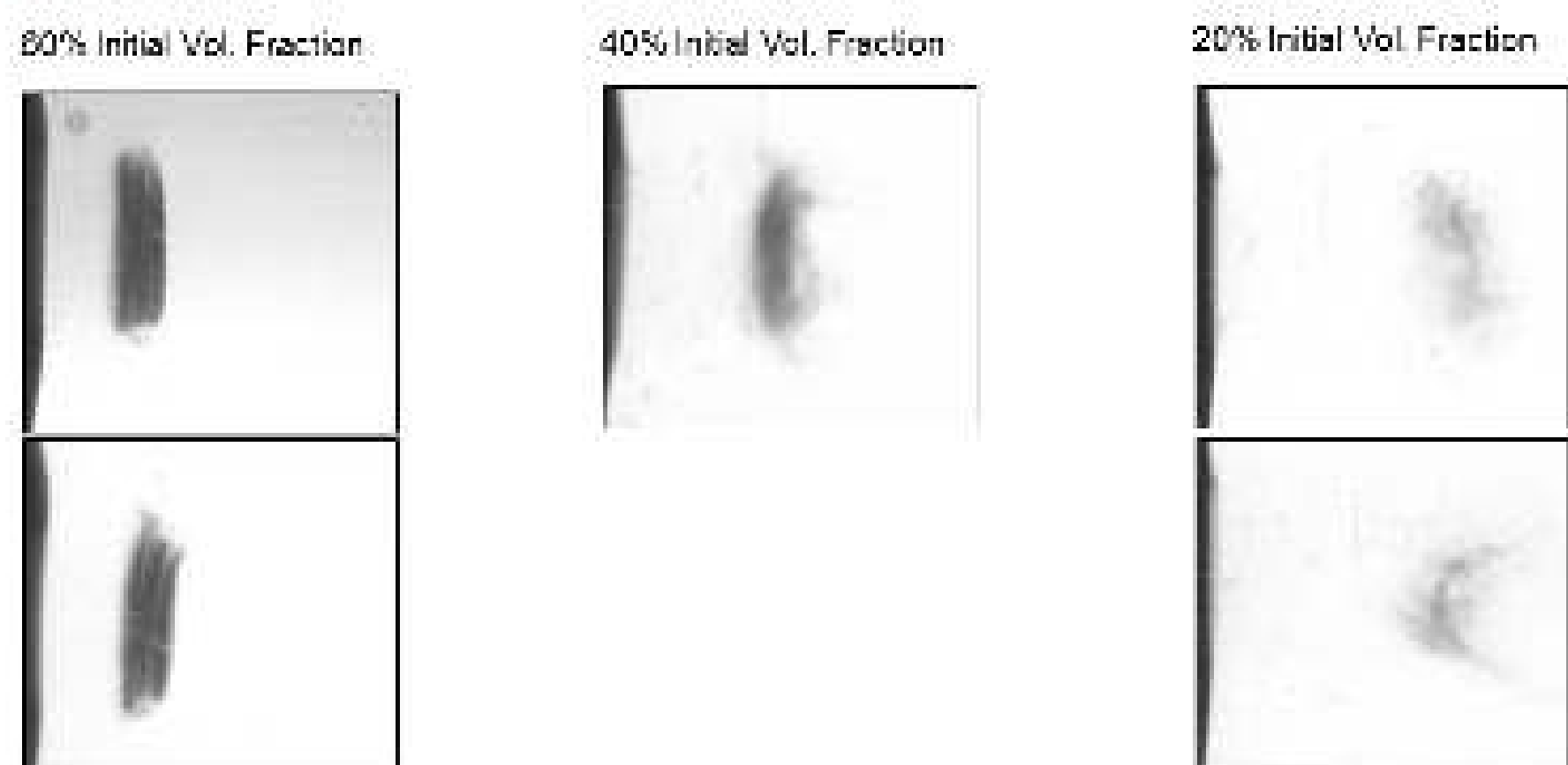


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Still Images - Transmission

- 60% moves in a piston-like motion, maintaining the 3-layer structure
- As the volume fraction is decreased, the structure becomes gradually more chaotic



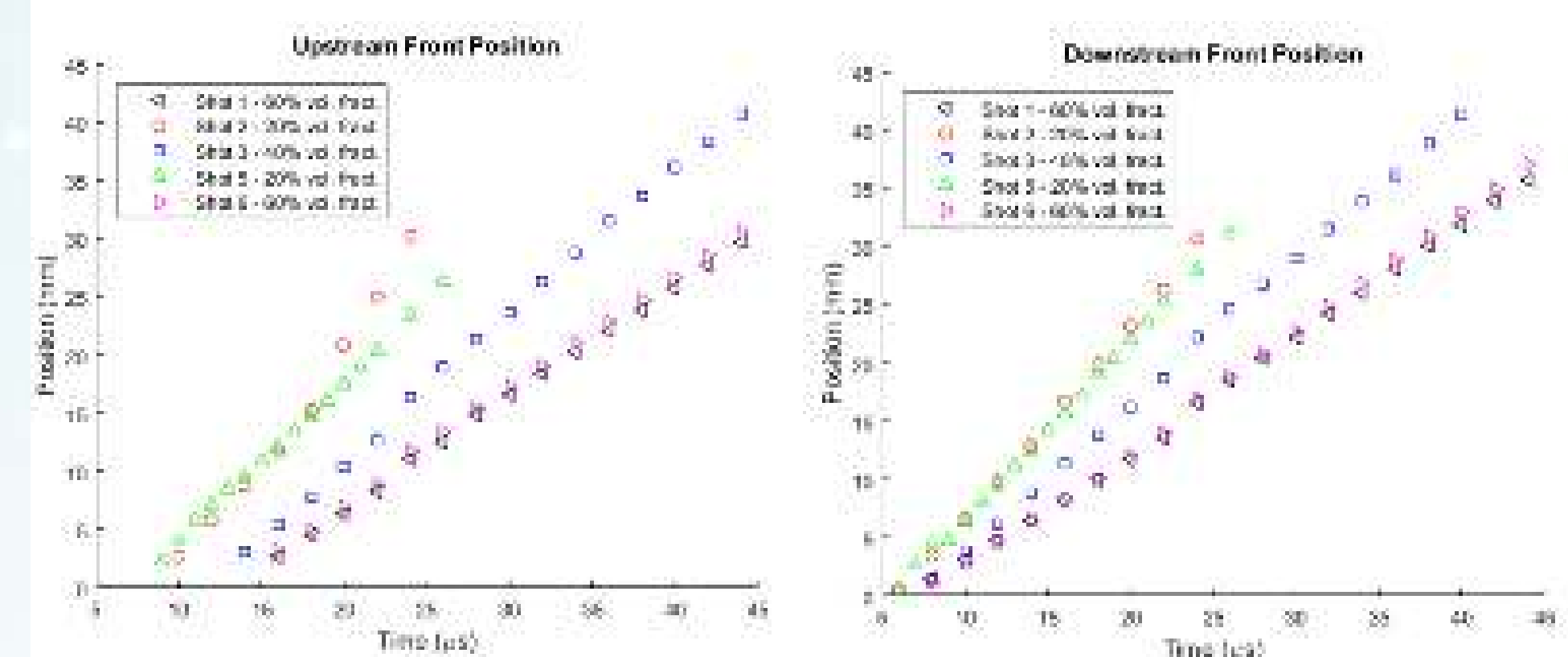
Proton radiography results at 20 μs after detonation

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Centerline Front Tracking Results

- Fronts calculated based on transmission falling below 90% of background value
- Relatively close agreement between repeated shots
- Decreasing mass leads to an increase in velocity for the lower volume fractions



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Uncertainty Quantification of ASU Shock Tube

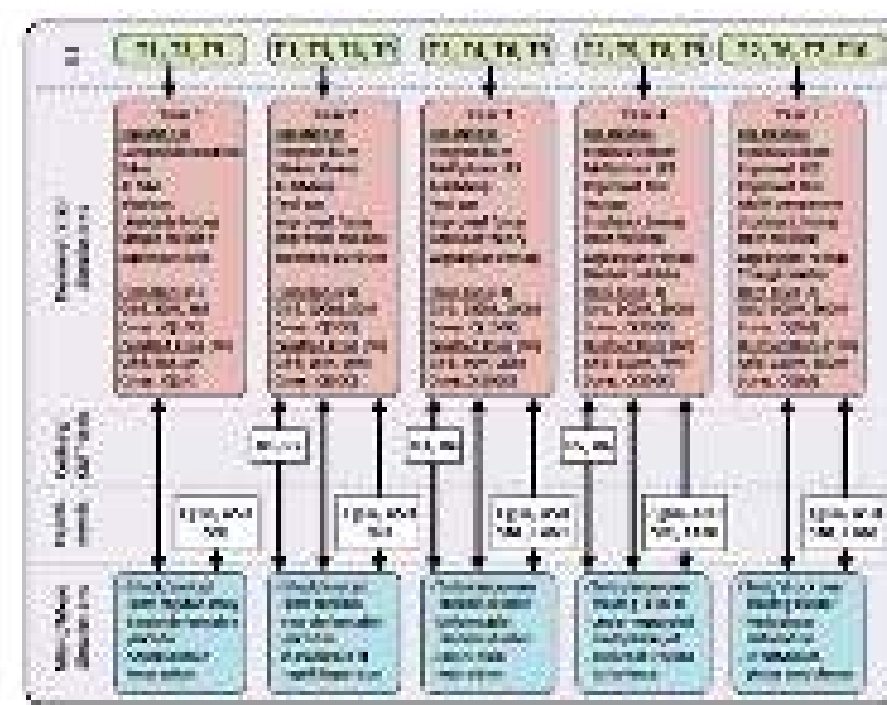
Tanner Jones

Advisor: Dr. Kim, Dr. Haftka, Dr. Park

Department: Mechanical and
Aerospace Engineering, UF

Goals

- Identify sources of uncertainty in experimental procedures
 - Propagate identified sources of uncertainty from experiments into simulations
 - Validate CMT-nek simulation capabilities
- #### Simulation roadmap
- Multiphase turbulence modeling and uncertainty
 - Conduct forensic UQ

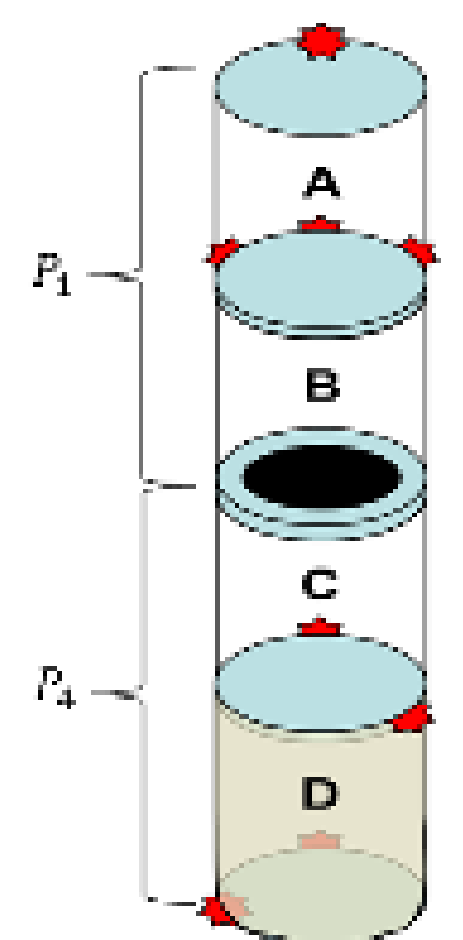


Simulation Roadmap

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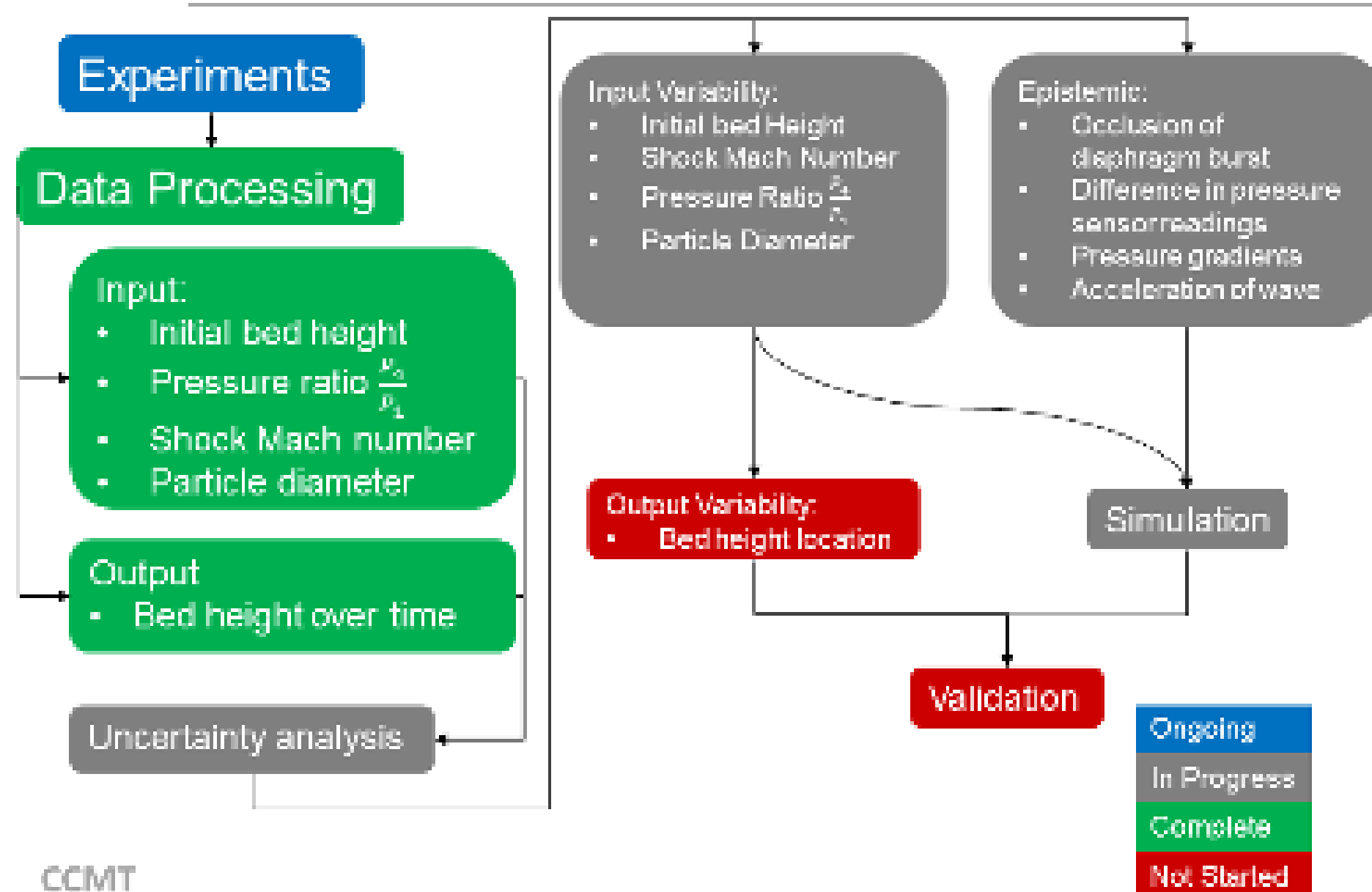
Motivation

- The study of measurement processes in shock tube experiments allows for uncertainty analysis of quantities of interest to be used in validating simulation code
- Uncertainty quantification reduces measurement processing uncertainties which leads to smaller simulation uncertainties
- A vertical shock tube is studied to characterize the input and output parameters used to validate turbulence models developed by the simulation team
- A particle bed is placed at the bottom of the Shock tube (D). A diaphragm is located above the particle bed, separating the shock tube into a high (P_4) and low (P_1) pressure region. Cameras and pressure sensors collect data on the movement of the particle bed and shock/expansion waves.



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ASU Shock Tube UQ



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ASU Input Variability

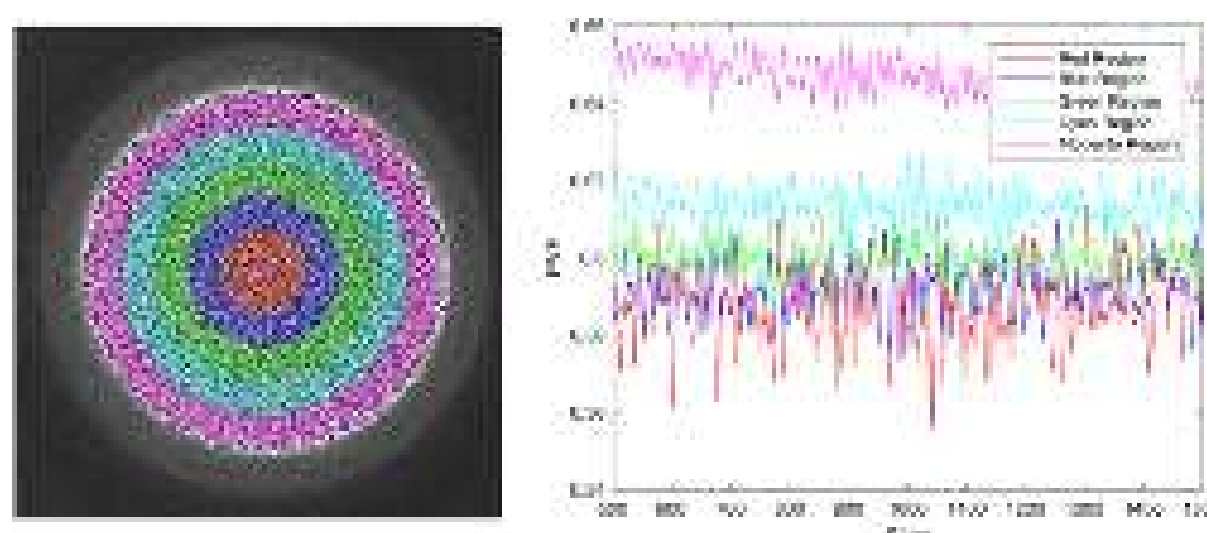
- Uncertainty originates because one quantity is measured which is used to calculate another. The time of pressure readings at two known distances are converted into velocity, which is then converted to a Mach number. The Mach number is then used to calculate the pressure ratio, $\frac{P_4}{P_1}$, in the shock tube.

Experiment	Measured Mach Number	Calculated Pressure Ratio $\frac{P_4}{P_1}$
09/20/2017 #4	1.17 ± 0.04	2.52 ± 0.38
09/20/2017 #5	1.65 ± 0.004	11.78 ± 0.15
09/20/2017 #6	1.52 ± 0.02	7.74 ± 0.62
10/12/2017 #3	1.67 ± 0.01	12.33 ± 0.57
10/12/2017 #4	1.57 ± 0.003	9.10 ± 0.11
10/12/2017 #5	1.48 ± 0.01	6.63 ± 0.26
10/12/2017 #6	1.28 ± 0.01	3.22 ± 0.10

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ASU Shock Tube Particle Characterization

- 4 samples of particles with nominal diameter ranges:
 - 45-90 microns, 90-150 microns, 150-212 microns, 211-297 microns
- SEM image processing shows particle diameters tending to the lower end of nominal ranges and that deformities and non-spherical particles were a rarity
- Pycnometer estimates of particle density averaged $2.46 \frac{g}{cm^3}$ for all particles with very low uncertainty. This is slightly lower than nominal $2.5 \frac{g}{cm^3}$ for glass.
- Average Particle Volume Fraction was found to be 0.6-0.61 using a CT scan. The Average Volume fraction was found to increase in the radial direction of the shock tube



These figures show the average volume fractions for each region over approximately 1500 horizontal slices taken from the CT scan along the vertical axis of the particle bed

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Summary and Future Work

- Data analysis and uncertainty quantifications of the input and output parameters are supplementing the simulation team
- Additional ASU Experiments
 - Probing epistemic uncertainty sources
- Simulation Validation
 - Experimental output will be compared with simulation output to validate CMT-nek simulation capabilities

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Center for Compressible Multiphase Turbulence

Compressible Multiphase Turbulence Modeling

Rahul Babu Koneru

Advisor: Dr. S. Balachandrar

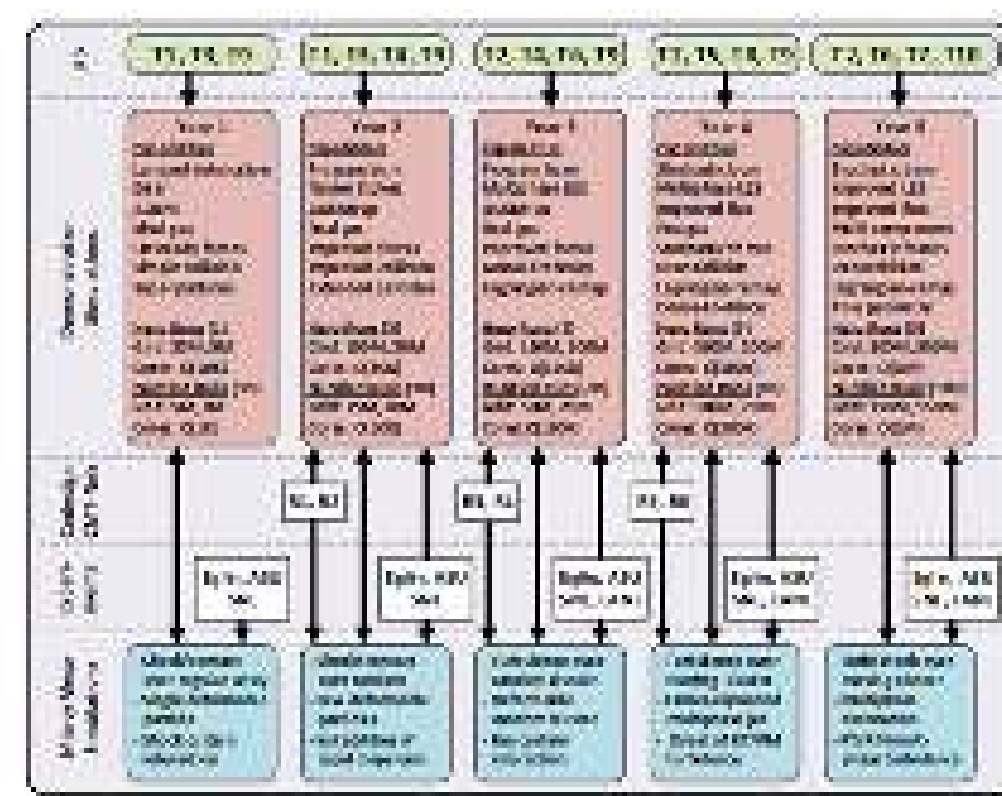
Department: MAE, UF

Goals

- Improve drag models at high Mach numbers and dense regimes
- Extend LES models to compressible multiphase flows
- Validation and integration into CMT-nek

Simulation roadmap

- Validate existing force models and develop new models
- Implement single phase LES and extend it to multiphase flows

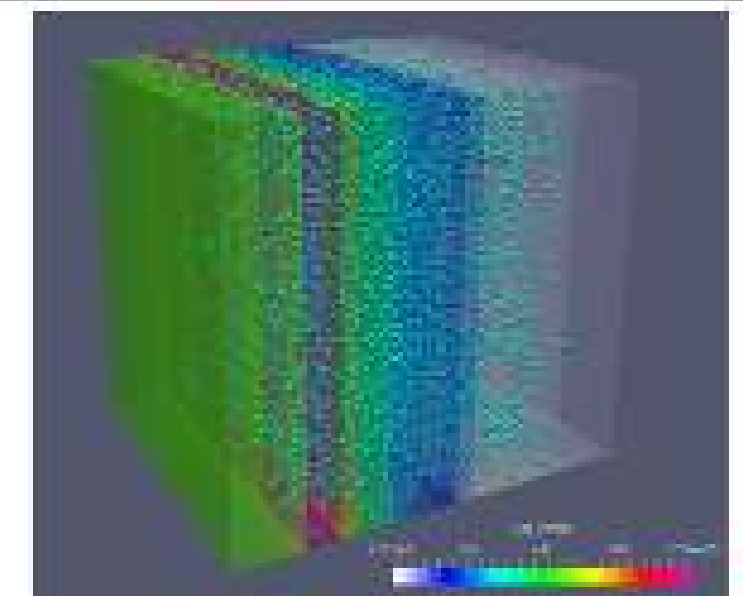
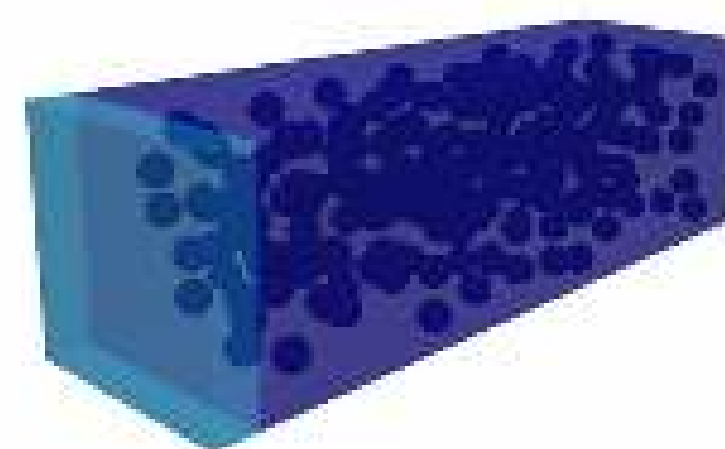


Simulation Roadmap

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1

Random Bed of Fixed Particles



Particle Resolved Simulations¹

M_s	3.0
$N_{p,LES}$	$O(10^2)$
$\phi_p(\%)$	10, 15, 20, 25
$d_p(\mu m)$	100

Point-Particle Simulations

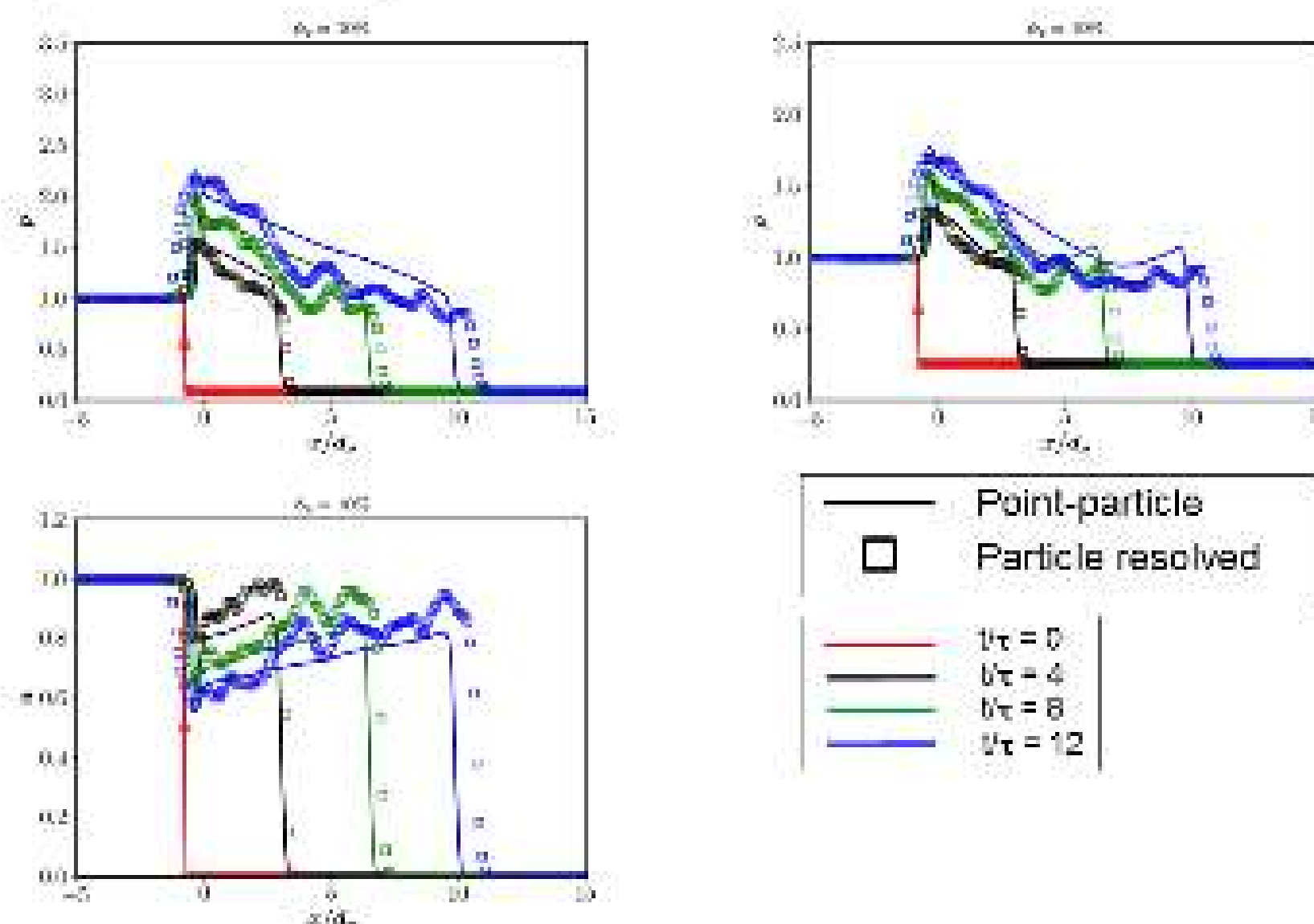
M_s	3.0
$N_{p,LES}$	$O(10^3)$
$\phi_p(\%)$	10, 15, 20, 25
$d_p(\mu m)$	100

¹Mehta, Y., et al. "Propagation of a strong shock over a random bed of spherical particles." *Journal of Fluid Mechanics* 839 (2018): 157-197.

