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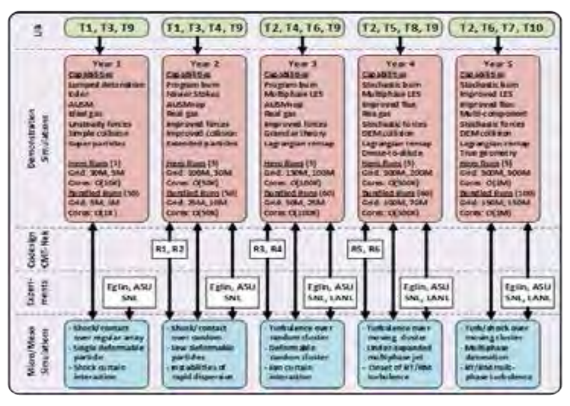
Center for Compressible Multiphase Turbulence

NGEE: Novo-G Exascale Emulator

Student Name: Carlo Pascoe
Advisor: Prof. Herman Lam
Department: ECE, UF

- Goals: Research & develop hardware-accelerated behavioral emulator to scale BE approach of system simulation up to Exascale while maintaining required performance (speed)
  - Explore methods of mapping BEOs onto systems of reconfigurable processors
  - Investigate use of large-scale reconfigurable supercomputing, RSC (e.g., Novo-G#, next-gen RSC) in emulation of Exa/extreme-scale systems

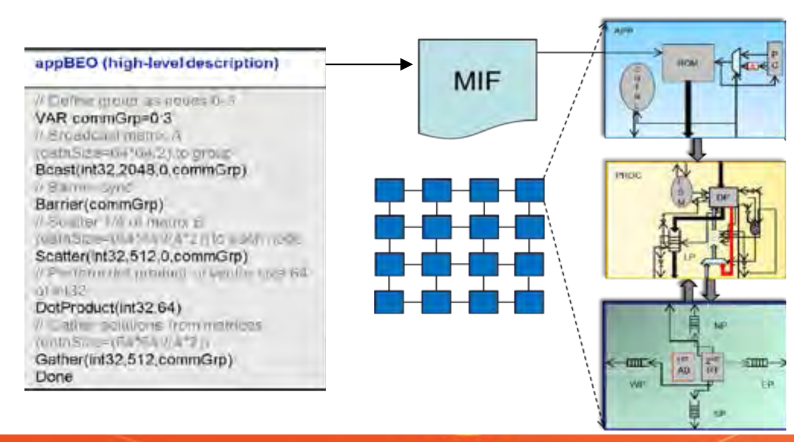


Simulation Roadmap

- Motivation: Behavioral emulation (BE) approach attempts to manage exascale complexity via abstraction of object behavior (BEOs) at multiple scales (micro, meso, and macro levels), but is it enough?
  - Ultimately, how do we simulate exascale without exascale?

Mapping BEOs onto a Single FPGA

- High-level appBEO script (abstraction of target app) mapped to custom machine code (MIF file)
  - Stream of instructions for procBEOs
- ProcBEOs as Lightweight processing elements to mimic "real" processor under study
  - Instruction decoding, timekeeping
  - No real computation: interpolation of compute operations
  - Generates tokens to emulate comm packets
- System-specific: fabric is explicit emulation of target architecture
  - Packets transferred contain characteristics of (not real) data



Current Single-FPGA Prototype: NGEEv1

Functioning prototype running on single FPGA of Novo-G

- No optimization (i.e., max-resource implementation)
- Current core density of 90 for Stratix IV, 256 for Stratix V
  - Each core contains one each of appBEO, procBEO, and commBEO
  - Stratix IV currently limited by FPGA block RAM, not logic
    - 9x10 mesh on Stratix IV: logic 19%, block memory 100%
  - Higher core density on Stratix V
    - 16x16 mesh on Stratix V: logic 94%, block memory 100%
- appBEO scripts stored in on-chip block RAMs as memory initialization files (MIFs)
- Proc interpolation resources replaced with MIF pre-processing
- Explicit emulation of target communication fabric without congestion modeling
- Separate management plane fabric collecting management tokens for postmortem analysis (e.g., simulation visualization)

NGEEv1 Performance Comparison: 3 Data Points

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

Next-gen

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

Anticipated

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

*Spectral Element Solver

Transitioning to Multiple FPGAs

With Novo-G# as target system architecture, requires modification of current design to allow communication between commBEOs instantiated on different FPGAs over direct FPGA interconnect

- Effect on current single-FPGA design?
  - Added communication infrastructure & overhead
  - Multi-layer communication protocol & virtual network fabric
  - Modified ISA, packet structure, management tokens, inter-device bandwidth allocation
  - General design considerations (e.g., arbitrary no. of resources vs. hardcoded limits of single FPGA)
  - Likely reduced BEO density
- Implications on speed/scalability?
  - BEO wait times
  - Inter-FPGA event queuing, flow controls, queuing size, event reordering
  - Sharing of BEO resources
  - Proposed scalability measurement & its use to inform multi-FPGA design decisions

Summary

Achievements

- Working single-FPGA prototype (NGEEv1) with max-resource implementation & management plane (no optimization)
- Beginning stages of performance optimization & scalability evaluation
- Initial planning for next NGEE design (NGEEv2)

Year 2 plans

- Prototype NGEEv1 platform operating on multiple FPGAs
- Extend SMP simulator performance comparison with NGEEv1 to new set of system architectures e.g.,
  - Anticipated Intel Xeon Phi KNL
  - New CMT-Nek centric app case studies
- Upgraded Novo-G# (4x4x4 torus) supporting BE
- Updated scalability experiments on Novo-G# incorporating results from multi-FPGA experiments

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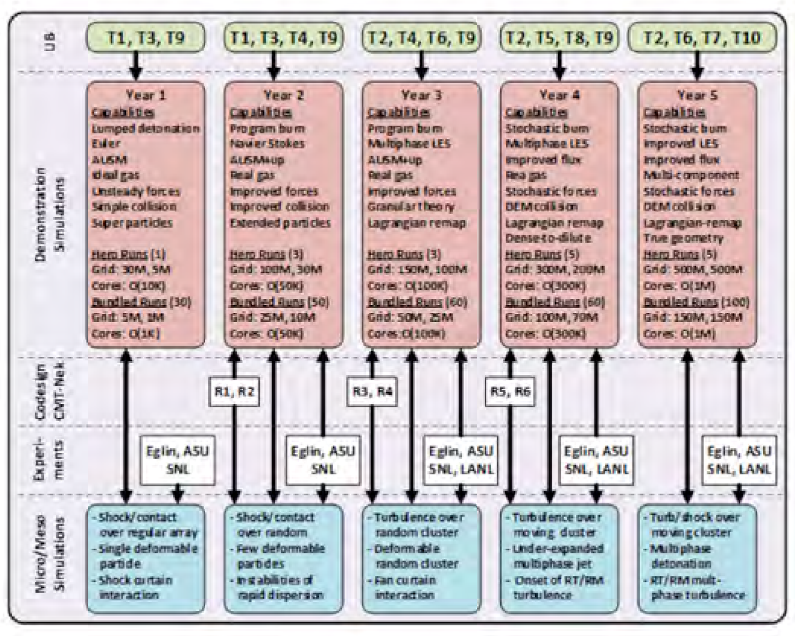
Uncertainty Budget for CMT Simulation

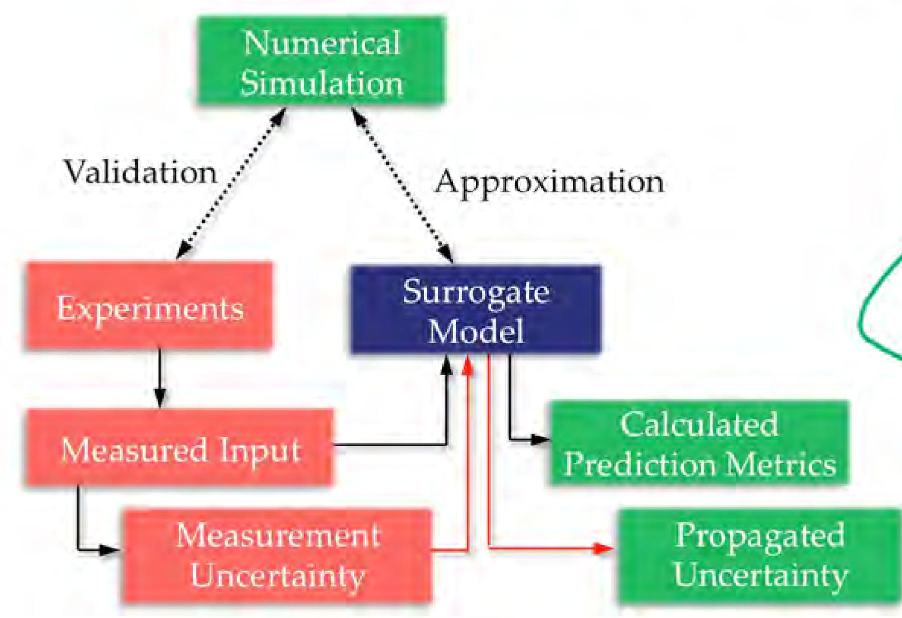
Dr. Chanyoung Park
Department: CCMT, UF

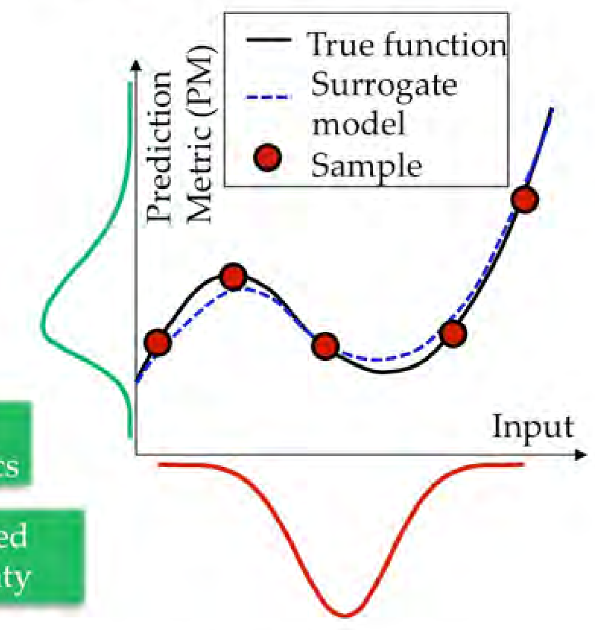
- Goals
  - V&V and UQ
  - Planning experiments and model developments for efficient uncertainty reduction
  - UQ tool developments
- Simulation roadmap
  - T4: Verification and validation of the shock tube simulation
  - T6: Finite Re, Ma and volume fraction model



Simulation Roadmap

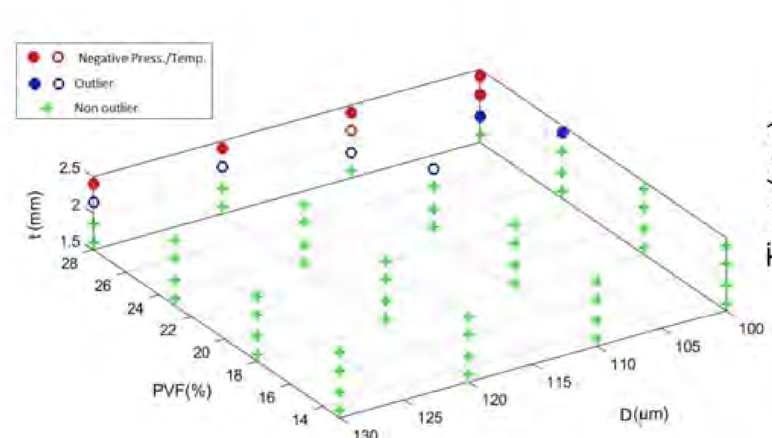
Computational Challenge of UQ

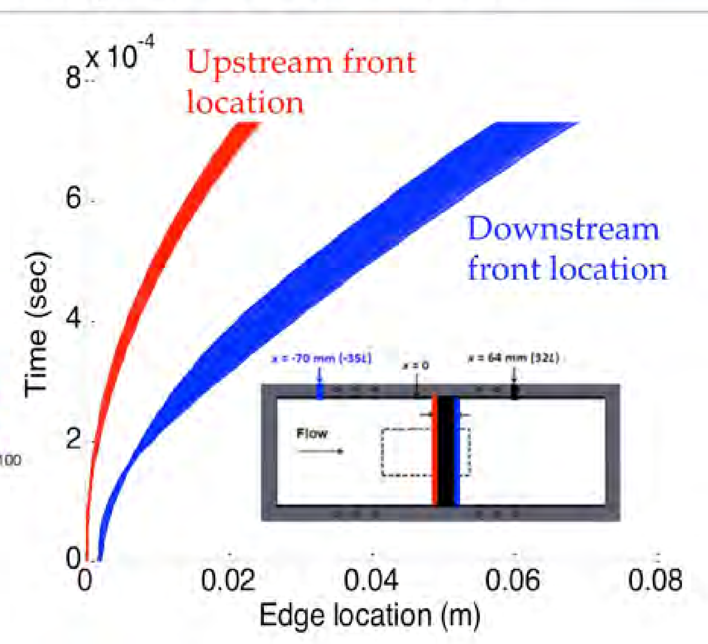




- General uncertainty propagation approach Monte Carlo method often requires thousands of simulations
- To avoid this large number of simulations runs, we use surrogate models built with a dozen of samples

Propagated Uncertainty of Meso Sim.

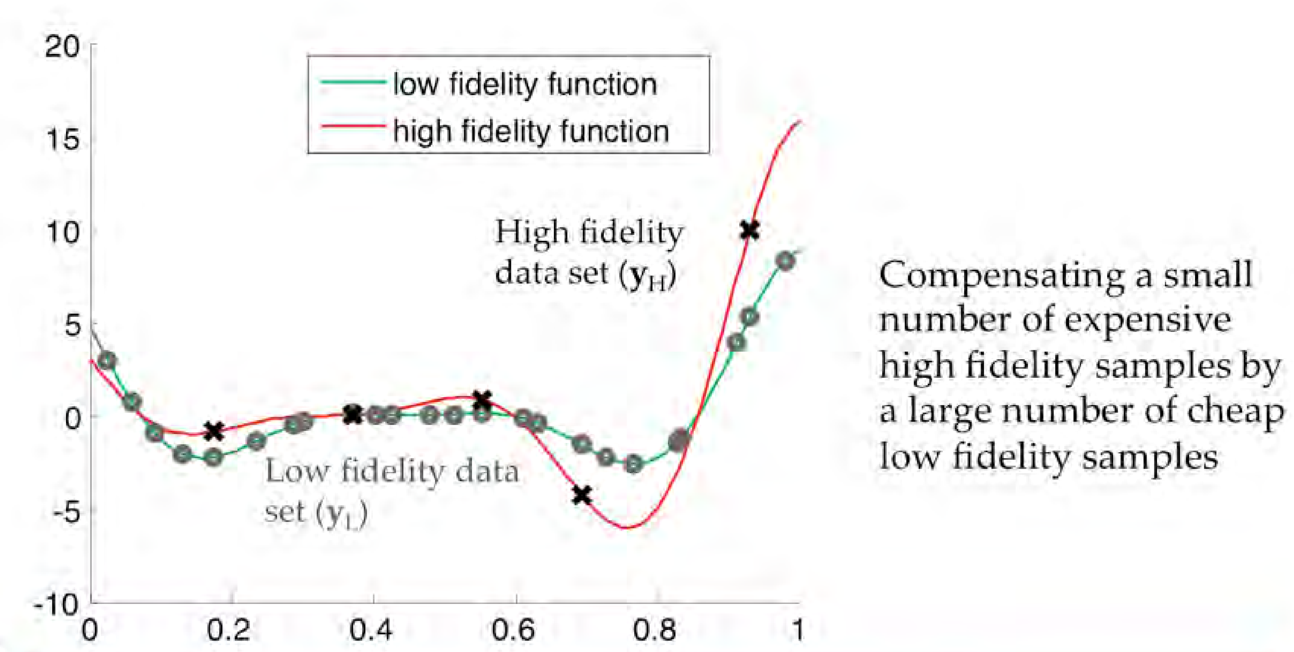




- Uncertainties in the curtain thickness, particle diameter and volume fraction are propagated through a Kriging surrogate
- 64 simulations were run for obtaining the edge location curves
  - DAKOTA was used to evaluate samples by managing simulation runs
  - Sampling also revealed the valid parameter domain of the simulation

Multi-Fidelity Surrogates (MFS)

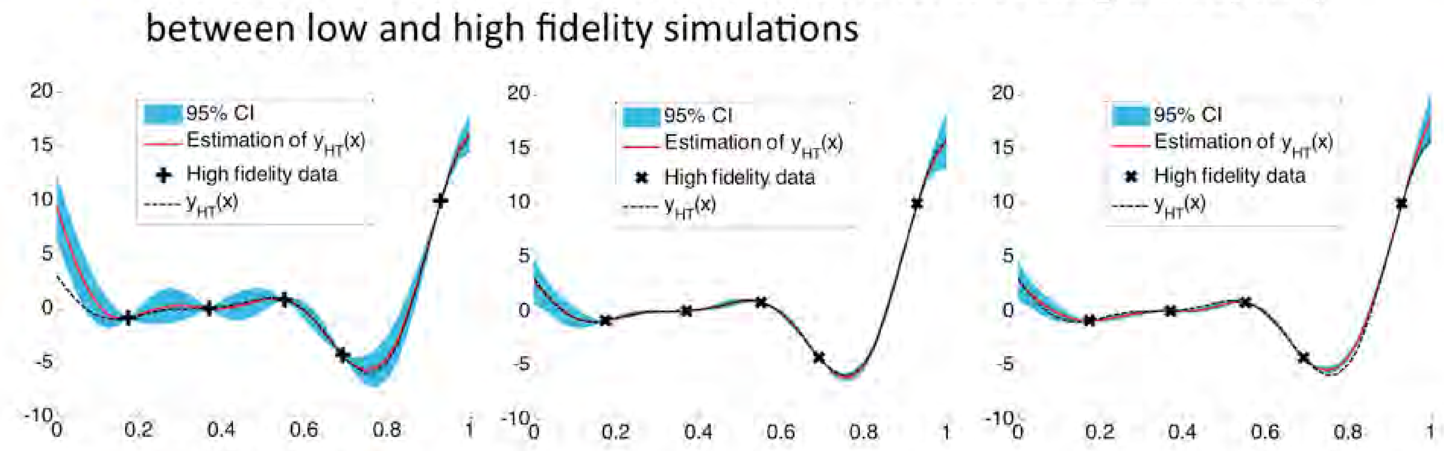
- UQ of computationally extremely intensive high fidelity simulations
- Building surrogate by combining samples from multi-fidelity simulations
  - UQ of macro scale 3D models using MFS based on 1D/2D/3D simulations
  - UQ of meso scale 3D models using MFS based on 1D/2D/3D simulations



Compensating a small number of expensive high fidelity samples by a large number of cheap low fidelity samples

Frameworks for Fitting MFS

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



$\hat{y}_H(x) = \rho\hat{y}_L(x) + \hat{\delta}(x)$ Discrepancy function based framework

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

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

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

Fitting Force Kernels from Microscale

- Inter-phase force coupling
- Hybrid approach using kernels:

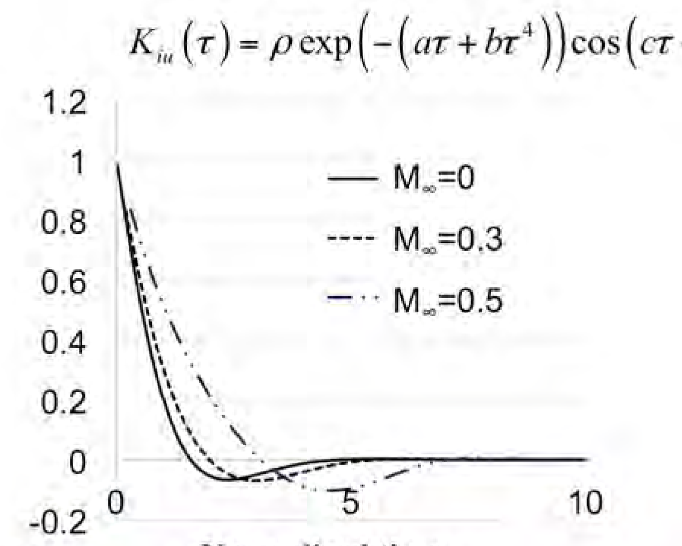
$$\mathbf{F} = \text{function of } \{C_D(\mathrm{Re}, \mathrm{M}, \phi), K_{iu}(\mathrm{M}, \phi), K_{vu}(\mathrm{Re}, \mathrm{M}, \phi)\}$$

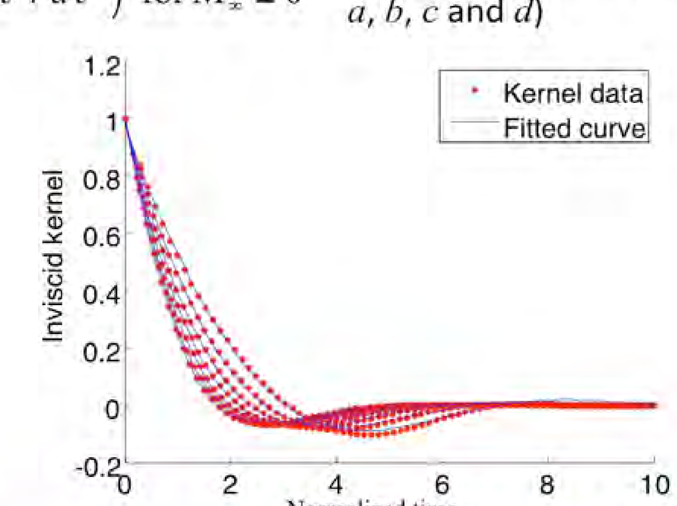
- Physical-algebraic hybrid surrogates were developed for fitting the inviscid unsteady kernel

$$K_{iu}(\tau) = \exp(-\tau)\cos(\tau) \quad \text{for } \mathrm{M}_\infty = 0$$

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

(Calibration parameters: *a*, *b*, *c* and *d*)





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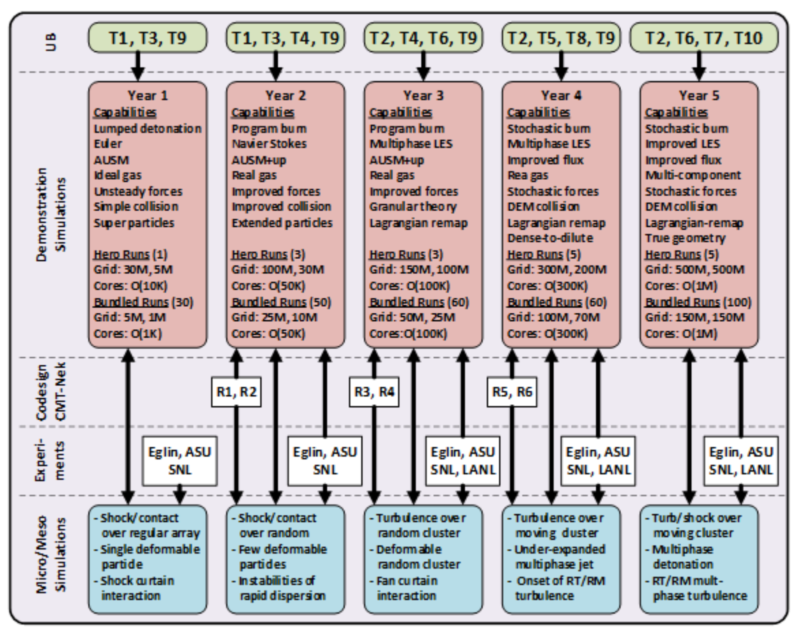
Error Analysis For Euler-Lagrange Formulation

Student: Angela Diggs

Advisor: Prof. S. Balachandar

Department: MAE, UF

- Goals
  - High-fidelity Euler-Lagrange coupling
  - Euler-Lagrange AUSM+-up
  - Validation against Sandia multiphase experiments
- Simulation roadmap
  - Rigorous error-estimation of Euler-Lagrange implementation (T9)
  - Critical evaluation of inter-particle collision model (T4) and volume fraction effects (T6)

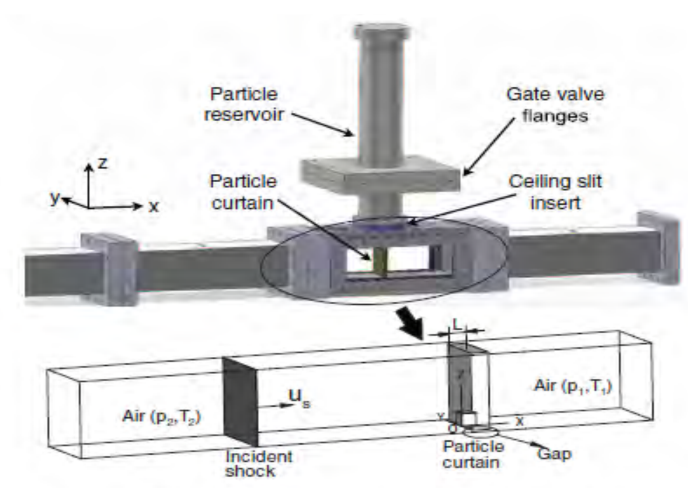


Simulation Roadmap

Motivation

- Shock Induced Particle Flow

- Simulation Setup
  - 1d shock tube
  - 100 µm particles
  - Mesoscale validation against Sandia experiments
  - Address all the fundamental challenges in Euler-Lagrange simulations of particle-particle interaction dominated flows