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2

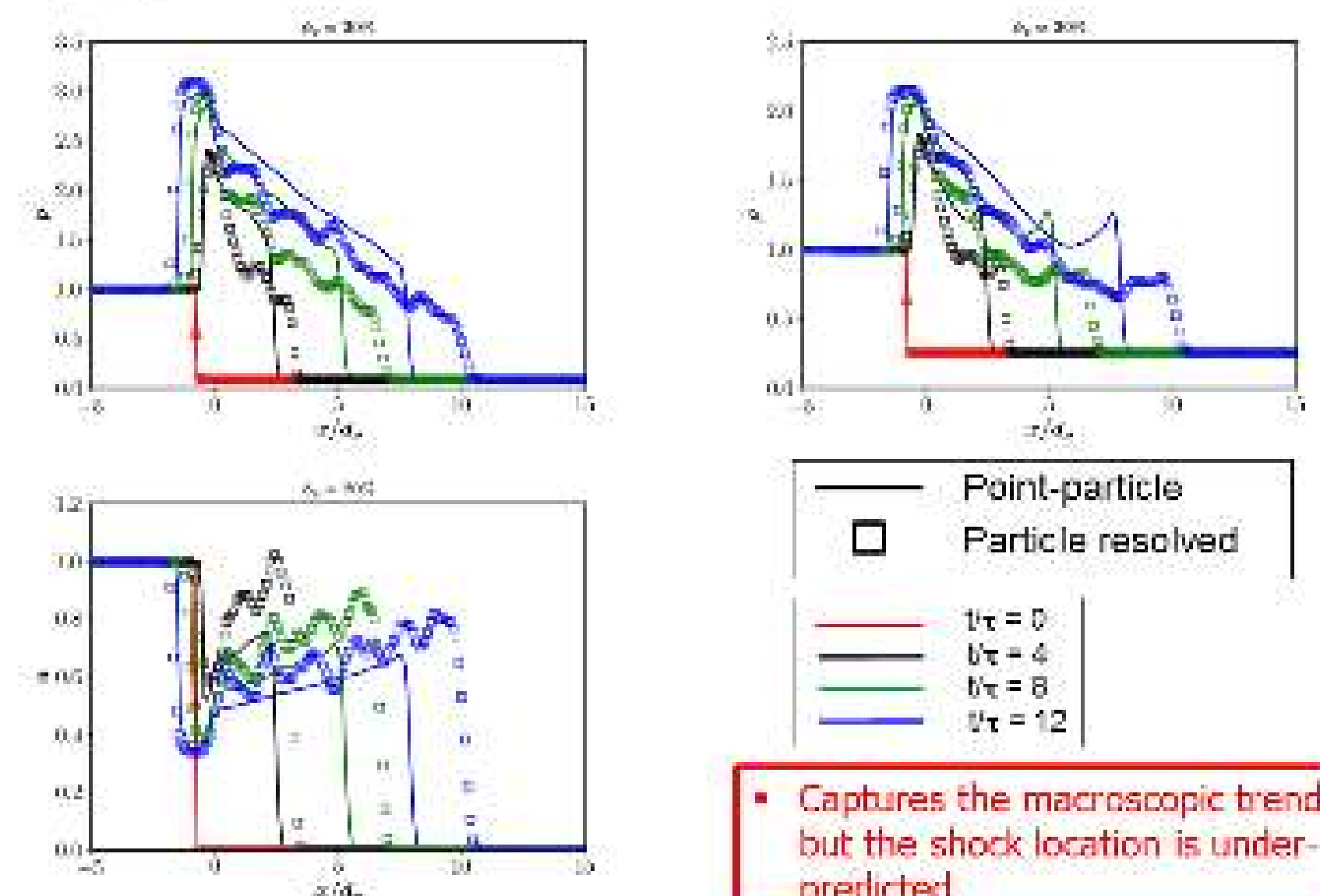
Results, $\phi_p = 10\%$...



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$\phi_p = 20\%$



• Captures the macroscopic trend but the shock location is under-predicted

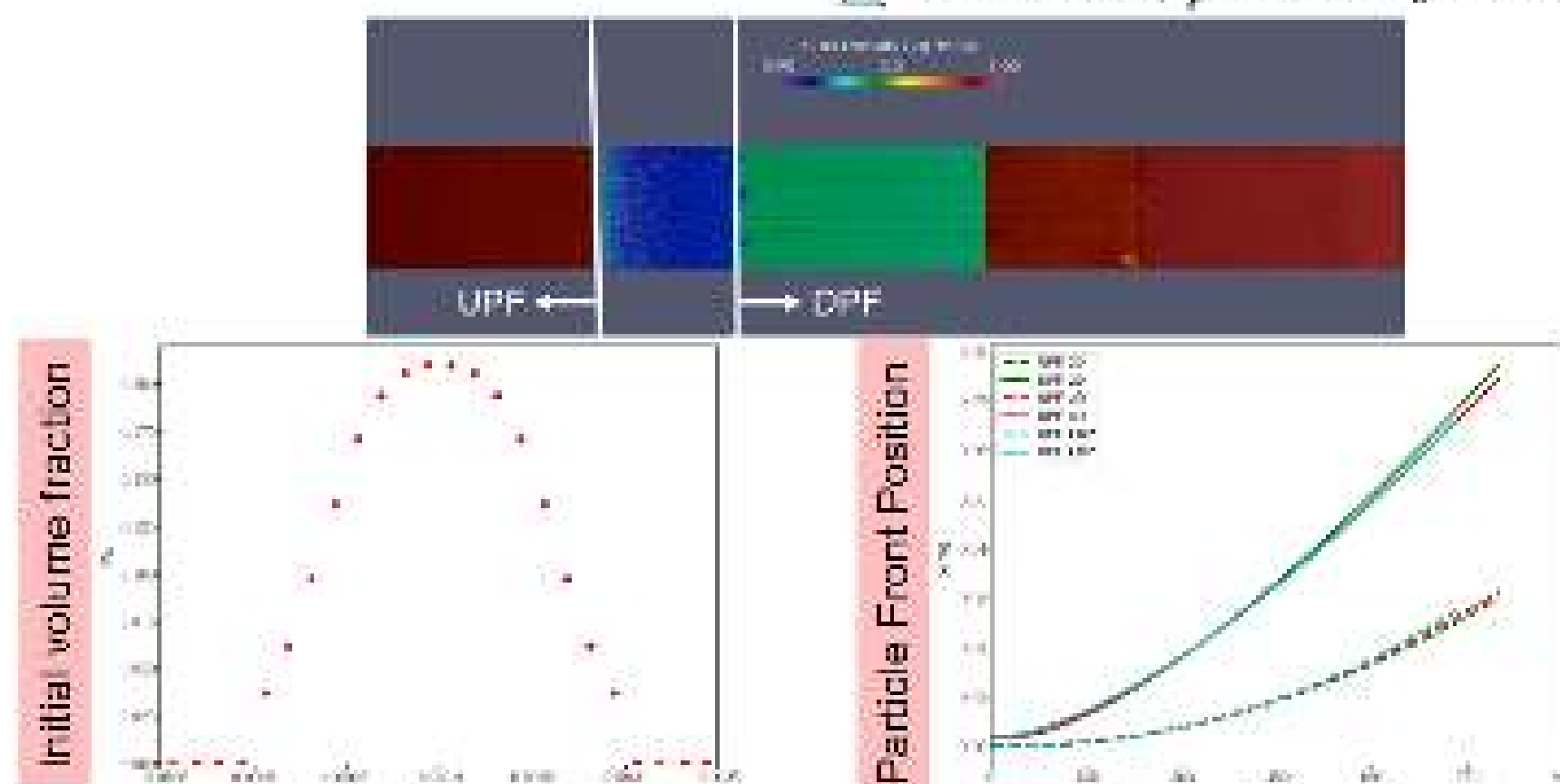
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4

Sandia MST Experiment

- Validation against experiments (Sandia MST)
- Effect of Initial particle volume fraction

$M=1.66$, $\phi_p=21\%$, $\delta_0=2mm$

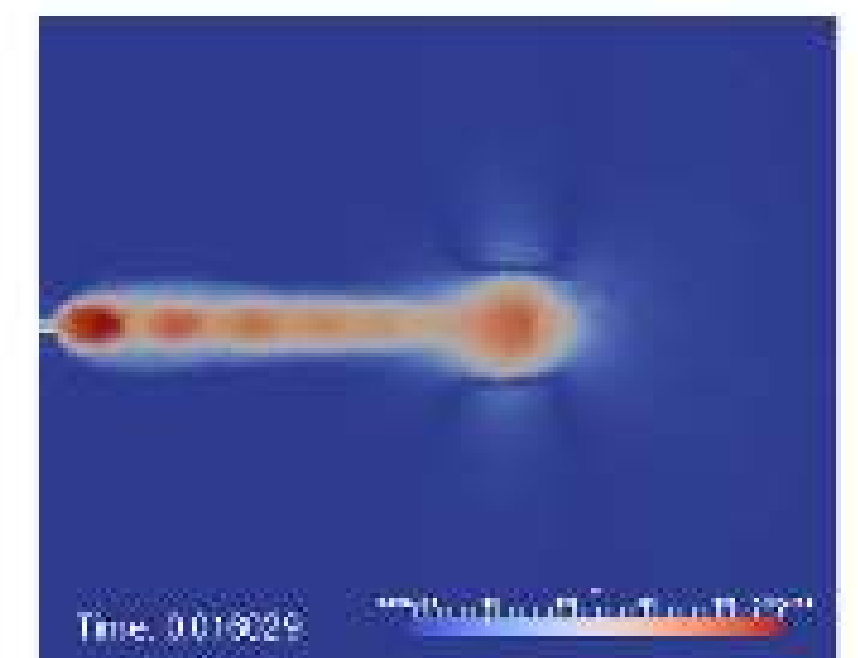
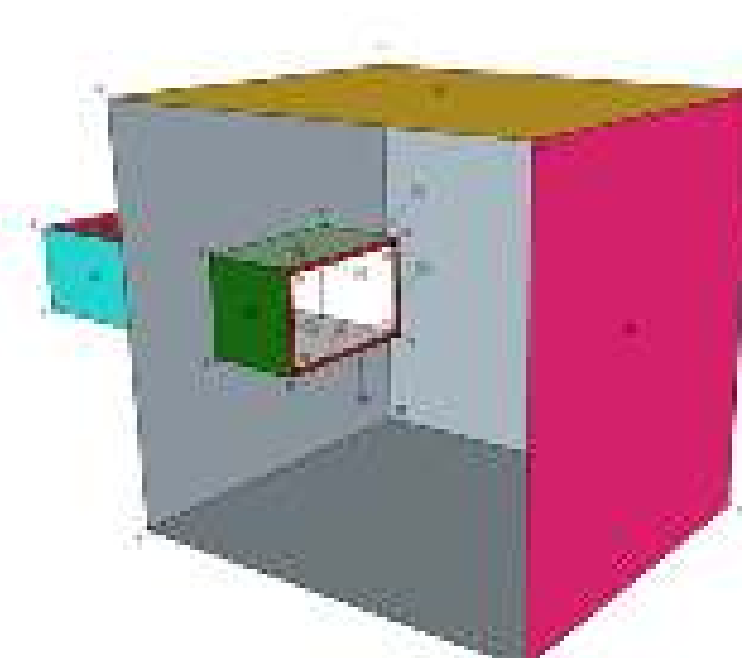


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5

Multiphase LES

- Performed simulations of single phase open-ended shocktube¹
- Integrated single-phase LES models in Rocflu
- Code verification and validation is in progress



¹ "Open Ended Shock Tube Flows: Influence of Pressure Ratio and Diaphragm Position", A. Haselbacher, S. Balachandrar and S. W. Keller, *AIAA Journal*

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CMT-nek Microscale Simulations

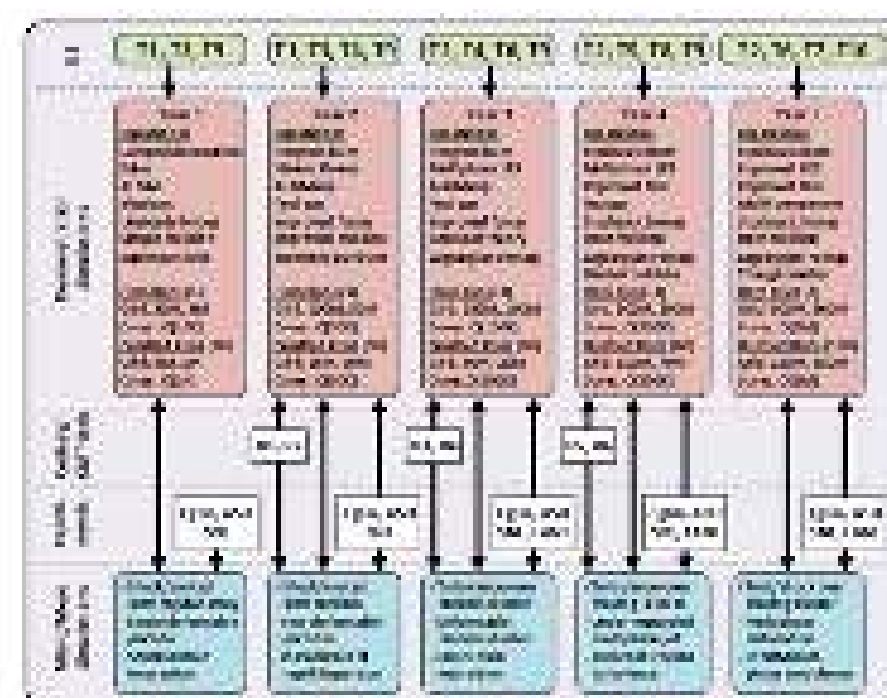
Goran Marjanovic

Advisor: Prof. Balachandar

Department: Mechanical & Aerospace Engineering, UF

Goals

- Demonstrate CMT-nek capabilities
- Validation
- Verification
- Simulation roadmap
 - Expansion wave propagating over particle beds



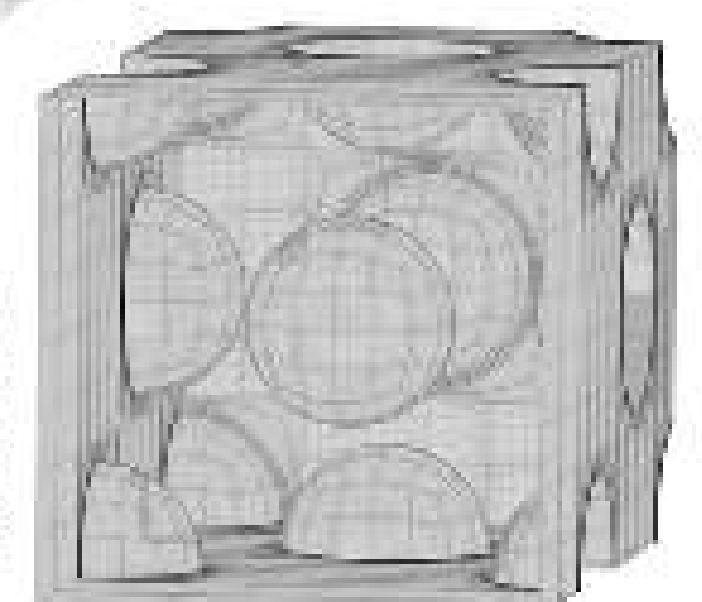
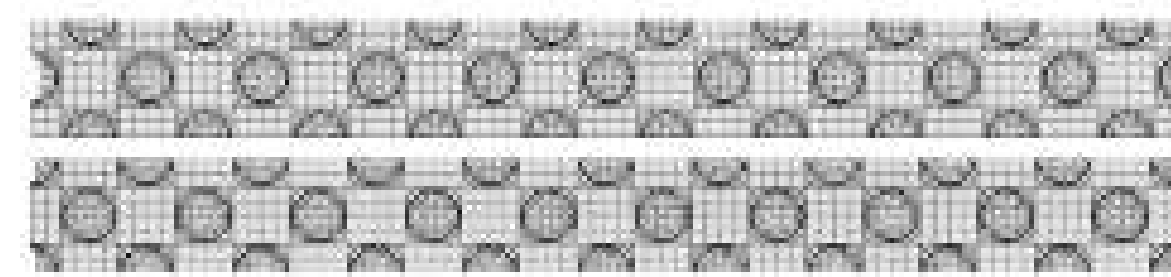
Simulation Roadmap

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Simulation Set-Up

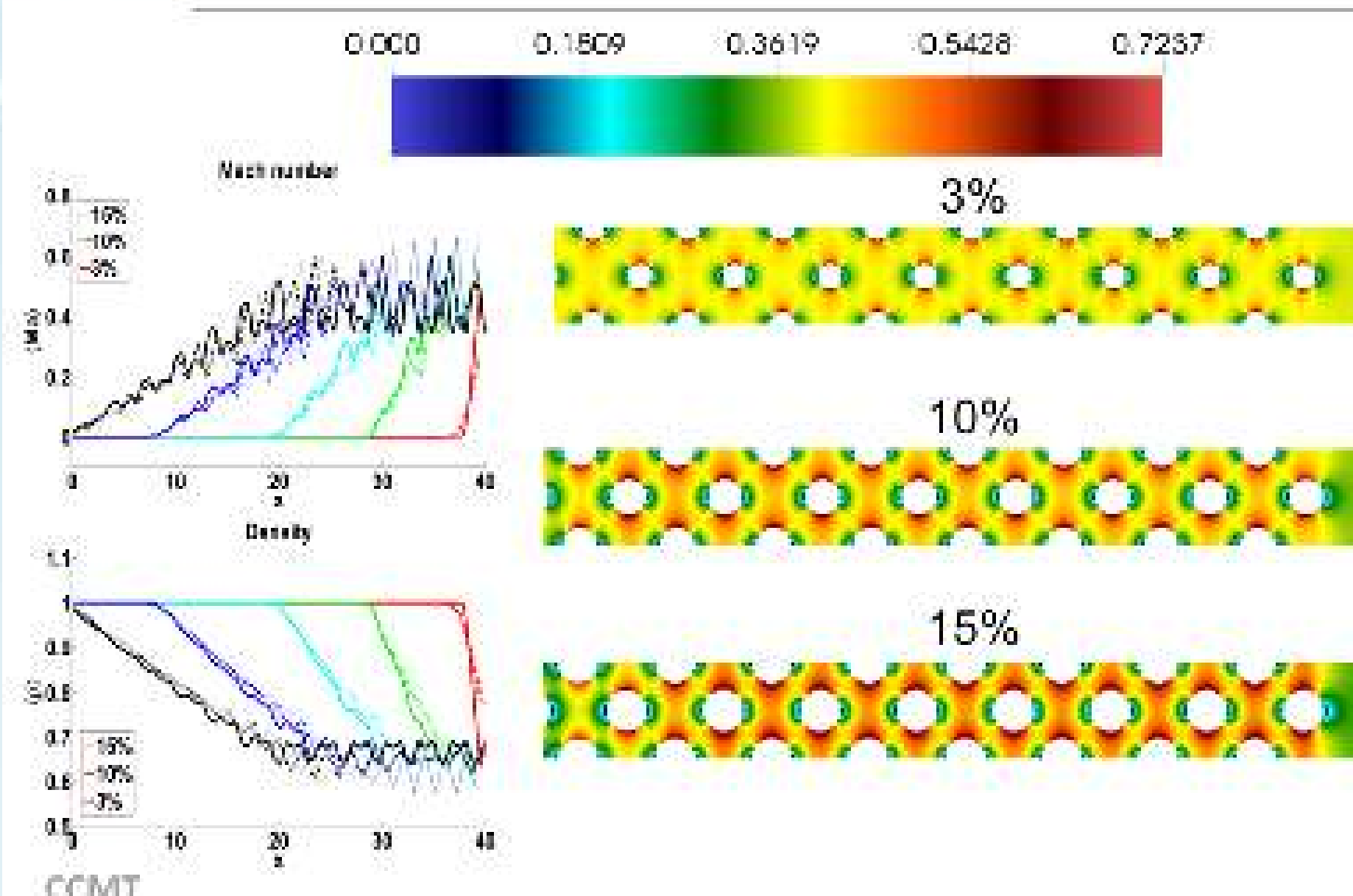
Volume Fractions	3%, 10%, 15%
Dimensions	126 x 4 x 4
Elements	29568
Polynomial order	12
DOF	64,960,896
Particle DOF	52,728-210,912
Pressure ratio	4.85
Head Mach number	0.4
Number of particles (obj)	95

- Particles are frozen in space (porous media)
- Inviscid



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Results – Mach Number

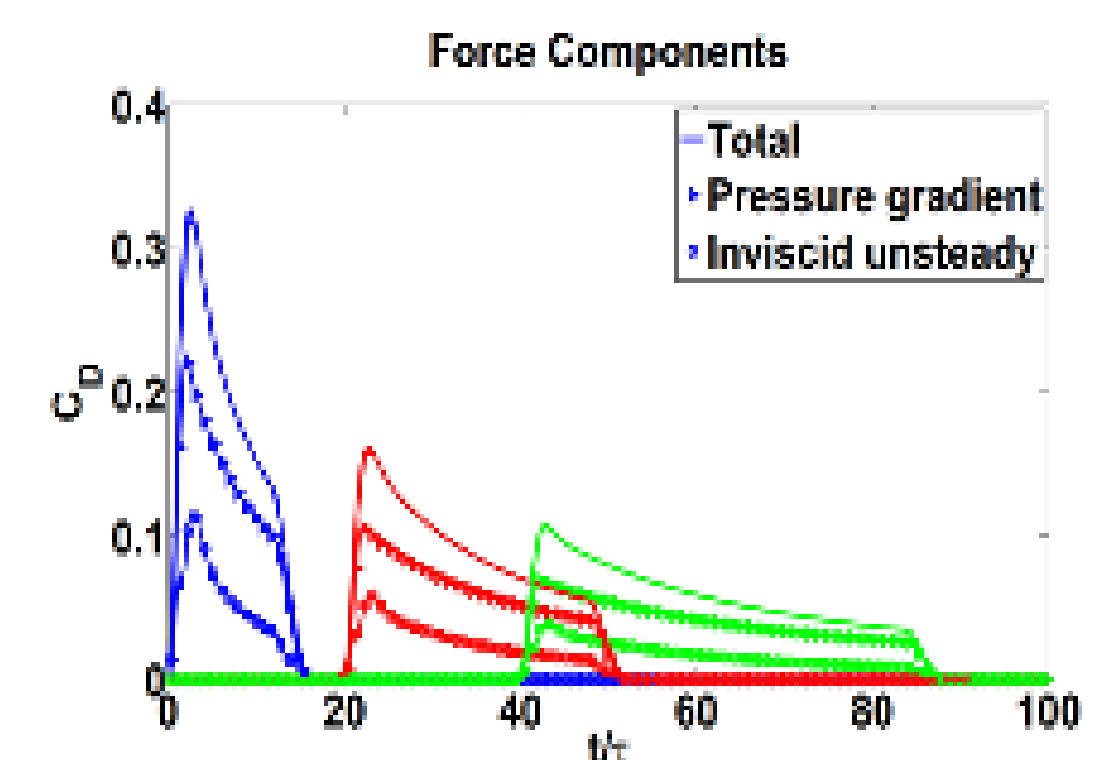


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Results – Drag Model

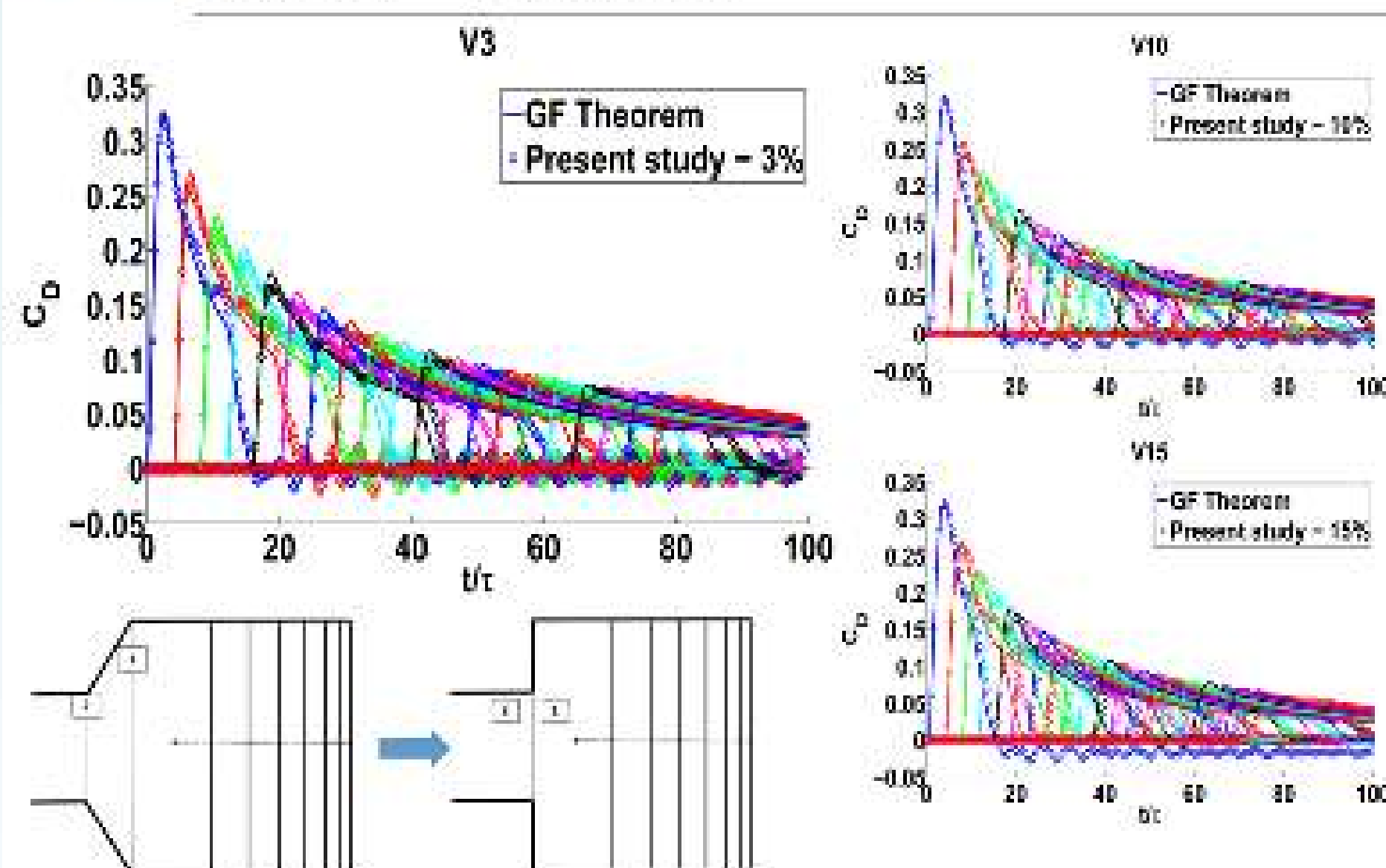
$$\mathbf{F}^{GF}(t) = \frac{4}{3}\pi R^3 \rho^{un} \frac{D\mathbf{u}^{un}}{Dt} + 4\pi R^3 \int_{\xi=-\infty}^t K_{in}(\bar{t} - \xi; M) \left[\frac{D}{Dt} (\rho \mathbf{u}_r)^{un} \right]_{t=\xi} d\xi$$

- Force models (single particle) for compressible flows
- Tested for shock-particle interaction
- Important feature
 - Better able to capture unsteady force effect
- Pressure gradient and inviscid unsteady forces



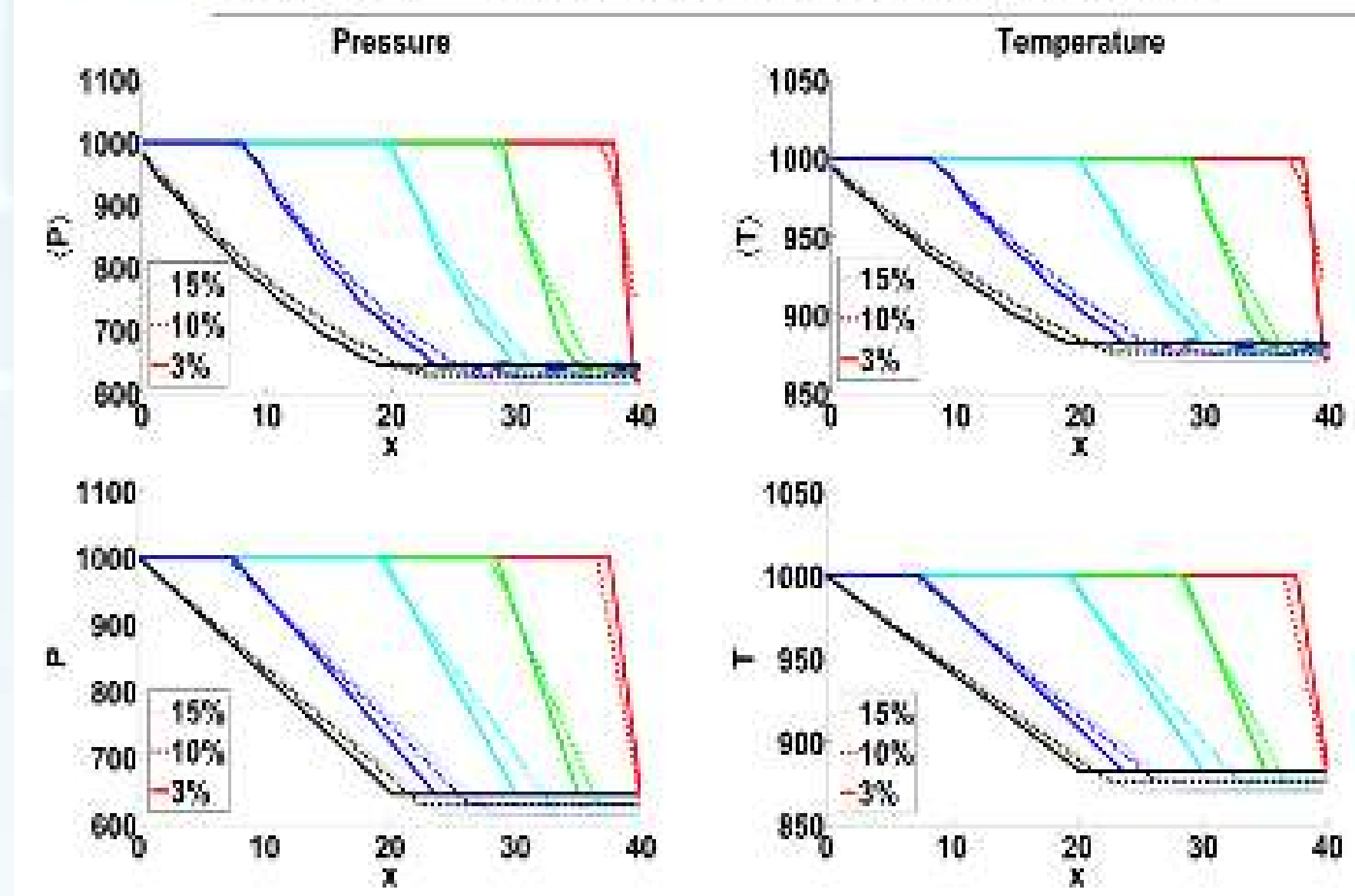
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Results – Drag Force



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Results – Pressure and Temperature



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Microscale – Shock Particle Interaction

Yash Mehta

Advisor: Prof. S. Balachander

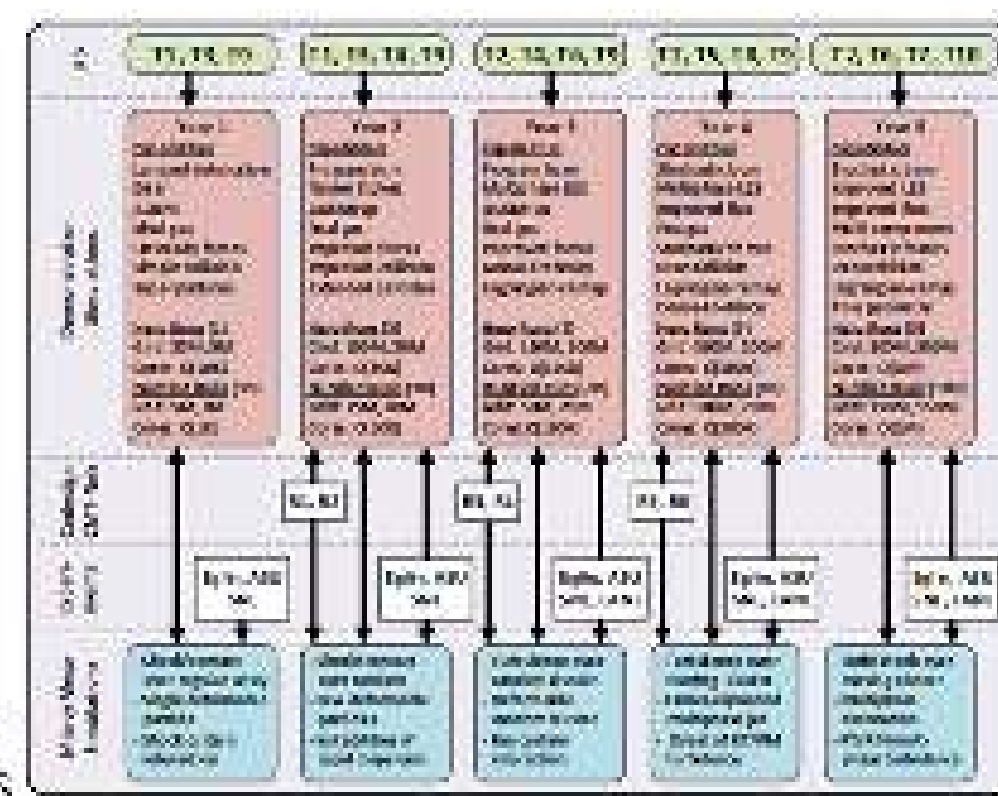
Department: MAE, UF

Goals

- Fully resolved DNS of shock interaction with particles
- Developing models for predicting particle motion and force history

Simulation roadmap

- Simulating shock interaction with random bed of particles
- Integration of force models in Meso-Macro scale simulations

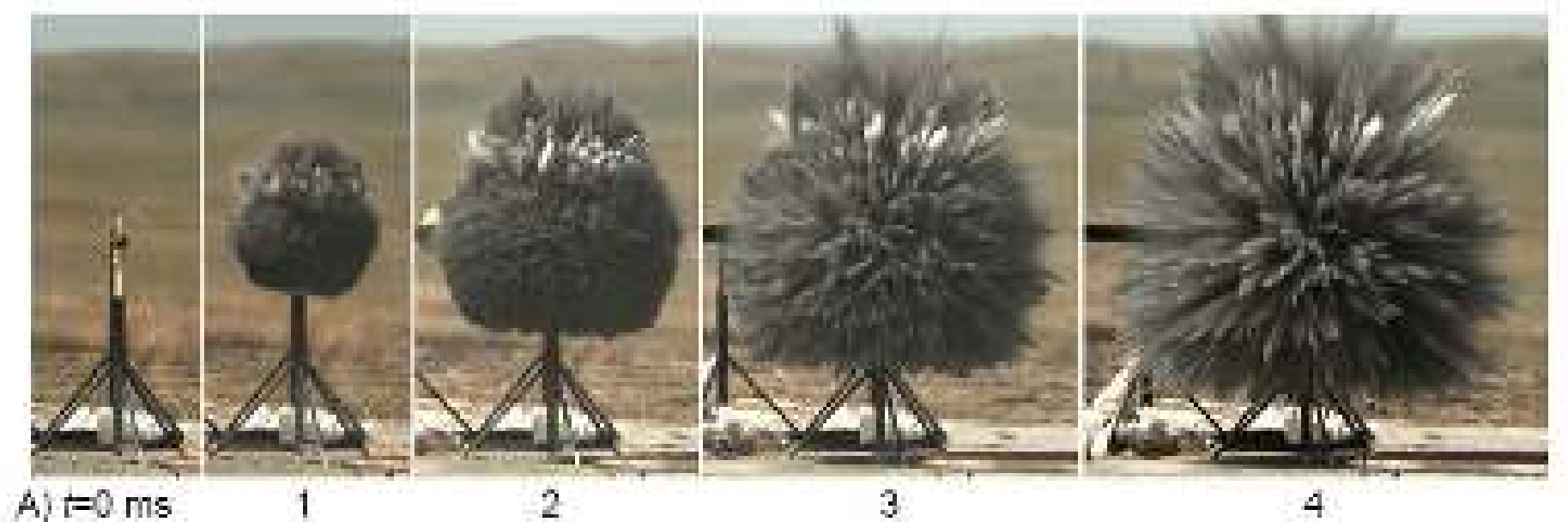


Simulation Roadmap

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1

Motivation

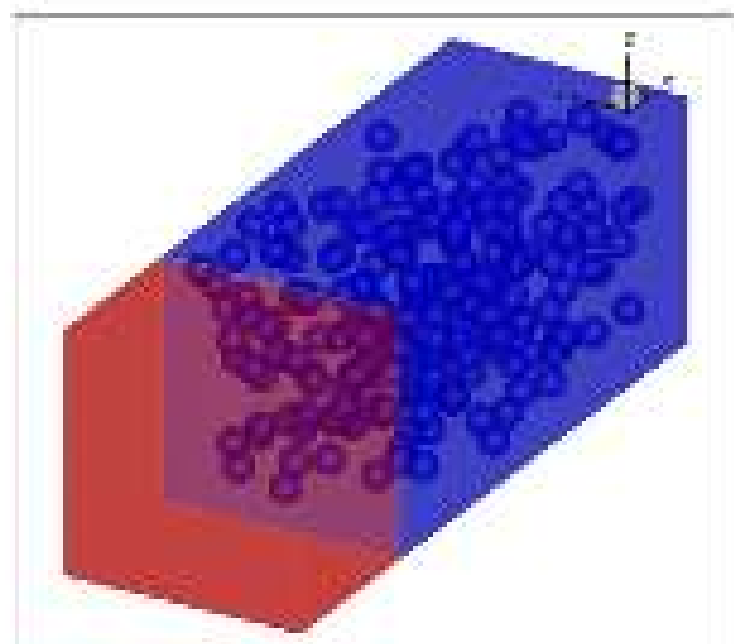


- There is a need for understanding the physics of high energy post detonation products interacting with particles
- Fully resolved inviscid numerical simulations are performed to understand the underlying physical mechanism at play during shock particle interaction
- Results from simulations are used to develop models for predicting the motion of particles in complex flows

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2

Shock interaction with random bed of particles



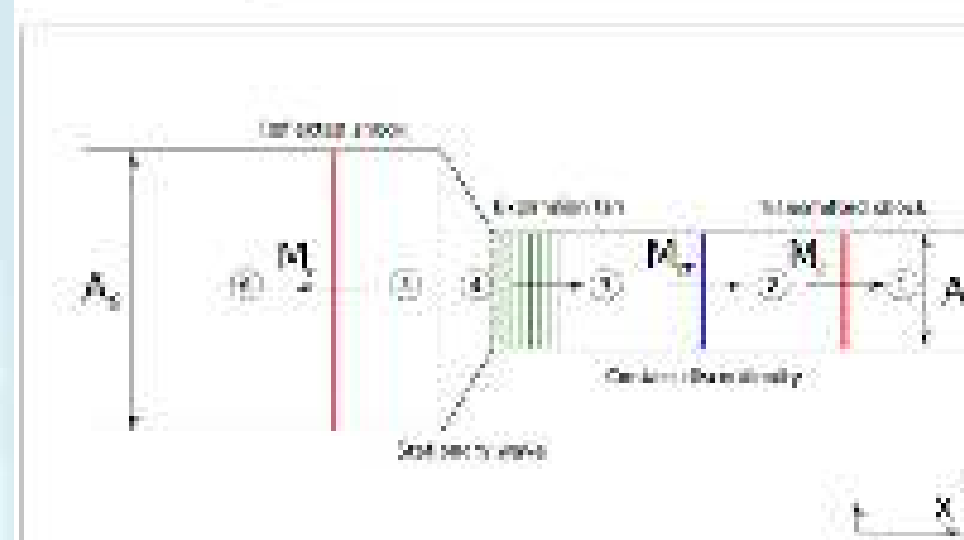
	$M_s = 1.22$	$M_s = 1.66$	$M_s = 3.00$
$\phi = 1.25\%$	RUN1	RUN2	RUN3
$\phi = 10\%$	RUN4	RUN5	RUN6
$\phi = 15\%$			RUN7
$\phi = 20\%$	RUN8	RUN9	RUN10
$\phi = 25\%$			RUN11

- Matrix of simulations were performed to understand the effect of shock Mach number and volume fraction
- Number of particles in the computational domain varied from 200 to 400
- Effect of viscosity and particle motion was neglected in these simulations

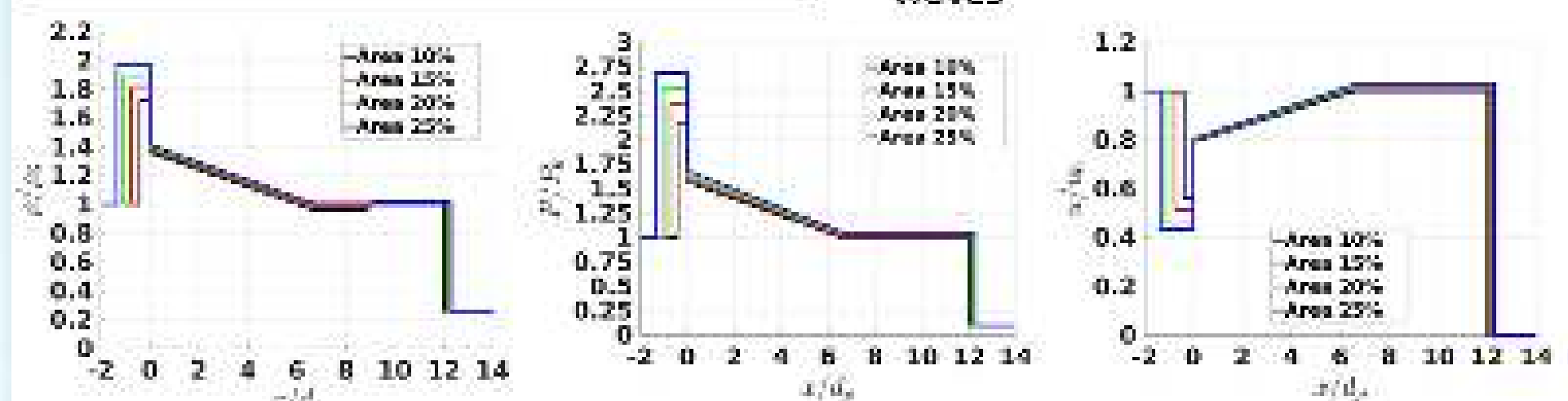
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3

1-D Riemann model



- Shock interaction with bed of particles can be modeled as shock interaction with an area change
- This is a standard Riemann problem with an area change
- Shock interaction with an area change leads to a unique solution with multiple different family of waves

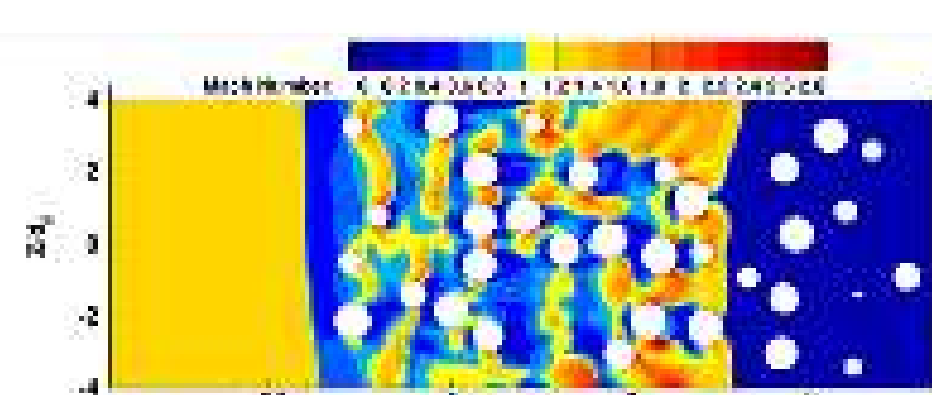


Flow properties predicted using 1-D Riemann model

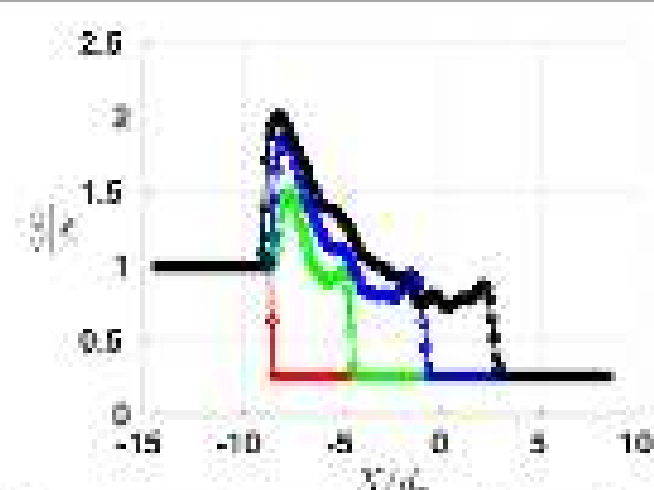
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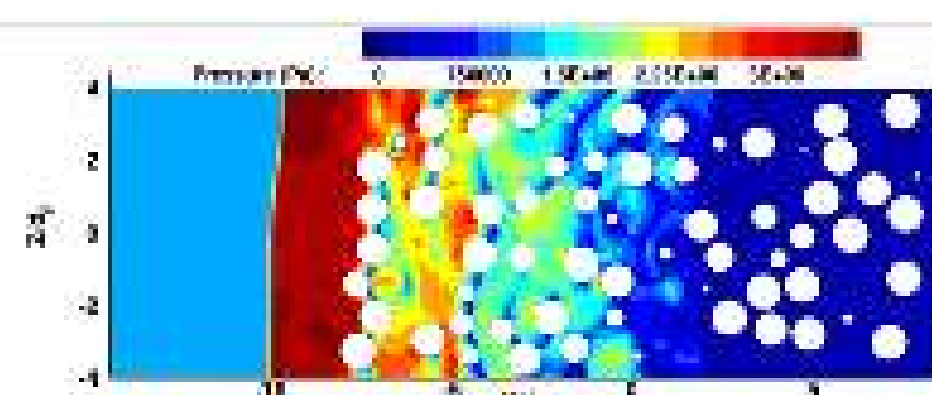
Flow properties



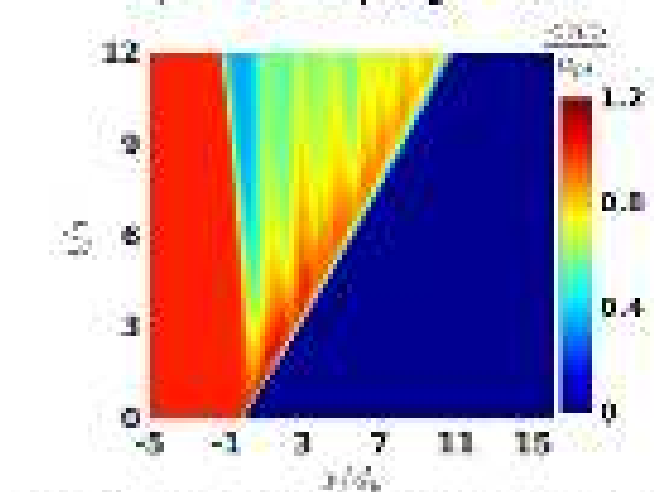
Mach number contour plot for $\phi = 10\%$; $M_s = 3.0$; $t/\tau = 12$



Stream-wise averaged density for $\phi = 15\%$; $M_s = 3.0$



Pressure contour plot for $\phi = 25\%$; $M_s = 3.0$; $t/\tau = 12$

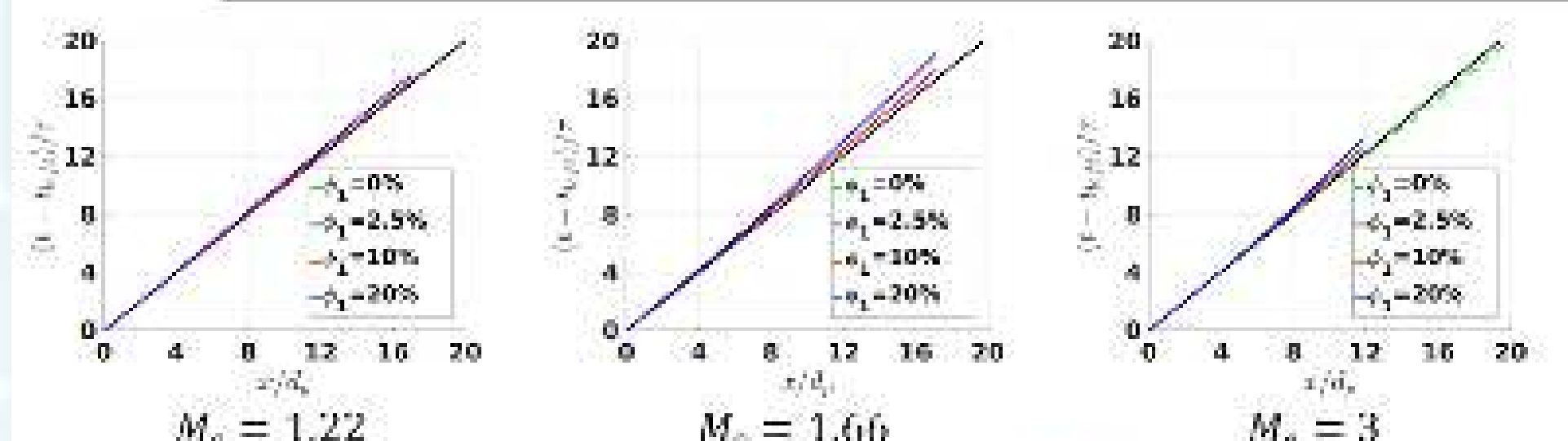


Stream-wise averaged velocity for $\phi = 20\%$; $M_s = 3.0$

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Slowing down of the transmitted shock



$M_s = 1.22$

$M_s = 1.66$

$M_s = 3$



Iso-surface of velocity magnitude

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Data-driven Point-Particle Force Modeling

W. Chandler Moore

Advisor: Prof. Balachandar

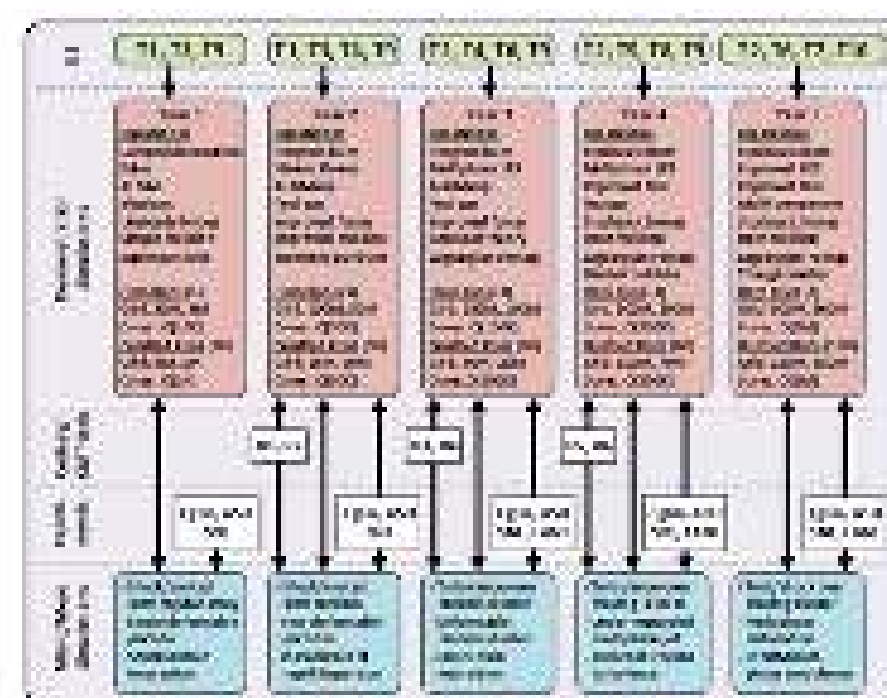
Department: MAE, UF

Goals

- Test the PIEP model at high volume fractions
- Improve the PIEP model using DNS data

Simulation roadmap

- This work uses data from microscale simulations to improve force models which bridge the gap between microscale simulations and the demonstration simulations.



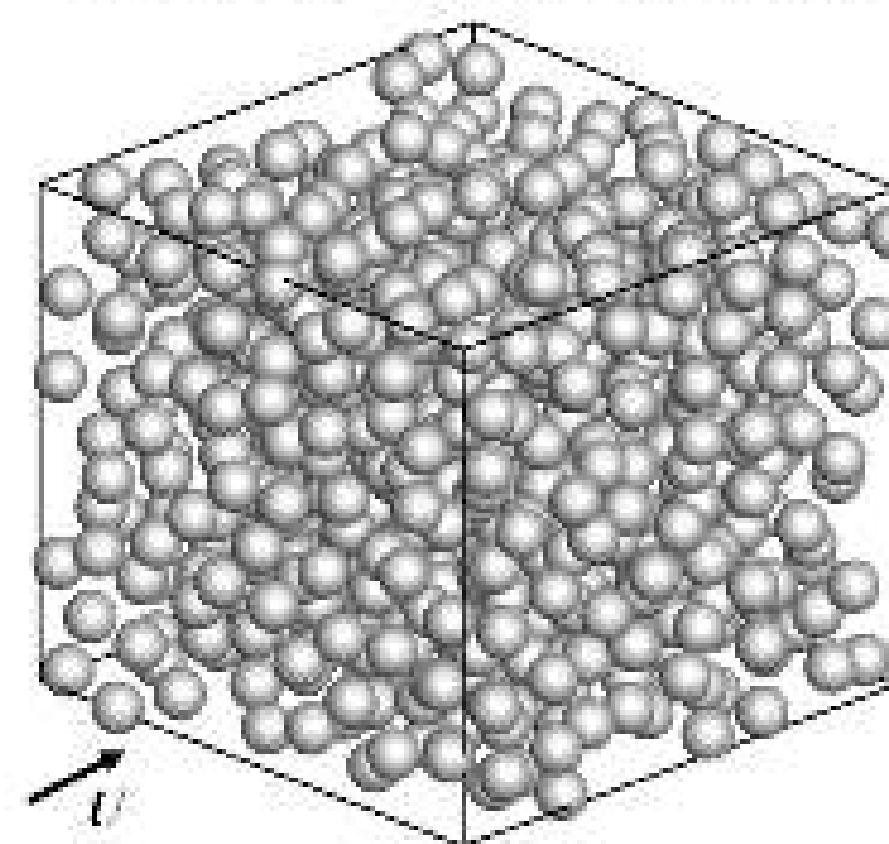
Simulation Roadmap

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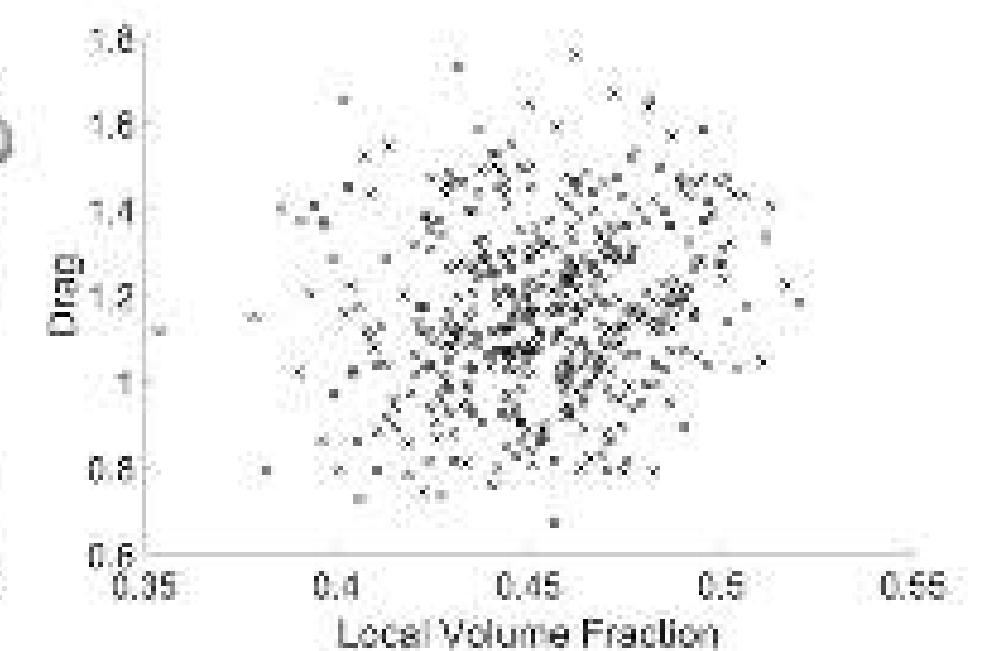
1

Motivation

Mean drag point-particle models are not sufficient for predicting microscale fluid mediated particle-particle interactions.



$\phi = 44\%, Re = 20, N = 459$



Drag law given by Tenneti et al. (2011)

$$\frac{F_D}{F_{Sto}} = f(Re, \phi) = \frac{1 + 0.15Re^{0.687}}{(1 - \phi)^3} + \dots$$

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2

PIEP Model at High Volume Fractions

The pairwise-interaction extended point-particle model loses accuracy at high volume fractions.

$$R^2 = 1 - \frac{\sum_{n=1}^{N_s} [F_{PIEP}(r_n) - F_{DNS}(r_n)]^2}{\sum_{n=1}^{N_s} [F_{DNS}(r_n) - \langle F_{DNS} \rangle]^2}$$

Case	Lift Force R^2 (DNS vs PIEP)
$\phi = 0.1, Re = 40$	0.67
$\phi = 0.2, Re = 16$	0.34
$\phi = 0.45, Re = 20$	0.09

To improve the PIEP model, introduce a data driven $F_{\phi,C}$ term.

$$F_{PIEP,Hybrid} = F_{PIEP} + F_{\phi,C}$$

$$T_{PIEP,Hybrid} = T_{PIEP} + T_{\phi,C}$$

where

$$F_{\phi,C} \equiv F_{\phi,C}(Re, \phi, r_1, r_2, \dots, r_N)$$

$$T_{\phi,C} \equiv T_{\phi,C}(Re, \phi, r_1, r_2, \dots, r_N)$$

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3

Postulated Functional Form

Postulated scalar functions for the drag (D), lift (L), and torque (T) due to a single neighbor:

$$D_{PIEP-data}(r_n, r_1 | Re, \phi) = \left(\sum_{m=1}^M \sum_{l=0}^L [a_{lm} \hat{r}_l(k_{lm} r) + b_{lm} \hat{r}_l(q_{lm} r)] Y_{lm}(\psi) \right) H(r)$$

$$L_{PIEP-data}(r_n, r_1 | Re, \phi) = \left(\sum_{m=1}^M \sum_{l=0}^L [c_{lm} \hat{r}_l(k_{lm} r) + d_{lm} \hat{r}_l(q_{lm} r)] Y_{lm}(\psi) \right) H(r)$$

$$T_{PIEP-data}(r_n, r_1 | Re, \phi) = \left(\sum_{m=1}^M \sum_{l=0}^L [e_{lm} \hat{r}_l(k_{lm} r) + f_{lm} \hat{r}_l(q_{lm} r)] Y_{lm}(\psi) \right) H(r)$$

Where j and n are the spherical Bessel and Neumann functions and

$$\psi = \tan^{-1}(r_1/r_2) \quad Y_{20}(\psi) = \sqrt{\frac{5}{4\pi}} P_2(\cos \psi) \quad \frac{\partial \hat{r}_l(k_{lm} r)}{\partial r} = 0 \quad \text{and} \quad \frac{\partial \hat{r}_l(q_{lm} r)}{\partial r} = 0$$

$a_{lm}, b_{lm}, \dots$ and f_{lm} make up the array of parameters to be determined by regression. M , and L are the hyper parameters that must be optimized using a second data set.