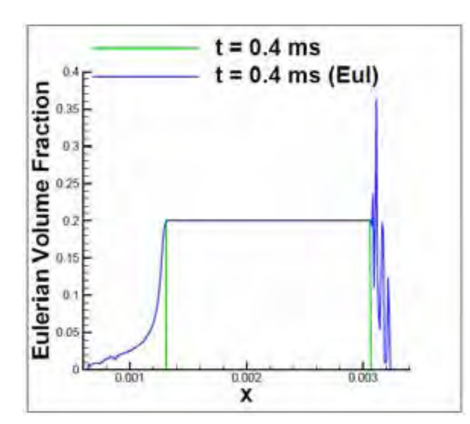


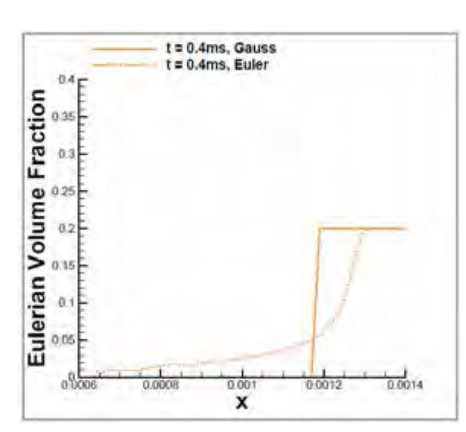
Flux Schemes For Multiphase Flows

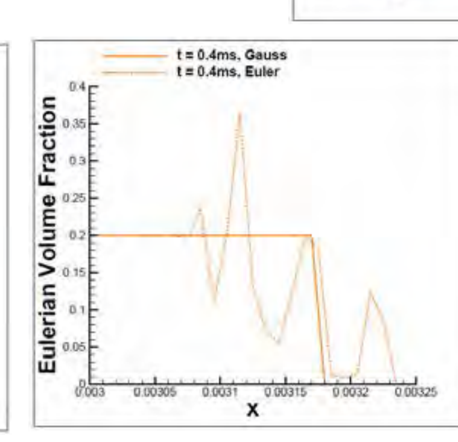
- AUSM+-up Flux Scheme
  - Developed by Liou, et al (2006)
  - Extension of AUSM (1993), AUSM+ (1996)
  - Eulerian-Eulerian formulation in literature; extended to Eulerian-Lagrangian
  - Rigorous verification using quiescent solid phase to emulate nozzle walls
    - Subsonic and supersonic flows
    - Match to isentropic properties
  - Investigate effect in shock tube (no analytic solution)
  - Discretization error will be established
- Observations
  - Desired resolution in volume fraction variation depends on use case
    - Nozzle requires a sufficiently smooth transition
    - Shock tube yields stronger shocks for sharp transition
  - Diffusion parameters (Ku, Kp) only effective after discontinuity
    - No apparent penalty for using
  - Use of non-zero interface pressure coefficient is not recommended

Euler-Lagrangian Coupling: Volume Fraction

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

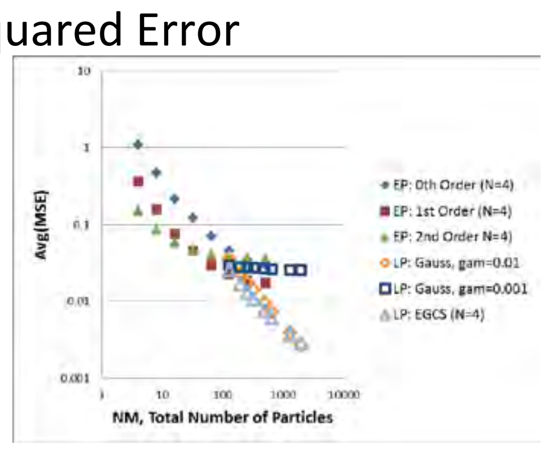


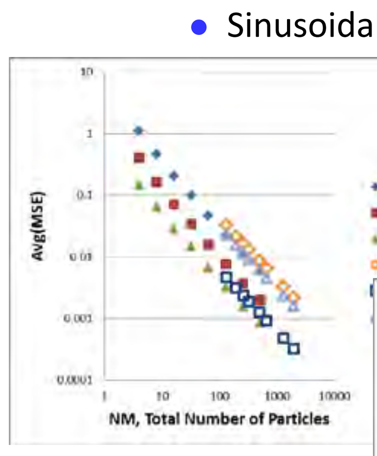


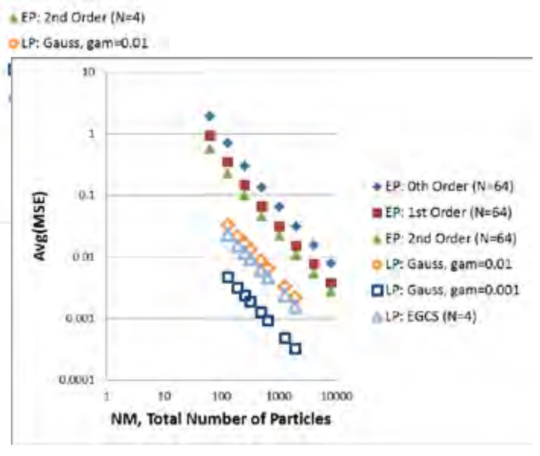


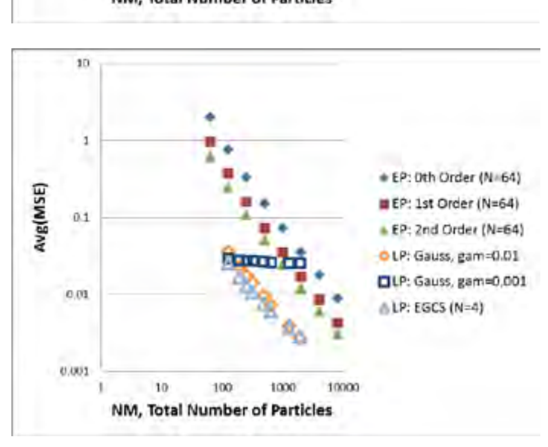
Von Neumann Error Analysis

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









Key Results and Future Work

- Discovery of new volume fraction instability
- Accurate way to compute volume fraction
- Consistent approaches to interpolation & projection
- Optimal number of computational particles per cell
- Improved fluxes for Euler-Lagrange simulations

- New approaches to Lagrangian remap
- Improved implementation of unsteady force and heat transfer
- Improved implementation of collisional-effects
- Validation against Sandia experiments and uncertainty quantification

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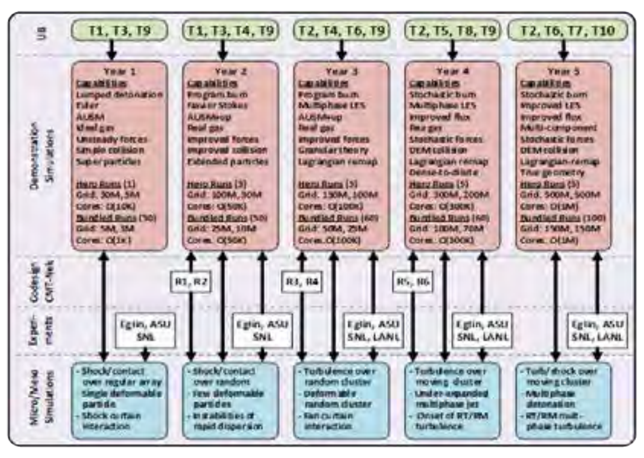
NGEE: Performance Modeling

Student Name: Dylan Rudolph
Advisor: Prof. Greg Stitt
Department: ECE, UF



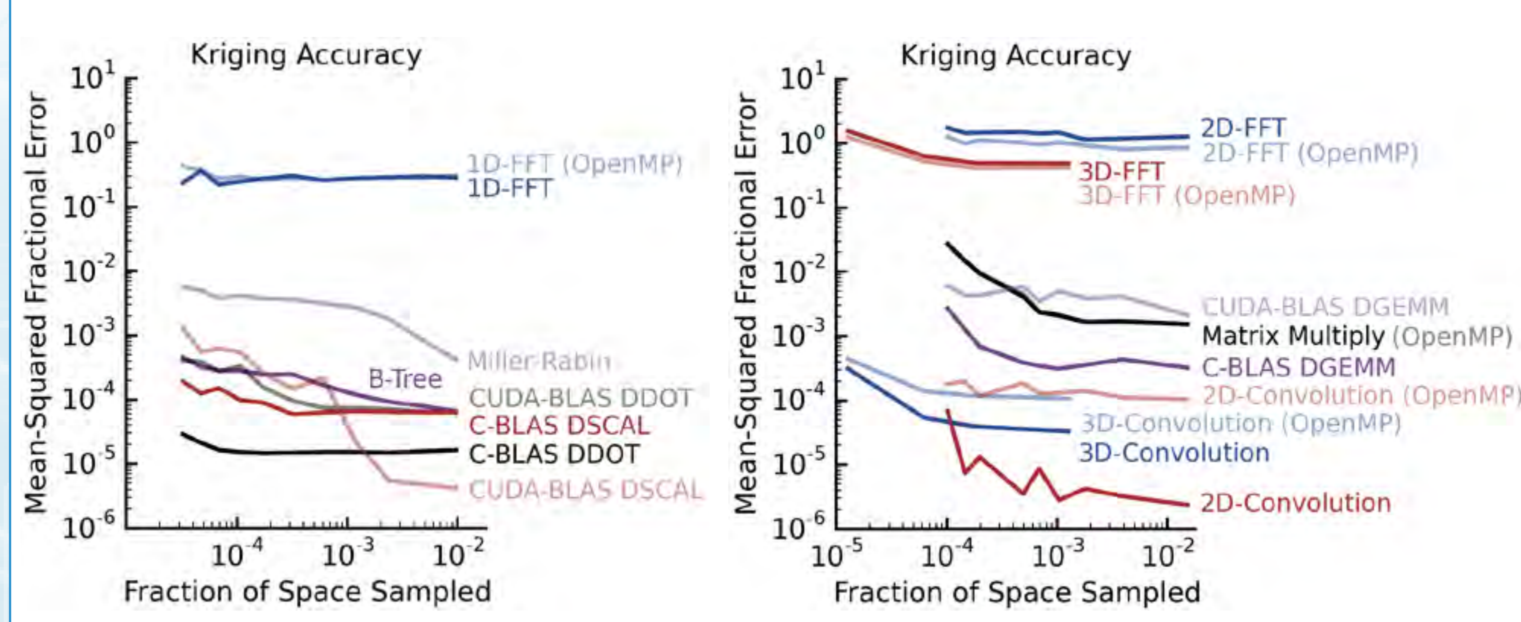
Simulation Roadmap

- Goals:
  - Estimate values of specific non-integral numerical parameters (e.g., computation time) before or during simulation without having access to real generators (e.g., the target CPU) of those parameters
  - Determine efficacy of possible surrogates in multi-dimensional domains
  - Perform uncertainty analysis to determine degree to which estimation is introducing error into the simulator
- Motivation:
  - Behavioral emulation necessitates that simulators do not perform cycle-accurate operations
  - Simulators must still know time required for an operation (e.g., Matrix Multiply) based on input sizes (e.g., [M, N, P] = [256, 100, 42])

Performance Modeling: Results

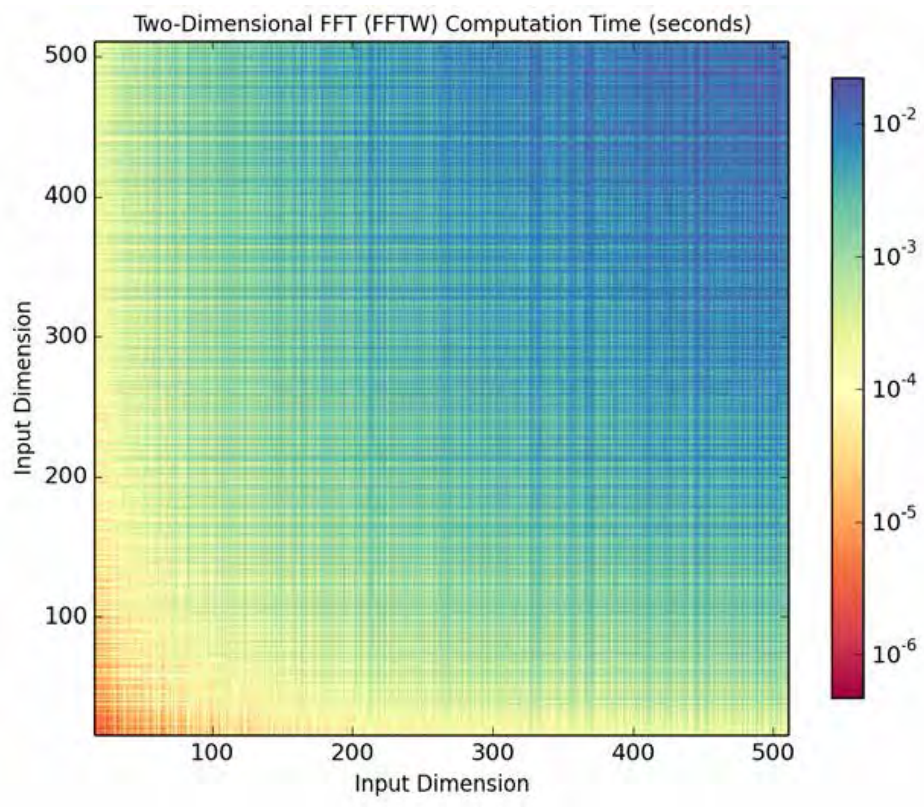
Absolute Accuracy of Kriging for Evaluation Benchmarks

Single-Dimensional Benchmarks (One Input Parameter) | Multi-Dimensional Benchmarks (Two and Three Input Parameters)



Performance Modeling: Sample Data

What do our data look like? (FFTW 2D FFT Routine)

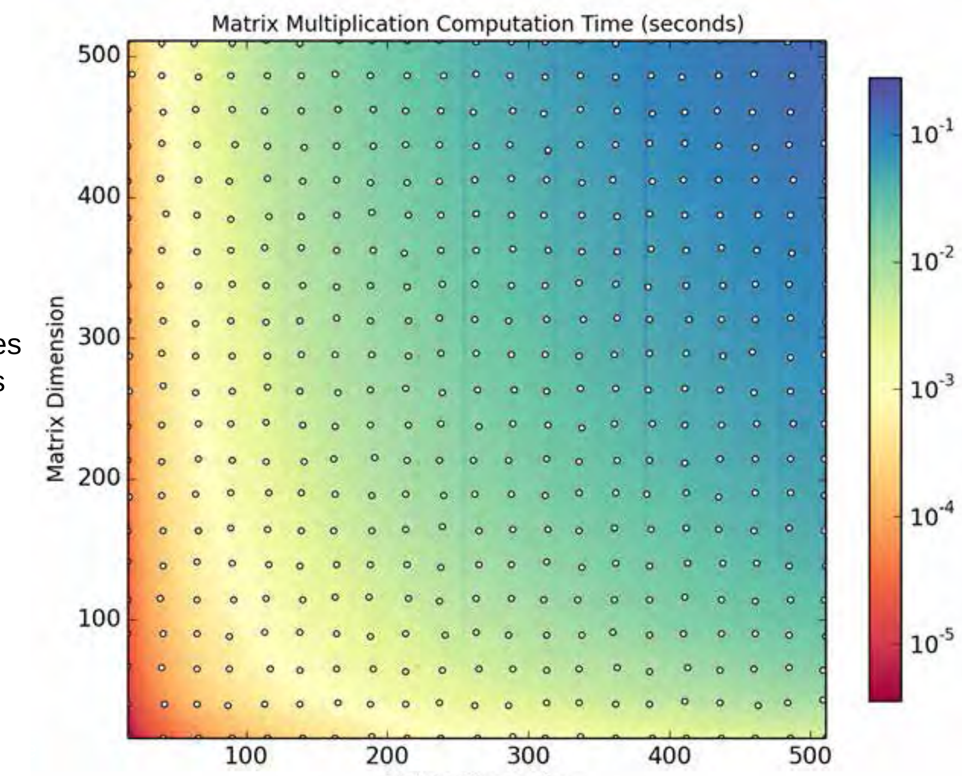


- FFTs (FFTW) are among the most difficult benchmarks
  - Computation time strongly related to how composite the input size is
  - Adjacent samples can jump by more than an order of magnitude
  - Interpolating to obtain an average error fraction of just below 1 is difficult
- Example details:
  - Platform: x86 Ivy-Bridge Quad
  - Single Core Used
  - FFTW
  - C, GCC, -O2

Performance Modeling: Process (1/3)

Step One: Obtain ordered, but slightly randomized samples within the domain

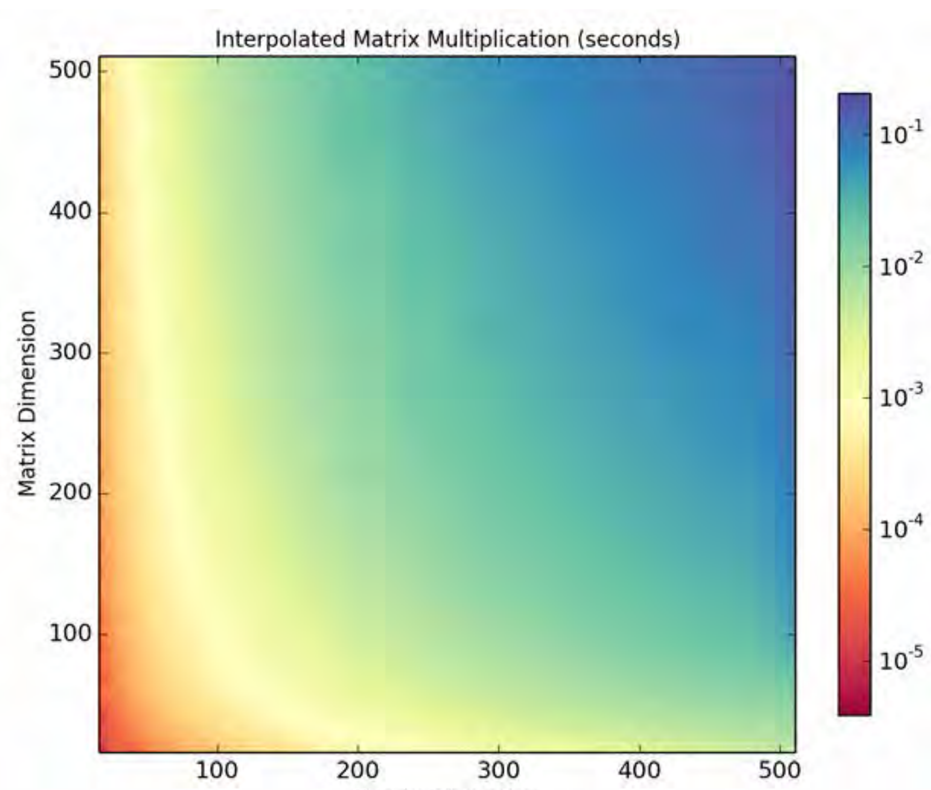
- Randomization prevents aliasing along areas of unusual time
- Determining the number of samples to use is one of the research goals
- Even sampling may not be ideal, but to do otherwise requires unavailable a priori knowledge
- Example details:
  - These samples cover 0.17% of the domain, a relatively small amount
  - Notably: they mostly missed the bands of high computation time



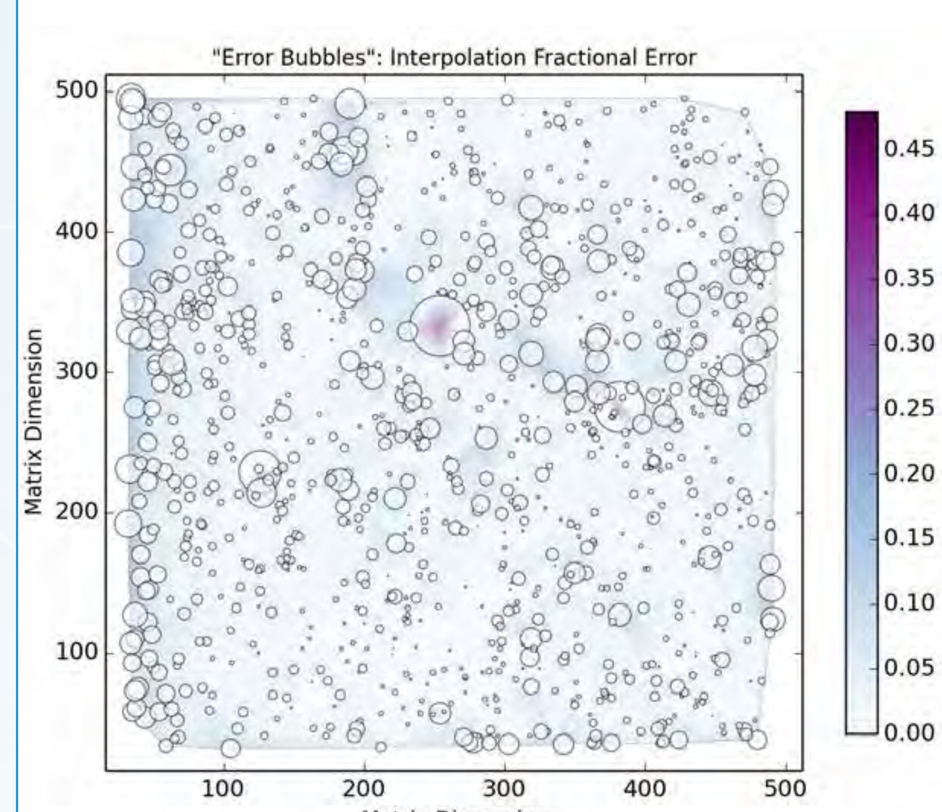
Performance Modeling: Process (2/3)

Step Two: Using those samples, construct an interpolation model

- After entering these parameters, we have a model which can substituted for the real data in the simulator (the surrogate)
- It will not be perfect, as it is subject to both the samples and the parameters
- For example: this model loses most of the banding of the original data



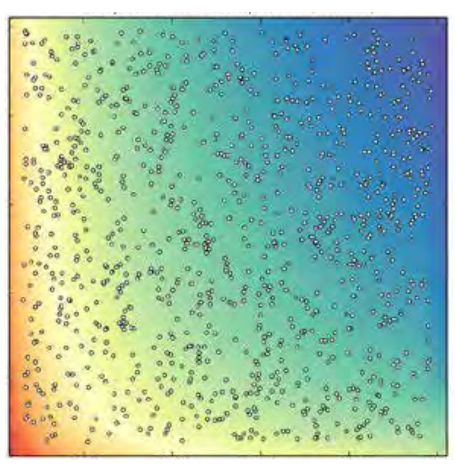
Performance Modeling: Process (3/3)



Step Three: Evaluate the model with another dataset and an error metric

- Test data are completely random within the domain
- Our Error Metric: average mean-squared fractional error

Step Four: Revise the model iteratively as needed.



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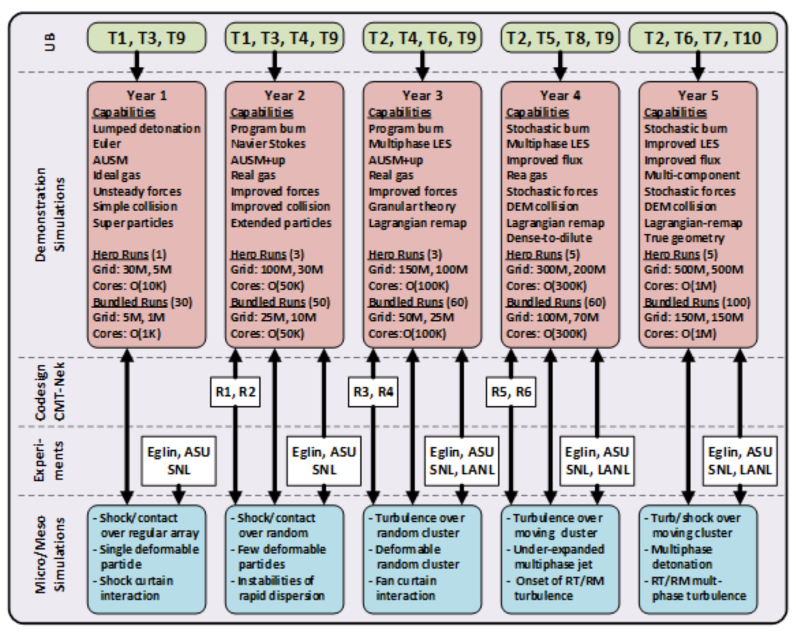
Early-Time Study of the Demonstration Problem

Student: Frederick Ouellet
Advisor: Dr. S. Balachandar
Department: MAE, UF

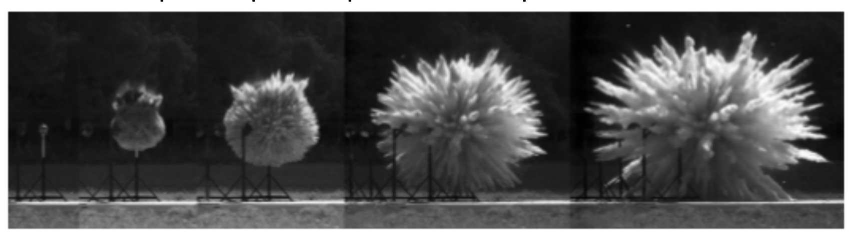
- Goals
  - Analyze the development of Rayleigh-Taylor (RT) and Richtmyer-Meshkov (RM) instabilities in explosively driven flows
  - Quantify the effects of particles and turbulence in RT/RM instabilities
- Simulation Roadmap
  - RT/RM development in the detonation problem
  - Analysis of RT/RM turbulence effects on particles and gas



Simulation Roadmap

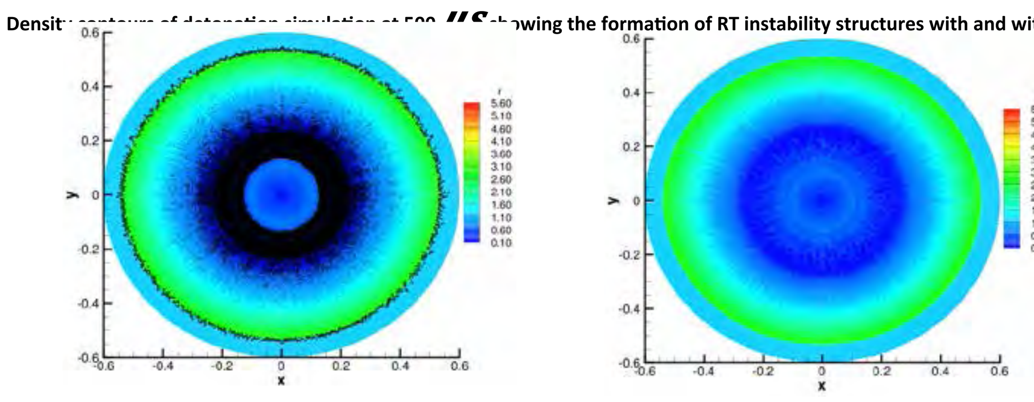
Motivation

Explosive dispersal of a packed bed of sand particles



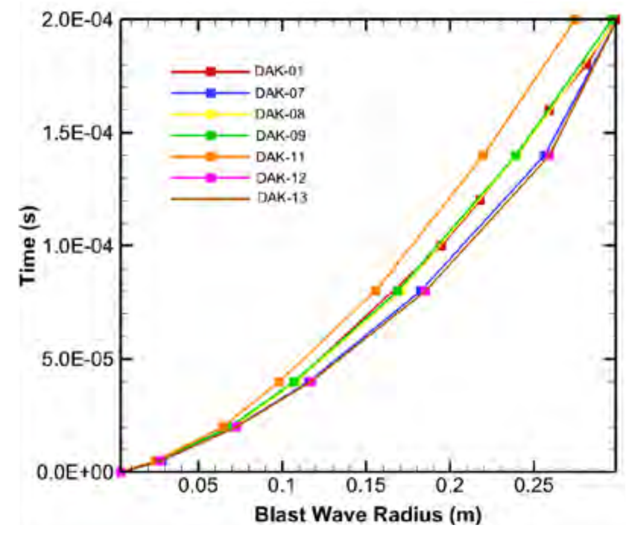
(D. L. Frost, Y. Gregoire, O. Petel, S. Goroshin, and F. Zhang, "Particle jet formation during explosive dispersal of solid particles," Physics of Fluids, vol. 24, no. 9, p. 1109, 2012.)

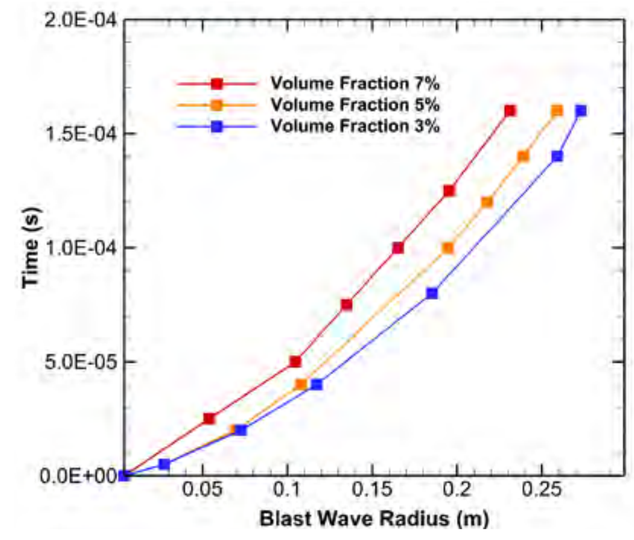
Density contours of detonation simulation at 500 μs showing the formation of RT instability structures with and without particles



- The pictures taken by Frost et. al during their detonation experiments show the formation of coherent jets at late time
- The images below show the development of the RT instability in the gas at early times. We believe that the jets shown above are related to these early time instabilities.

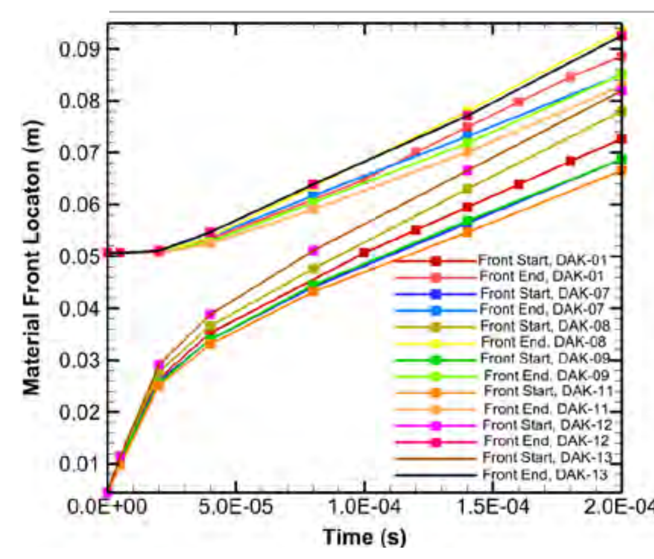
Blast Wave Speed

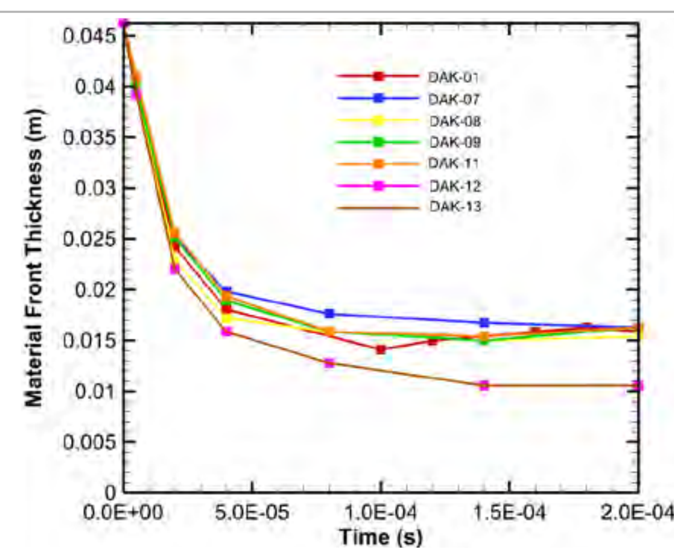




- Higher particle volume fractions lead to a slower blast wave. The particle bed acts like an obstacle to the shock wave.
- Note: The Frost video shows the blast wave radius to be 0.25 m at 200 μs while our cases will hit that mark earlier, i.e., our blast waves are faster. Possible reasons for this include:
  1) We are still assuming an ideal gas and are not using real gas relations.
  2) The particle volume fractions that are being run are still much lower than those used in the experiment.

Sensitivity to Initial Conditions



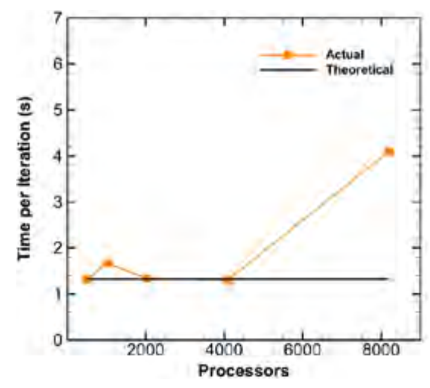


Case #	Particle Distribution	Volume Fraction	N_{CP} (millions)	Particle Diameter (μm)	Density ($\frac{kg}{m^3}$)	Total Energy ($\frac{J}{m^3}$)
1	Cell Centroid	5 %	5	100	2500	1.01×10^{10}
7	Cell Centroid	5 %	5	150	2500	1.01×10^{10}
8	Cell Centroid	5 %	5	100	2200	1.01×10^{10}
9	Cell Centroid	5 %	5	100	2800	1.01×10^{10}
11	Cell Centroid	5 %	5	100	2500	5.57×10^{9}
12	Cell Centroid	3 %	5	100	2500	1.01×10^{10}
13	Cell Random	5 %	5	100	2500	1.01×10^{10}

- Increasing the initial particle diameter will increase the thickness of the material front while decreasing the initial particle volume fraction will decrease the front thickness.

Scaling Studies

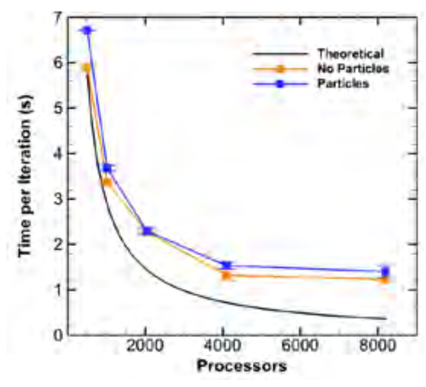
Weak Scaling:

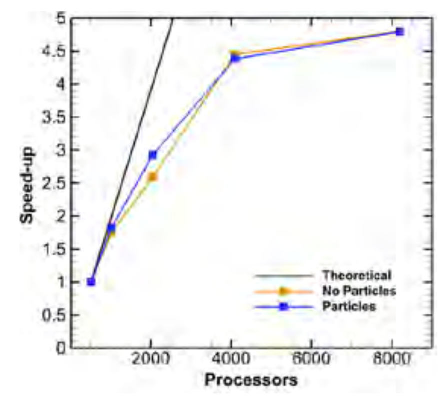


- Weak Scaling conditions: Demonstration problem grid, ratio of grid points to number of processors is 7068.
- Relative Scaling conditions: Demonstration problem grid, 30 million grid points, 5 million particles.

Relative "Strong" Scaling:

(Per definition, a strong scaling study computes the speed-up relative to a sequential run. Our reference run uses 512 processors.)





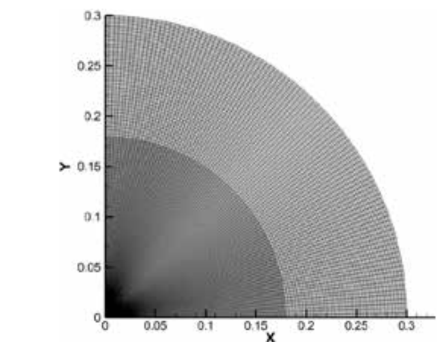
- **The relative scaling speed-up is roughly linear until 4096 processors, where it then flattens out.**
- **We believe the 8192 processor case for the weak scaling is slow due to too much communication among processors.**

Summary

- Analyzed the sensitivity of demonstration problem in early times to changes in initial conditions.
- Performed scaling studies of the demonstration problem.

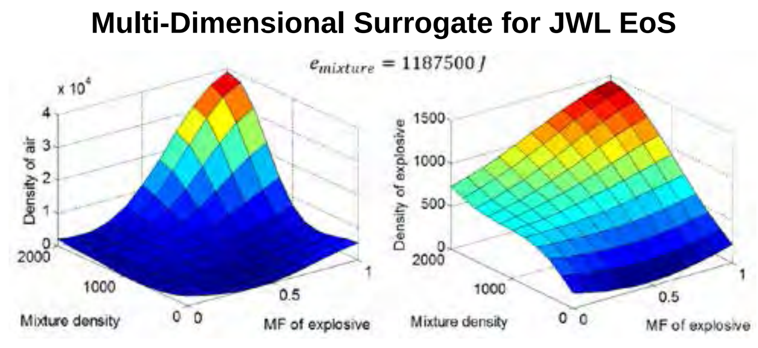
Future Work

Mesoscale Demonstration Problem Grid



- Mesoscale simulations of the demonstration problem will study the details of instability driven mixing and multiphase turbulence.

Multi-Dimensional Surrogate for JWL EoS



- Developing a surrogate model for real gas behavior in collaboration with UB team.

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Uncertainty Quantification in the 1D Code

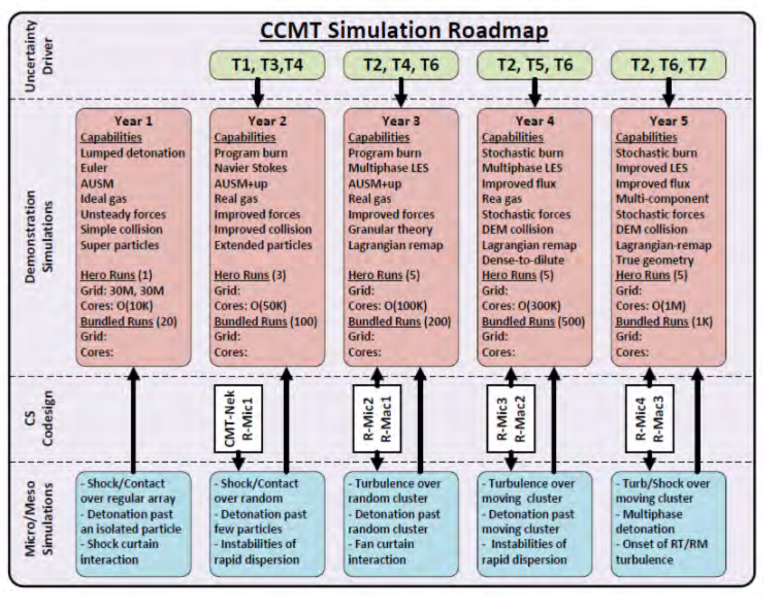
Student: M. Giselle Fernandez

Advisors: Dr. Raphael T. Haftka

Dr. Nam Ho Kim

Department: MAE, UF

- Goals:
  - Validation, uncertainty quantification, and detecting anomalies in the 1D shock tube simulation
- Simulation roadmap:
  - T4: Validation and uncertainty quantification in mesoscale simulations



Simulation Roadmap

Motivation

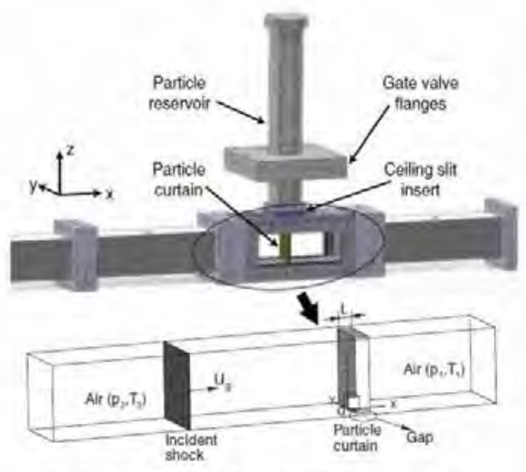


Figure 1. Sandia Laboratories multiphase shock tube experimental setup.

- 1-D shock tube simulation: planar shock wave interacting with a dense particle curtain
- Takes in account the effects of compressibility and particle volume fraction, unsteady force contributions and inter-particle collision
- Can afford to quantify uncertainty and detect anomalies using high number of simulations

- Main purpose: shock-particle interaction
- Prediction metrics (PM): edge locations of upstream and downstream particle curtain

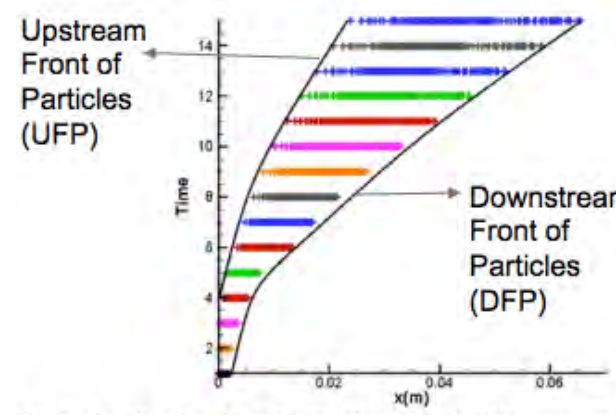


Figure 2. Prediction Metric (PM) used. In different colors are shown the particles at different times after the shock-particle interaction

Detecting Anomalies from Groups of Runs

- When we perform a single simulation, we can detect problems with the model or software when the results are obviously wrong
- In our case, negative pressures and temperatures did that job
- Performing groups of runs allows detecting suspect simulations even if each one singly does not look obviously wrong, see example in Figure 3

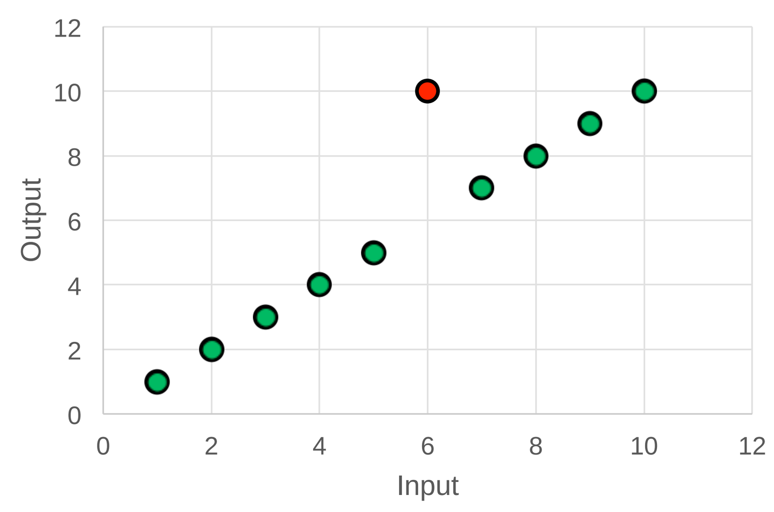


Figure 3. Examples of anomaly detection by comparison.

1D Code: 64 design points in the domain

- Particle diameter (D), initial particle curtain thickness (t) and particle volume fraction (PVF) have the largest effect on uncertainty
- The PM were calculated as these parameters were varied over their range of uncertainty in a 4x4x4 grid
- High PVF values (around 28%), usually led to negative pressures
- Weighted least squares linear regression fit was used to recognize outliers (anomalies)
- Figure 5 shows that all the outliers are at least on one boundary
- Since outliers are on boundary, outlier detection is based on extrapolation
- Extrapolation results will be compared with an improved simulation code or future experimental results.

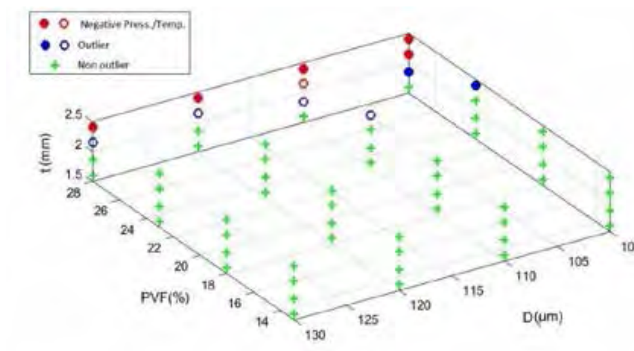


Figure 4. Schematic distribution of outliers (blue dot), bad runs (red dot) and non outliers points(green cross). The filled dots indicate that the point share more than one extreme location.

Detecting Additional Anomalies

- Diameter of particles (D), the initial particle curtain thickness (t) and PVF were varied to predict results at a point fingered as an outlier
- Unexpected anomalies were found that are not related to extrapolation
- PVF was varied from 13% to 23%, the particle diameter from 100µm to 110µm and the initial particle curtain thickness from 1.6mm to 2.4mm

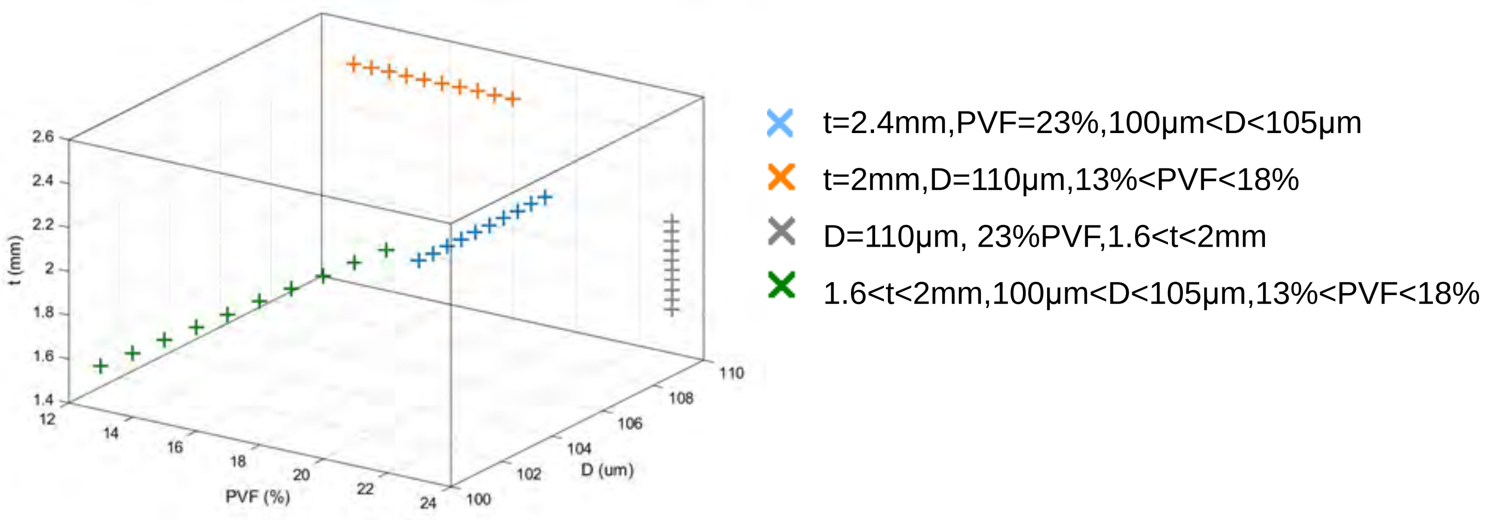


Figure 5. Points selected to perform the code runs for extrapolation. The points are distributed in 4 lines, each line has 10 equally distributed points.