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4

Prediction Results

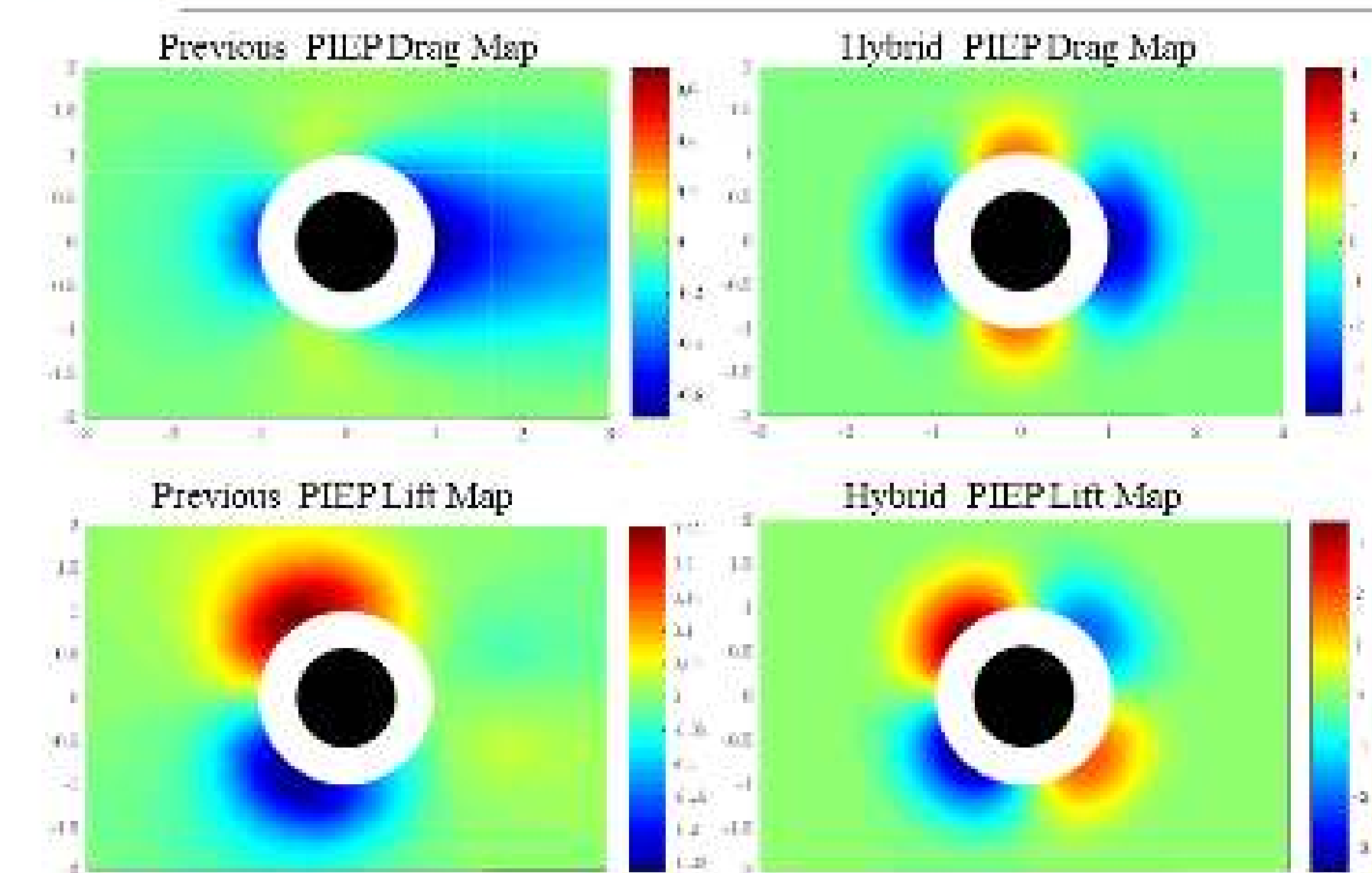
Results from testing data set:

R ² Values:		Previous PIEP			Hybrid/Data-Driven PIEP		
ϕ	Re	Drag	Lift	Torque	Drag	Lift	Torque
0.1	40	0.66	0.67	0.75	0.66	0.73	0.80
0.1	70	0.61	0.67	0.65	0.62	0.70	0.72
0.1	173	0.33	0.55	0.45	0.43	0.58	0.60
0.2	16	0.51	0.34	0.48	0.74	0.75	0.72
0.2	89	0.60	0.48	0.72	0.73	0.62	0.78
0.45	20	0.12	0.09	0.47	0.64	0.59	0.76
0.45	115	0.24	0.19	0.51	0.67	0.57	0.65

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Resulting Force Maps ($\phi = 0.45$ & $Re = 20$)



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Center for Compressible Multiphase Turbulence

Multi-fidelity Surrogate Modeling for Co-design

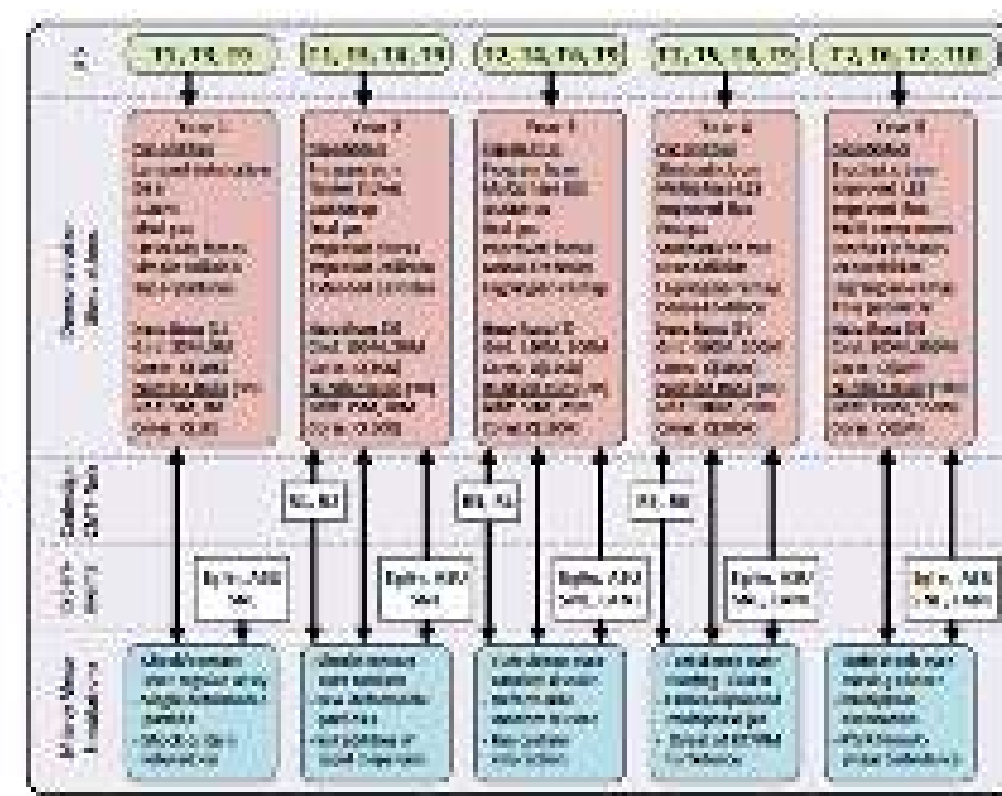
Aravind Neelakantan
Advisor: Dr. Lam, Dr. Stitt
Department: ECE, UF

Goals

- Reduce computational budget of HPC codes (parent app)
- Low-cost model validation over larger design space
- Extrapolation of parent app towards large scale run

Simulation roadmap

- MFS and BE helps in simulating CMT-nek on exascale systems (notional architectures)



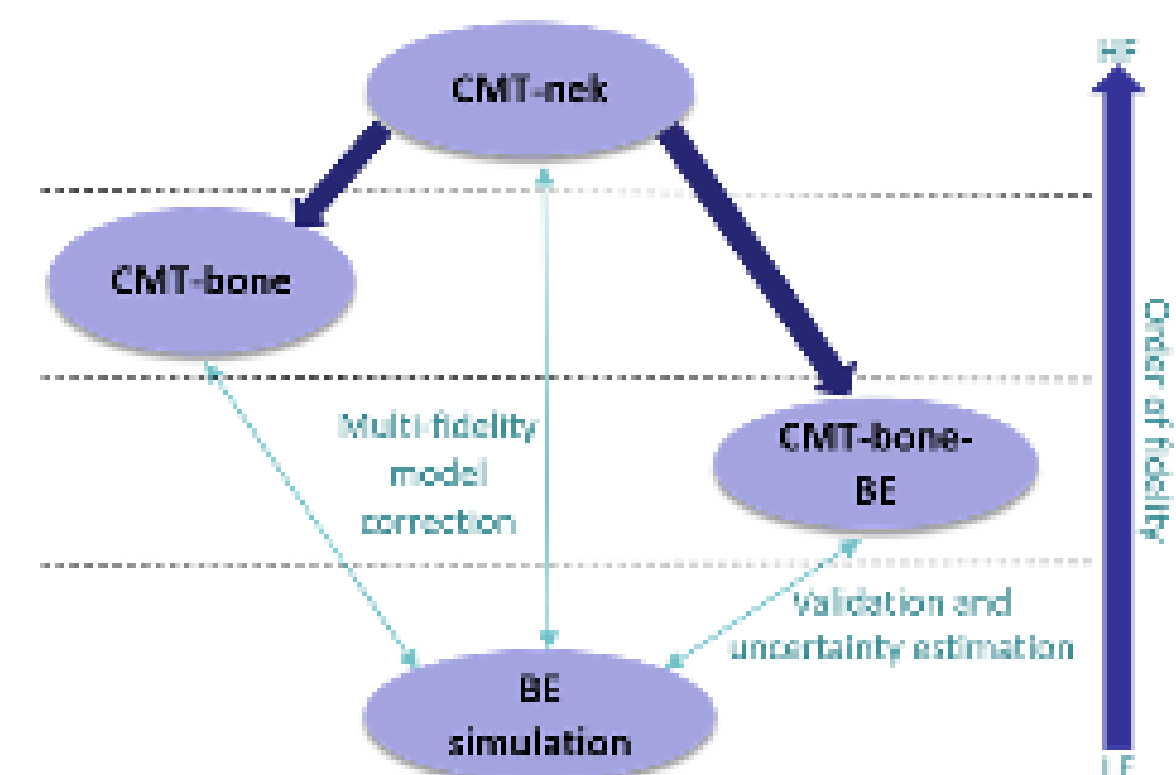
Simulation Roadmap

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Behavioral Emulation with MFS

Objective

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



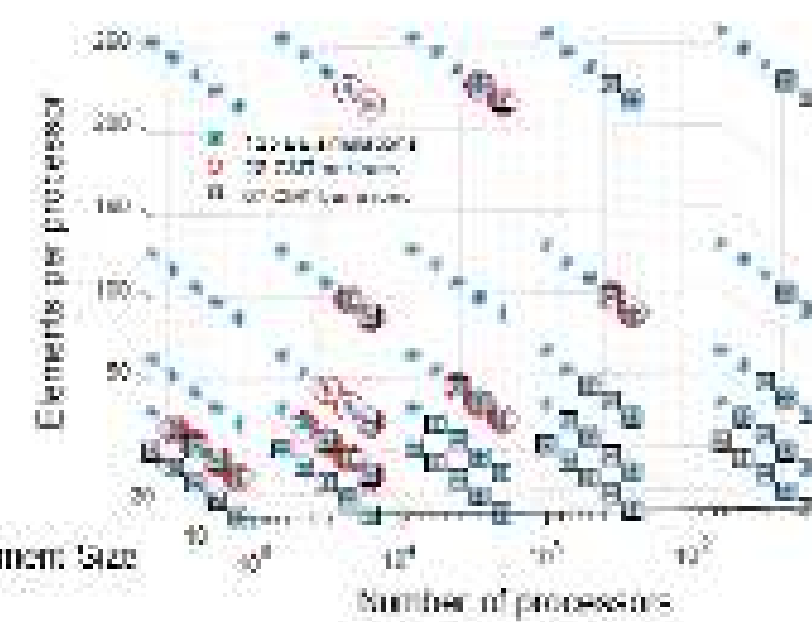
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Developing MFS: Experimental setup

- Design of experiment (DOE)
 - Element size (ES) = 5,9,13,17,21
 - Elements per processor (EPP) = 8,32,64,128,256
 - Number of processors (NP) = 16,256,2048,16384,131072

125 total data points

- BE simulation: all 125 runs
- CMT-nek: 22 runs
- CMT-bone: 67 runs



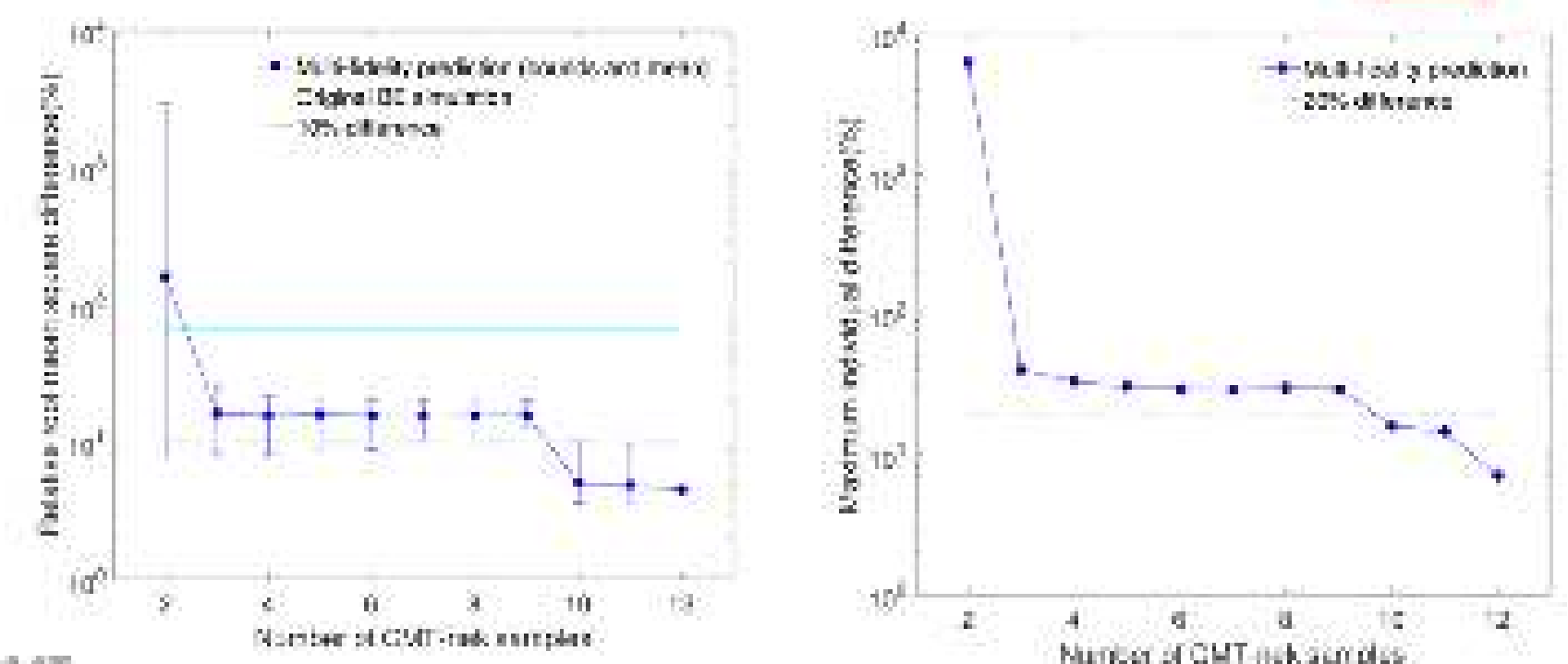
Multi-fidelity surrogate model

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

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MFS: CMT-nek (HF) vs BE simulation (LF)

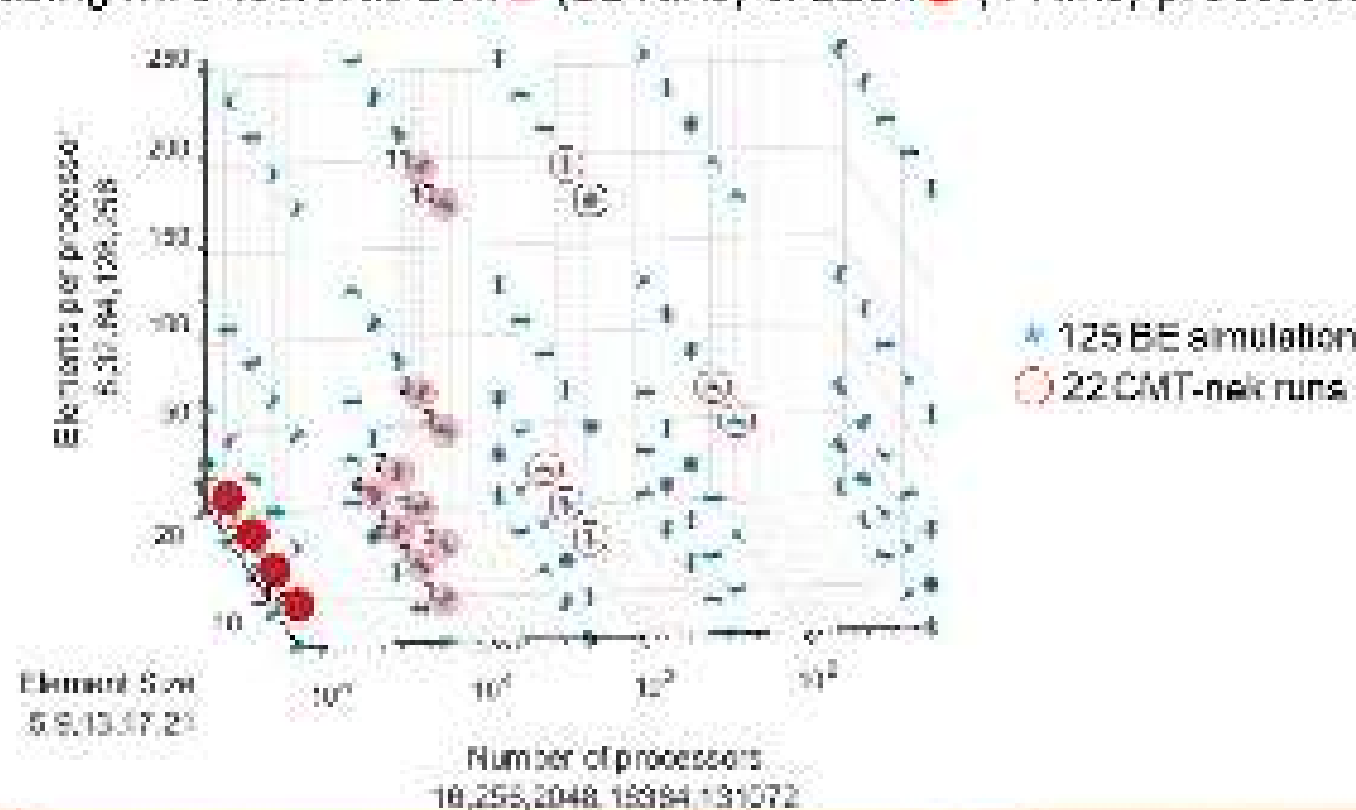
- Accuracy of corrected BE simulation at 10 left-out CMT-nek test points
 - Overall error (RMSE) is less than 8% with 10 or more nek data (left figure)
 - Max error is less than 15% with 10 or more CMT-nek data (right figure)



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Extrapolation Towards Large-scale Runs

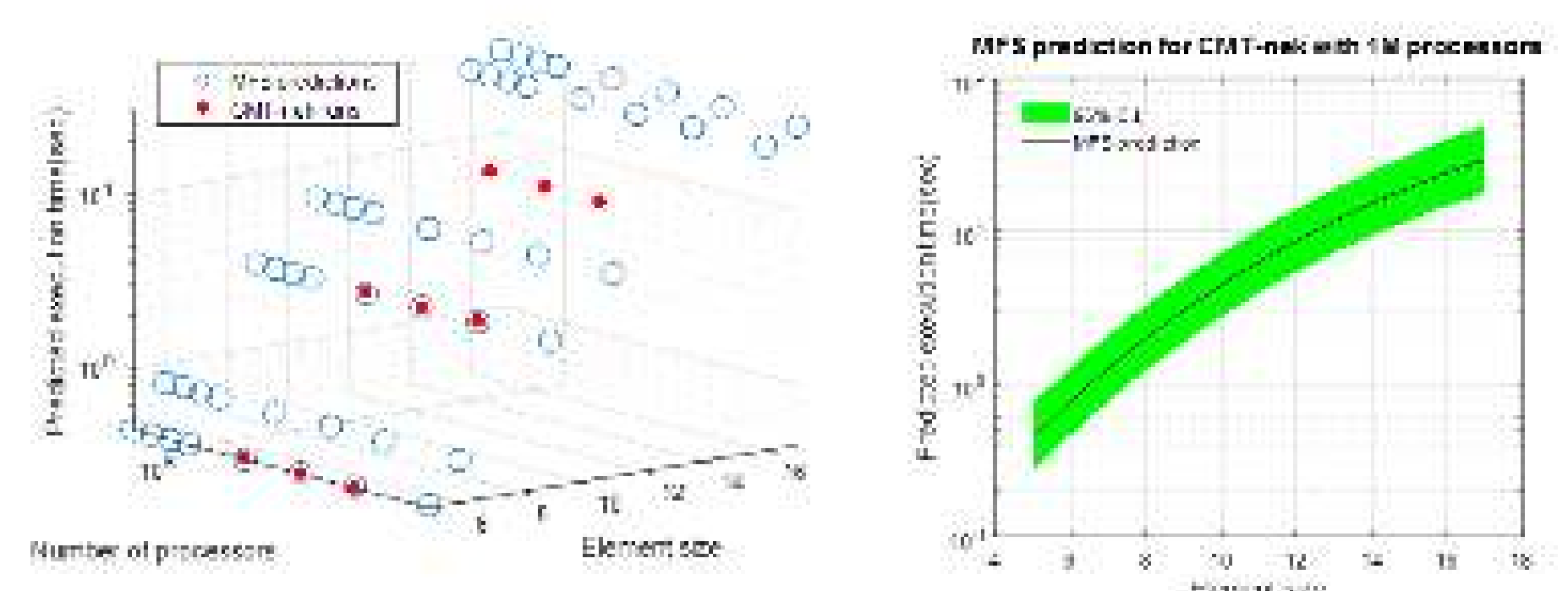
- Extrapolation necessary for exascale prediction
 - But challenging due to limited runs
- Develop MFS using:
 - 7 (out of 22) runs of CMT-nek (high-fidelity), at 256 and 2k processors
 - All 125 BE simulations (low-fidelity)
- Extrapolate using MFS towards 16k (11 runs) & 128k (4 runs) processors



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Extrapolation: Prediction of CMT-nek

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



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Discretization Error in Euler-Lagrange Simulation

Samaun Nili

Advisor: Prof. Kim, Haftka & Balachandar

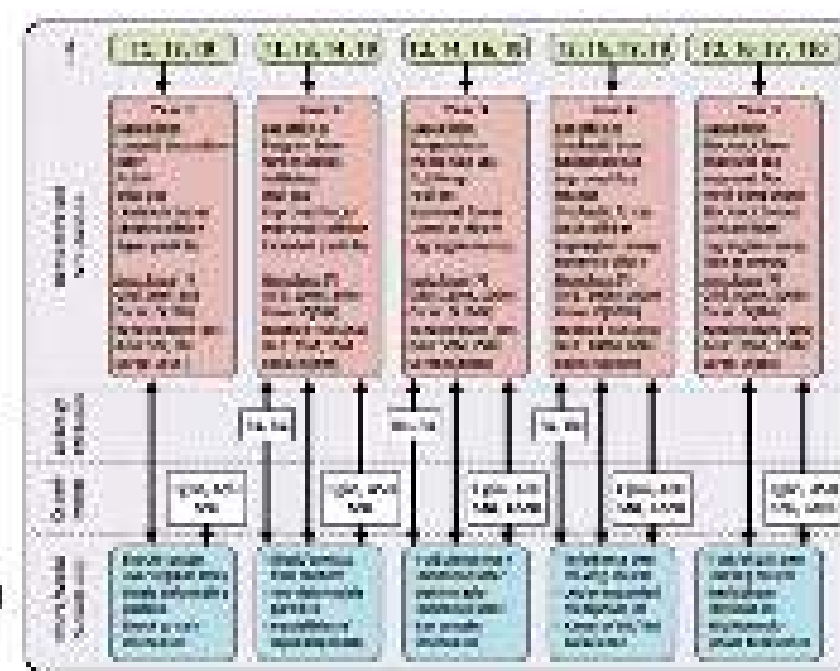
Department: MAE, UF

Goals

- To estimate the discretization error in a 1D Euler-Lagrange simulation of an interaction between the shock wave and particle-laden
- To achieve mesh convergence for 1D shock particle-laden interaction problem via model implementation improvement

Simulation roadmap

- T4: Verification and validation of the shock tube simulation
- Uncertainty reduction via model implementation improvement



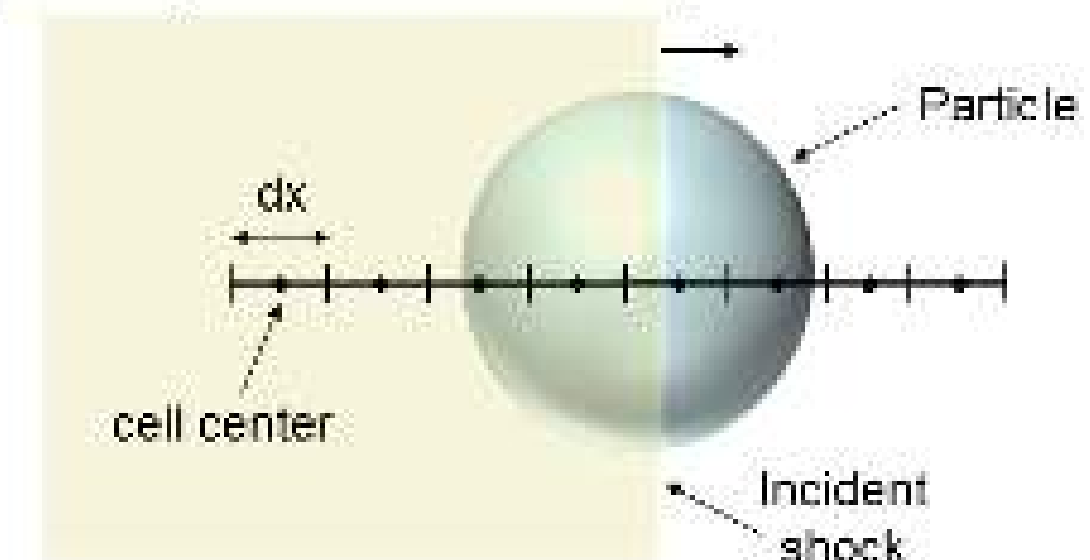
Simulation Roadmap

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1

Challenge in Point Particle Model

- Standard Euler-Lagrange point particle methods fail to provide grid-independent predictions for the interphase momentum exchange

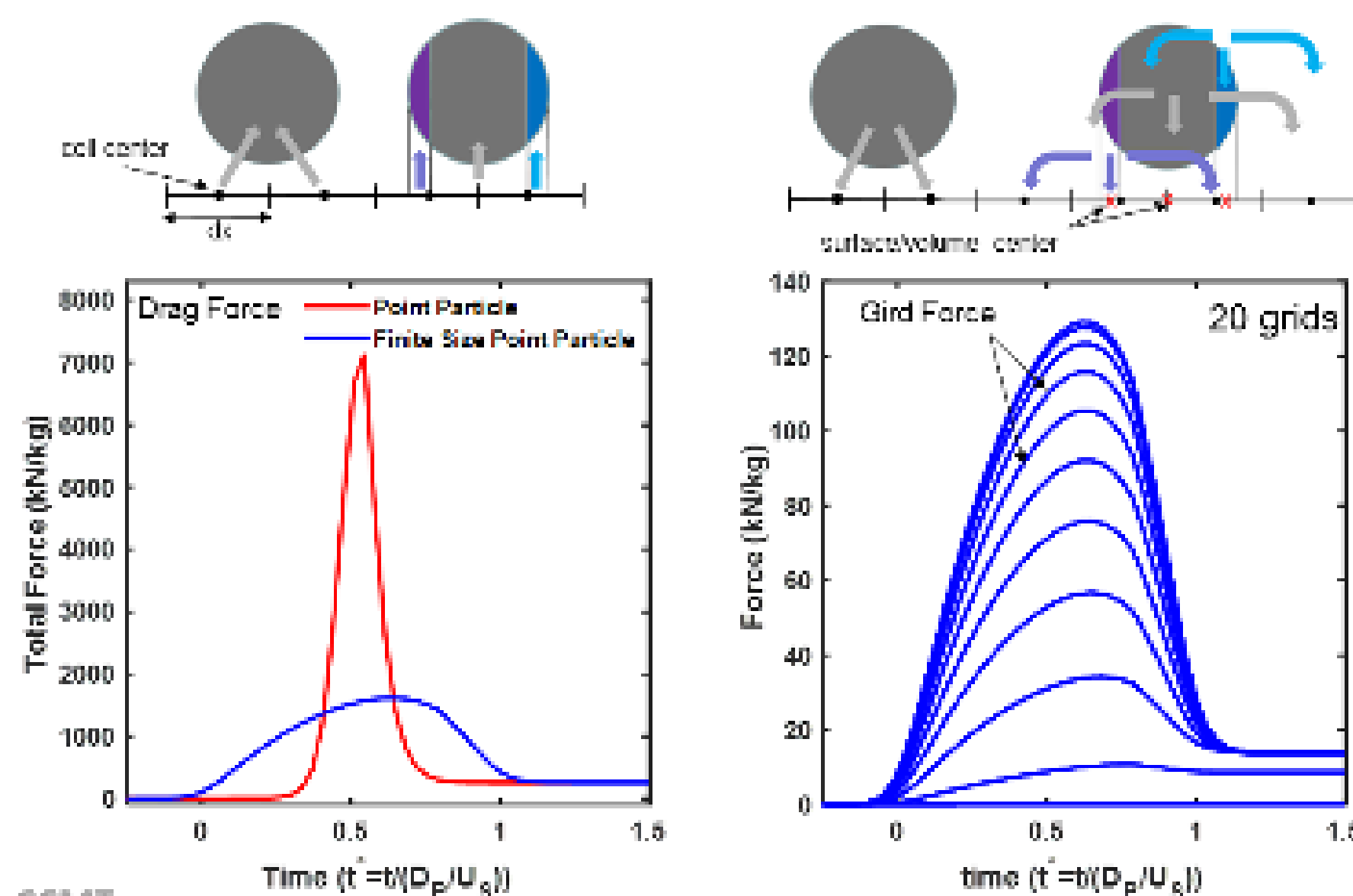


- The particle feels the shock only if the shock reaches to the cell where particle center is located
- Since particle diameter is larger than grid size, it causes an unrealistic sudden change in the particle force
- The peak force increases as we reduce the grid size