Detected Additional Anomalies

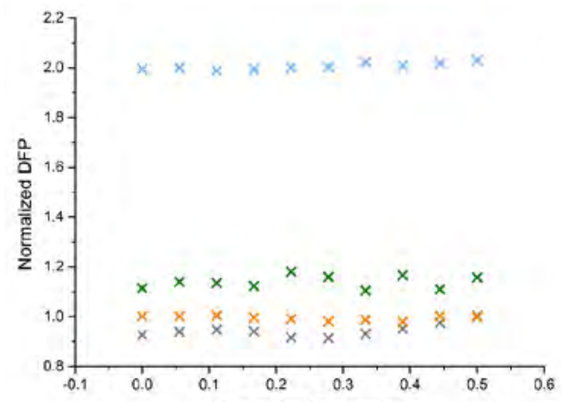


Figure 6. DFP vs. parameter variation

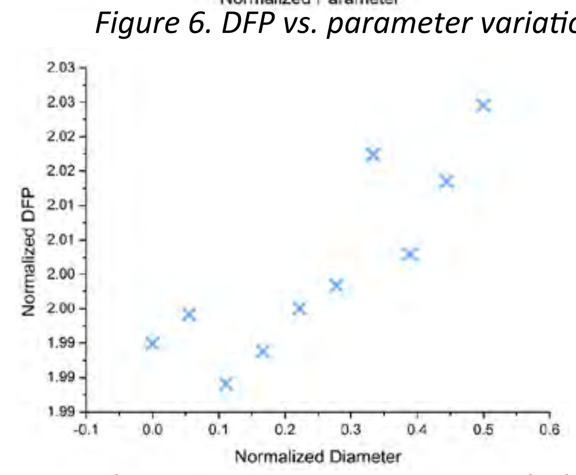


Figure 7. DFP vs. parameter variation

- Normalized results for points in Figure 5 are shown in the left plots
- The results show the DFP location at 50µs after the shock-particle interaction
- Parameters variation was normalized to [0,1] and DFP location to the central point (PVF=18%, D=105µm and t=2mm)
- Figure 6 shows that the diameter variation line (PVF=23%, t=2.4mm) stands out from the other 3 lines indicating possible problems with this combination of PVF and t
- Figure 7 zooms on that line and shows substantial noise in the DFP location that need to be investigated

t=2.4mm,PVF=23%,100µm<D<105µm
t=2mm,D=110µm,13%<PVF<18%
D=110µm, 23%PVF,1.6<t<2mm
1.6<t<2mm,100µm<D<105µm,13%<PVF<18%

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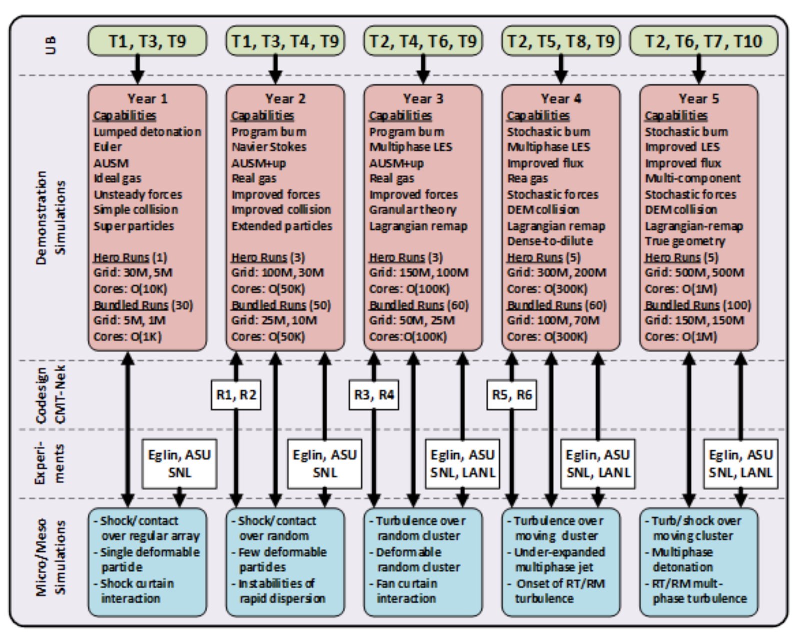
Multiphase Turbulent Jets

Student: Goran Marjanovic
Advisor: Dr. Balachandar
Department: MAE, UF

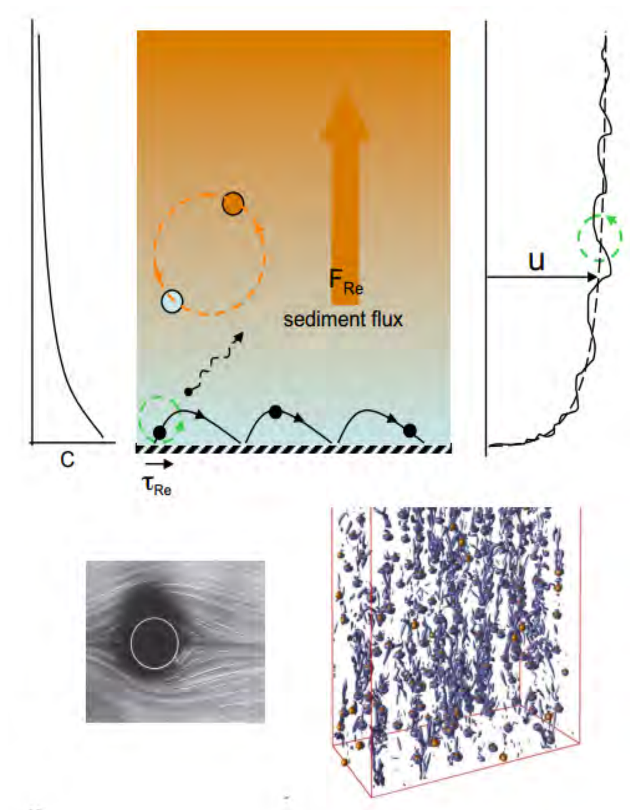
- Goals
  - Eulerian-Eulerian
  - Lagrange Point Particle Tracking
  - LES
- Simulation roadmap
  - Year 2: Eulerian-Eulerian & LPP simulations
  - Year 3: LES simulations, implement LPP, LES in to CMT-Nek
  - Year 4: Refine LES models, scalability



Simulation Roadmap

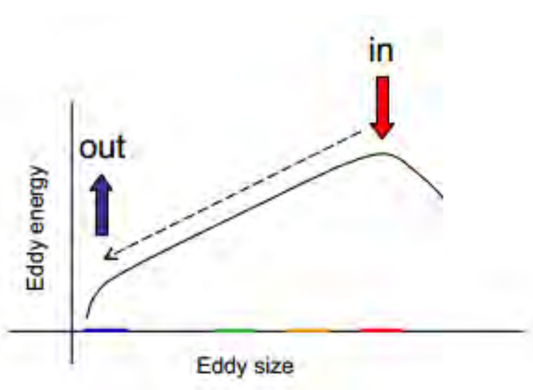
Motivation - Physics

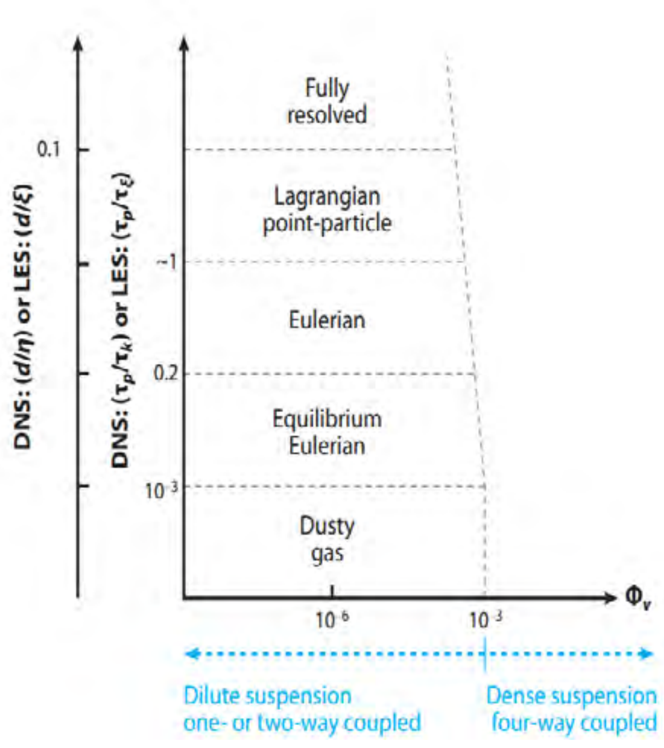
- Jet-like structures
- Entrainment
- Turbulence modulation
- Preferential particle accumulation



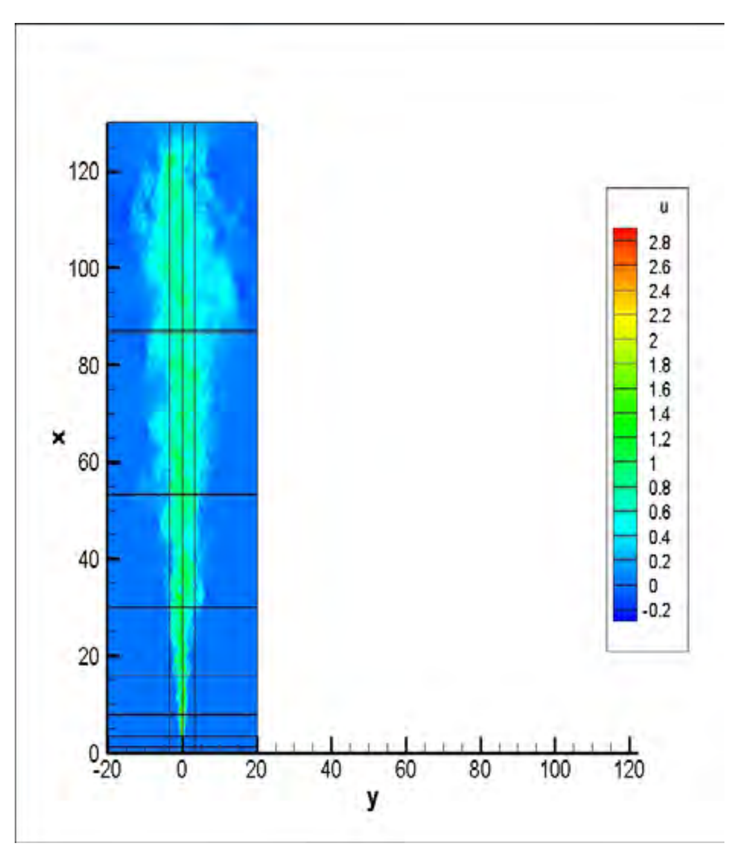
Motivation - Numerical

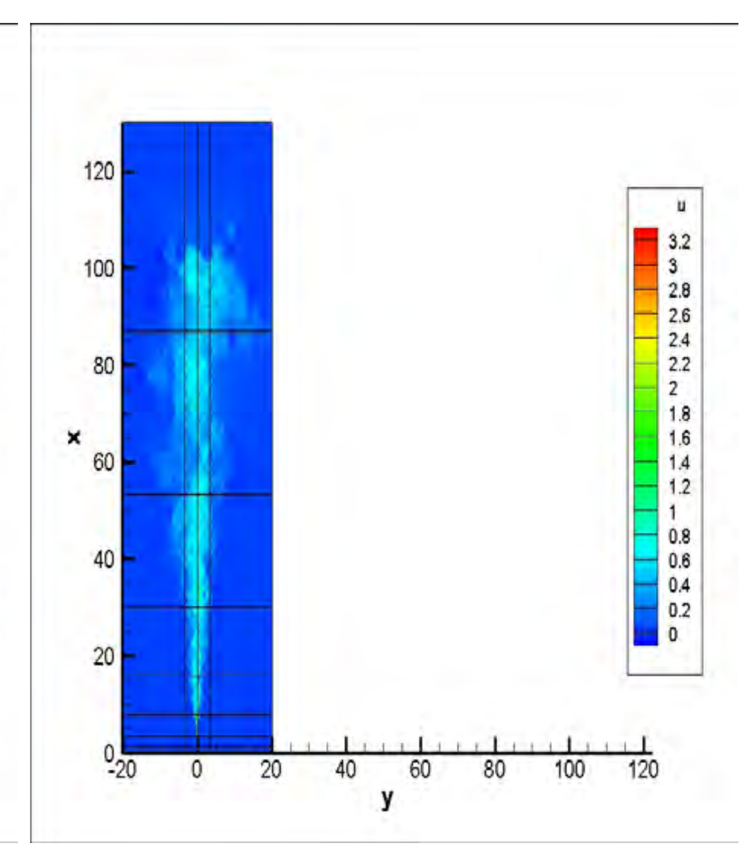
- Understand and facilitate implementation of Lagrange point particle tracking and LES capabilities for CMT-Nek
- Symbiotic relationship with CMT-Nek and Nek5000
- LES models for multiphase turbulent jets



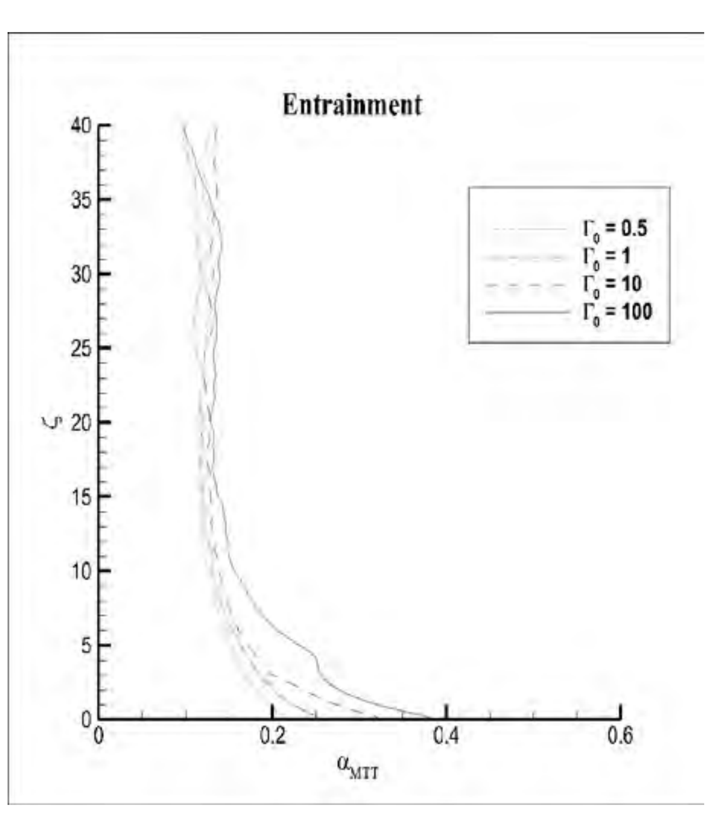


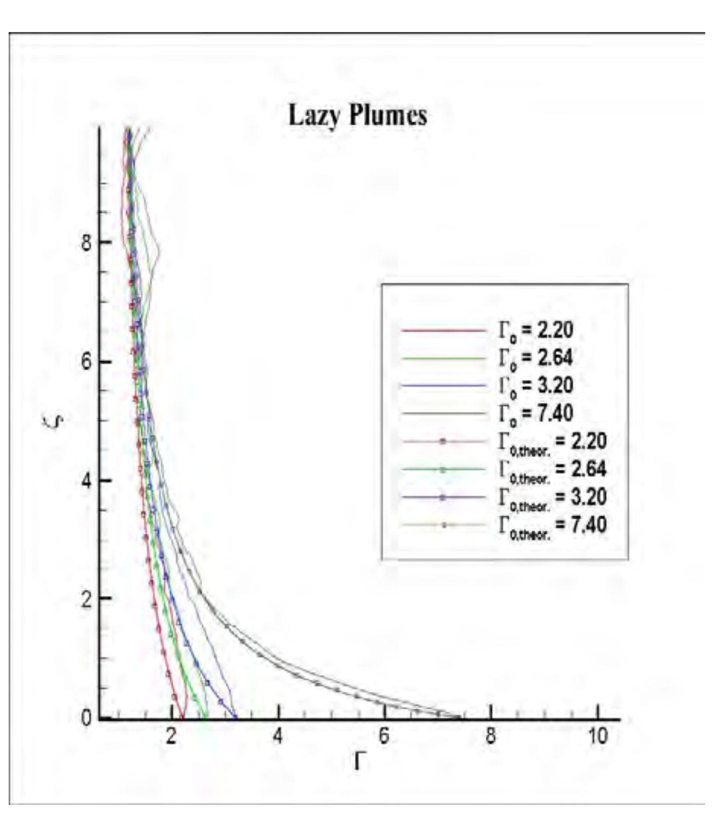
Preliminary Single Phase Results



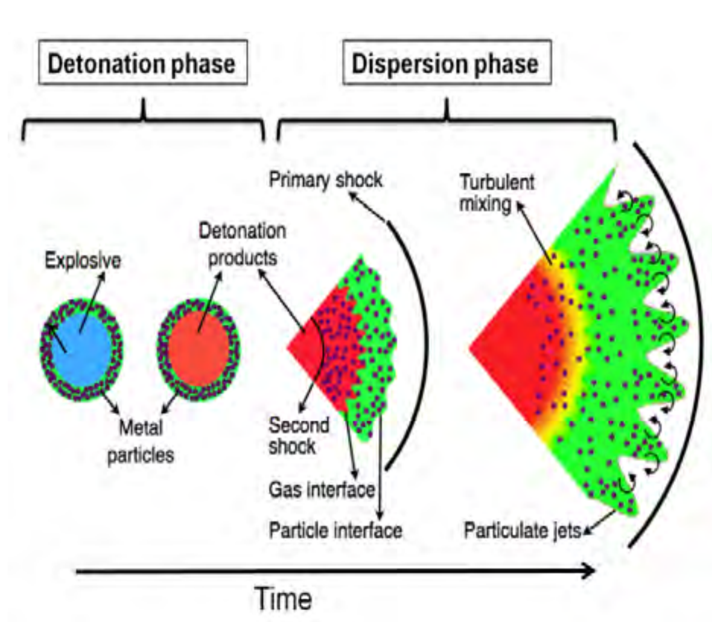


Preliminary Single Phase Results





Summary



- Eulerian-Eulerian simulations year 2
- Understand and implement Lagrange point particle tracking year 3
- Develop LES capabilities and LES multiphase models year 3
- Better understanding of the physics of multiphase turbulent jets
  - Structures
  - Entrainment
  - Turbulence Modulation
  - Preferential Particle Accumulation

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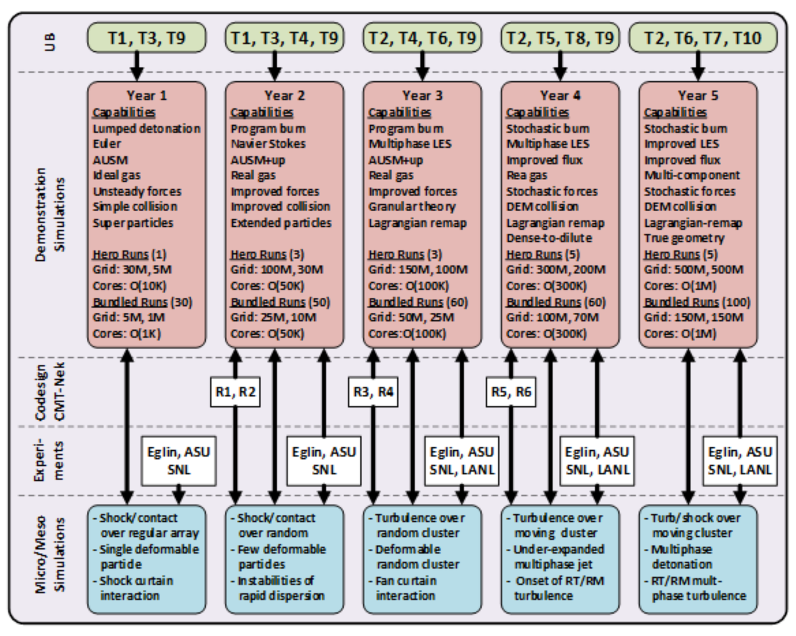
Center for Compressible Multiphase Turbulence

CMT-nek development – Formulation

Dr. Jason Hackl
Dr. Mrugesh Shringarpure
Department: MAE, UF

- Goals
  - Framework of CMT-nek
  - Implement explicit Euler solver
  - Verify and demonstrate capabilities of CMT-nek
  - Develop CMTBone for codesign of CMT-nek
- Simulation roadmap
  - Develop scalable code for compressible multiphase turbulence for exascale simulation of demonstration problem



Simulation Roadmap

Motivation

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

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

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

CMT-nek governing equations

- CMT-nek solves the compressible multiphase flow equations
- We have implemented the terms in red
- *E* is total energy per unit mass

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial}{\partial x_j}\mathbf{H}_j = \mathbf{R}$$

$$\mathbf{U} = \phi_g \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{bmatrix}, \quad \mathbf{H}_j = \mathbf{H}_j^{\text{conv}}(\mathbf{U}) + \mathbf{H}_j^{\text{visc}}(\mathbf{U}, \nabla \mathbf{U}) \quad \mathbf{R} = - \begin{bmatrix} \mathcal{C}_{gp} \\ p\partial\phi_p/\partial x_1 + \mathcal{M}_1^{gp} \\ p\partial\phi_p/\partial x_2 + \mathcal{M}_2^{gp} \\ p\partial\phi_p/\partial x_3 + \mathcal{M}_3^{gp} \\ pu_k^p \partial\phi_p/\partial x_k + \mathcal{E}_{gp} \end{bmatrix}$$

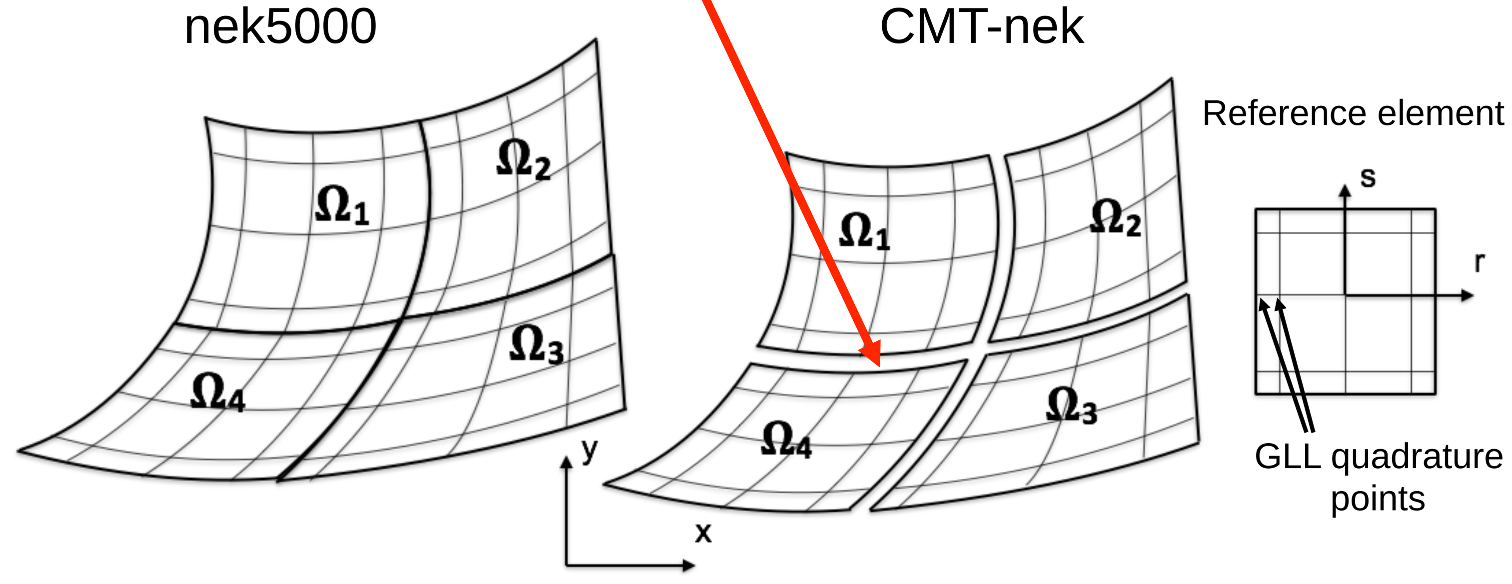
$$\mathbf{H}_j^{\text{conv}} = \phi_g \begin{bmatrix} \rho u_j \\ \rho u_1 u_j + \delta_{1j} p \\ \rho u_2 u_j + \delta_{2j} p \\ \rho u_3 u_j + \delta_{3j} p \\ (\rho E + p) u_j \end{bmatrix}, \quad \mathbf{H}_j^{\text{visc}} = -\phi_g \begin{bmatrix} 0 \\ \tau_{1j} \\ \tau_{2j} \\ \tau_{3j} \\ u_k \tau_{jk} + \kappa \frac{\partial T}{\partial x_j} \end{bmatrix}$$

g: gas
p: particle
gp: gas-particle coupling
k: thermal conductivity
ϕ: volume fraction

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

Discontinuous Galerkin formulation

$$\frac{\partial}{\partial t}\int_{\Omega_\kappa} \psi U_i dV - \int_{\partial\Omega_\kappa} \psi \left(H_{ij} - H_{ij}^*\right) n_j dA + \int_{\Omega_\kappa} \psi \frac{\partial H_{ij}}{\partial x_j} dV = \int_{\Omega_\kappa} R_i dV$$



Hesthaven J.S. and Warburton T. (2008) *Nodal Discontinuous Galerkin Methods: Algorithms, Analysis and Applications* Springer.

Spectral element DG approximation

$$U(\xi) \approx \sum_{n=0}^{N} U(\xi_n)\psi_n(\xi)$$

- Unknowns are nodal values on GLL quadrature points
- Galerkin/weighted-residual method assures orthogonality of this approximation to the function space containing Ψ

$$\psi_n(\xi) = \frac{-1}{N(N+1)} \frac{1-\xi^2}{\xi - \xi_n} \frac{L_N'(\xi)}{L_N(\xi_n)}$$

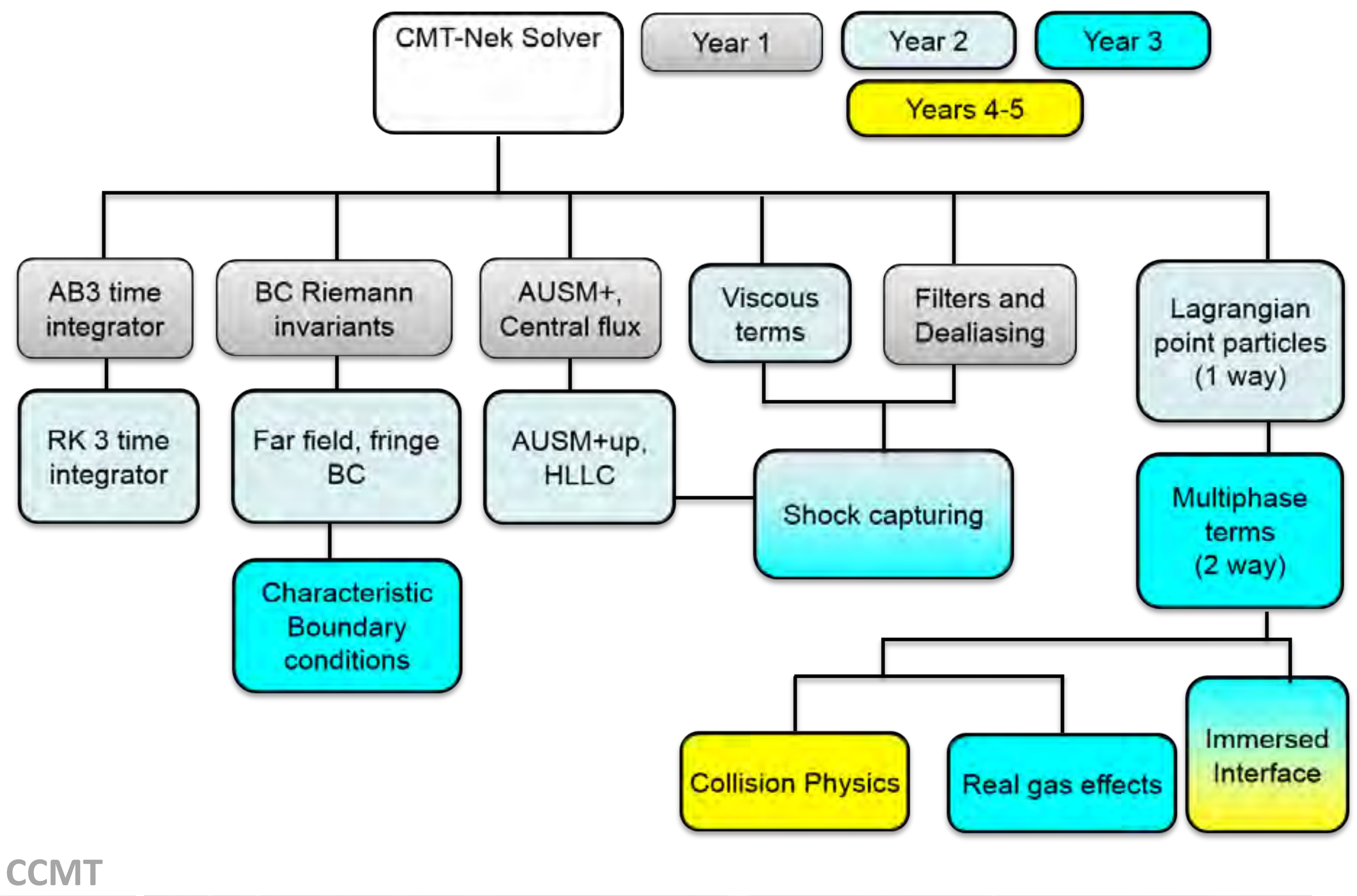
- Basis is Lagrange interpolant
- Approx. diagonal mass matrix
- Convergence depends on smoothness; shocks will need mollification or a different basis

$$\mathbf{H}_j^{*\text{conv}}$$

- Numerical flux for convective terms: Advection Upstream Splitting Method (AUSM+) of Liou
- Any Riemann solver can be used

Deville, Fischer and Mund (2002) *Higher-Order Methods for Incomp. Flows* Cambridge
Ronquist and Patera (1987) *Intl. J. Numerical Methods Engrg.* **24**, 2273-2299
Liou (1996) *J. Comp. Phys.* **129**, 364-382

Capabilities and timeline



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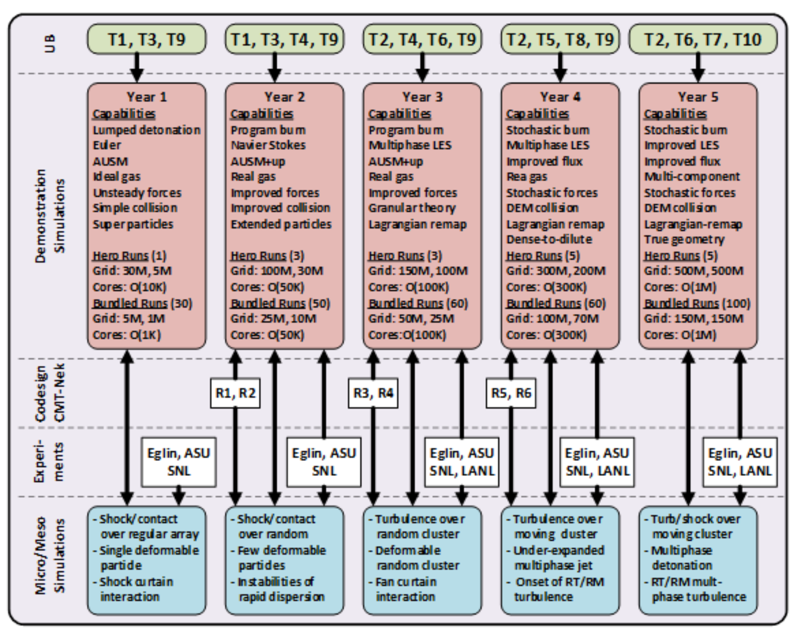
CMT-nek development - Verification

Dr. Mrugesh Shringarpure
Dr. Jason Hackl
Department: MAE, UF

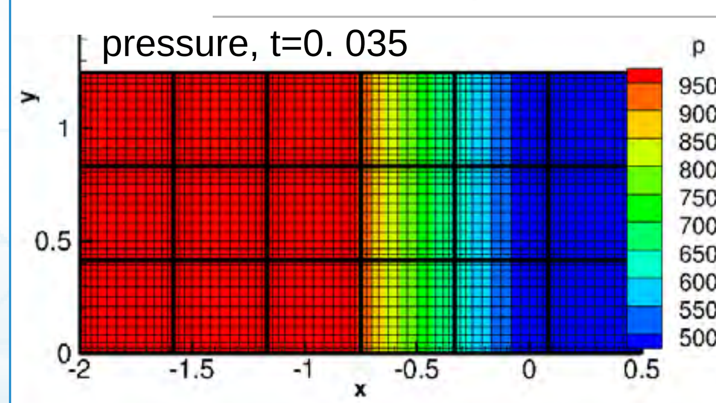
- Goals
  - Framework of CMT-nek
  - Implement explicit Euler solver
  - Verify and demonstrate capabilities of CMT-nek
  - Develop CMTBone for codesign of CMT-nek
- Simulation roadmap
  - Develop scalable code for compressible multiphase turbulence for exascale simulation of demonstration problem



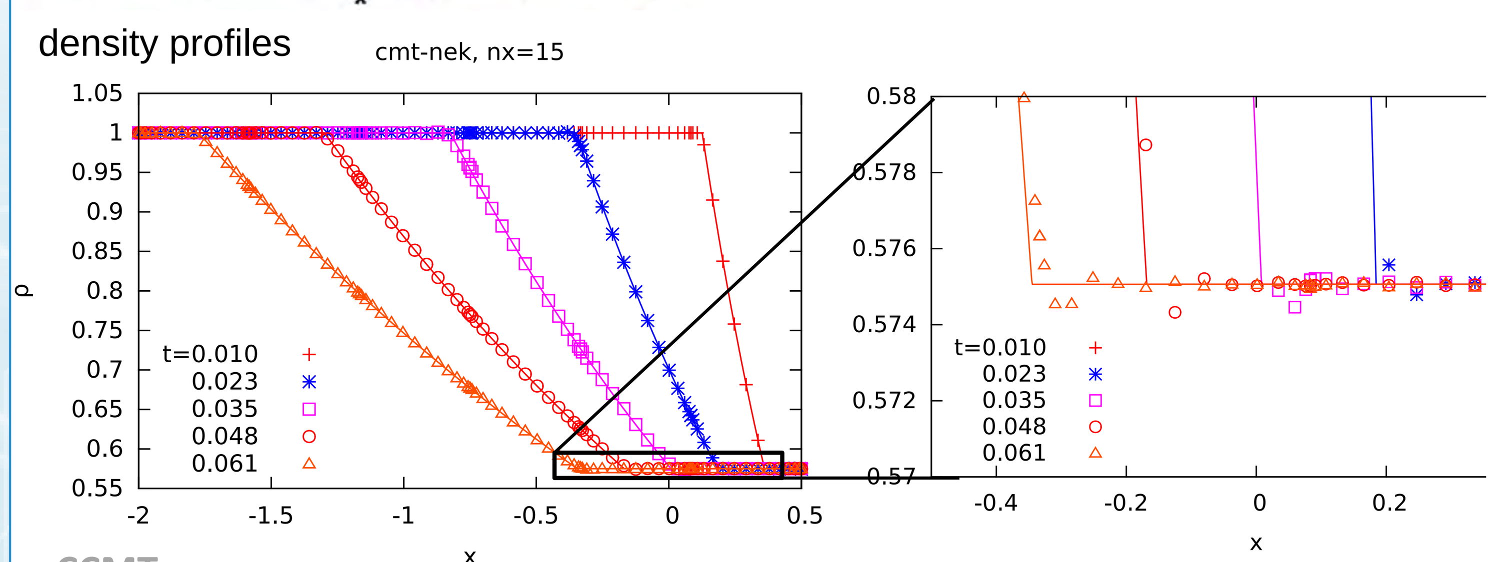
Simulation Roadmap

CCMT 1

Unsteady 1D rarefaction in 2D



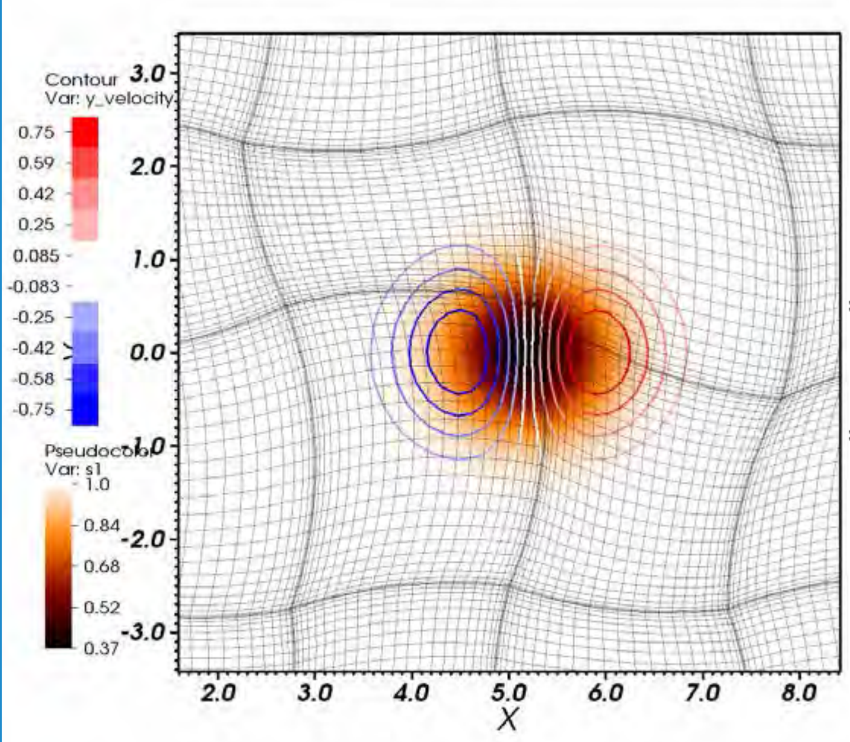
- Solution close to that of "exact" RS
  - But C1 discontinuity introduces Gibbs oscillations in solution
- Coupling elements, equations, terms
  - But no spectral convergence

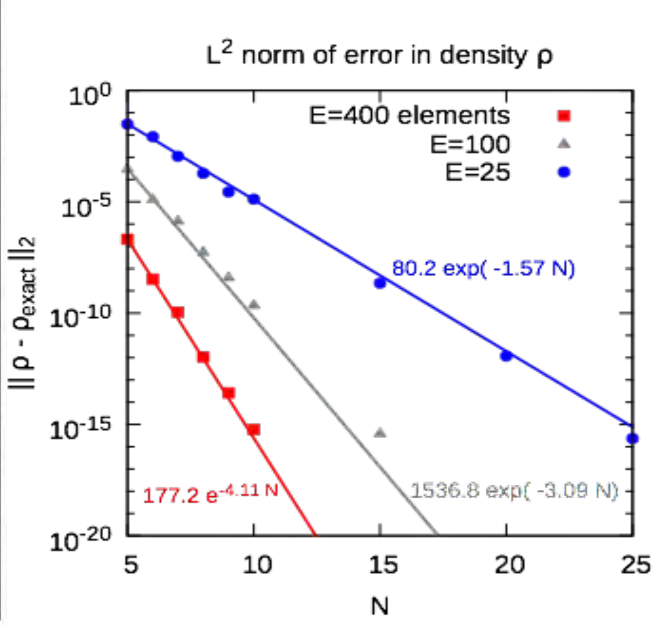


CCMT T1-2

Inviscid Isentriopic vortex

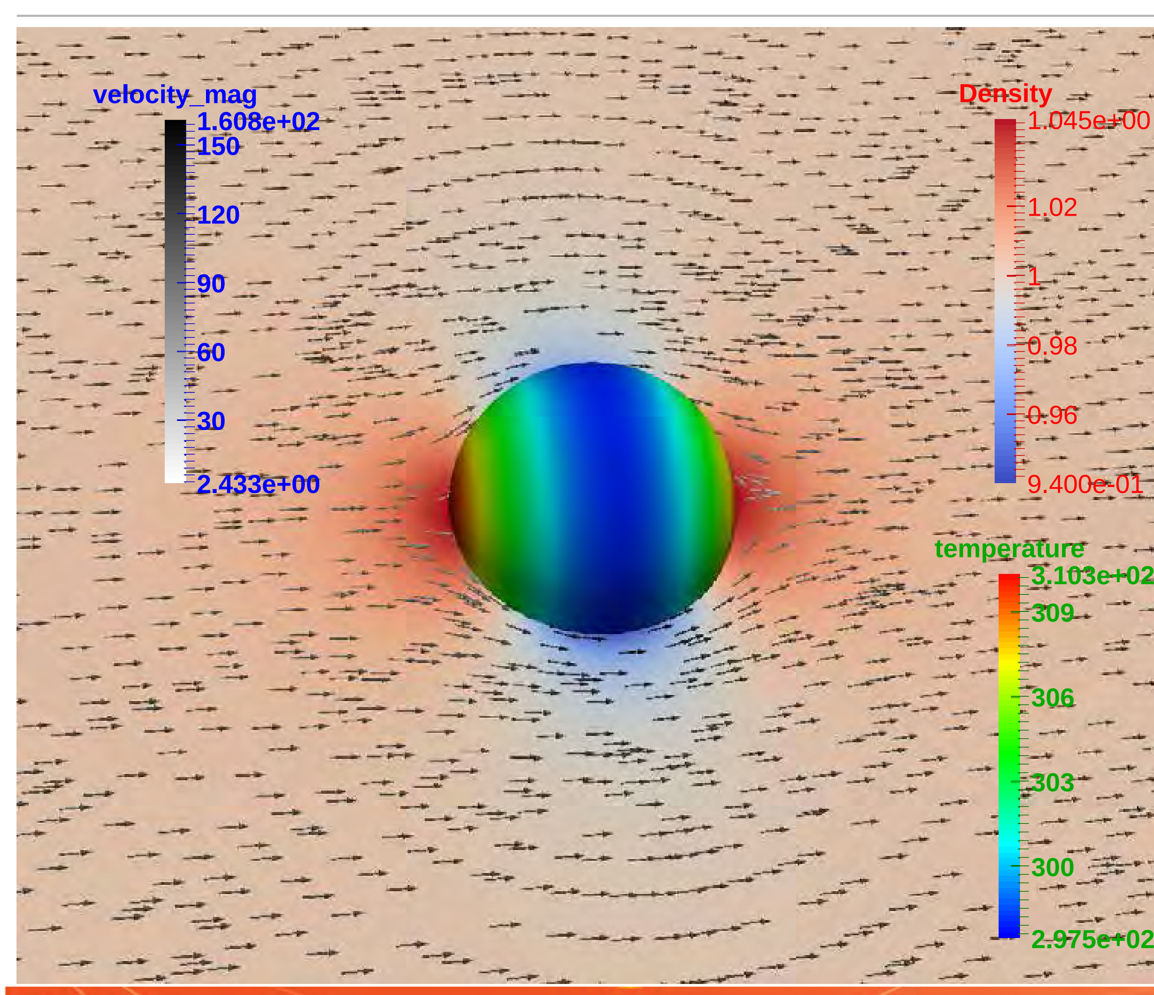
Yee, Vinukor & Djomehri (2000) *J. Comp. Phys.* **162**





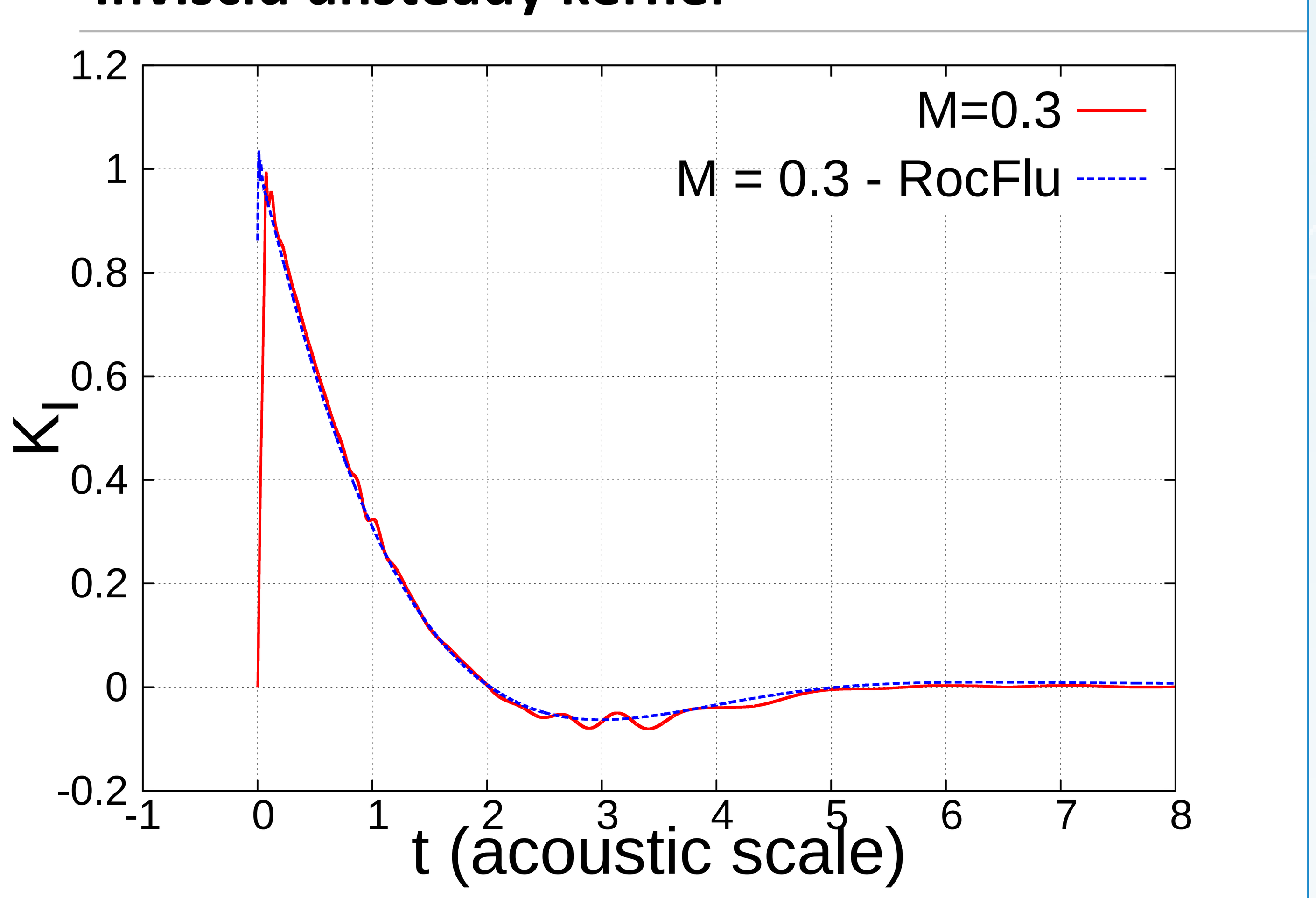
CCMT 3

M=0.3 flow over a sphere



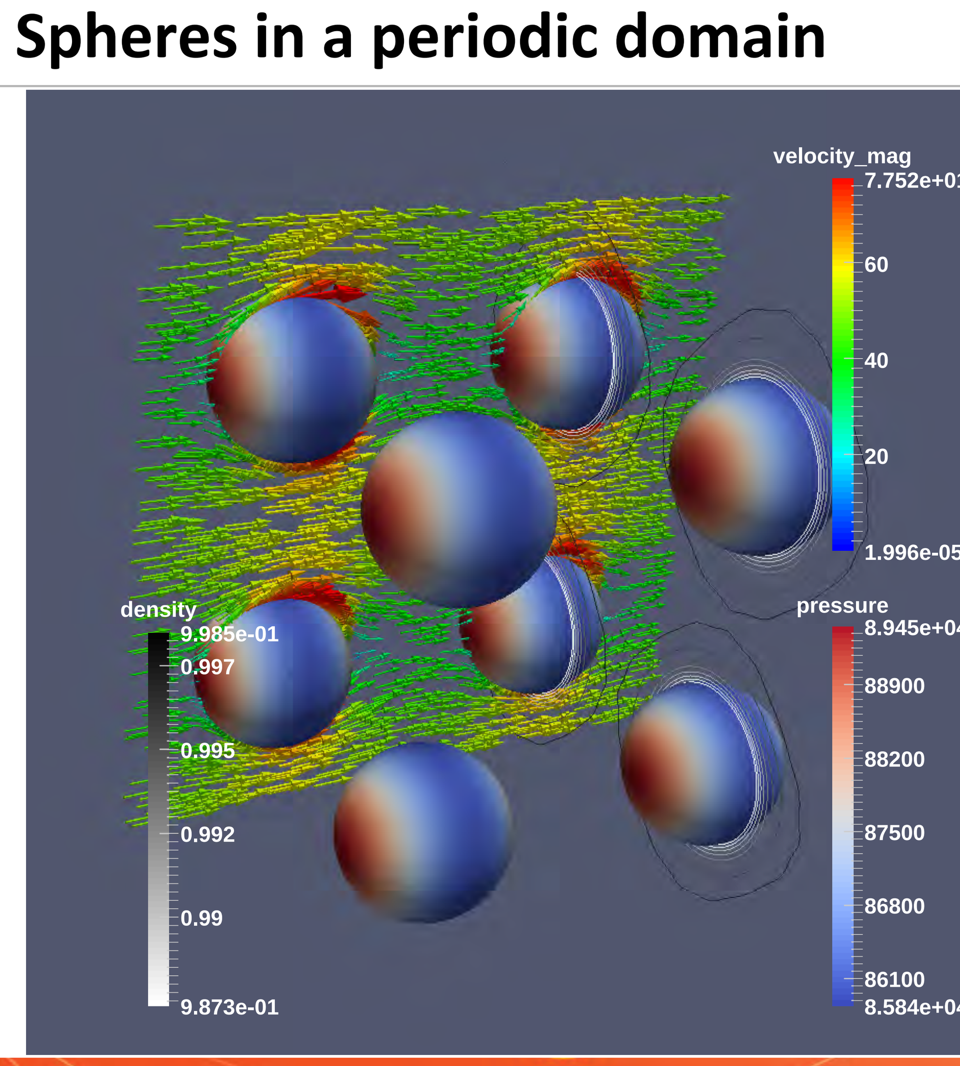
CCMT 4

Inviscid unsteady kernel



CCMT 5

8 Spheres in a periodic domain



CCMT 6

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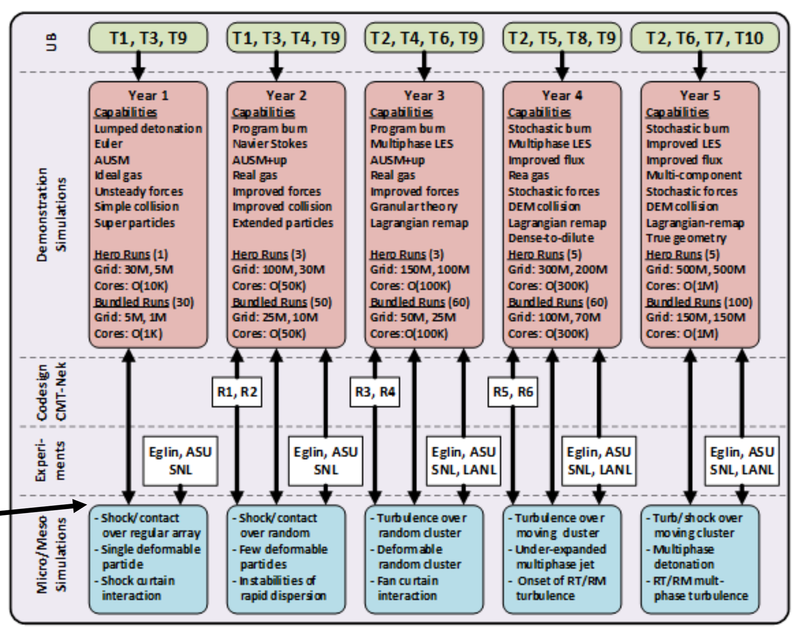
Center for Compressible Multiphase Turbulence

Shock & Contact Particle Interactions

Student: Christopher Neal
Advisor: Prof. S. Balachandar
Department: MAE, UF

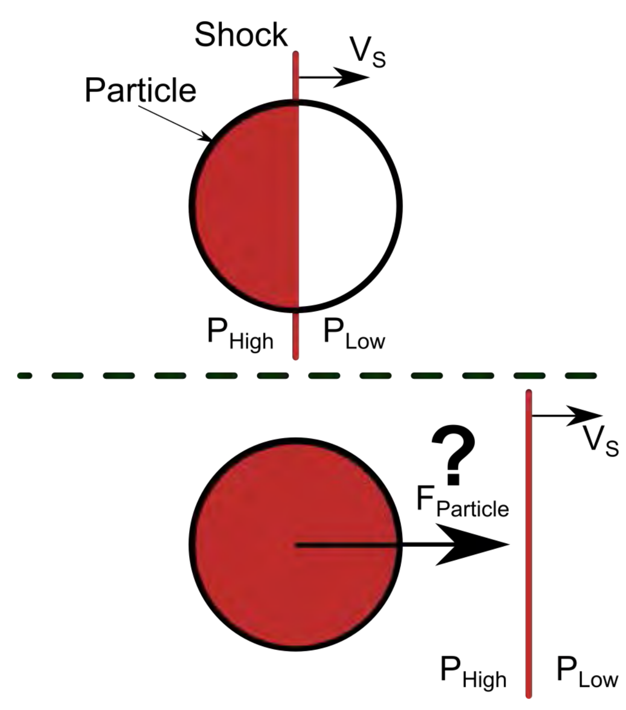
- Goals
  - Develop Point-Particle Models
  - Multiple Particle Shock Interaction Simulations
  - Contact-Interface Simulations
- Simulation roadmap
  - This simulation work contributes data for the impinging shock & contact(density gradient) over single & arrays of particles to be used for advanced point-particle models.