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2

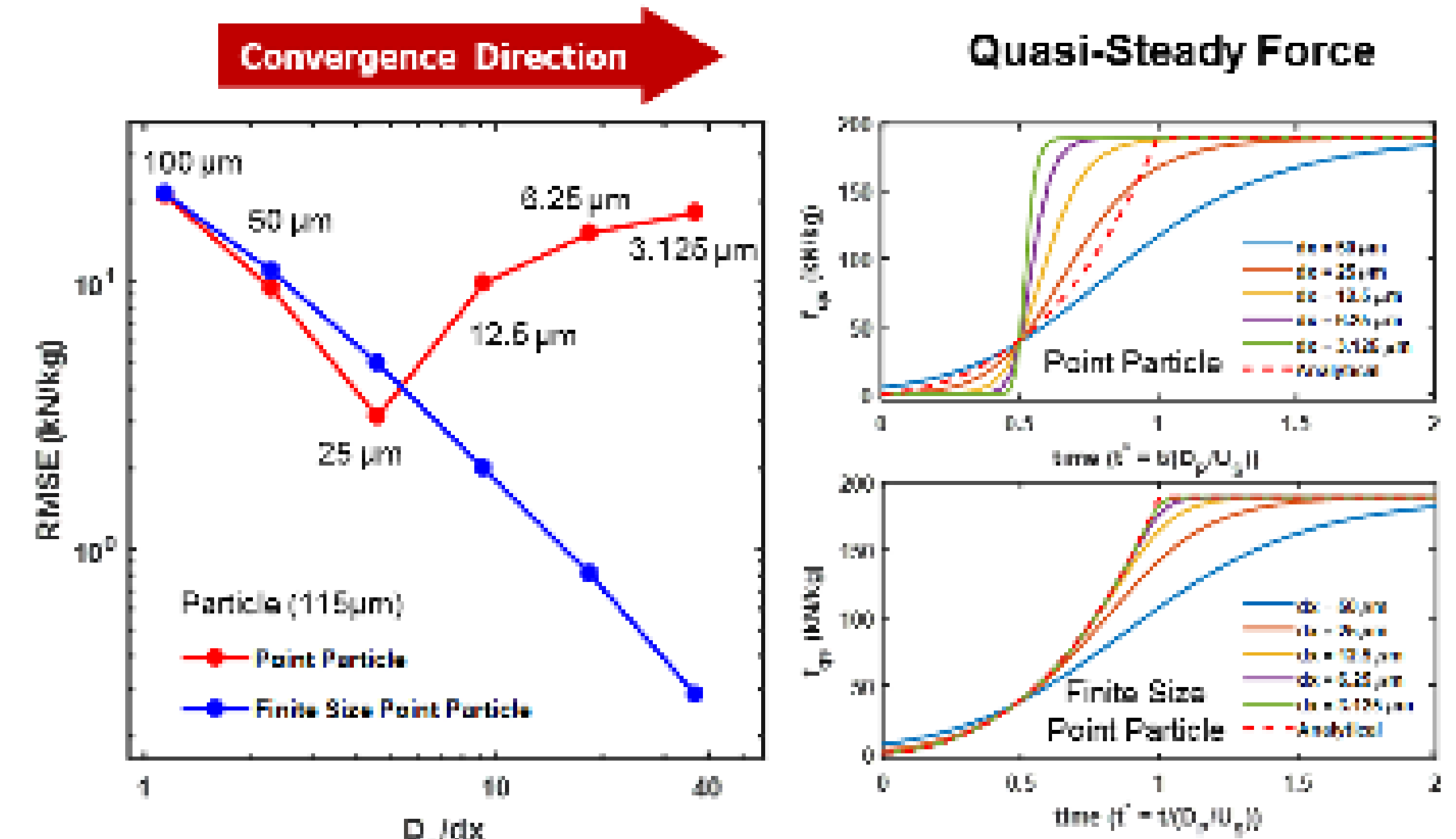
Finite Size Particle vs. Point Particle



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3

Quasi-Steady Force Convergence

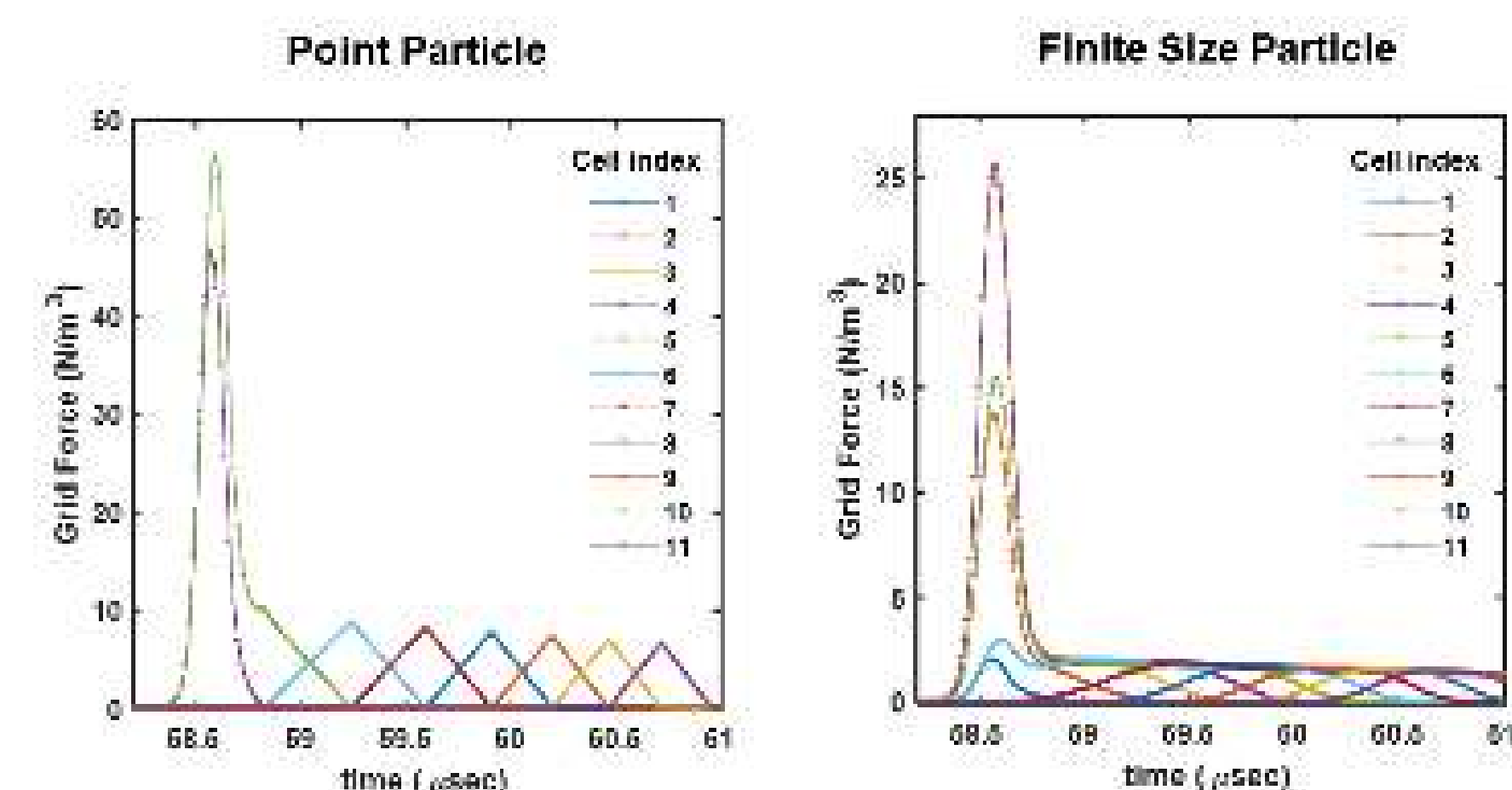


Root Mean Square Error (RMSE) between the numerical and analytical solution over the time for different grid resolution

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4

Projected Force for a Moving Particle



$dx = 25 \mu m$, $D_p = 115 \mu m$

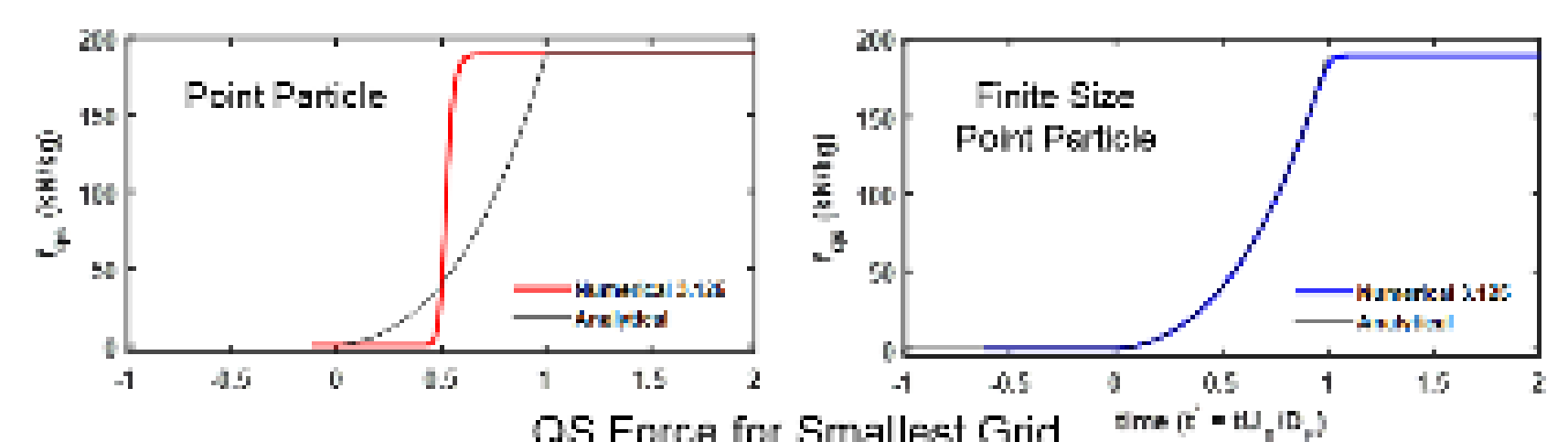
Particle/Fluid density ratio = 10

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5

Summary

- Convergence is achieved for a well-formulated force model and back coupling for finite size particles for a single stationary particle



Next Steps

- Apply finite size particle model for a one-dimensional model of shock propagation through a particle-laden field at moderate volume fraction
- Comparison with DNS will be used to check if the approach also improves accuracy compared to the point particle model

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Surrogate Modeling of the Equation of State

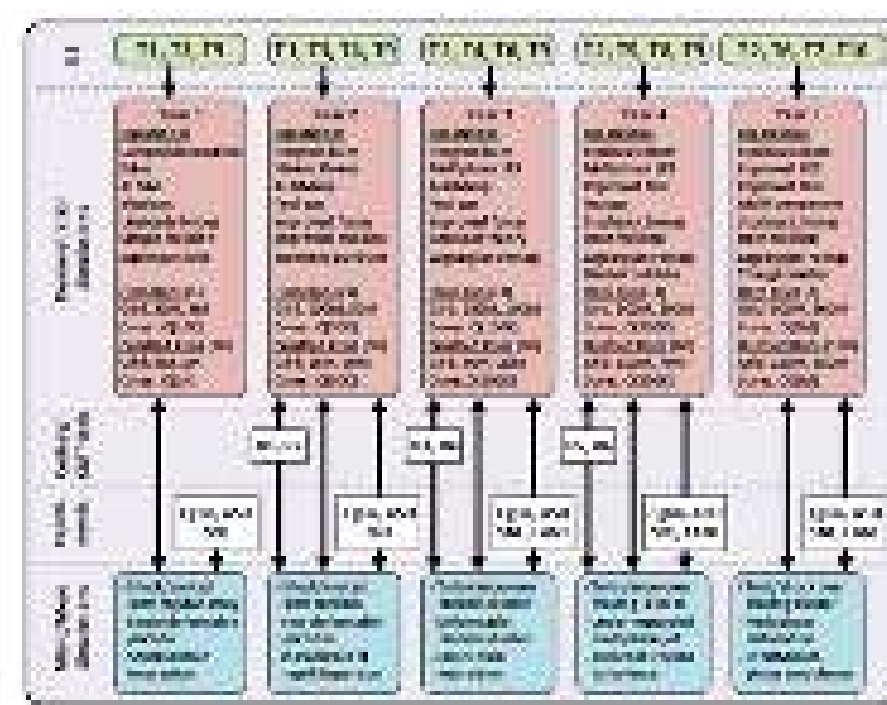
Frederick Ouellet

Advisor: Dr. S. Balachandrar

Department: MAE, UF

Goals

- Develop surrogate models for use in evaluating equations of state (EoS) in mixed air/product cells
- Perform and analyze macroscale simulations of the Frost and Eglin blastpad experiments
- Simulation roadmap
 - Real gas equation of state capabilities in code
 - Analysis of instabilities of rapid dispersion



Simulation Roadmap

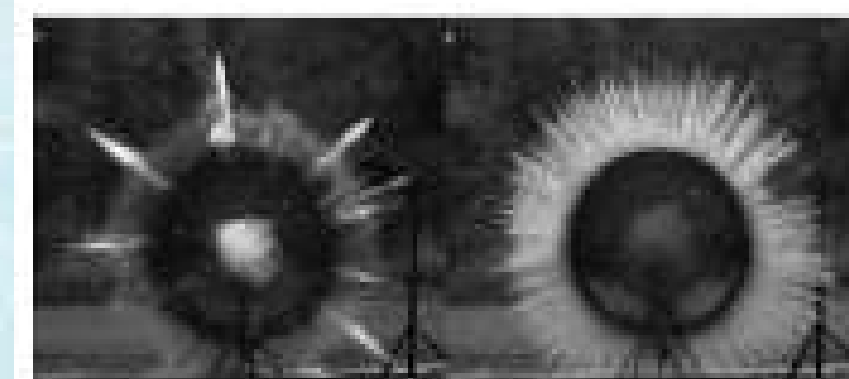
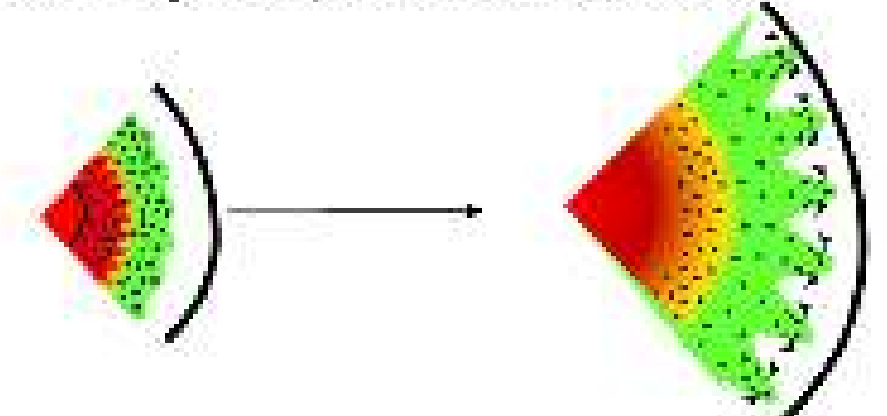
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1

Motivation

Equation of State	Initial PETN Detonation Temperature (K)
Ideal Gas	7944.25
JWL	4501.40
Experimental Result	4140

- A real gas EoS must be used to accurately model the gaseous products of a detonation



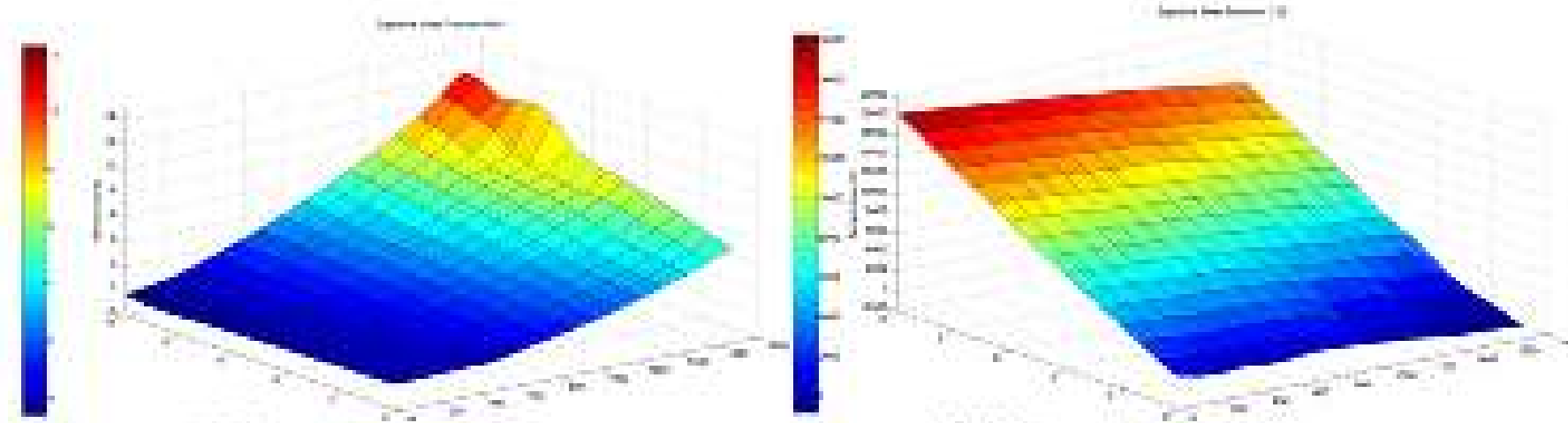
(D. L. Frost, Y. Geng, D. Fata, S. Gossard, and F. Zhang, "Frost et al. (2018) Detonation wave structure and instabilities", *Journal of Computational Physics*, vol. 358, pp. 1048-1068, 2018.)

- As the products are swept outward by the blast, a mixture region forms where the new EoS must be in equilibrium with the EoS used for the ambient gas
- Commonly used iterative approaches to handle these mixture cells are computationally expensive
- A faster alternative would be beneficial for the macroscale simulations to be performed at the center

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2

Surrogate Model – Development



Surfaces of surrogate model for pressure (left) and temperature (right) at an explosive inert fraction of 0.55 using 200 sampling points

- Bayesian Kriging used to generate models for mixed-cell pressure and temperature, in terms of P_{det} , E_{det} and V_{det} using 50-800 sampling points (chosen via adaptive sampling)
- Models replace an iterative, Brayden's Method solver with functions of the form:

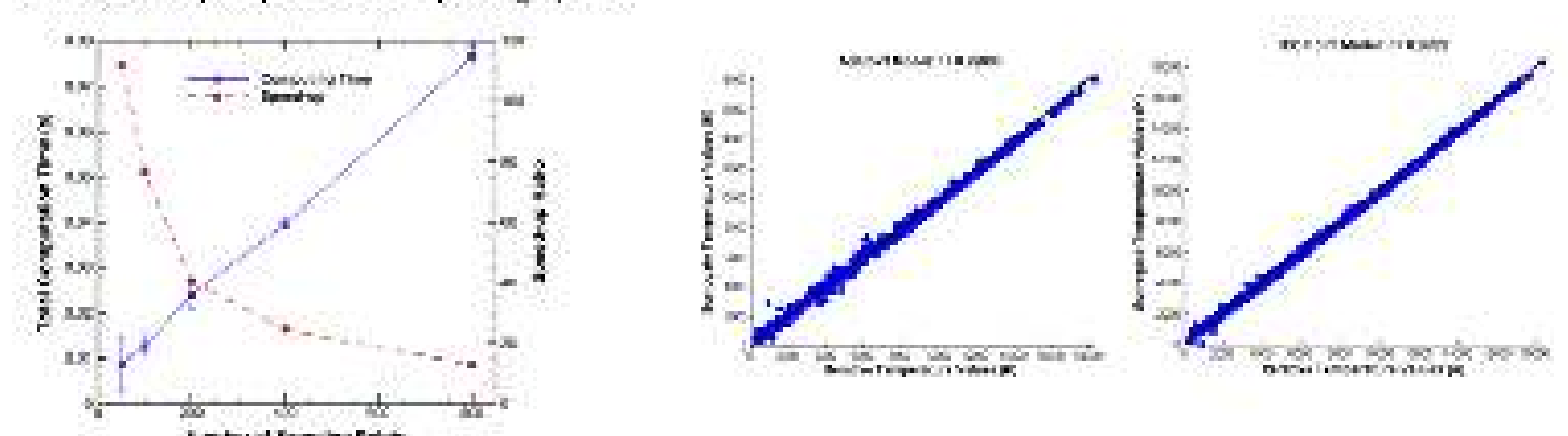
$$f(\mathbf{x}) = \sum_{i=1}^N \beta_i \phi_i(\mathbf{x}) + \sum_{j=1}^M \gamma_j \psi_j(\mathbf{x}) + \sum_{k=1}^L \delta_k \chi_k(\mathbf{x}) + \epsilon^2 f_{\text{mean}}$$
 which have operation counts that scale only with the number of sampling points

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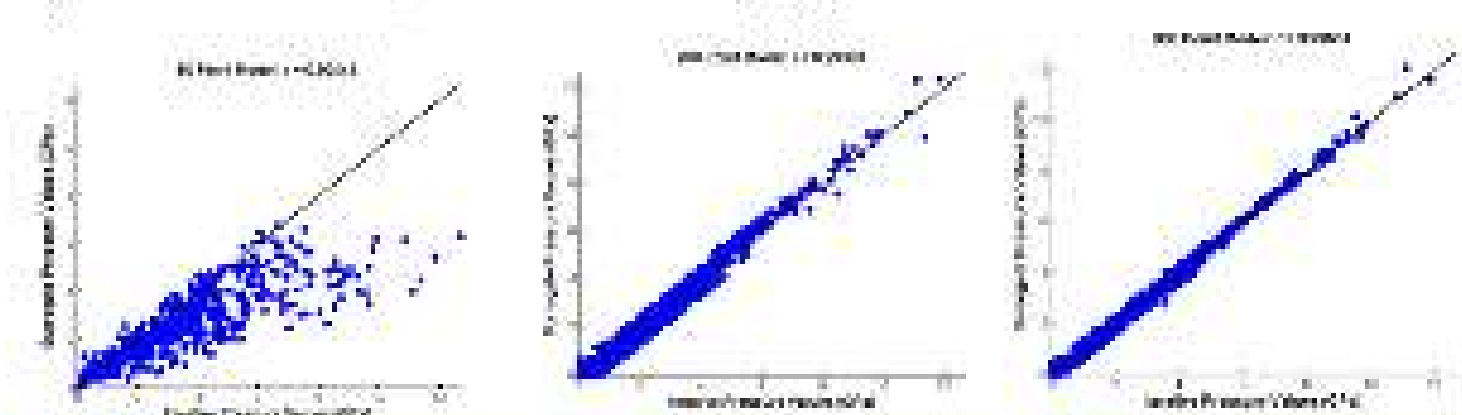
3

Surrogate Model – Testing

- Timings of the different surrogate models compared to the iterative solver to calculate the mixture EoS for 1000 points shows substantially improved computing speed
- Accuracy tests show that the temperature models are highly correlated with the iterative solver for even low numbers of sampling points



- The pressure models require additional sampling points to reach a similar correlation



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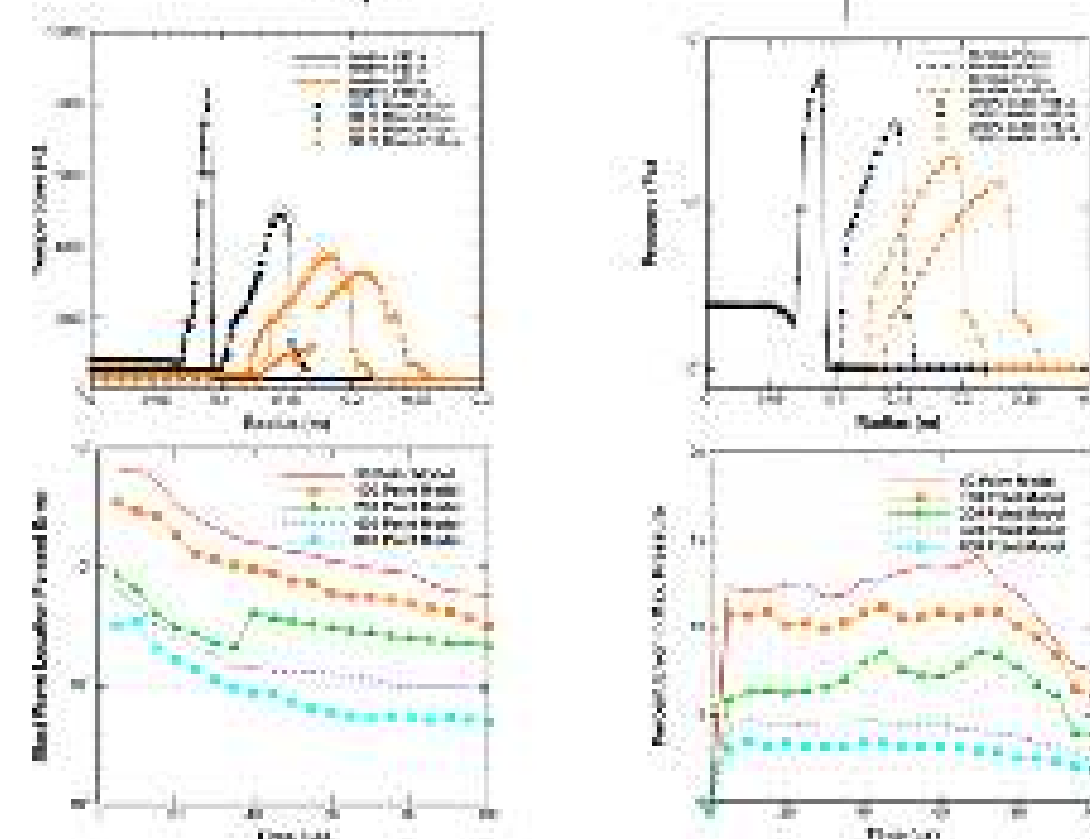
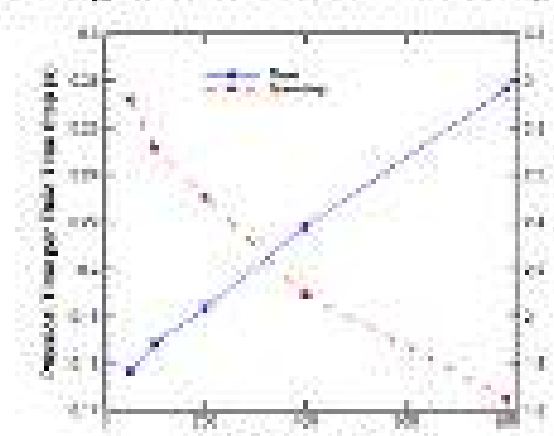
4

Surrogate Model – Hydrocode Testing

- Timings for the full fluid solver using the models compared to the iterative mixture EoS solver also shows a significant decrease in computing time

Test Simulation Description

- 2D, Quarter Cylinder grid
- Outer radius = 0.3 m
- 400,000 cells
- Gas Only, multispecies Euler Eqs.