Simulation Roadmap

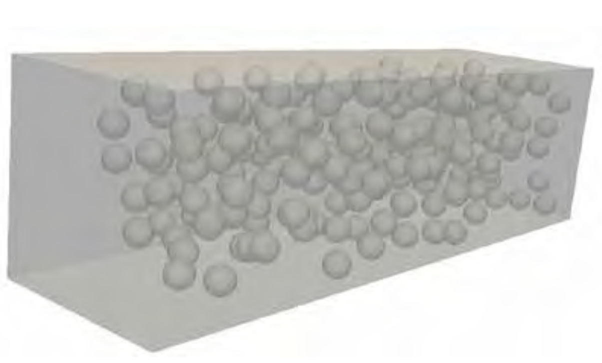
Why do We Need Point-Particle Models?

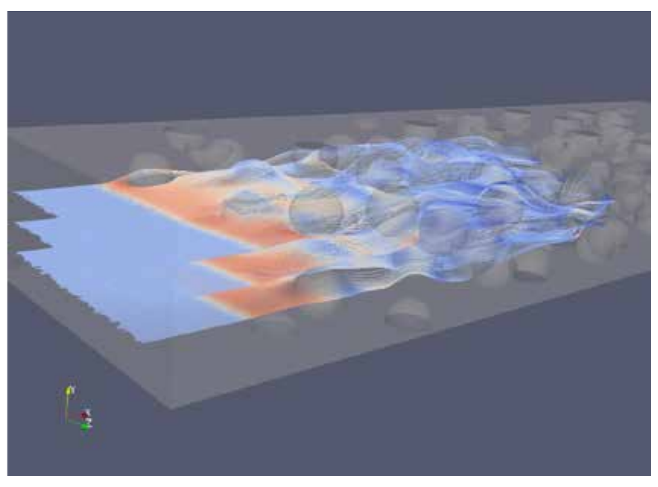
- There is a need Point-particle models to approximate the force that a particle in a flow will feel under different conditions
- The models reduce the need for complete flow resolution around particles and are necessary for simulations with many particles or simulations that have large spatial resolutions
- Work for point-particle models has focused on the force that an isolated particle in an incompressible or weakly(Ma~1.0) compressible flow experiences
- There is little discussion in literature about the particle force contribution from a strong density gradient in a compressible flow

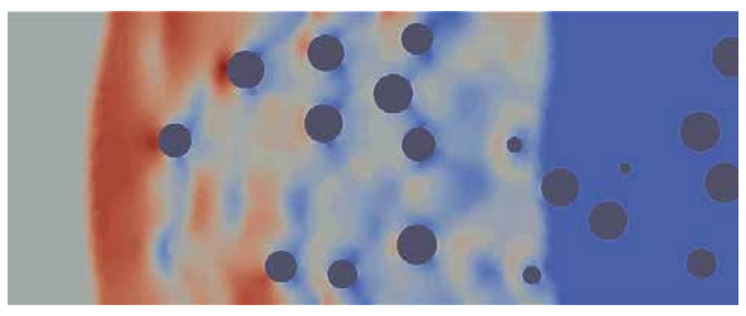


Random Particle Shock Results

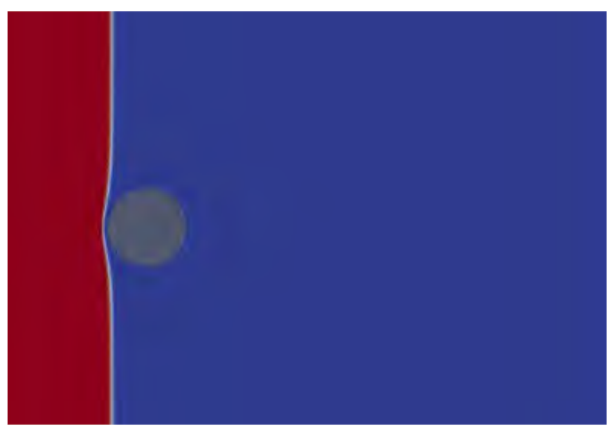
- A randomly packed domain with 200 stationary particles with a total volume fraction of 10 percent was subjected to an impinging shock with a Mach number of 3.0
- The goal was to examine the force fluctuations that the particles feel
- A large coalesced bow shock formed on the leading edge of the particle pack

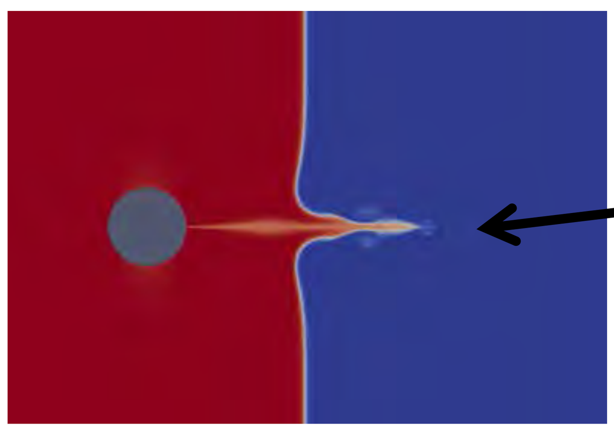






Contact Interface Results





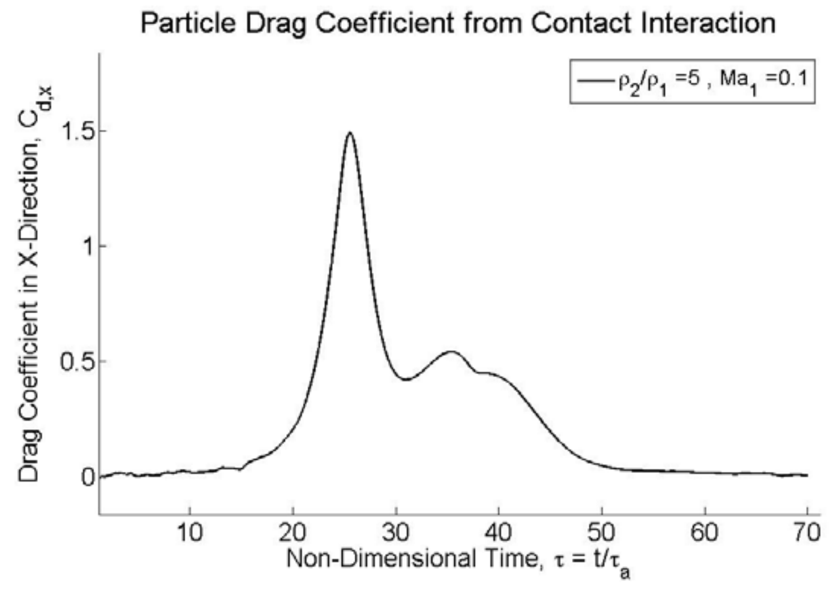
- Wake structure behind particle as contact interface reconnects
- The density jump across the interface had a ratio of 5.0. Strong shock problems have greater density ratios across the interface.

This phenomenological effect is not unexpected

- How does this change as Mach number is increased?
- How does it affect force history?

* http://images.fineartamerica.com/images-medium-large/1-water-droplet-jet-dustin-k-ryan.jpg

Contact Interface Results



- The presence of a secondary peak that is seen from the direct numerical simulation was not initially expected
- The current force models do not account for this additional force behavior during a contact interface interaction

Future Work

- Develop a methodology to statistically examine the force fluctuations in the random packs of particles & compare to single particle results
- Continue random pack simulations with different volume fractions and Mach numbers & use Voronoi tessellation to determine an approximate local volume fraction for the particles within the random packs
- Continue my work with comparing the forces from contact interface(density gradients)-particle interactions with current point-particle models
- Examine the particle force for a single particle experiencing supersonic flow behind a contact interface
- Simulate contact interface interactions with density ratios that are representative of what would be present in the demonstration problem

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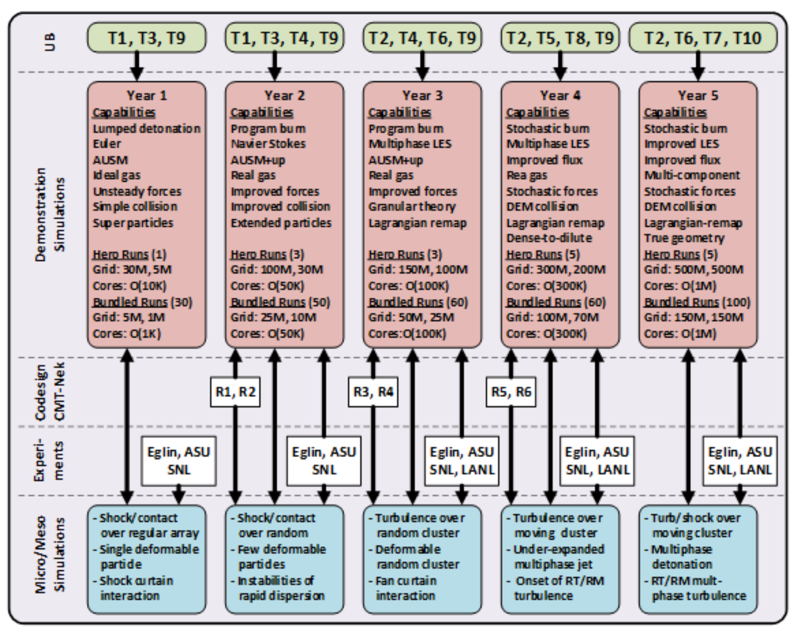
RocSDT: Shock-Particle Interaction in Air

Student: Prashanth Sridharan
Advisor: Dr. S. Balachandar
Department: MAE, UF

- Goals
  - Investigate aluminum spherical particles under various shock loading conditions
  - Find differences between single particle and a 1-D array
  - Produce transient drag coefficient curves for a single particle and 1-D particle array
- Simulation roadmap
  - Develop transient force/drag histories for the Demonstration Problem



Simulation Roadmap

Motivation/Background

- **Purpose:** quantify momentum exchange of a particle under shock loading through the imparted transient drag coefficient curve, which can be used to create correlations, for point-particle force models, and kernels for larger scale simulations
- The present work focuses on early time behavior of shock-particle interaction, which is dominated by inviscid mechanisms
- The particle and medium are governed by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \qquad p = (\gamma - 1)\rho e - \gamma P^{\infty}$$

$$\frac{\partial (\rho \vec{u})}{\partial t} + \nabla p + \nabla \cdot (\rho \vec{u}\vec{u}) = 0$$

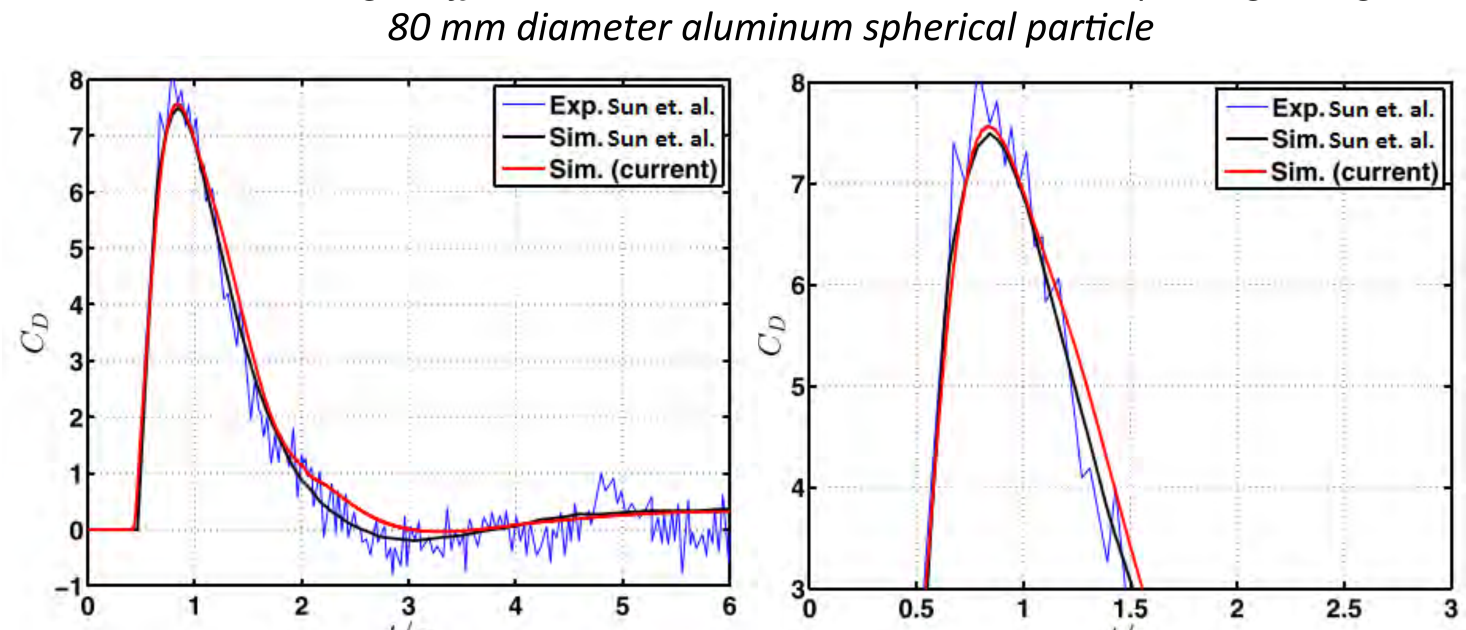
$$\frac{\partial E}{\partial t} + \nabla \cdot ((E + p)\vec{u}) = 0$$

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0$$

Results – Single Particle Validation

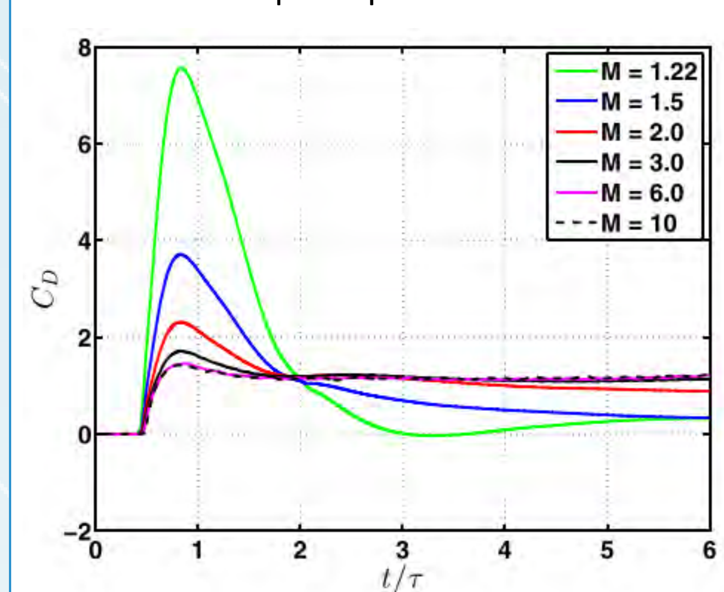
- Grid resolved simulation is validated, with excellent agreement, with published experimental results [Sun et. al., Shock Waves **14**, 3 (2005)]

Transient drag coefficient curve due to Mach 1.22 shock impacting a single 80 mm diameter aluminum spherical particle



Results – Single Particle

- Once validated, simulations are conducted at incident shock Mach numbers up to 10
  - The peak drag coefficient is found to decrease with increasing Mach number
  - A drag coefficient correlation, as function of Mach number, is created for point-particle models



$$C_{D,model} = C_{D,pg} + C_{D,am}A(M)e^{-B(M)t/\tau} + H(M - M_{cr})\,C(M)(1 - e^{-D(M)t/\tau})$$

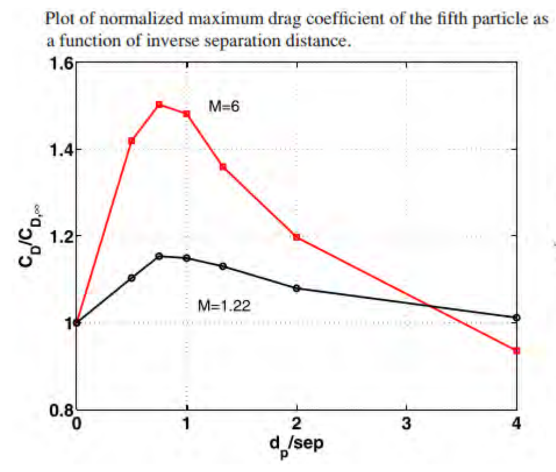
Calibrated values of *A*, *B*, *C*, and *D* as a function of Mach number.

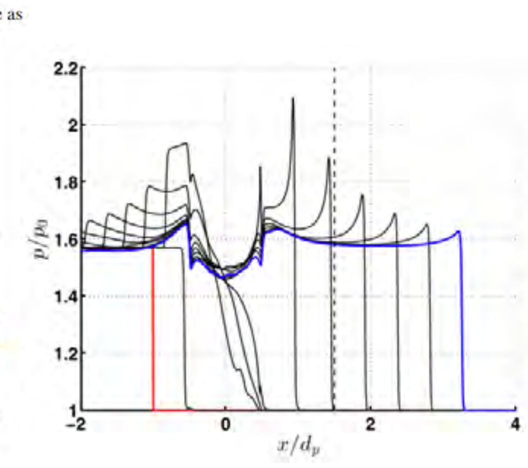
M	A	B	C	D
1.22	1	0	...	...
1.5	1.1	0.2	0.3709	2.0
2.0	1.8	1.8	0.9317	1.7
3.0	2.8	2.8	1.0952	1.7
6.0	5.0	5.0	1.1260	3.2
10.0	8.0	8.0	1.4460	5.0

Results – 1-D Particle Array

- Simulations of a five particle array undergoing shock loading at Mach numbers of 1.22 and 6 at various inter-particle spacings are conducted
  - Pressure overshoot occurs after the shock passes over each particle, which causes subsequent particles to experience larger peak drag coefficients
  - Peak drag coefficient increase, which is influenced by the incident shock Mach number and inter-particle spacing, is found to asymptote around the 5th particle
  - Ratio of 5th particle's peak drag coefficient to a single particle has a maximum at an inter-particle spacing of about one particle diameter
  - As inter-particle spacing goes to zero this ratio drops below one

Plot of normalized maximum drag coefficient of the fifth particle as a function of inverse separation distance.





Plot of nondimensional pressure along the centerline $r = 0$ as a function of x/d_p at various times and for Mach number $M = 1.22$. The initial and final times are shown in red and blue, respectively. The vertical dashed line at $x/d_p = 1.5$ corresponds to one particle diameter downstream of the aluminum particle with center located at $x/d_p = 0$.

Additional Notes/Future Work

- The following is a non-comprehensive list of recommended numerical investigations for future work:
  - Particle deformation effect on transient drag coefficient curves for a single particle and 1-D particle array
  - Initial particle shape's effect on transient drag coefficient curves for a single particle and 1-D particle array
  - Investigation of particle medium combinations on transient drag coefficient curves for a single particle and 1-D particle array
- The present work has been published:
  - Journal of Applied Physics **117**, 075902 (2015); doi: 10.1063/1.4913217

UNIVERSITY of FLORIDA

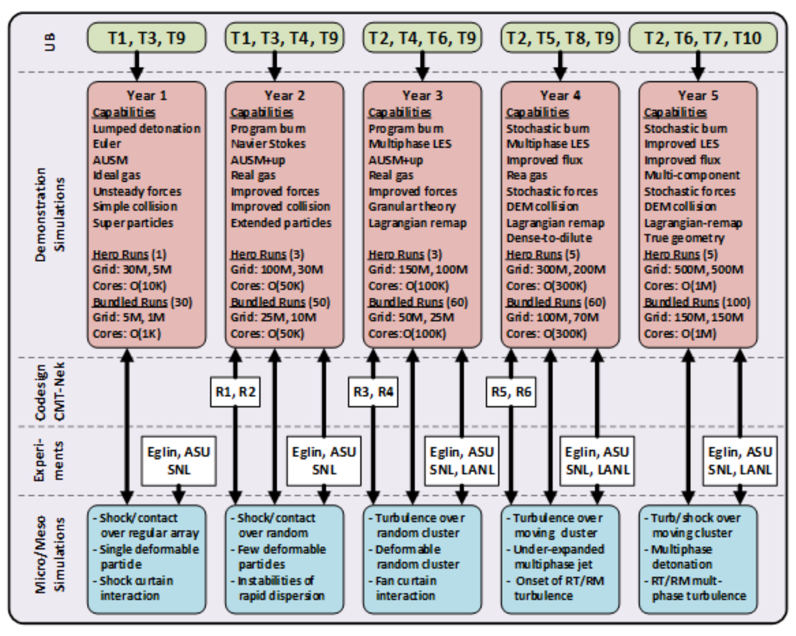
CCMT

Center for Compressible Multiphase Turbulence

Multiphase Turbulence Modeling

Student: Rahul Babu Koneru
Advisor: Dr. S. Balachandar
Department: MAE, UF

- Goals
  - Develop multiphase compressible LES model
  - Integration into Rocflu and CMT-nek
  - Validation of the model
- Simulation roadmap
  - Under-expanded jet behavior will be studied using LES in single phase and multiphase flows
  - Mesoscale simulation of the signature problem
  - This model will be incorporated into the existing code



Simulation Roadmap

Governing Equations – LES Formulation

- Favre averaged single phase LES equations.

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\widetilde{u_i}}{\partial x_i}=0 \qquad \textbf{Note: } \overline{(.)} = \text{Filtered quantity, } \widetilde{(.)} = \text{Favre-averaged quantity}$$

$$\frac{\partial \bar{\rho}\widetilde{u_i}}{\partial t}+\frac{\partial \bar{\rho}\widetilde{u_i}\widetilde{u_j}}{\partial x_j}+\frac{\partial \bar{p}}{\partial x_i}-\frac{\partial \dot{\widetilde{\sigma_{ij}}}}{\partial x_j}=-\frac{\partial \tau_{ij}}{\partial x_j}+\frac{\partial}{\partial x_j}[\overline{\sigma_{ij}}-\dot{\widetilde{\sigma_{ij}}}]$$

$$\frac{\partial \bar{\rho}\widetilde{E}}{\partial t}+\frac{\partial (\bar{\rho}\widetilde{E}+\bar{p})\widetilde{u_j}}{\partial x_j}+\frac{\partial \dot{\widetilde{q_j}}}{\partial x_j}-\frac{\partial \dot{\widetilde{\sigma_{ij}}}\widetilde{u_j}}{\partial x_j}=-\frac{\partial}{\partial x_j}[A_j+B_j-C_j+D_j]$$

Filtered pressure $\bar{p}=(\gamma-1)\left[\bar{\rho}\widetilde{E}-\frac{1}{2}\bar{\rho}\widetilde{u_i}\widetilde{u_j}-\frac{1}{2}\tau_{ii}\right]$

Favre averaged temperature $\widetilde{T}=\frac{(\gamma-1)}{R}\left[\widetilde{E}-\frac{1}{2}\widetilde{u_i}\widetilde{u_j}-\frac{1}{2\bar{\rho}}\tau_{ii}\right]$

Shear stress in terms of averaged quantities, $\dot{\widetilde{\sigma_{ij}}}=\mu(\widetilde{T})\left[\left(\frac{\partial \widetilde{u_i}}{\partial x_j}+\frac{\partial \widetilde{u_j}}{\partial x_i}-\frac{2}{3}\frac{\partial \widetilde{u_k}}{\partial x_k}\delta_{ij}\right)\right]$

Heat flux in terms of averaged quantities, $\dot{\widetilde{q_j}}=-k(\widetilde{T})\frac{\partial \widetilde{T}}{\partial \widetilde{x_j}}$

Sub-grid scale terms,

$$A_j=\bar{\rho}\left[\widetilde{Eu_j}-\widetilde{E}\widetilde{u_j}\right], \qquad B_j=\bar{p}\,[\overline{u_j}-\widetilde{u_j}]$$

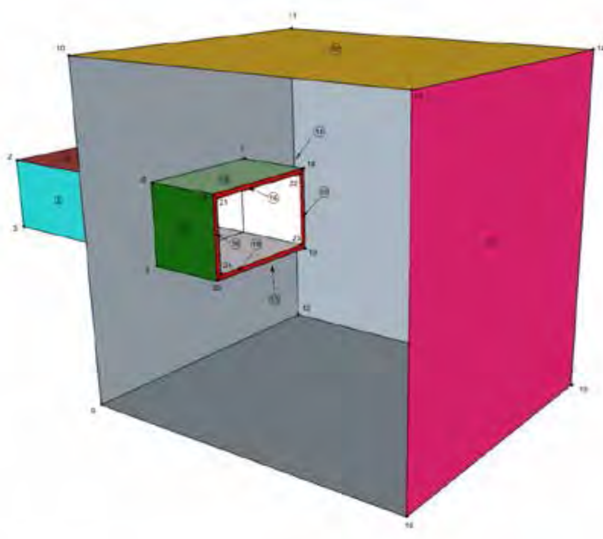
$$C_j=\overline{\sigma_{ij}u_j}-\dot{\widetilde{\sigma_{ij}}}\widetilde{u_j}, \qquad D_j=\overline{q_j}-\widetilde{q_j}, \qquad \tau_{ij}=\bar{\rho}\,[\widetilde{u_iu_j}-\widetilde{u_i}\widetilde{u_j}]$$

Open Ended Shock Tube – 3D Configuration

- The setup consists of a long channel/shock-tube from which the flow expands into far-field domain
- The test cases being simulated are taken from '*Open-Ended Shock Tube Flows: Influence of Pressure Ratio and Diaphragm Position*', A. Haselbacher, S. Balachandar and S. W. Keifer, AIAA Journal.

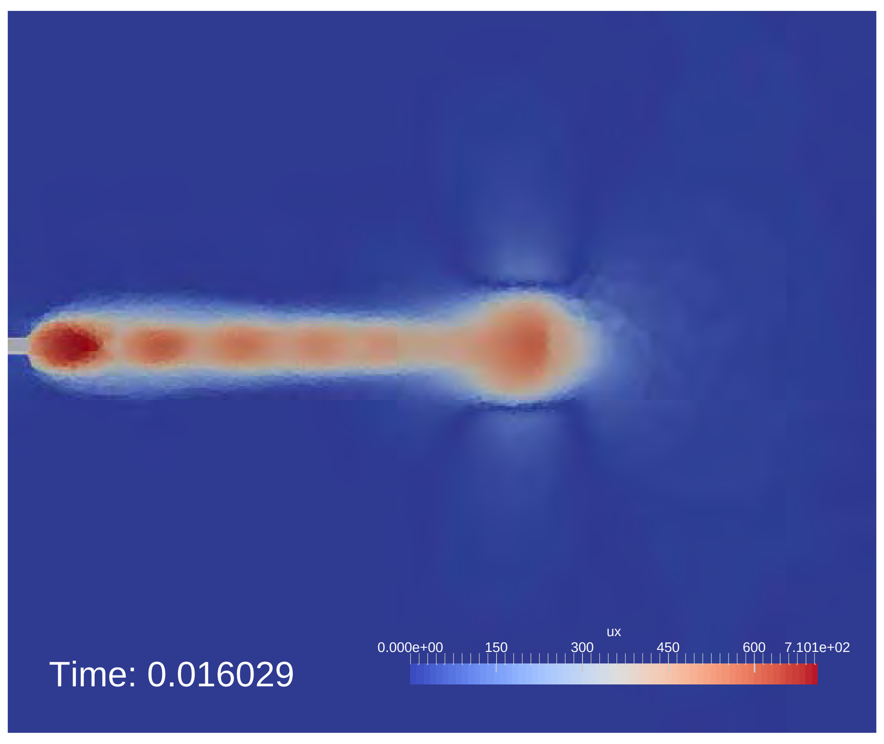
Table 1 Summary of initial conditions for open-ended shock tubes cases. All cases use $u_1 = u_4 = 0$ and $\gamma_1 = \gamma_4 = 1.4$

p_4/p_1	ρ_4/ρ_1	x_D/d
7.25	6.58	−1.0
50.0	28.74	−1.0
50.0	28.74	0.0



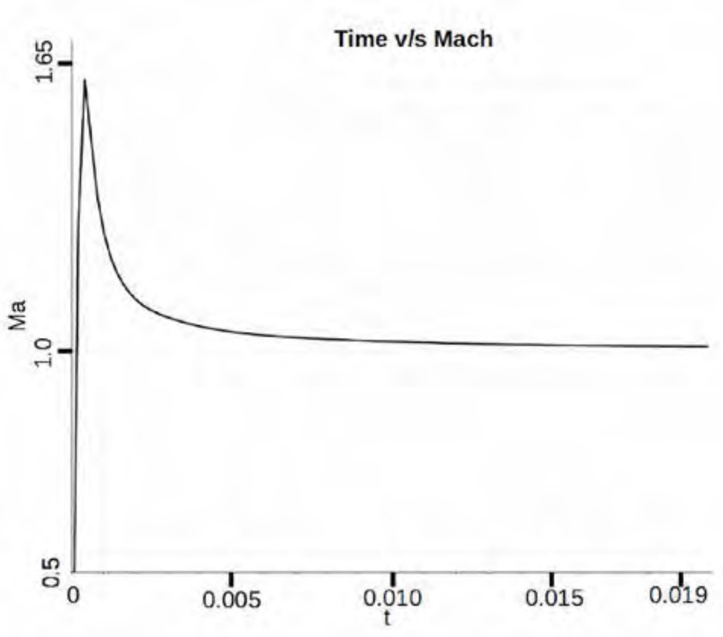
Velocity Field at a Late Time

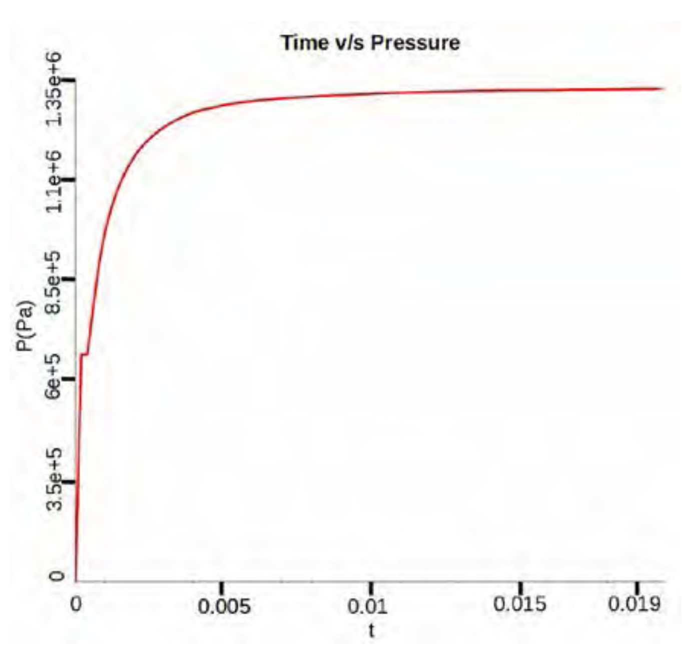
- Below shown is an under-expanded jet of air expanding into ambient
- Initial pressure and density ratios across the diaphragm are 50 and 28.74 respectively



Results

- The Mach number and pressure behind the contact at the exit plane are plotted against time





Summary

- Simulations of single-phase jets with no turbulence model have been performed
- Work is in progress to incorporate LES model into the code to further study single-phase under-expanded jets

Future Work

- After a successful implementation of the turbulence model for single phase flows, it will be extended to simulate dilute (~20% volume fraction)multi-phase flows
- Further, models will be developed to study flows with higher particle volume fractions

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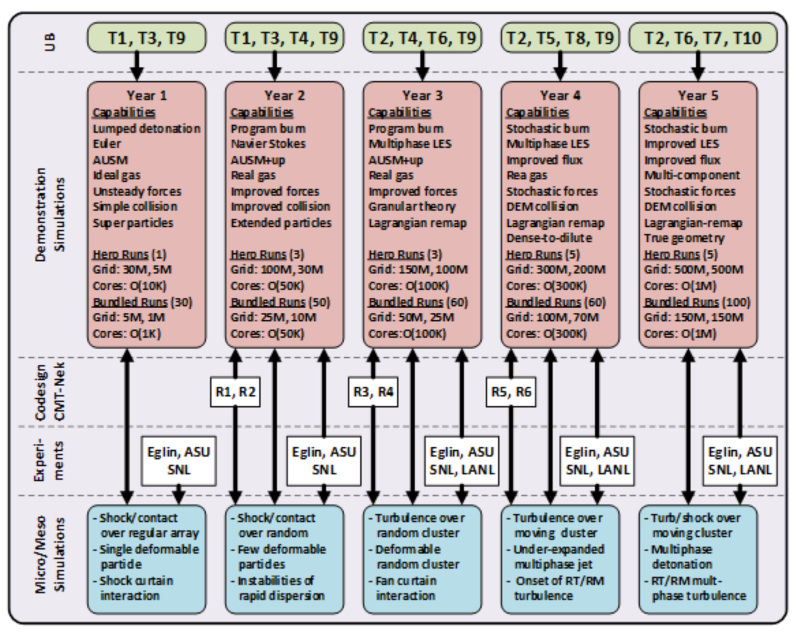
Center for Compressible Multiphase Turbulence

Mesoscale Shock – Particle Curtain Simulations

Student: Saptarshi Biswas
Advisor: Prof. S. Balachandar
Department: MAE, UF

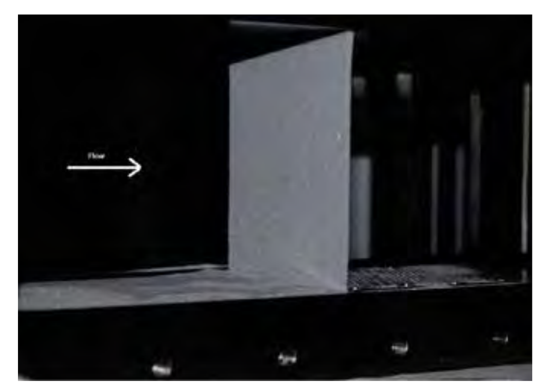
- Goals
  - Study the Shock-Particle Curtain Interaction
  - Study the Shock/Contact over random array of particles and instabilities caused due to rapid dispersion
- Simulation roadmap
  - Validate the Uncertainty Quantification Methodology
  - Validate the Microscale force modeling in an application context



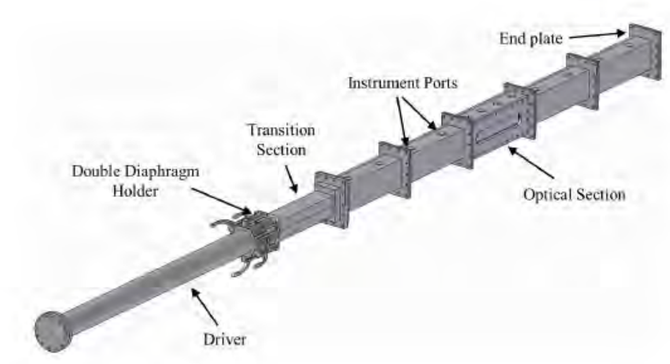
Simulation Roadmap

Motivation

- Particle dispersal by shock waves is an ubiquitous phenomenon characterized by highly nonlinear coupled physics of compressible flow, turbulence, and multiphase flows
- Accurately predicting the shock-particles interactions in the demonstration problem is essential for its prediction



Photograph of the particle curtain acquired with test section wall removed

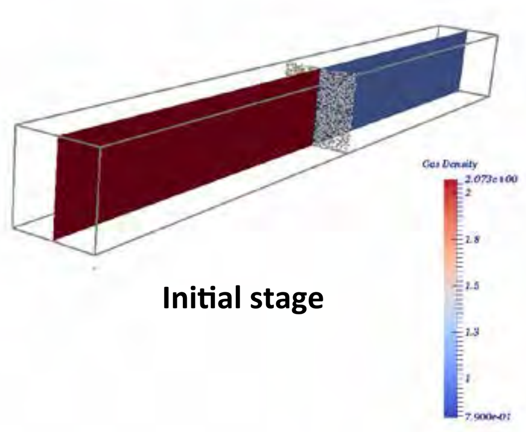


Experimental apparatus for the particle curtain experiment

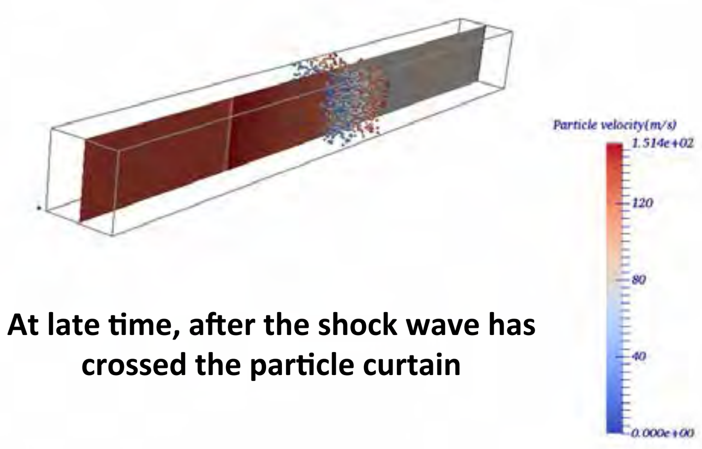
Wagner et al.," multiphase shock tube for shock wave interactions with dense particle fields" Exp. Fluids **52**, 1507–1517 (2012).

Particle Curtain Simulation

- The particle velocity profile at later instant of time shows that, the downstream front moves at a faster rate than the upstream front (positive velocity gradient of the particles). This is because of the increase in the velocity gradient of the gas within the curtain after the passage of the transmitted shock.



Initial stage

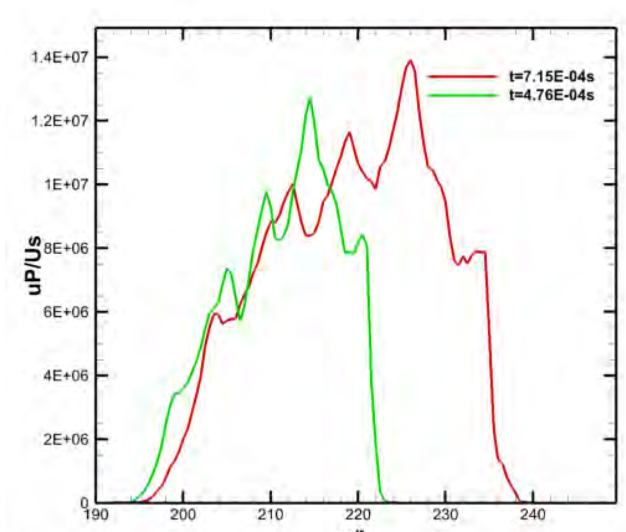


At late time, after the shock wave has crossed the particle curtain

Domain Size: 0.8X0.08X0.08(m) (5 million grid cells)
Mach number of Shock : 1.66
Volume Fraction of particles : 5%
Number of Particles (glass particles) : 1 million
Particles Diameter: 100 µm

Particle Velocity Profile

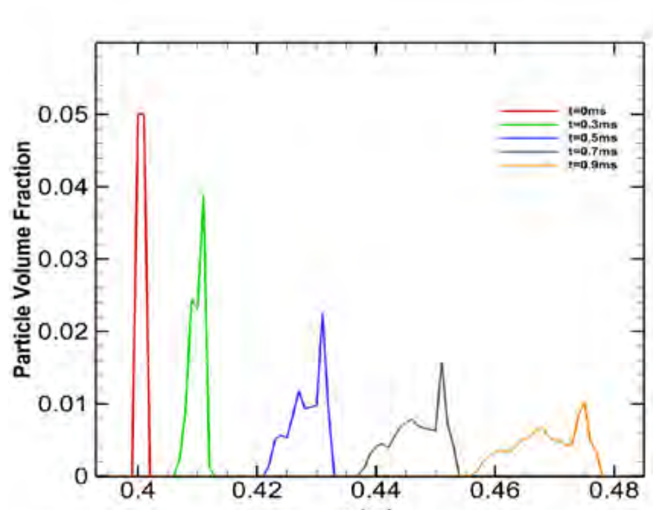
- The upstream front of the particle curtain starts to move downstream immediately following the arrival of the shock wave. This results in a negative velocity gradient and a compression of particle curtain at earlier times. The particle curtain then starts to expand following the decrease in volume fraction which is shown by the positive particle velocity gradient in the plot below.



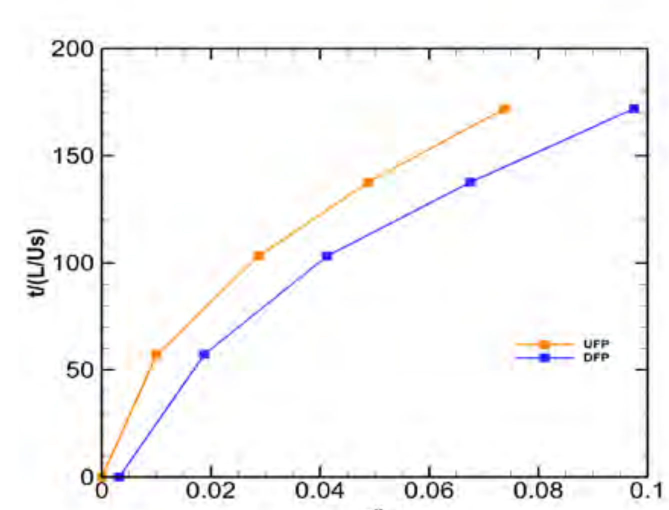
Time evolution of particle velocity with respect to stream wise direction.
L= width of the particle curtain (0.002m) , uP=particle velocity, Us= shock velocity.

Volume Fraction Evolution

- It is seen that particle volume fraction decreases over time as the curtain expands



Time evolution of particle volume fraction as a function of stream wise direction.



Trajectories of the upstream and downstream fronts of the particle curtain.
L=width of the particle curtain(0.002m)
Us=shock velocity.

Future Work

- Study the effect of shock wave Mach number on the particle curtain behavior
- Study the effect of particle distribution and particle sizes in the curtain
- Study the effect of re-shocking the particle curtain
- Run simulations at a realistic volume fraction distribution

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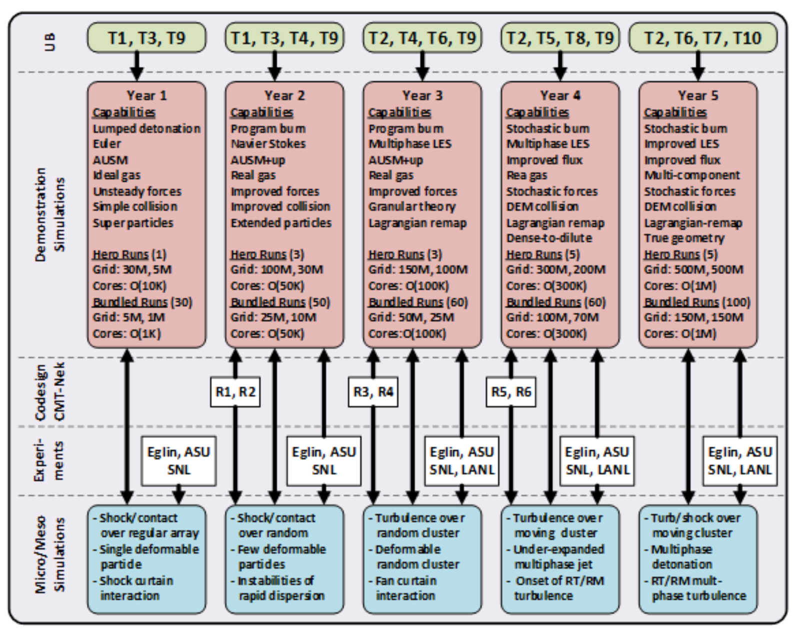
Center for Compressible Multiphase Turbulence

Generalized Faxén's Theorem and Detonation Sensitivity

Dr. Subramanian Annamalai
Department: MAE, UF

- Goals
  - Analytical model to compute force on a particle due to interaction with a planar shock
  - Effect of non-uniformity in initial detonation products and particle volume fraction
- Simulation roadmap
  - Develop improved forces models (Microscale)
  - Detonation sensitivity (T1)
  - Particle jetting behavior through RT/RM instabilities (Meso/Macro)



Simulation Roadmap

Motivation

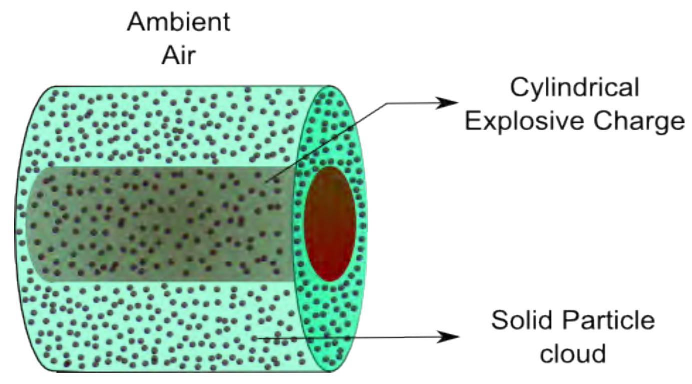


Fig .1a Sketch of initial cylindrical charge surrounded by an annulus of particles.

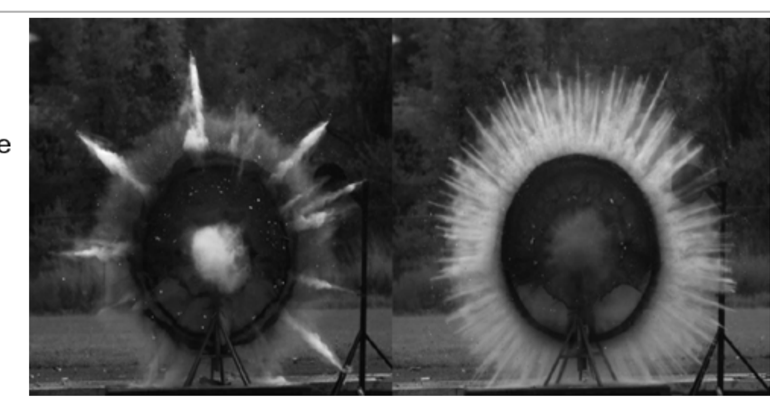


Fig .1b Formation of particulate jets (dry and wet glass particles) after detonation [†]

On detonation of the cylindrical charge (Fig. 1a), the particles surrounding the charge form jet-like patterns (Fig. 1b)

To understand why these needle-like structures form and predict it using computer simulations we need to

- Develop force models that can track these particles accurately
- Study the effect of initial particle distribution and initial non-uniformity in detonation products in forming these patterns

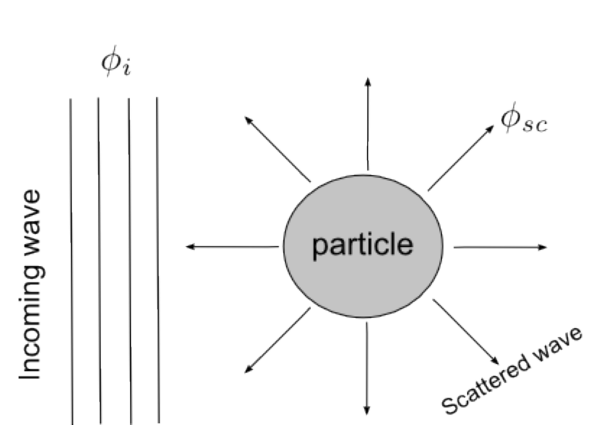
CCMT [†] Frost DL, Gregoire Y, Petel O, Goroshin S, & Zhang F, 2012. *Phys. Fluids*, 24(9).

Shock-Particle Interaction

For steady, uniform and incompressible flows over a sphere, one could use the standard Stokes drag given by $6\pi\mu R(\mathbf{u}-\mathbf{v})$ to compute the force on a particle.
For steady, non-uniform and incompressible flows, the force is given by $6\pi\mu R(\overline{\mathbf{u}}^{S}-\mathbf{v})$ (Faxén's drag) where the fluid velocity is averaged over the particle surface.

However unsteady, non-uniform and compressible flows occur when a **shock wave/contact interface** passes over a particle.