- The models track the blast wave efficiently for increasing numbers of sampling points but they do not capture the peak values of the state variables in the domain as effectively

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Summary & Future Work

- Summary
 - Developed surrogate models using varying numbers of input sampling points to calculate the EoS of a mixture of detonation products and ambient air
 - Models show good agreement with an iterative approach above roughly 200 sampling points and demonstrate a significant decrease in required computing time
- Future Work
 - Extend model platform to mixtures containing more than two different gases and base equations of state and test their speed and accuracy trade-off
 - Incorporate the currently constructed models into CMT-nek for use in the future simulations of the demonstration problem (Eglin Blastpad)
- This work is being prepared for publication as:
 - F. Ouellet, C. Park, R. Rollin, R.L. Haftka and S. Balachandrar, "A Multi-Fidelity Surrogate Model for Handling Gas Mixture Equations of State", *Journal of Computational Physics* (2018)

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Center for Compressible Multiphase Turbulence

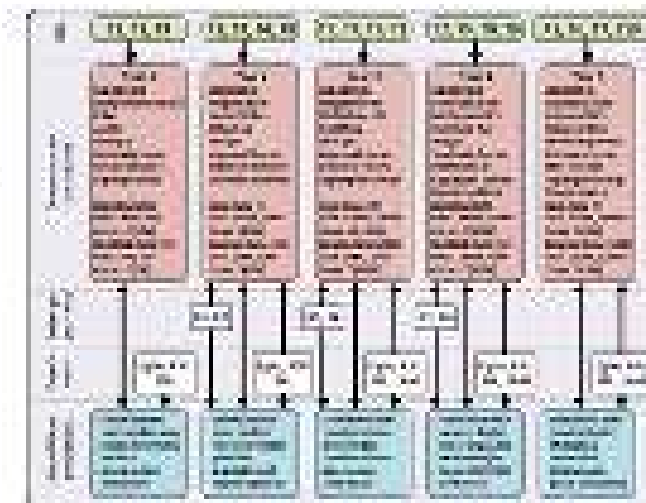
FPGA Pipelined Simulations for CMT-nek

Carlo Pascoe

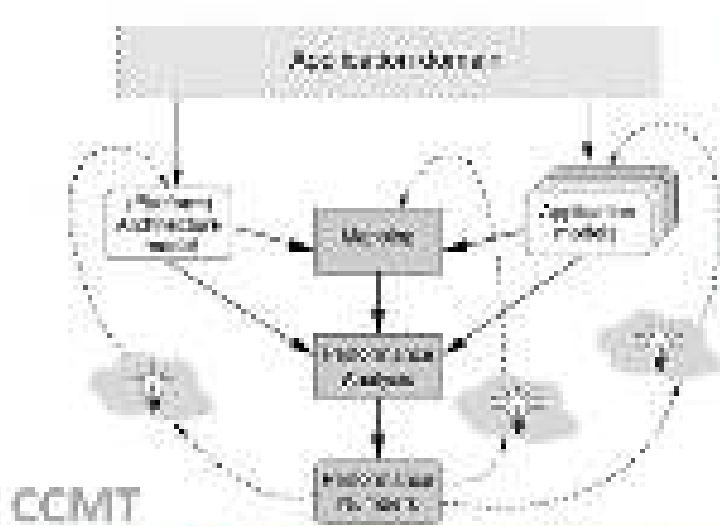
Advisors: Dr. Herman Lam, Dr. Greg Stitt

- Design-space exploration (DSE) critical in optimization of CMT-nek for potential Exascale architectures

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



Simulation Roadmap



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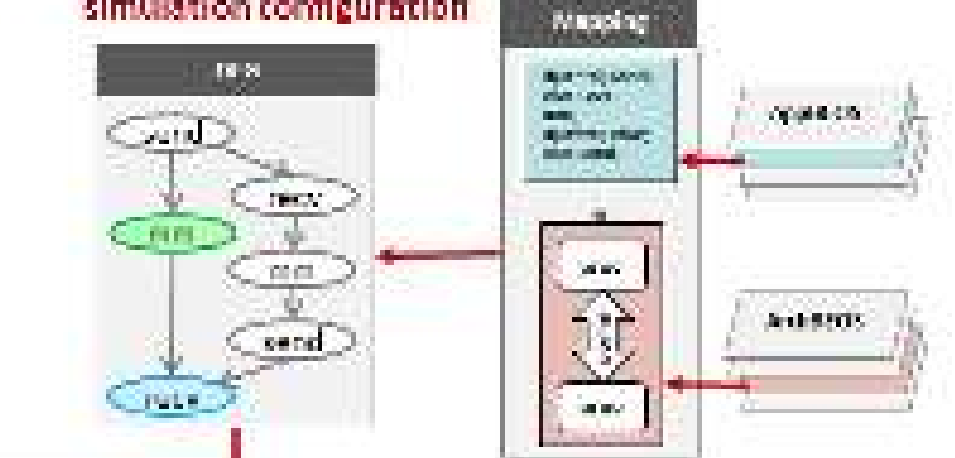
1

Fully-Expanded Pipeline

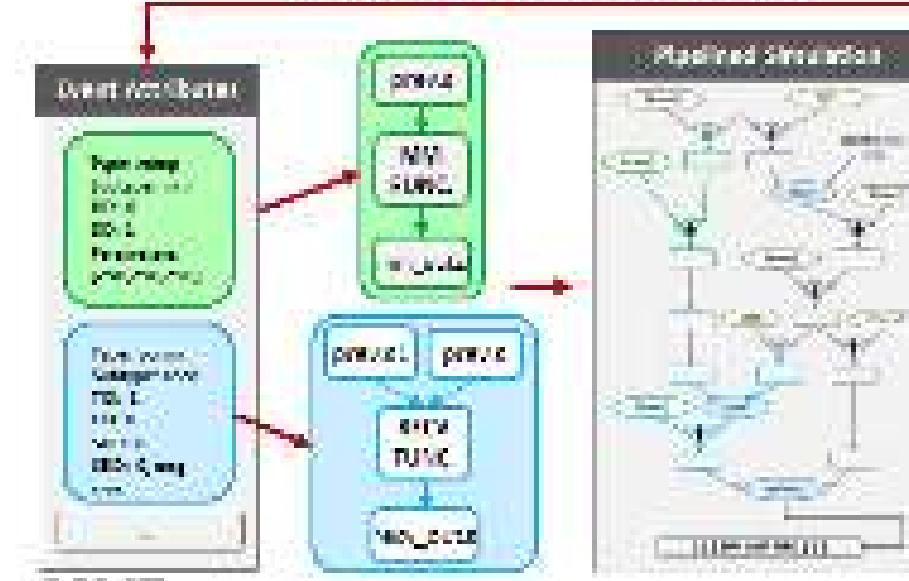
- Construct data flow graph (DFG) from simulation configuration

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

- Extracting DFG from BE simulation configuration



- Mapping DFG to FPGA Pipeline



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- Map DFG to pipeline circuit

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

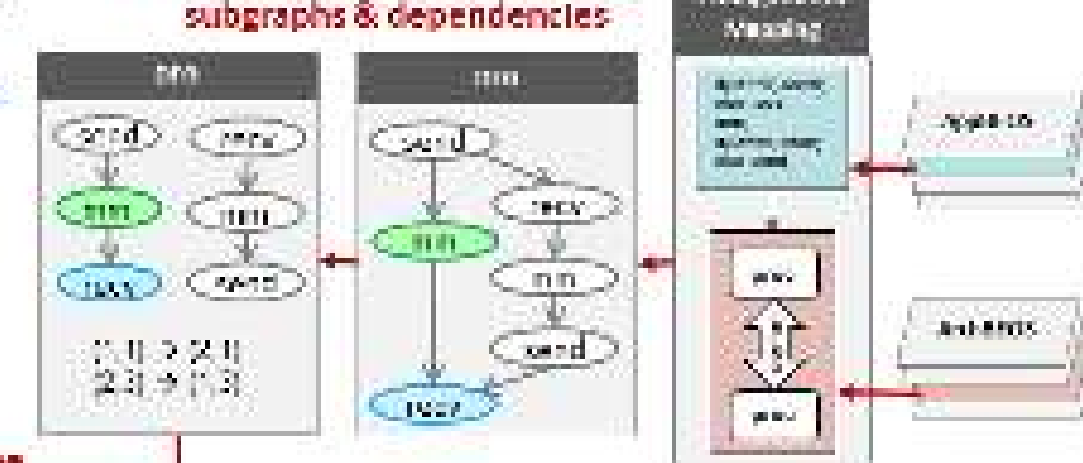
Because each instruction (from sim) mapped to independent HW (no resource sharing), each vertex able to start next sim 1 cycle after current sim

Collapsed Pipeline

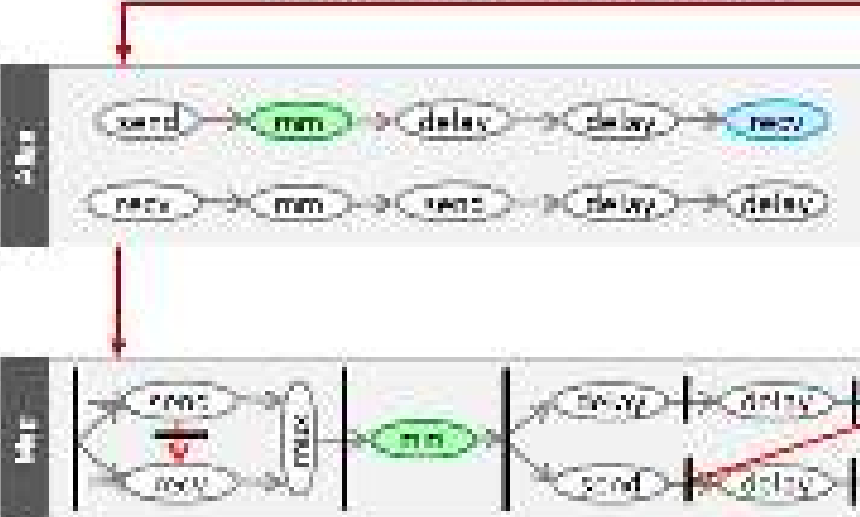
- Construct Data Flow Graph (DFG) from simulation configuration

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

- Extracting DFG, then identify subgraphs & dependencies



- Mapping DFG to FPGA Pipeline



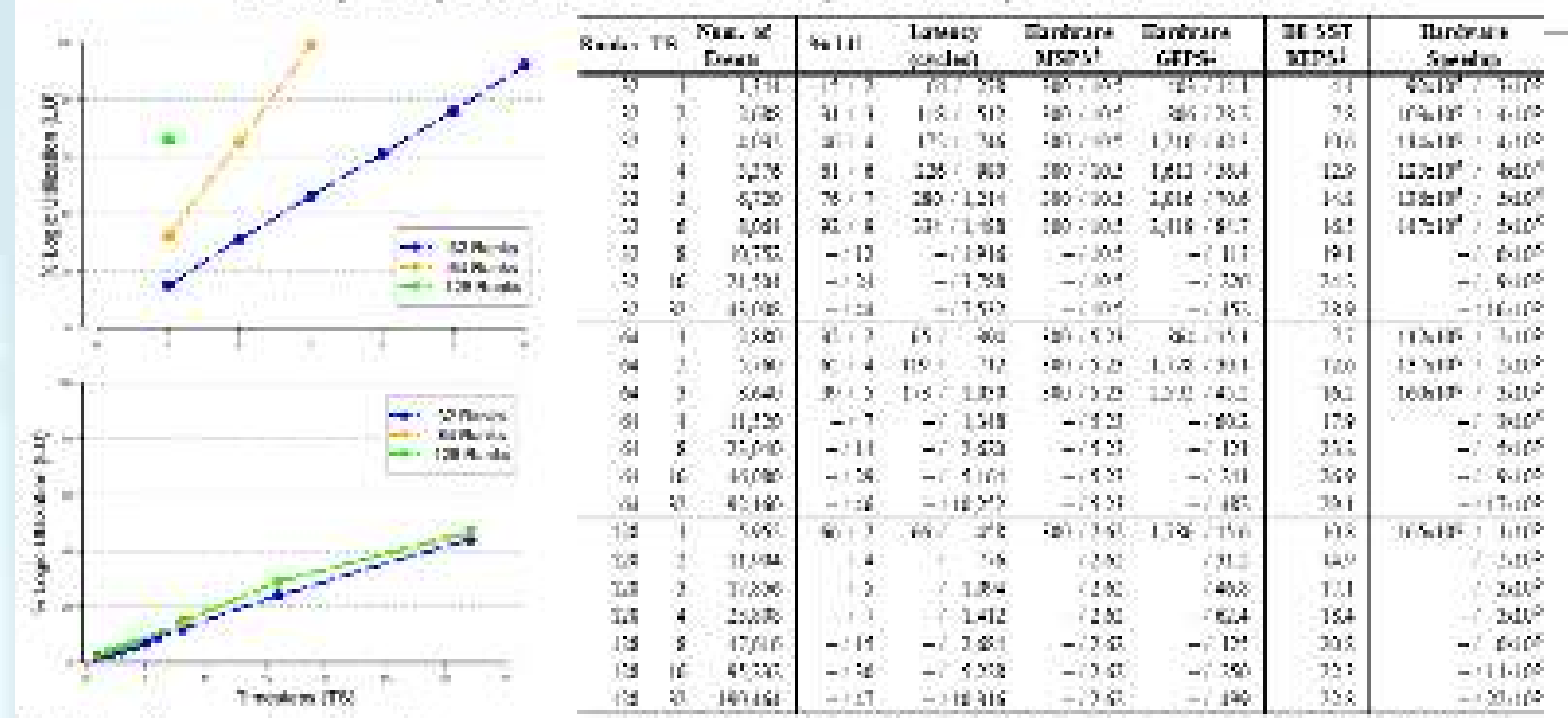
- Map DFG to pipeline circuit

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

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

3

Fully-Expanded & Collapsed Pipeline Tradeoffs



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Center for Compressible Multiphase Turbulence

BE-SST Simulator

Rajashekar Rajagopalan
Trokon Johnson

Advisor: Dr Herman Lam,
Dr Greg Stitt

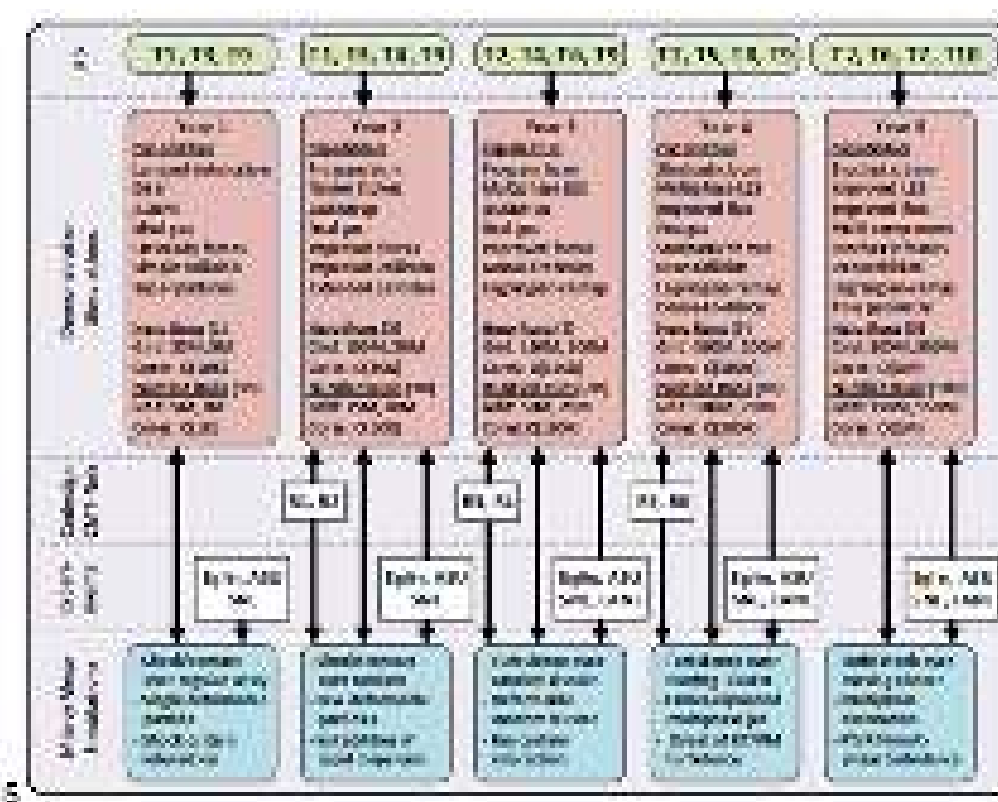
Department: ECE, UF

Goals

- Use SST framework to develop BE methods and run parallel, scalable simulations
- Simulations and validations of large HPC systems
- Improve communication models and Interpolation API

Simulation roadmap

- BE-SST simulator enables scalable Design Space Exploration on exascale systems

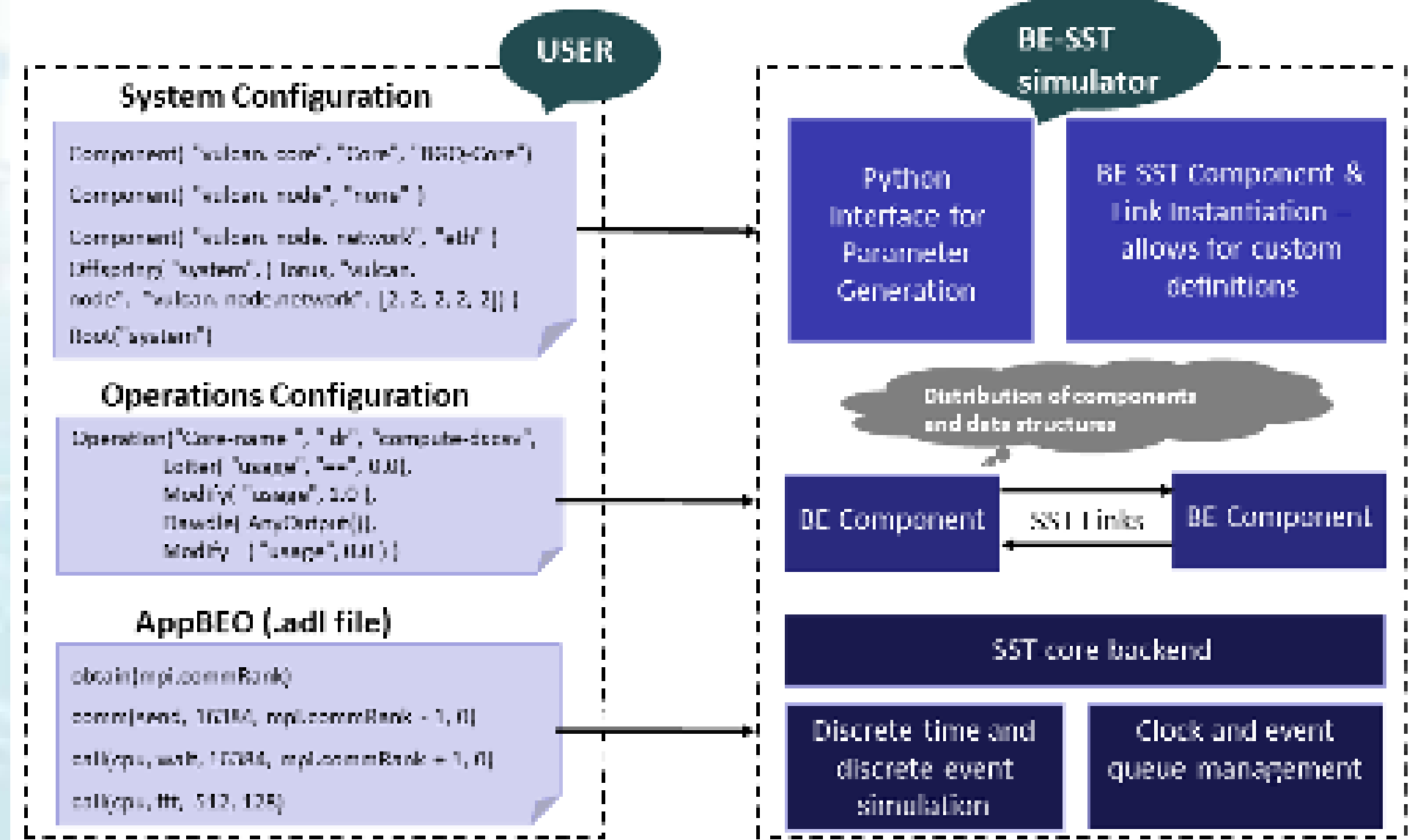


Simulation Roadmap

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BE-SST Features



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Results – Dynamic Routing

- Improved BE scaling as large static routing table was not required with increase in the number of cores being simulated (Fig. 1)
- Configuration build-time was not a bottle-neck for large simulation (Fig. 2)

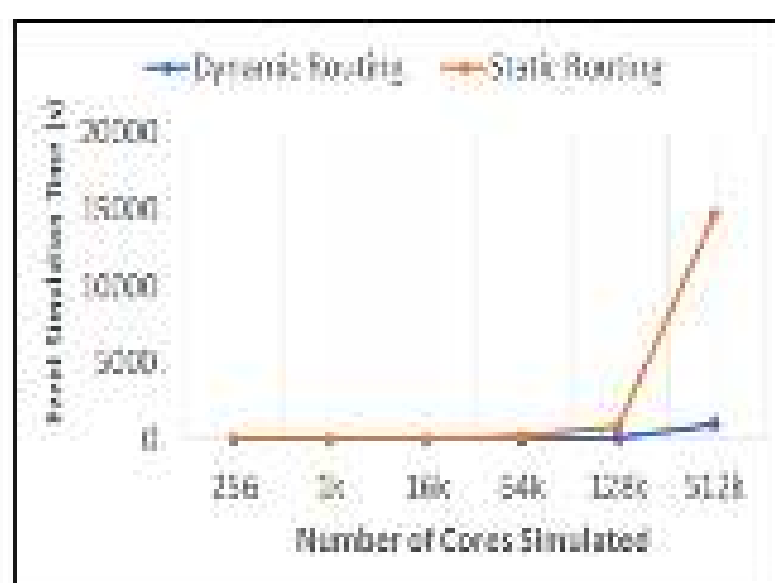


Fig. 1 Static vs. Dynamic Routing

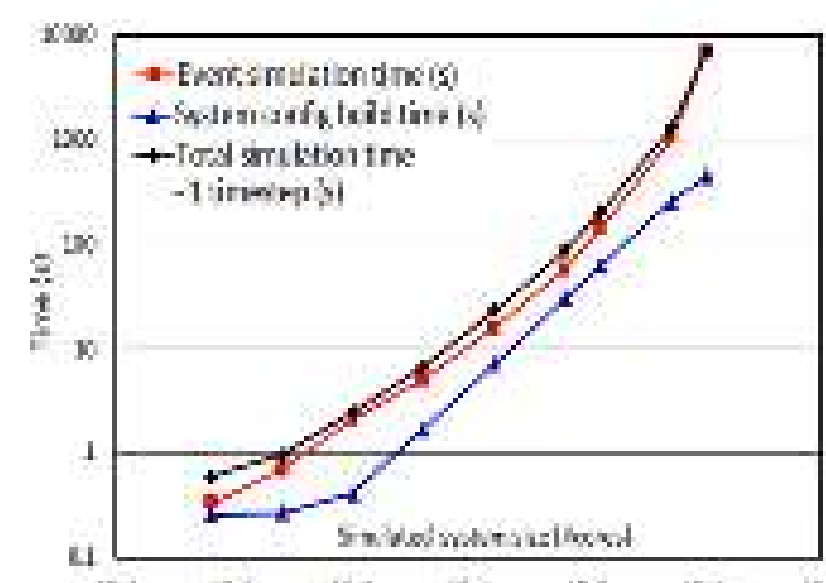


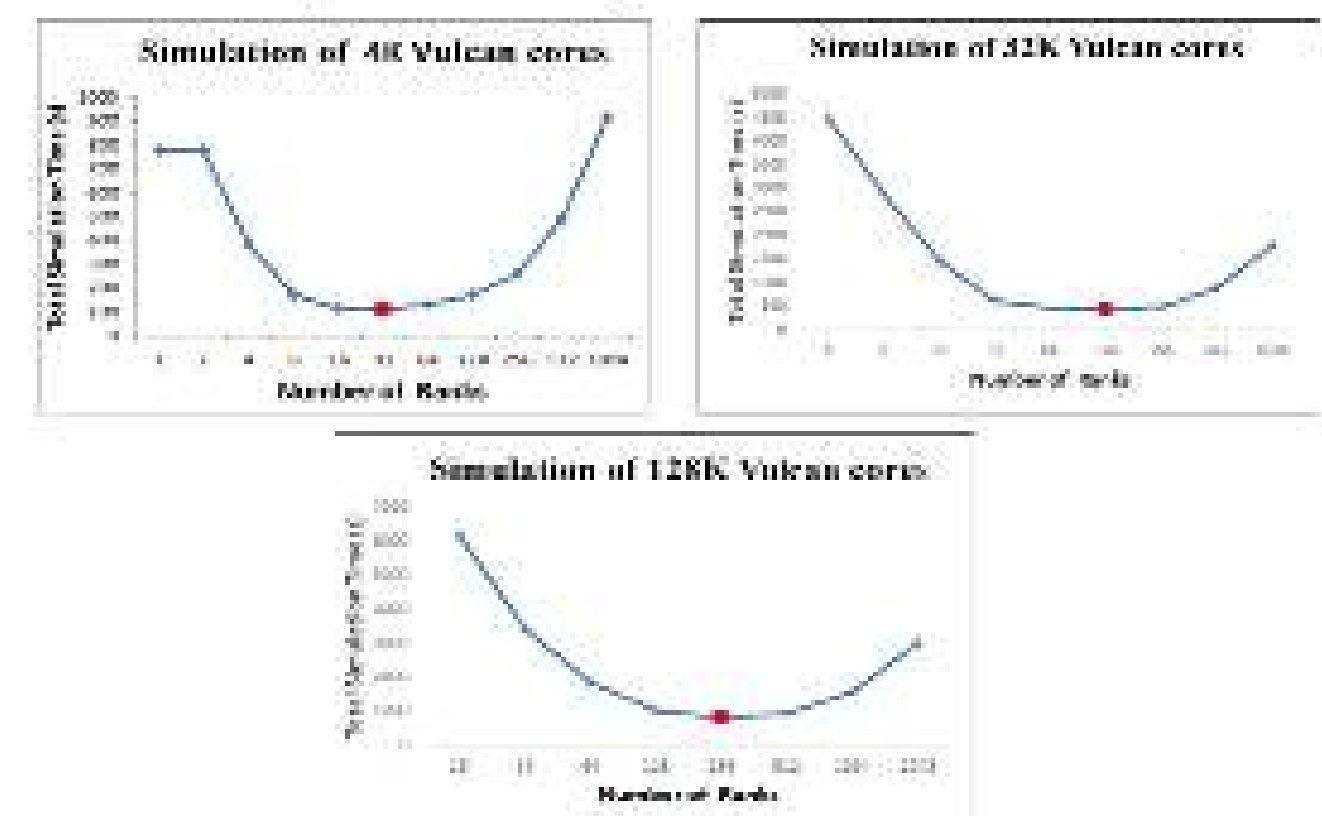
Fig. 2 BE-SST parallelized on 64 cores on HiperGator @UF

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Results – Parallel Performance of BE-SST

- Simulations of Vulcan system with 5-D torus topology using dynamic routing
- Simulations were run using BE-SST installed on Titan
 - Here, 3 Vulcan systems with 4k, 32K & 128K cores were simulated and the simulations were parallelized using BE-SST

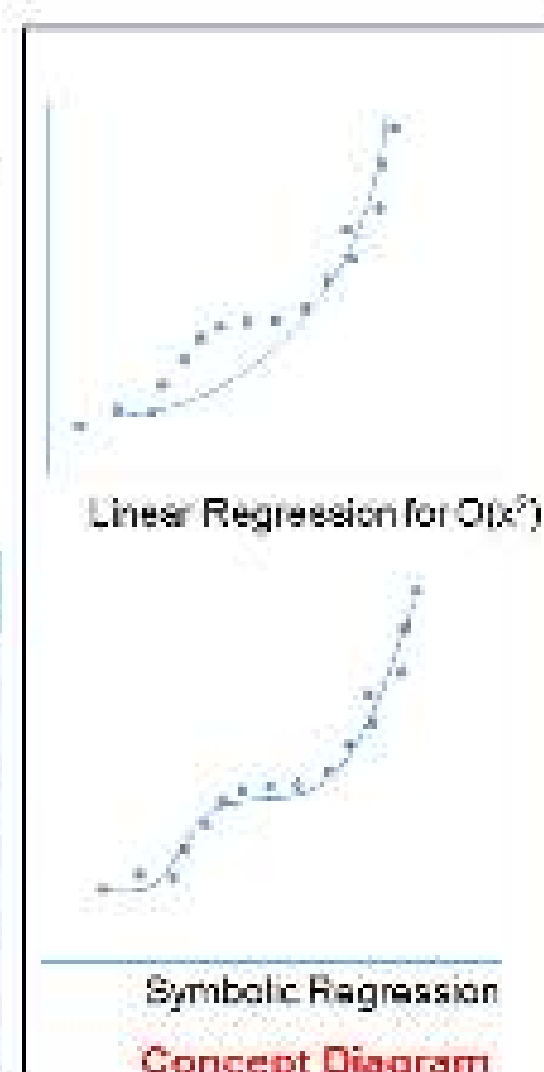


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Results - Symbolic Regression

- Approach
 - Evokes "trees" from mathematical primitives
 - Multiple optimization goals: minimize error, minimize error given tree size constraint, minimize tree size given error constraint, etc.
- Advantages
 - Captures machine-specific performance behaviors
 - Requires no prior knowledge of the kernel
 - Enables trade-offs between accuracy vs computational complexity



* Root Mean Square Error
** Mean Absolute Percentage Error

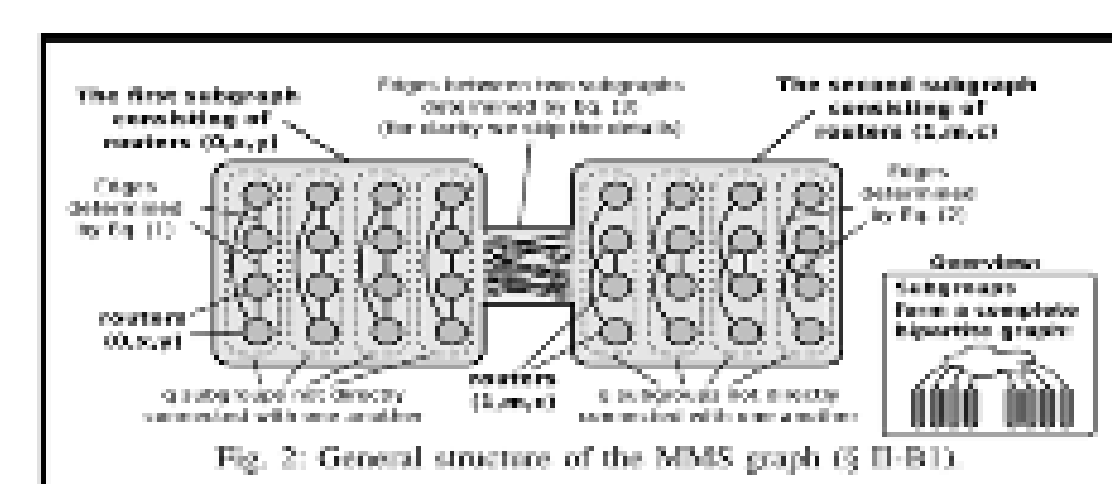
Particle solver variant	RMSE	MAPE	RMSE	MAPE	RMSE	MAPE
Old solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.20E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%
adaptive_particle_solver	1.10E-02	3.2%	1.20E-02	1.8%	1.30E-02	2.4%

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Abstract Machine Modeling

- Goal: Add additional network topologies to BE-SST to enable :
 - Modeling of notional large-scale architectures
 - Facilitates additional architectural design space exploration
- Slim Fly: notional network modeling
 - Scalable, low diameter network topology
 - Maximize endpoints for a given diameter and router radix
 - Improve latency, cost, energy, and resiliency (common HPC architecture concerns)



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Center for Compressible Multiphase Turbulence

Dynamic Load Balancing for CMT-nek

Keke Zhai

Advisor: Prof. Sanjay Ranka

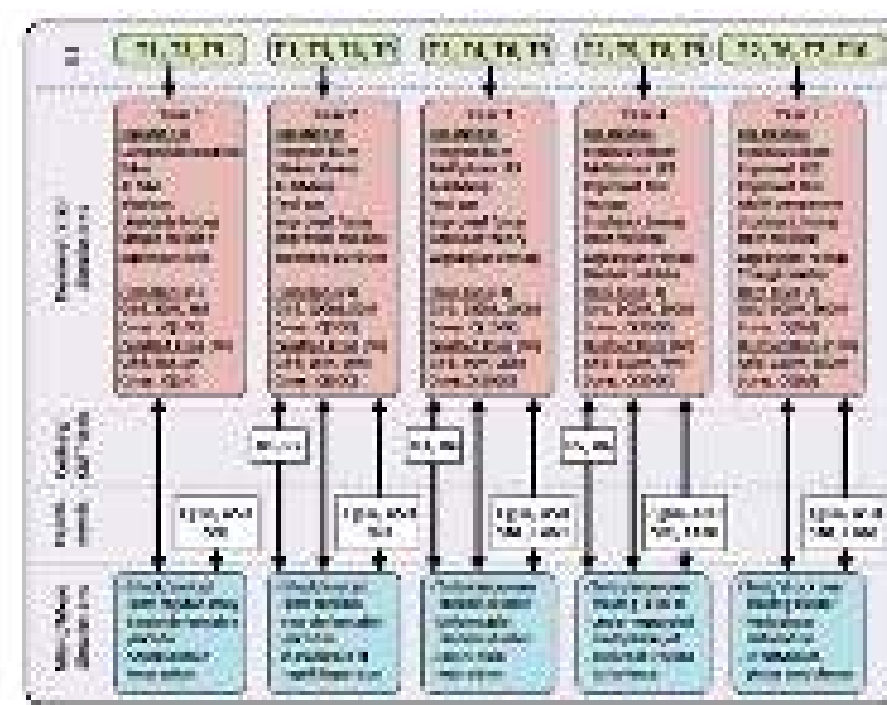
Department: CISE, UF

Goals

- To reduce simulation time and decrease power consumption on CMT-nek by utilizing dynamic load balancing algorithms

Simulation roadmap

- This simulation includes moving particles and gas to simulate the actual particle movement within a fixed box



Simulation Roadmap

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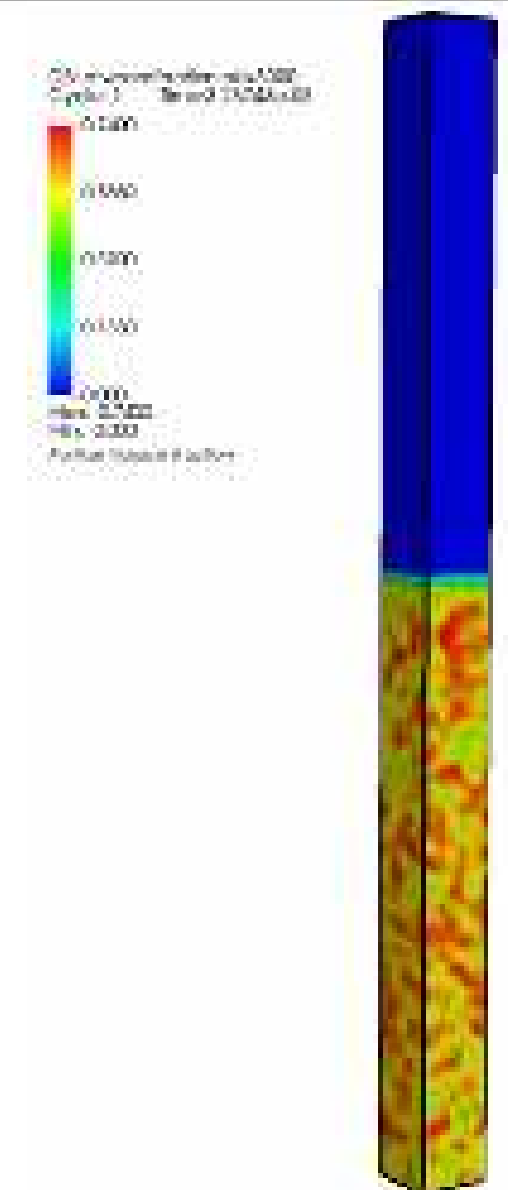
Background

Simulation test case — Expansion fan

- box size
 - x: [-2.208, 6]
 - y: [0, 0.0802]
 - z: [0, 0.0802]
- Particles are initially placed at the bottom of the box
- percent of elements that have particles are about 6.1% of total number of elements

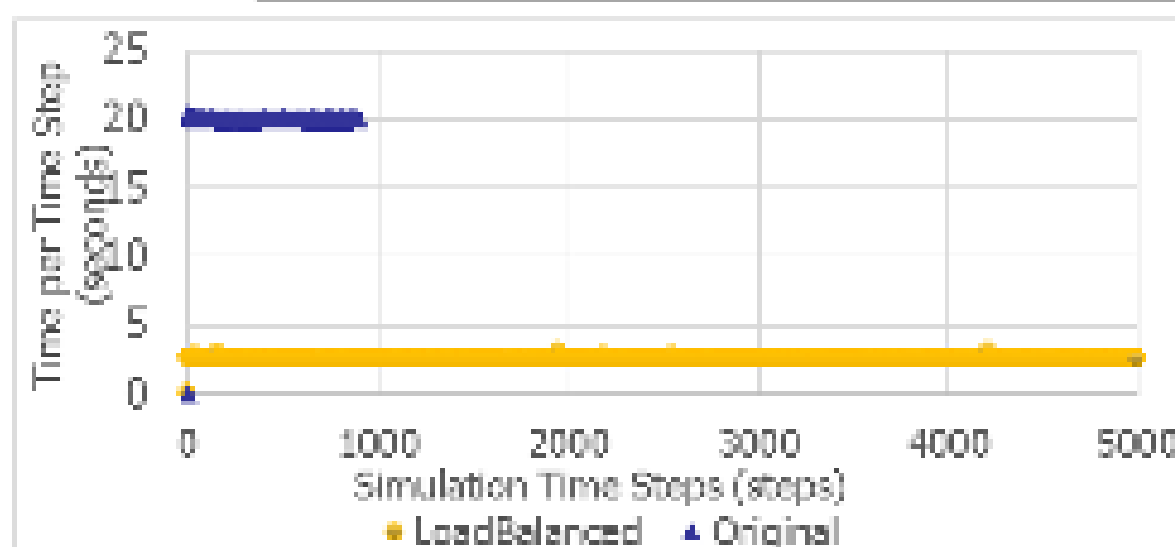
Platform

- Vulcan: IBM BG/Q platform
- Quartz: Intel Xeon (Broadwell)



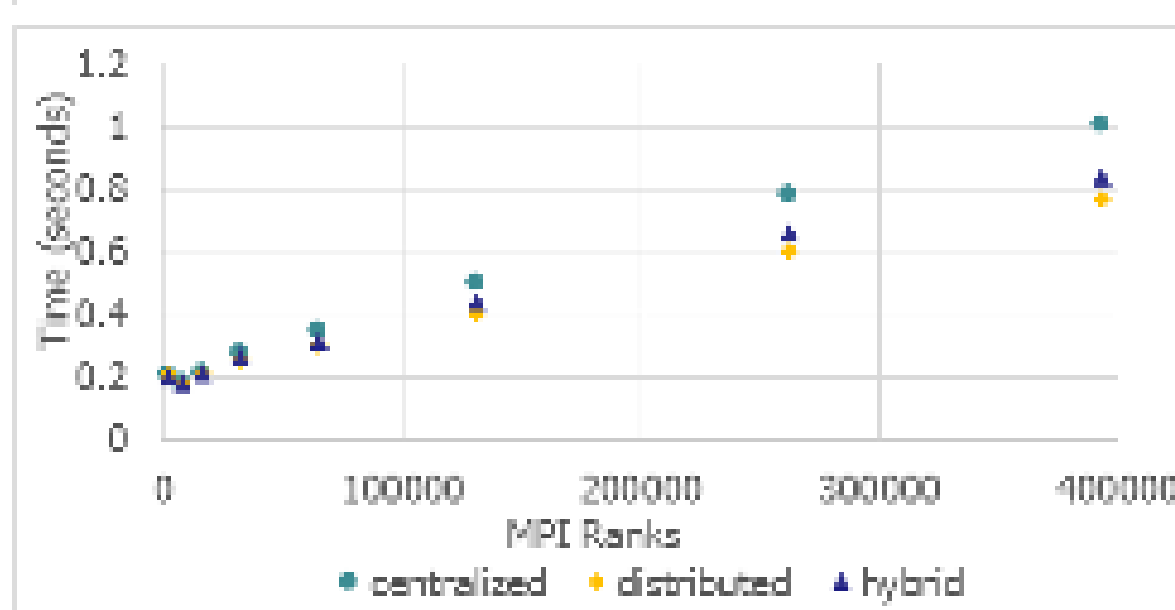
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Load Balancing Results on Vulcan



LB vs. original

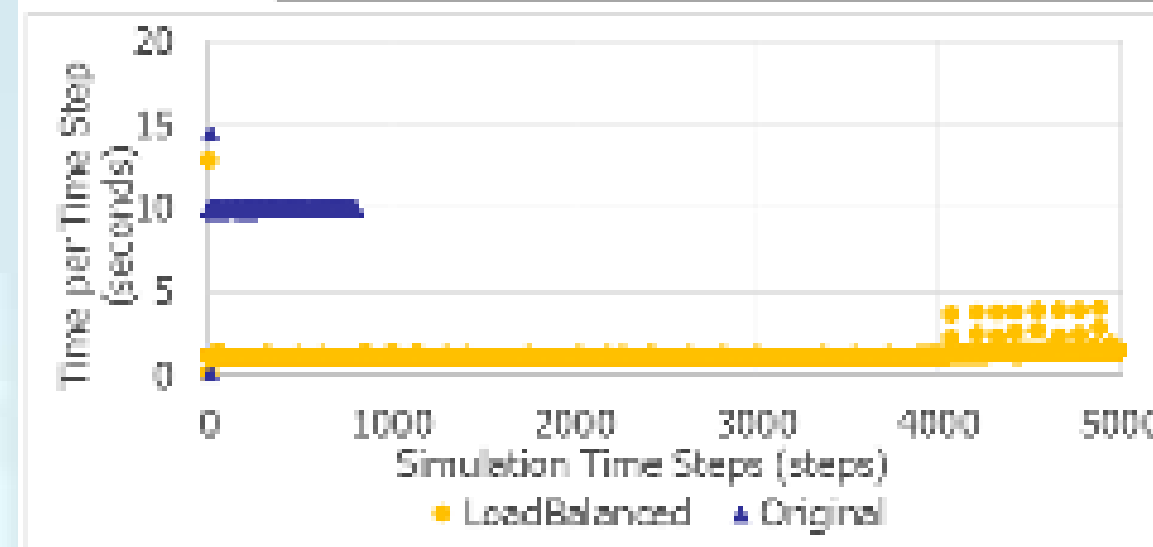
- 20.00 s for the original code
- 2.52 s for the load balanced code
- 7.9x improvement in performance



Overhead for load balancing

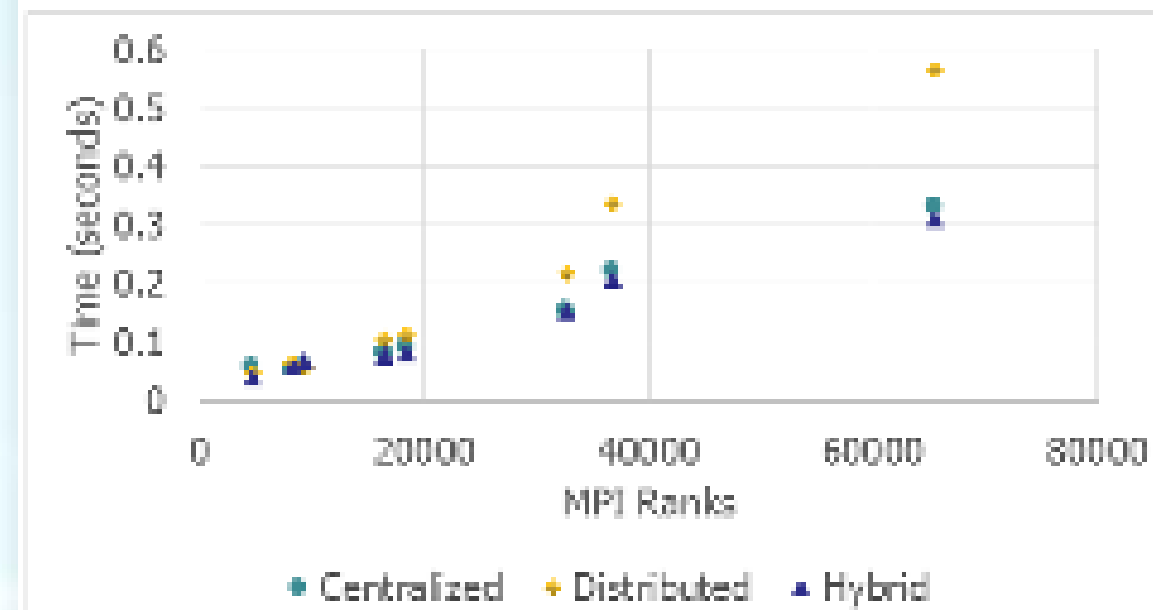
- Overhead expressed as number of time steps:
- 1.00 for the centralized
- 0.77 for the distributed,
- 0.84 for the hybrid algorithm
- overhead for load balancing is very small

Load Balancing Results on Quartz



LB vs. original

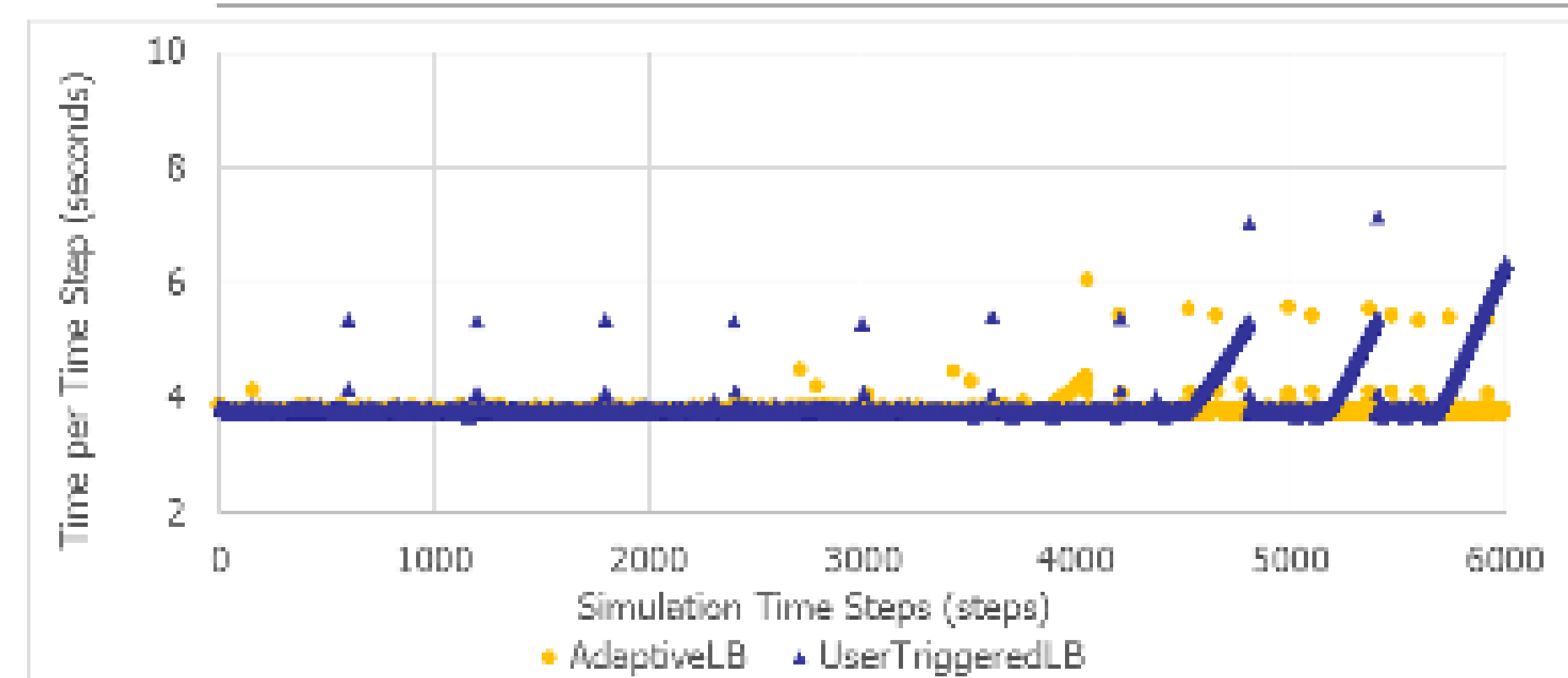
- 9.92s for the original code
- 0.995s for the load balanced code
- 9.97x improvement in performance
- Adaptive load balancing first happened at 4077 time step



Overhead for load balancing

- Overhead expressed as number of time steps:
- 1.94 for the centralized
- 3.35 for the distributed
- 1.82 for the hybrid algorithm
- overhead for load balancing is very small

Adaptive Load Balancing on Vulcan



- User-triggered load balancing algorithm: load balance every 500 time steps
- Adaptive load balancing algorithm: first load balance after 4000 time step
- Time per time step from step 4,000 to 6,000 for adaptive and user-triggered load-balancing algorithms was 3.78 s and 4.17 s, respectively
- Giving us an overall improvement of 9.4%

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Summary

- The load balancing results of CMT-nek running on Vulcan and Quartz have been presented
- Using load balancing algorithm, the total execution time can be saved by up to 10 times compared to the original
- The load balancing overhead is pretty small, so this has the potential to scale to a million or 10 million ranks in the future
- Future Work:
 - Investigate on the initial mapping algorithm to see if it would make the load balancing algorithm faster
 - More test cases will be added to make this algorithm more robust

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Adaptive Sampling For Design Space Exploration Using Behavioral Emulation

Yiming Zhang

Advisor: Prof. Raphael T. Haftka

& Prof. Nam H. Kim

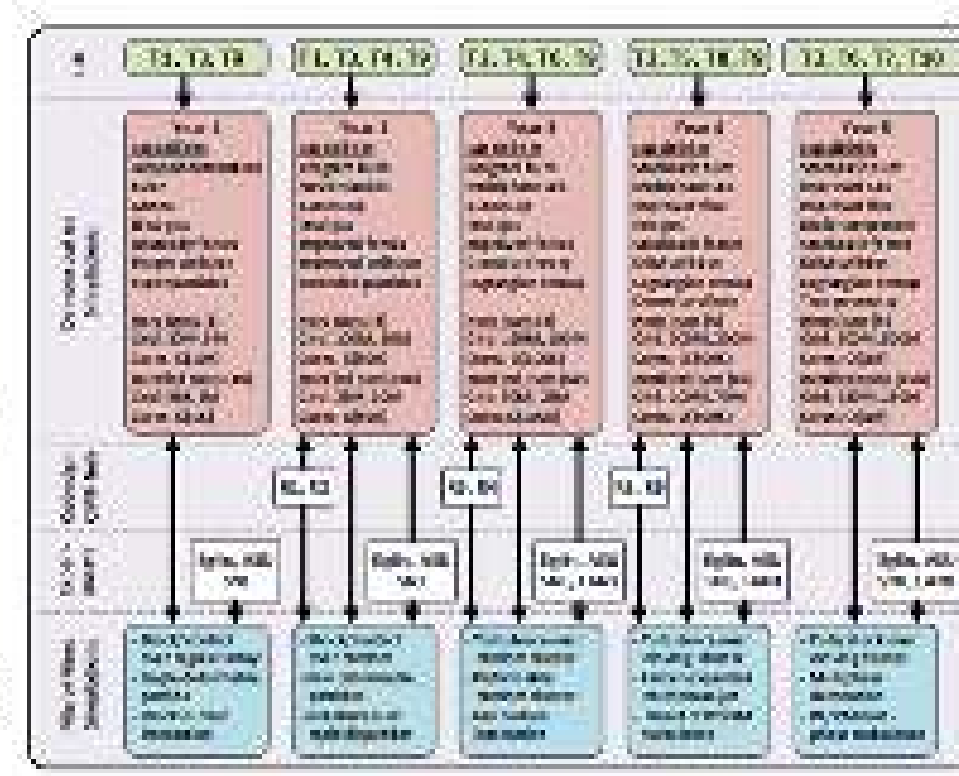
Department: Mechanical Engr. /UF

- Goals

- Produce sampling plans and predictions using probabilistic models for the validation and usage of Behavioral Emulation of HPC architectures

- Simulation roadmap

- Assist validation and usage of Behavioral Emulation for algorithmic & architectural design-space exploration at different stages



Simulation Roadmap

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Motivation and Progress

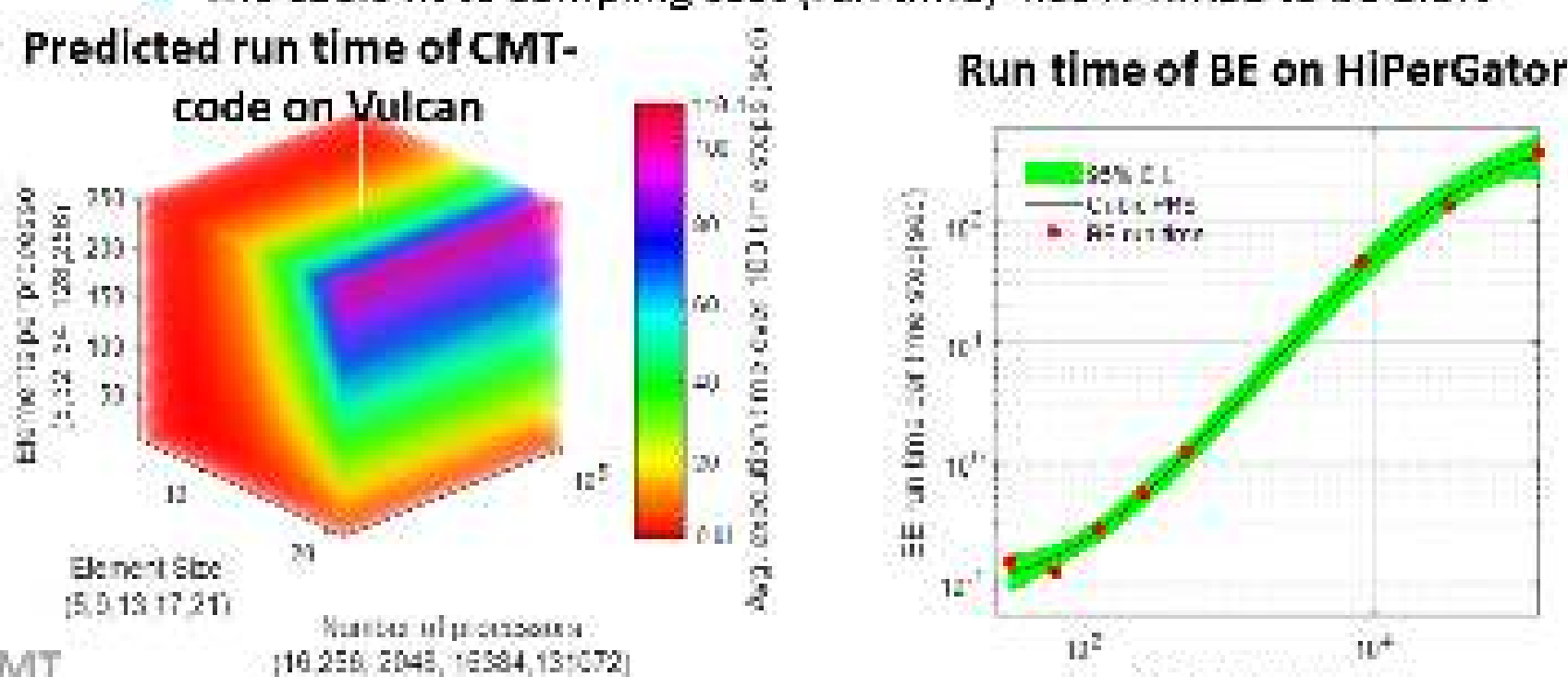
- **Behavioral emulations to predict run time of CMT-nek code on Vulcan**
 - Allow algorithmic & architectural design-space exploration for CMT-code and the notional architecture
 - The emulations are being validated on Vulcan and performed on H1PerGator
 - Three identified design variables for the CMT-nek code: element size, number of processors, element per processors
- **Where to run the behavioral emulations for algorithmic & architectural design-space exploration (DSE)?**
 - Emulations are expensive to run. Surrogates are introduced based on existing runs for prediction at untested configurations
 - The run time (cost) varies in the design space and challenges classical sampling plans which assume constant cost(run time)
 - Developed adaptive sampling with surrogate model for approximation with quantified uncertainty

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Adaptive Sampling to Explore Design Space

- **Synthesize the test function based on the 125 BE runs for the study of different sampling plan**
 - Used a cubic polynomial to fit the 125 BE runs, the normalized root-mean-square error (N-RMSE, normalized by the range of function values) is 0.9%
 - The cubic fit to sampling cost (run time) has N-RMSE to be 1.0%



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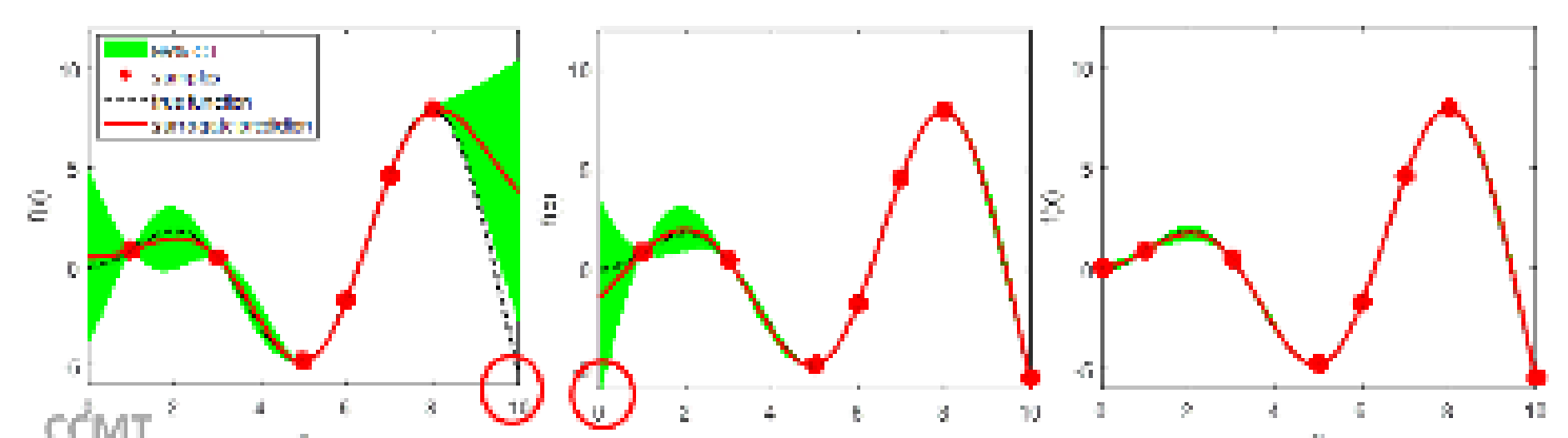
Adaptive Sampling to Explore Design Space

- Is it possible to improve design space exploration using BE?
 - Adaptive sampling versus all-at-once sampling
 - Current sampling plans implicitly assume constant sampling cost. Need revise the standard sampling plans to incorporate varying cost(run time)
- Key procedures for the typical adaptive sampling (AS) without varying cost

Step1: Generate initial samples with partial budget

Step 2: Iteratively add samples at points with large uncertainty

Step 3: Update surrogate predictions until desired



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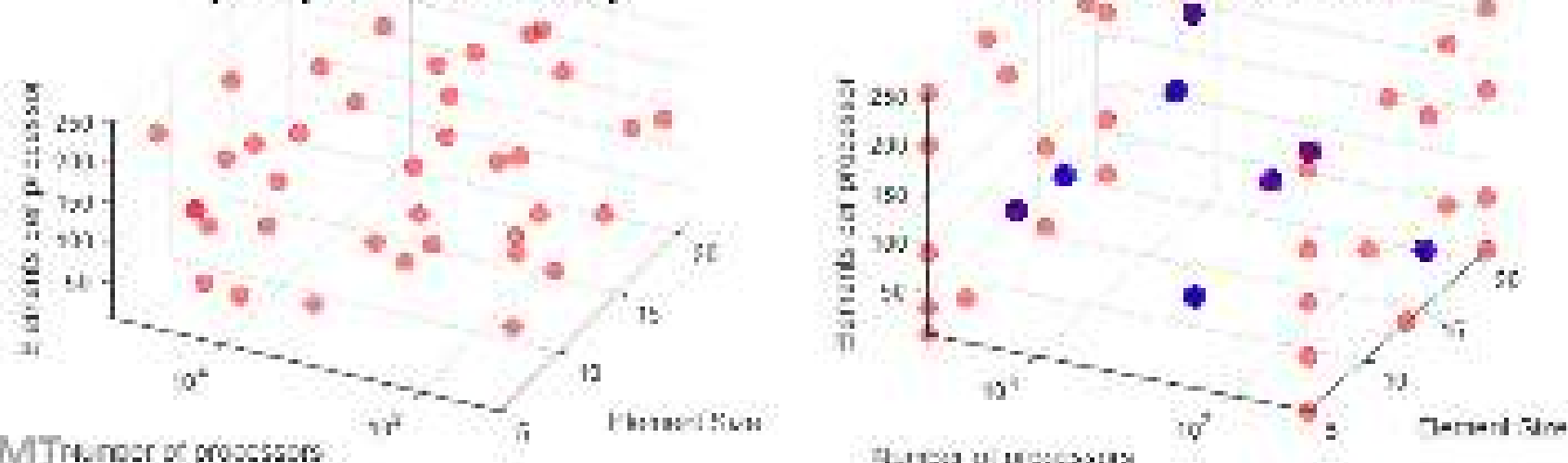
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Adaptive Sampling to Explore Design Space

- **Adaptive sampling was preferred than all-at-once sampling using 38 runs**
 - Three design variables for the CMT-code: element size, number of processors, element per processors. 38 runs(samples) were used.
 - Adaptive sampling started from 8 runs, ended with 38 runs, the N-RMSE (normalized by function range) is 1%
 - All-at-once sampling using latin hypercube sampling, the N-RMSE is 5%, much inferior to the adaptive sampling

All-at-once sampling
(red points are runs)

Adaptive sampling
(initial runs in blue)

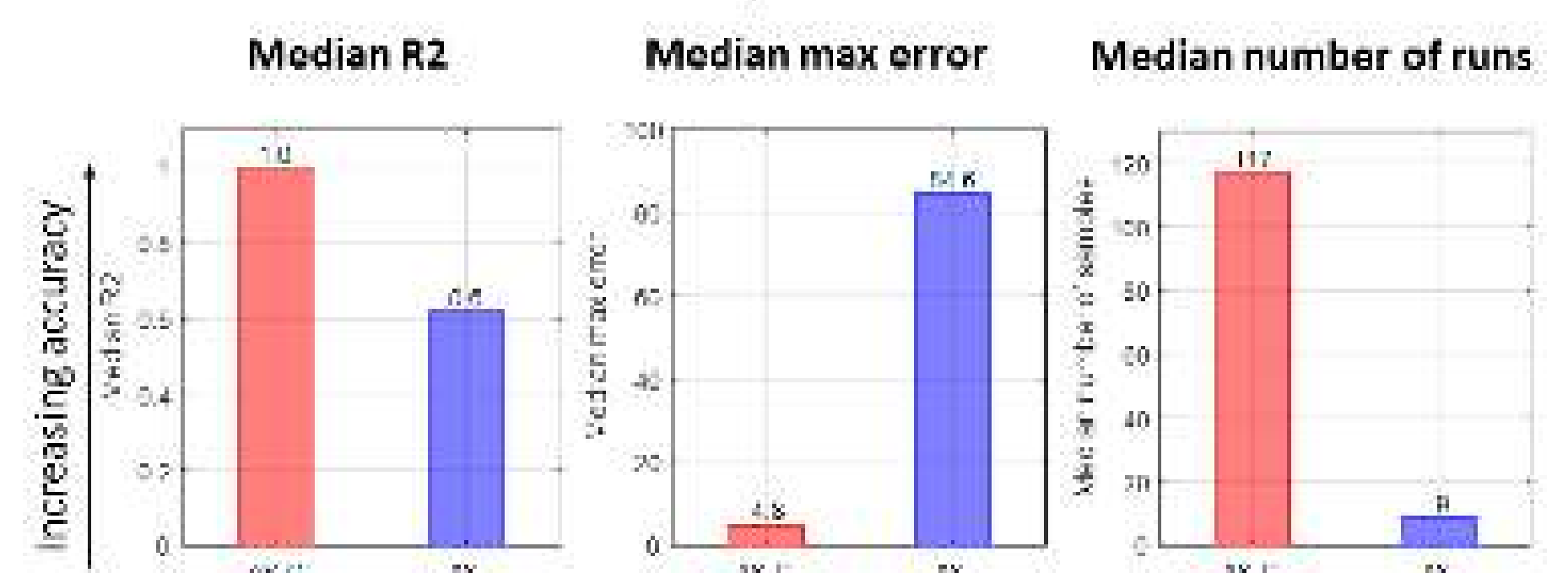


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Adaptive Sampling to Explore Design Space

- **The proposed adaptive sampling with varying cost (AS-C)**
 - AS-C is developed based on two surrogates for objective and cost
 - 100 sets of initial samples(8), sampling budget is up-to 800seconds
 - AS-C ended with more cheaper runs and lead to accurate estimation



AS-C: adaptive sampling with varying cost
AS: standard adaptive sampling

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Gas-Particle Mixtures Under Sudden Expansion

Heather Zunino

Advisor: Prof. Ronald Adrian

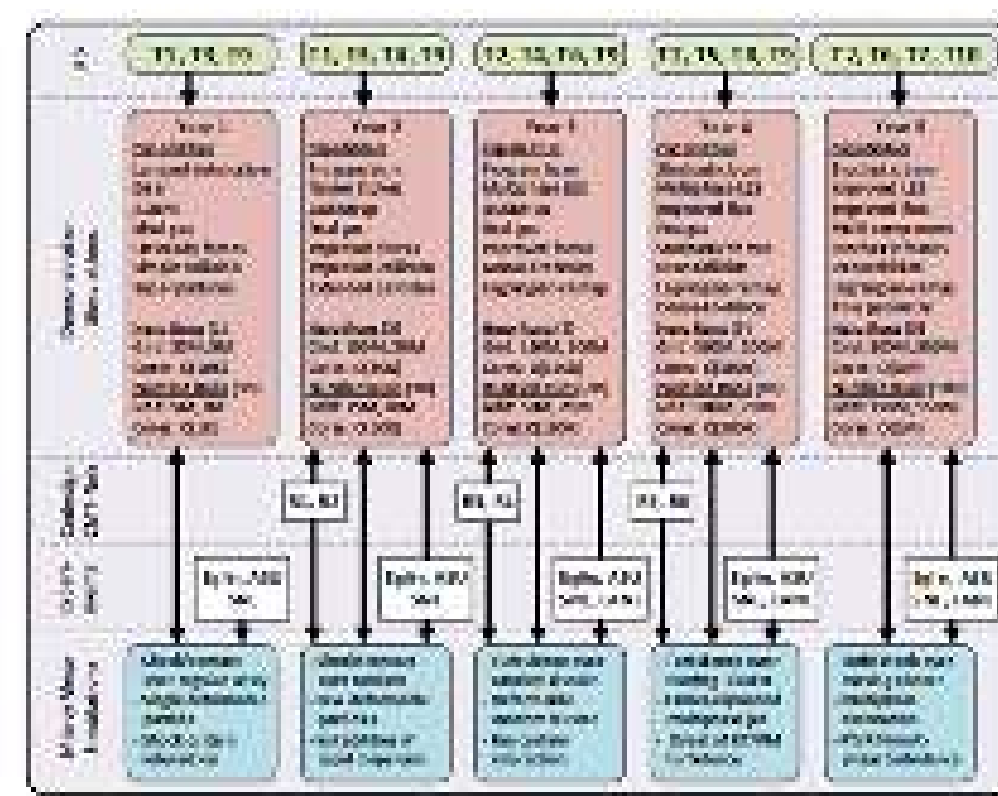
Department: SEMTE, ASU

Goals

- Perform repeatable experiments on a vertical shocktube at ASU
- Examine expansion fan, flow structures, and instabilities
- Provide data for validation of computational codes

Simulation roadmap

- The shocktube experiment at ASU will provide data for validating the codes being developed at UF.

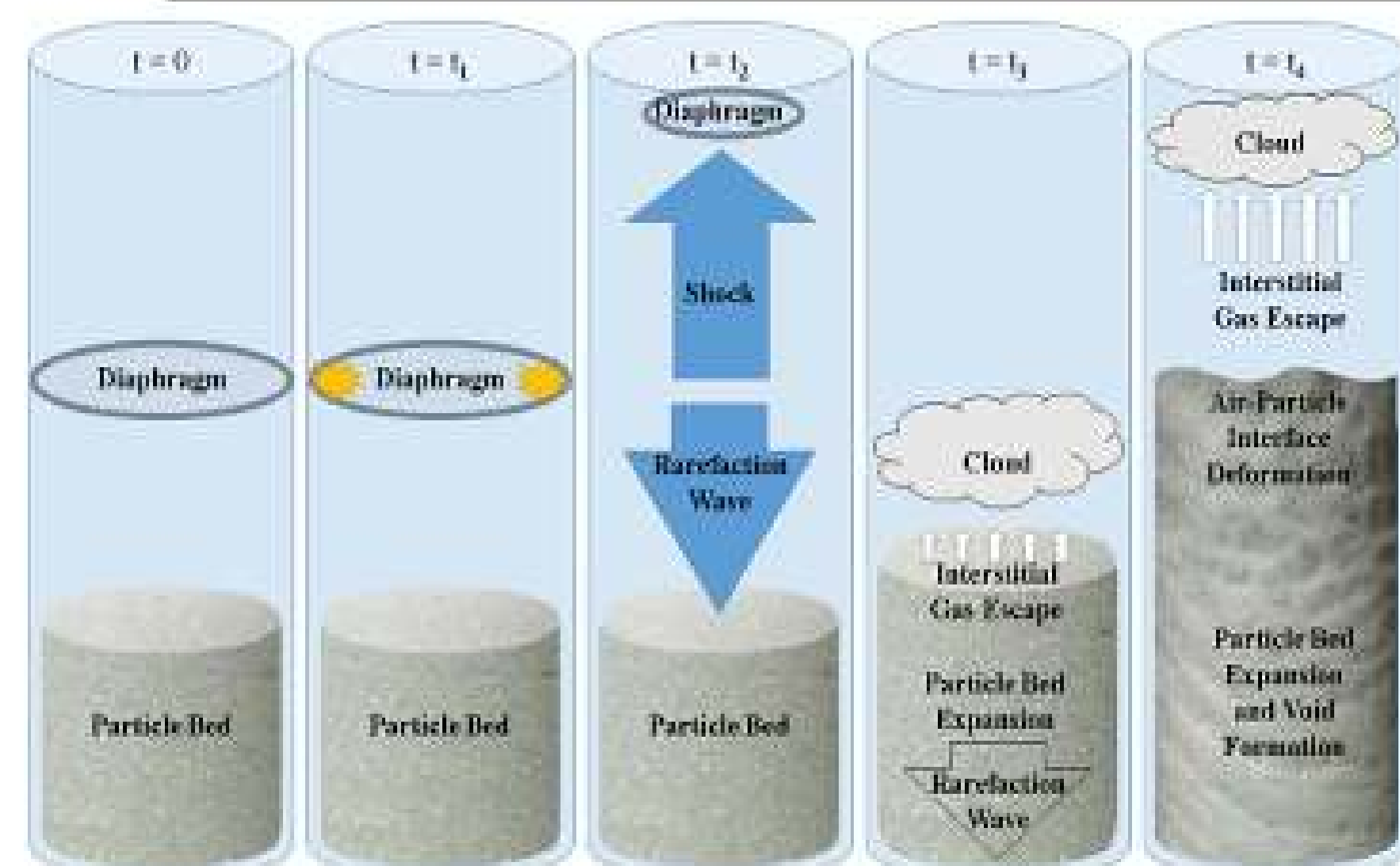


Simulation Roadmap

Motivation

- 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 cylindrical 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

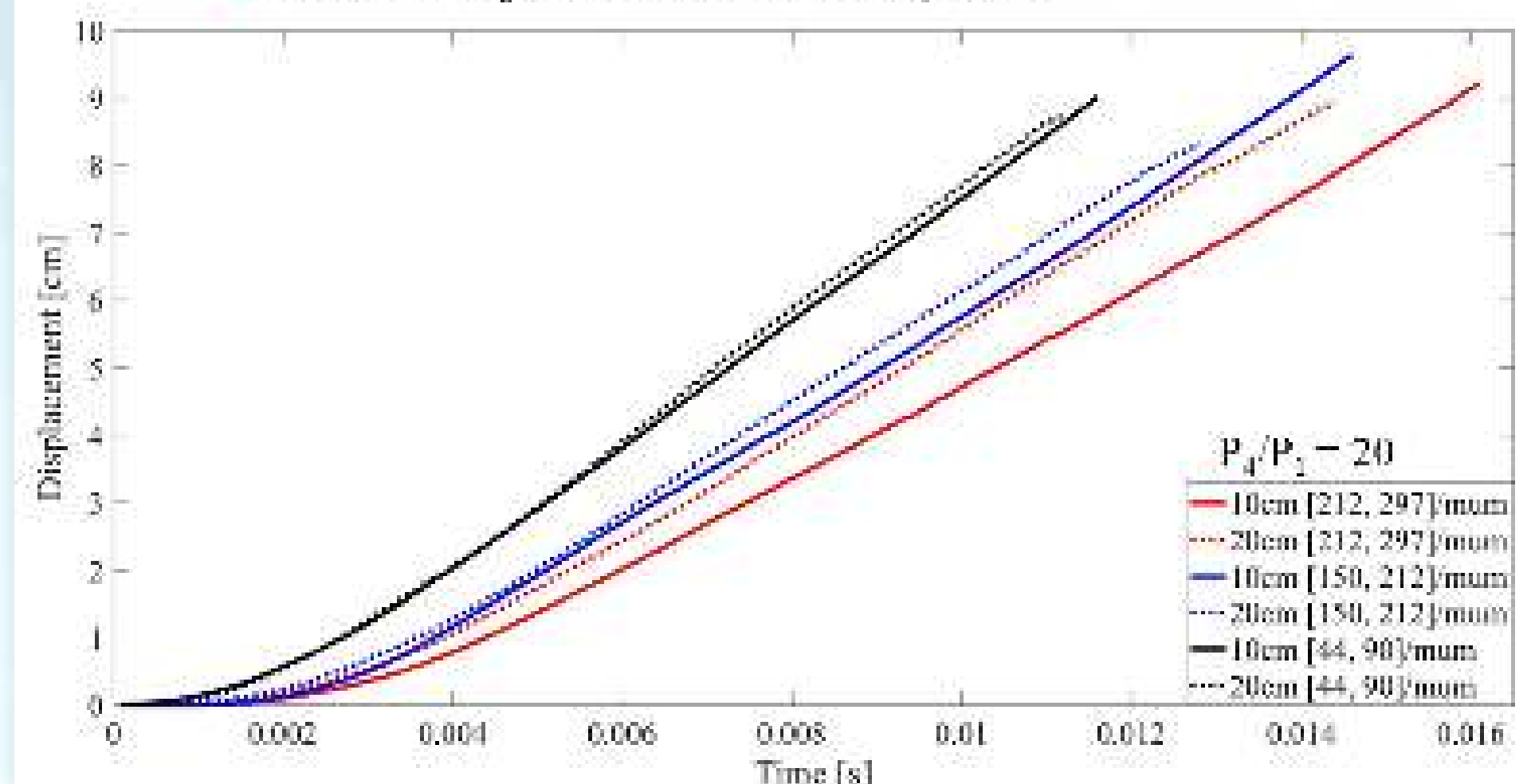
Results



Stages of Experiment

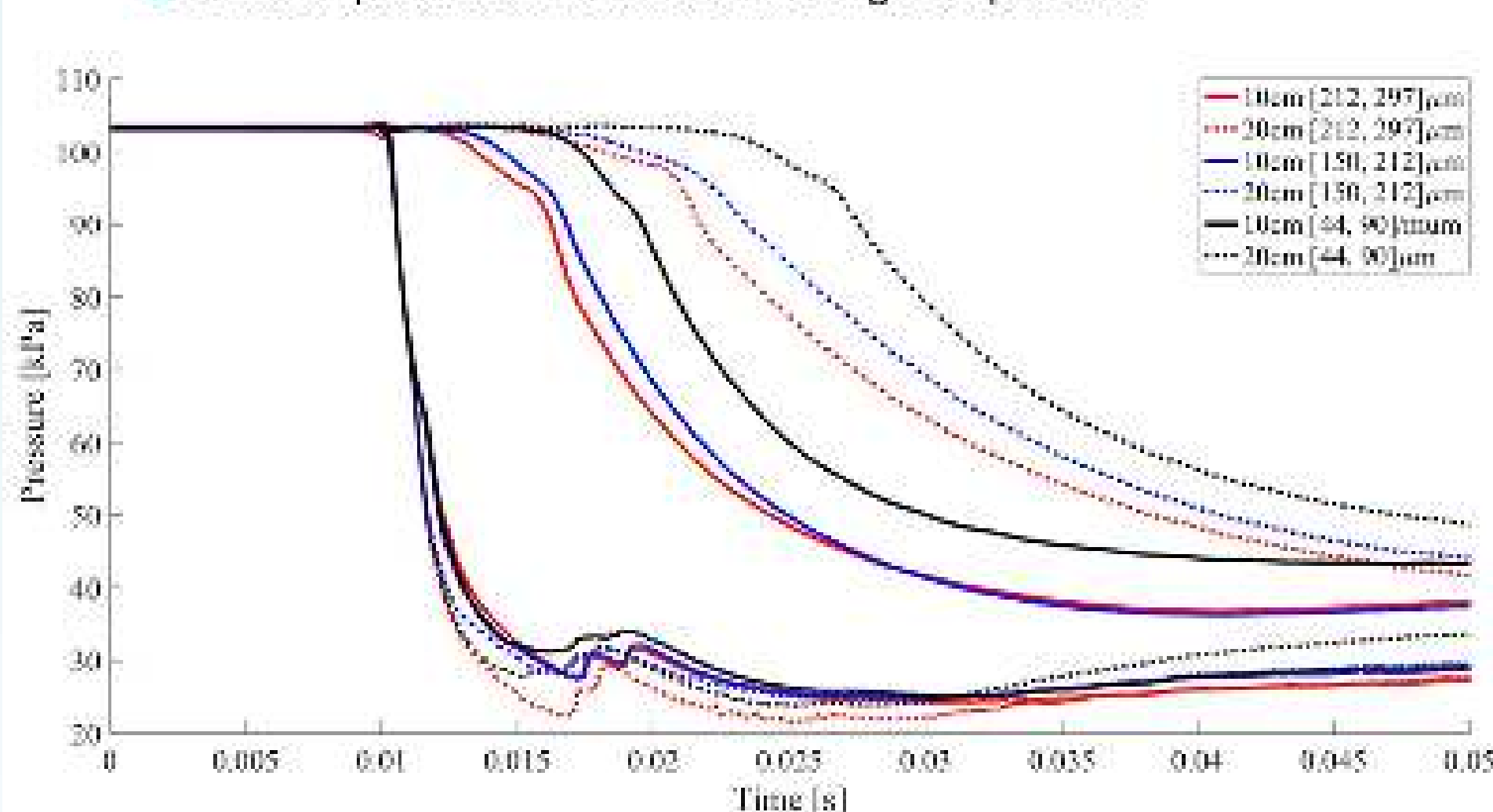
Results

- Effect of particle size and initial bed height on bed displacement
 - Ensemble average of 5 realizations for each experiment



Results

- Effect of particle size and initial bed height on pressure



Summary

- Bed height
 - Beds composed of smaller particles rise more quickly
 - Taller beds rise more quickly
 - This effect is magnified as particle diameter is increased
- Pressure
 - The rarefaction wave travels more slowly through beds composed of smaller particles
 - This effect is magnified as initial bed height is increased
 - The pressure above the particle bed interface drops more rapidly when the particle bed interface is closer to the diaphragm (i.e. the bed is taller)

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Center for Compressible Multiphase Turbulence

Simulations of Fine Powder Decompression

David Zwick

Advisor: Prof. Balachandrar

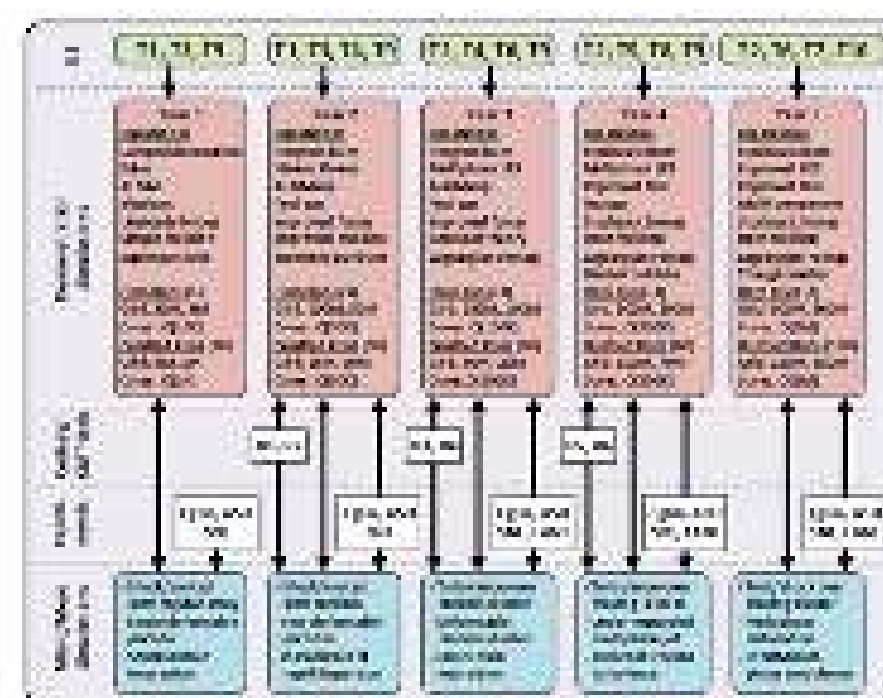
Department: MAE, UF

Goals

- Development of state-of-the-art Eulerian-Lagrangian capabilities in CMT-nek
- Understanding the physics of particles interacting with expansion waves

Simulation roadmap

- Detailed modeling of particle simulations of ASU experiment in CMT-nek



Simulation Roadmap

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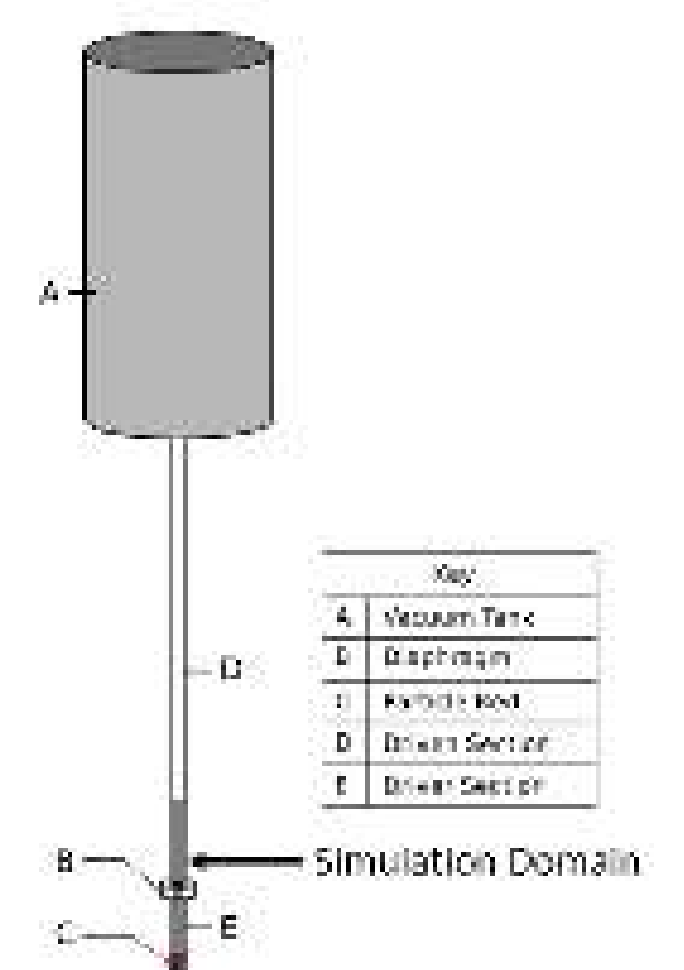
Motivation

Multiphase shock tube is a surrogate used for laboratory-scale volcanic eruptions



- Problem consists of a vertical shock tube with particle bed in driver section
- Particle bed swells upwards due to rapid decompression when diaphragm bursts
- Results are compared with Cagnoli et al. (2002) experiments

Experimental Setup



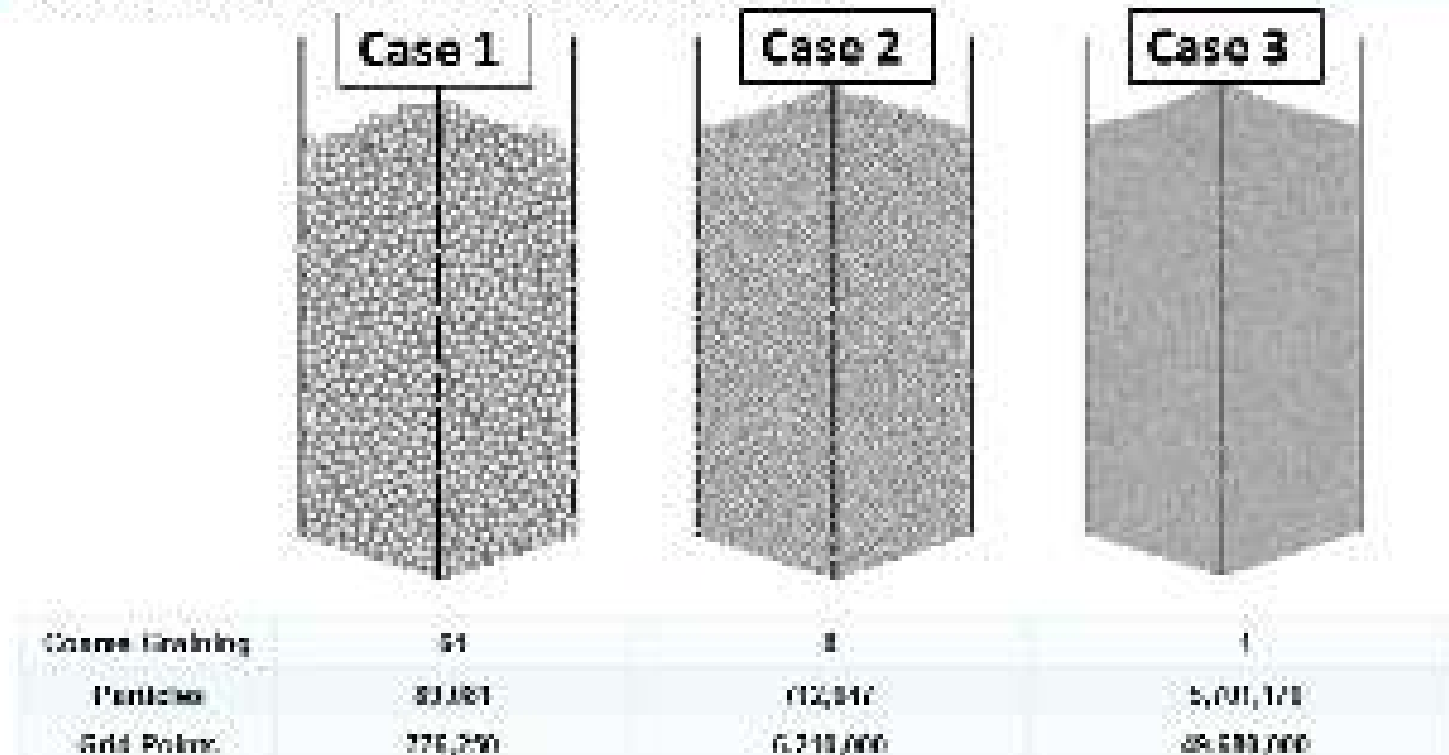
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Multiphase Refinement

- Grid refinement in multiphase flow is not well defined
- We consider two types of refinement:
 - Fluid refinement (grid resolution)
 - Particle refinement (coarse graining)
- Three cases of increased refinement:

Coarse graining:
The number of real particles that each computational particle represents



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Simulation Setup

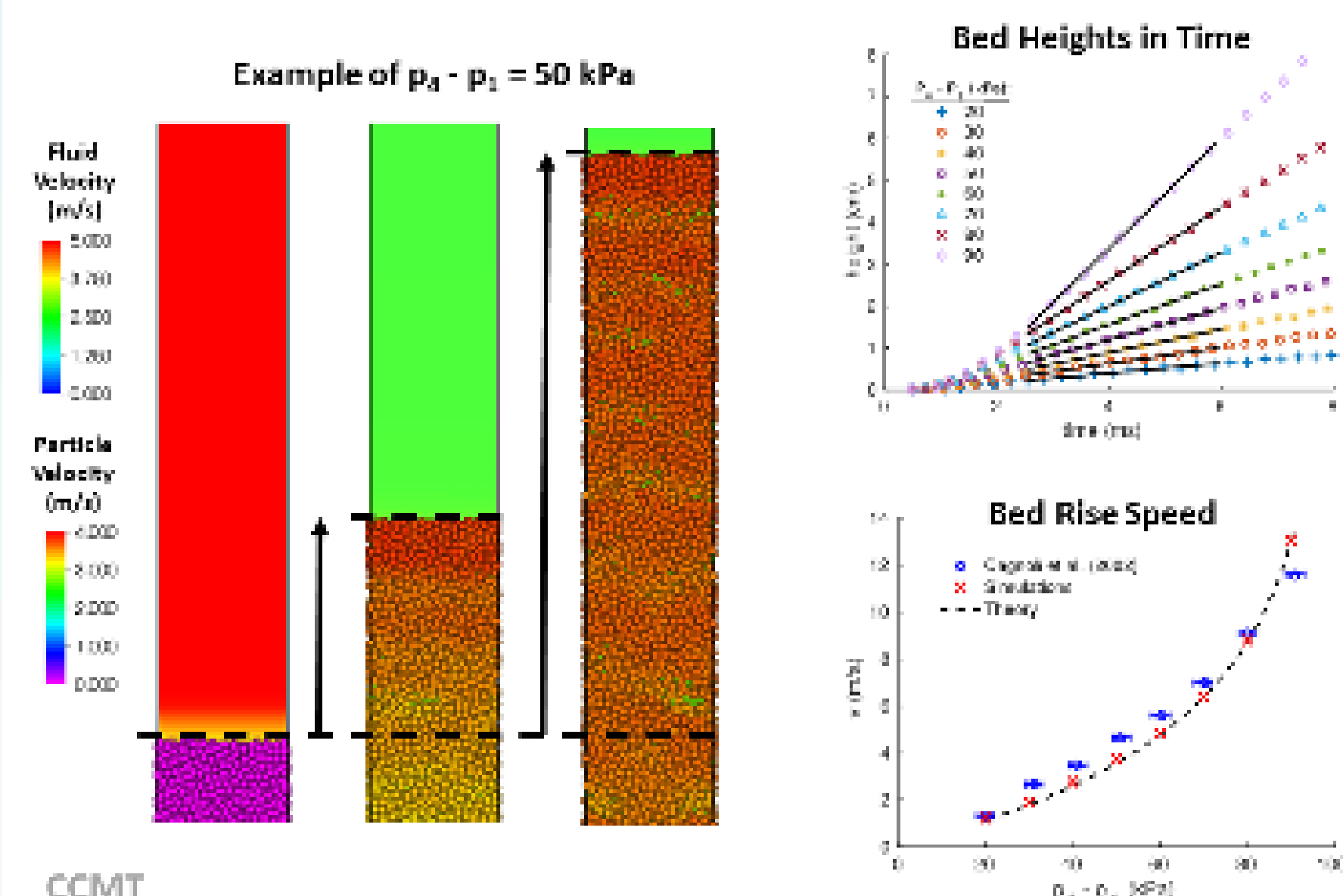
Geometry			Particles		
	Experiment	Simulation		Experiment	Simulation
$L(\text{cm})$	23	23	$d_p(\mu\text{m})$	38	38
$D_0(\text{cm})$	0.2	3.8	$\rho_p(\text{kg/m}^3)$	2,500	2,500
$h_0(\text{cm})$	6.5	6.5	N_p	$\sim 2 \times 10^9$	89k, 713k, 6701k
			$\mu_p(\text{kg/s}^2)$	-	80, 40, 20
			σ_n	-	0.9
Grid			Initial Conditions		
	Simulations			Experiment	Simulation
N_p	6k, 50k, 400k		$p_0(\text{kPa})$	Laboratory	101
N	5		$T_0(\text{K})$	Laboratory	293
$\Delta x(\mu\text{m})$	167, 83, 42		$\Delta p(\text{kPa})$	20 - 80	20 - 80
$\delta_f/\Delta x$	2.5		$T_0(\text{K})$	Laboratory	293
δ_f/D_0	2.85				

Simulations are performed with CMT-nek

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Case 1 Results: Particle Front Movement



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Future Work

- Quantifying the effect of numerical parameters
- Determining the shape/structure of the particle bed front
- Effect of volume fraction dependent drag models in void formation
- Validation with ASU experiments

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