A model to predict the force is presented and expressed as averages over particle surface/volume using the procedure below



An acoustic wave of a given amplitude and frequency is assumed to pass over the particle in a stationary medium.

$$\mathbf{u} = Ue^{i(kz-\omega t)}\mathbf{e_z}$$

Flow-field is decomposed using a scalar and vector potential, and further into incoming and scattered potentials.

$$\mathbf{u} = \nabla\phi + \nabla\times\mathbf{\Psi}$$

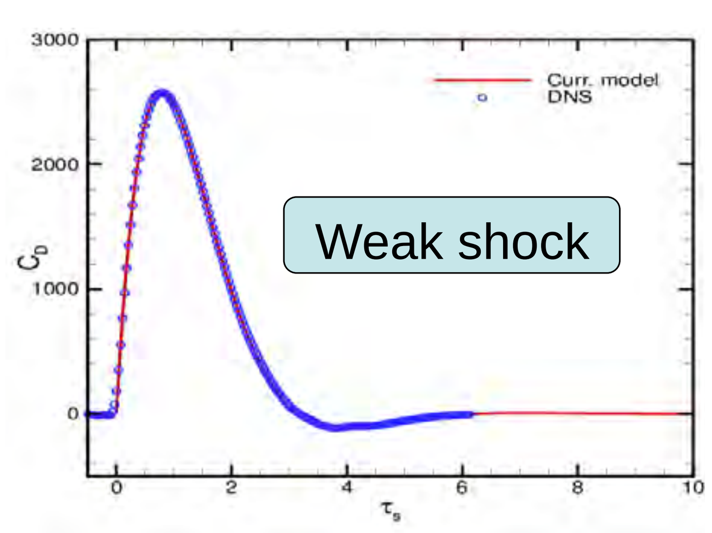
First-order perturbation theory is used to solve for velocity potentials in wavenumber space.

The force is then transformed to time-domain.

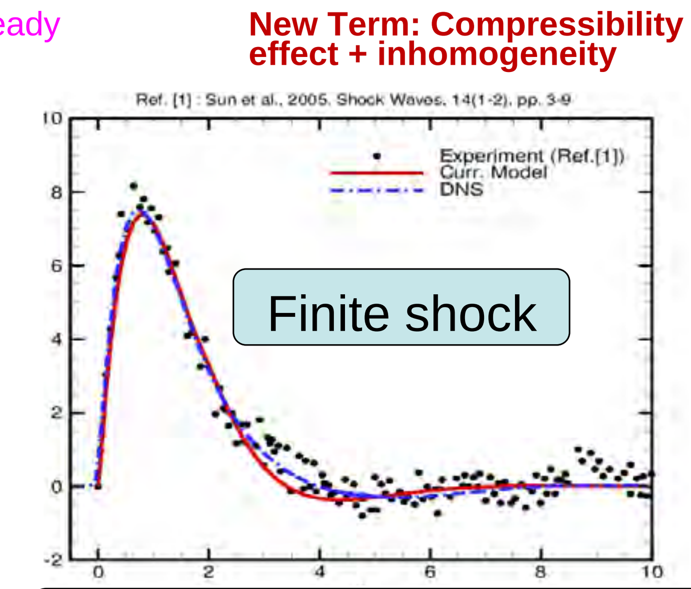
Generalized Faxén's Theorem

$$\mathbf{f_1} = \int_{\Omega} p_1\mathbf{n}\,\mathrm{d}\Omega = \rho_0\overline{\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t}}^{V} + \int_{\xi=-\infty}^{t} \mathrm{e}^{-\tau}\cos(\tau)\left[\overline{\frac{\mathrm{D}(\rho_0\mathbf{u})}{\mathrm{D}t}}^{V} + \overline{\frac{\mathrm{D}(\mathbf{r}\nabla\cdot(\rho_0\mathbf{u}))}{\mathrm{D}t}}^{V}\right]_{t=\xi}\frac{c_0}{R}\,d\xi$$

Pressure Gradient — Inviscid-unsteady kernel — **New Term: Compressibility effect + inhomogeneity**



The model precisely predicts the force in the limit of negligible Mach number



Model also captures the force for finite shock Mach numbers (M_s=1.22)

Minor variation from experiments due to usage of zero Mach number inviscid kernel

Detonation sensitivity (T1)

We consider three cases to study T1:
Case 0: No perturbation in gas density and particle volume fraction
Case 1: Perturbation only in gas density (mode 24) as seen in Fig 2a
Case 2: Perturbation only in particle volume fraction (mode 24) as seen in Fig 2b

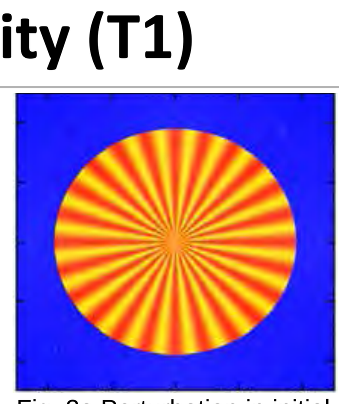


Fig .2a Perturbation in initial high density gas

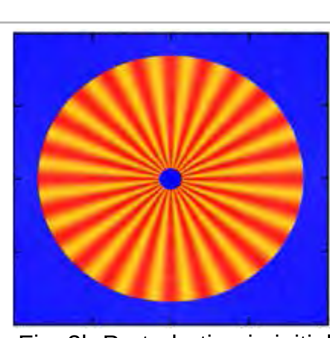
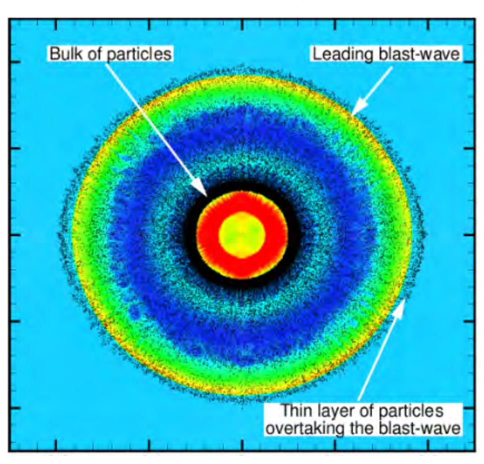
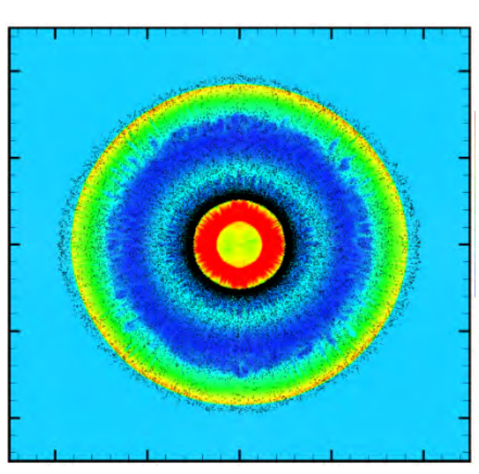


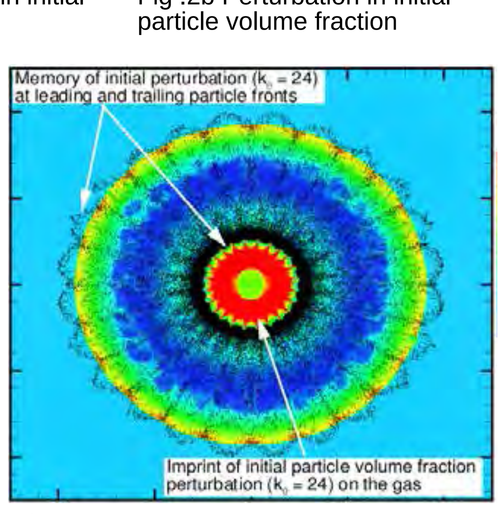
Fig .2b Perturbation in initial particle volume fraction



Case 0: Particles overtake the blast wave



Case 1: Behavior identical to "no perturbation case"(Case 0)



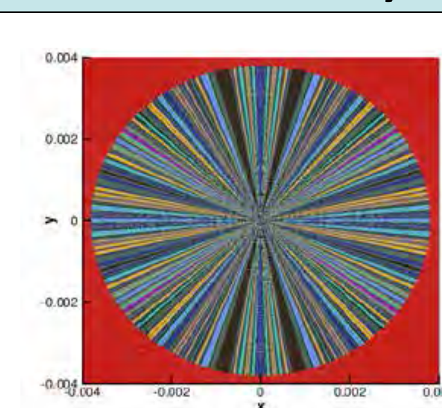
Case 2: Initial perturbation lingers for late times

Summary & Future Work

Shock-Particle Interaction

- Developed an analytical model to compute the force on a particle situated in a viscous, compressible, unsteady and non-uniform flow.
- The model accurately predicts the force for both zero Mach number and shock strengths of relatively finite Mach numbers.
- Need to improve the generalized Faxén's theorem by using improved kernels for finite Mach numbers.

Detonation Sensitivity and particle-jet formation



- The perturbation in particle volume fraction lingers for a longer period of time and possibly leads to the formation of particle jets.
- The perturbation in detonation products decay over time and therefore our assumption of homogeneous charge is justified.
- Extend the single-mode perturbation analysis to multi-mode (random) perturbation and better understand detonation sensitivity (T1).

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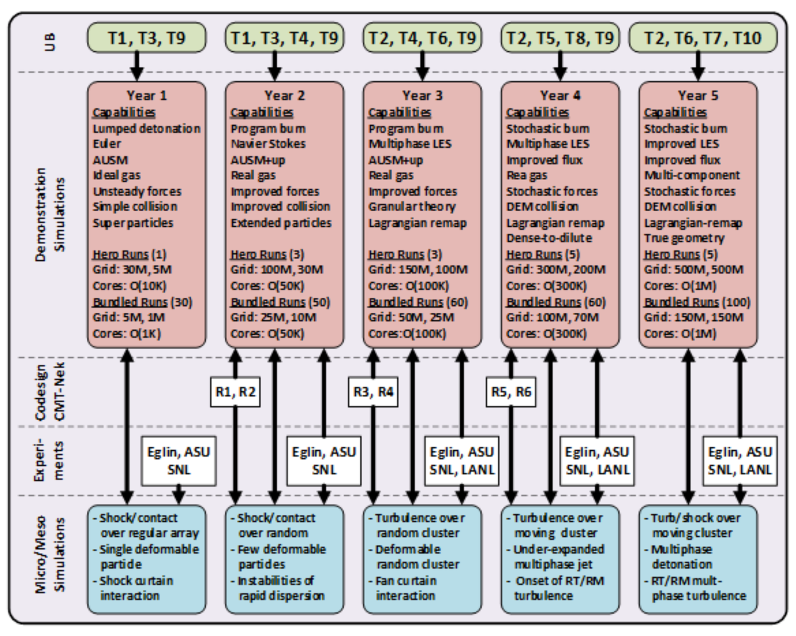
Center for Compressible Multiphase Turbulence

Performance, Energy and Thermal Research

Dr. Tania Banerjee
Department: CISE, UF

- Goals
  - Performance, energy and thermal optimization framework applied to CMT-nek on a variety of platforms.
  - Provide performance data to Exascale team for modeling
  - Load balancing algorithms for particulate applications applied to CMT-nek
- Simulation roadmap
  - Our research roadmap is closely tied with CMT-nek development



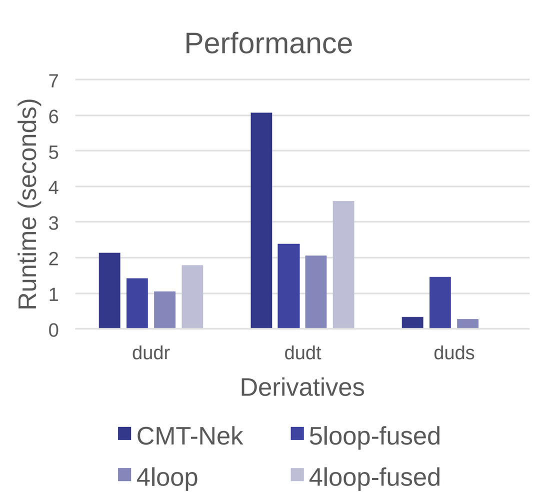
Simulation Roadmap

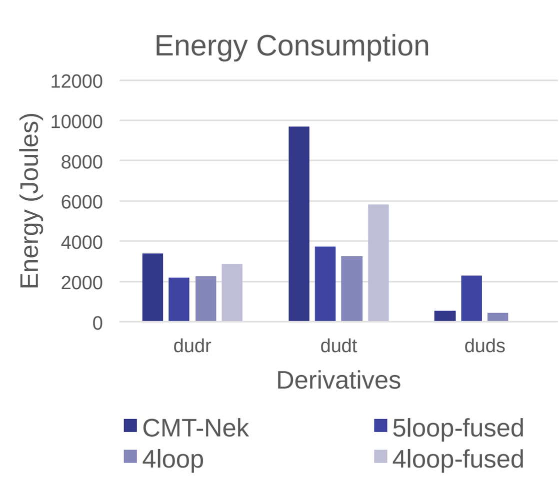
Motivation

- CMT-nek target kernels:
  - Derivative computing kernel
  - Dealiasing kernel
  - Both the kernels use matrix multiplication
- Optimization scheme: Autotuning driven by genetic algorithms
- Autotuning:
  - Empirical and platform independent method of code optimization
  - Exploration of the design space of an algorithm to determine the most performance efficient version.
- Genetic Algorithms
  - Provides an alternative to exhaustive design space exploration
  - Does not guarantee distance from optimal solution, but from our experiments, we got very close to optimal results.

Results (IBM BG/Q)

- Exhaustive run on IBM BG/Q
- Matrix size: 16x16x16, 25 elements





- 61% improvement versus CMT-nek (~2.53 times)
- 56.8% reduction in energy versus CMT-nek

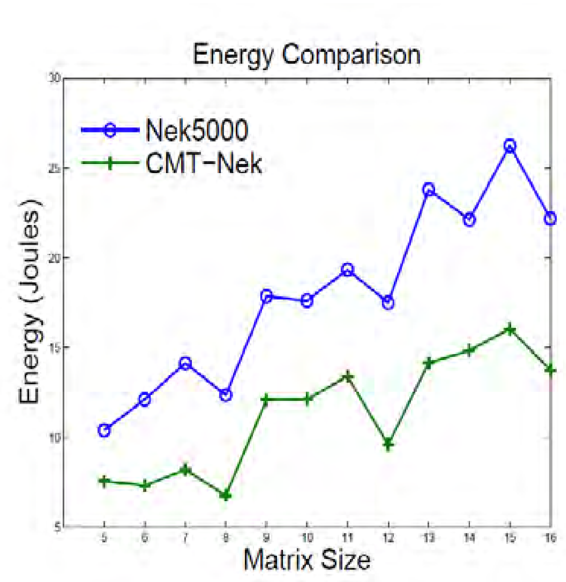
Results (AMD Opteron)

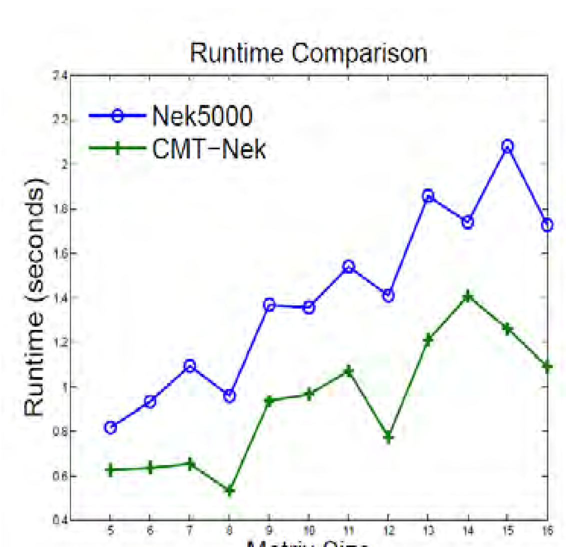
- Comparison of results from exhaustive run versus genetic algorithm
- Matrix size: 10x10x10, 100 elements
- Nearly 100,000 variants of matrix multiplication for exhaustive run

Derivative	Minimum Time	Nek5000 Time	CMT-Nek Time	Number of variants analyzed
$\partial u/\partial r$	0.39 s	0.62 s	0.41 s	444 variants
$\partial u/\partial s$	0.18 s	0.31 s	0.20 s	393 variants
$\partial u/\partial t$	0.45 s	0.88 s	0.45 s	446 variants

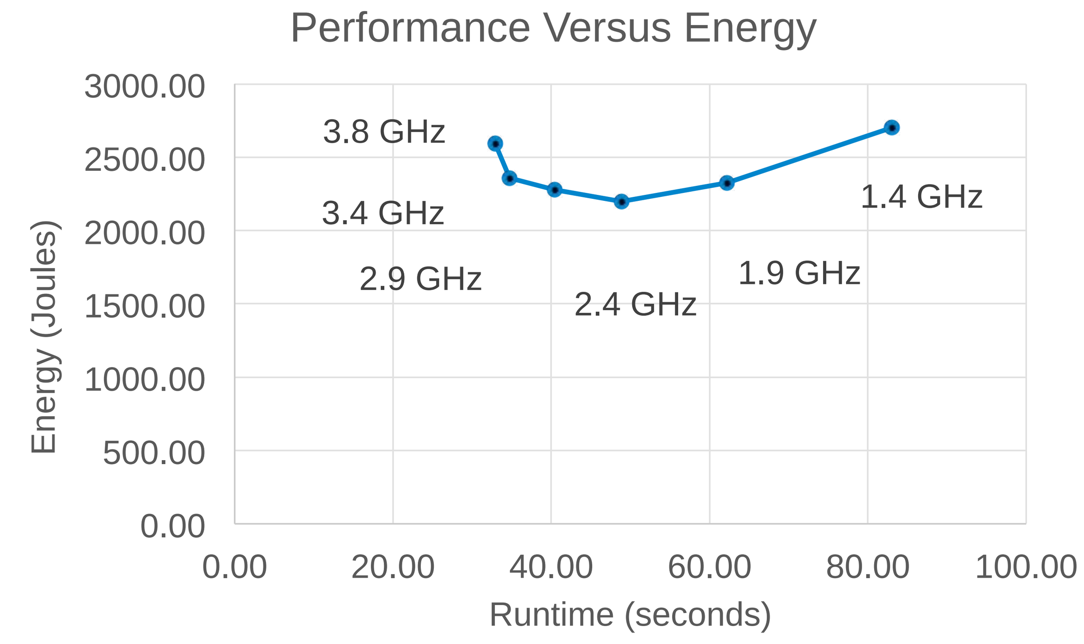
Results (AMD Fusion)

- For different matrix sizes, energy and runtime improvement
- Up to 45% improvement in runtime and energy consumption
- Faster variants are also more energy efficient variants
- Frequency: 3.8 GHz





Results (AMD Fusion)



- Results of frequency scaling on the basic matrix multiplication version
- At the highest frequency runtime is the least
- However, energy consumption is least at 2.4GHz

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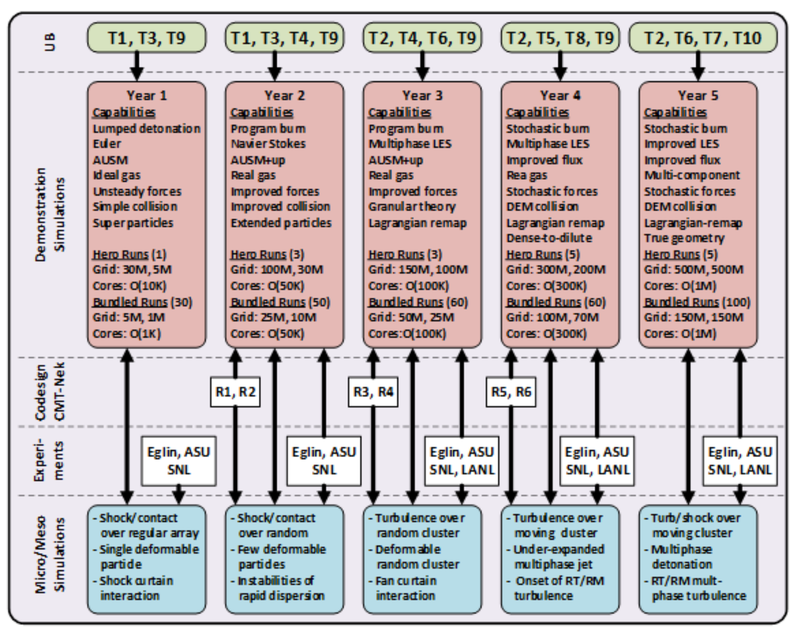
Microscale – Shock Particle Interaction

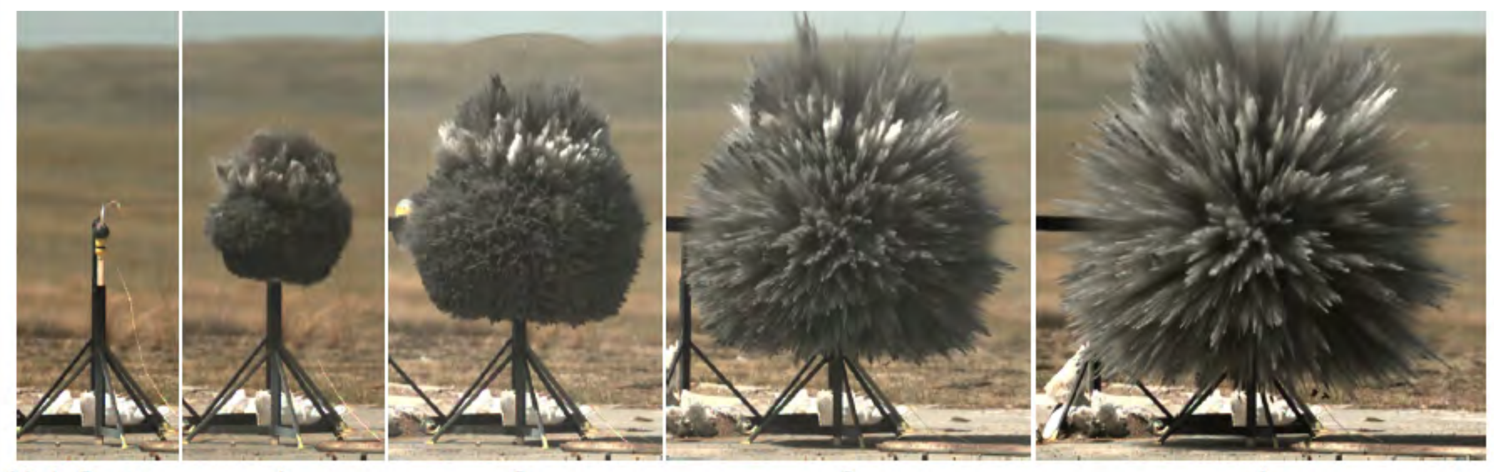
Student: Yash Mehta
Advisor: Prof. S. Balachandar
Department: MAE, UF

- Goals
  - Fully resolved DNS of shock particle interaction
  - Developing point particle models for predicting force history on particles
- Simulation roadmap
  - Shock Particle Interaction for regular array and random distribution of particles
  - Integration of point particle models in Meso-Macro scale simulations



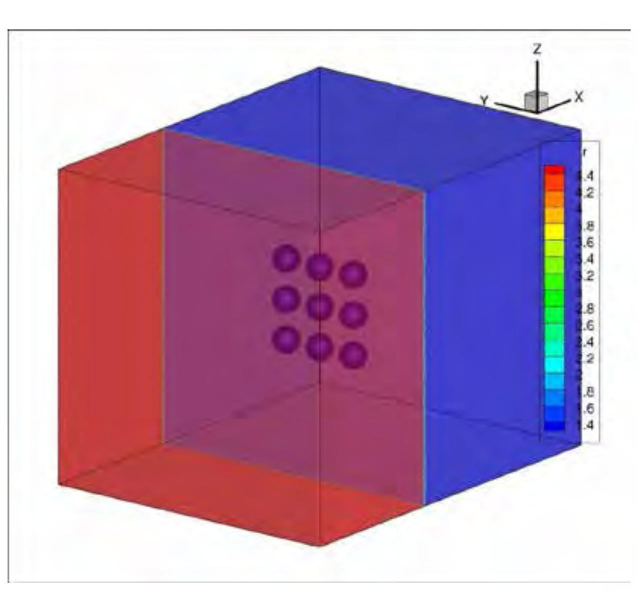
Simulation Roadmap

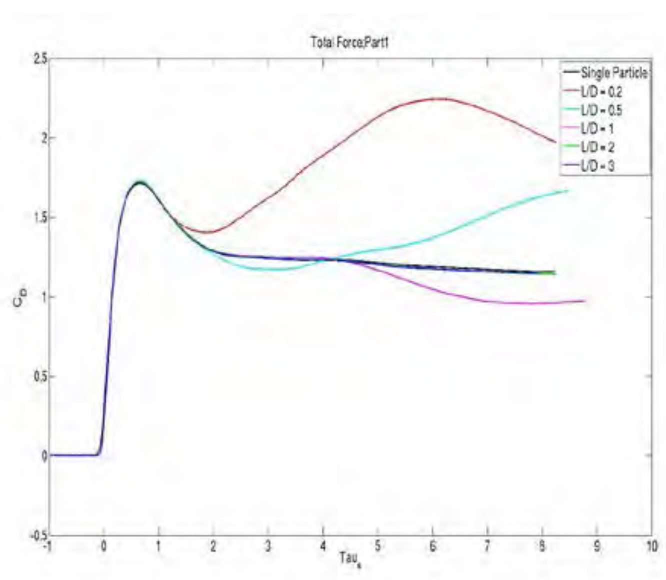
Motivation



- There is a need for understanding the interaction of high pressure - high temperature flow, with the particles
- Micro scale simulations – fully resolved DNS will be used to obtain force history on the particles for different conditions
- Results from DNS will be used to develop point particle models

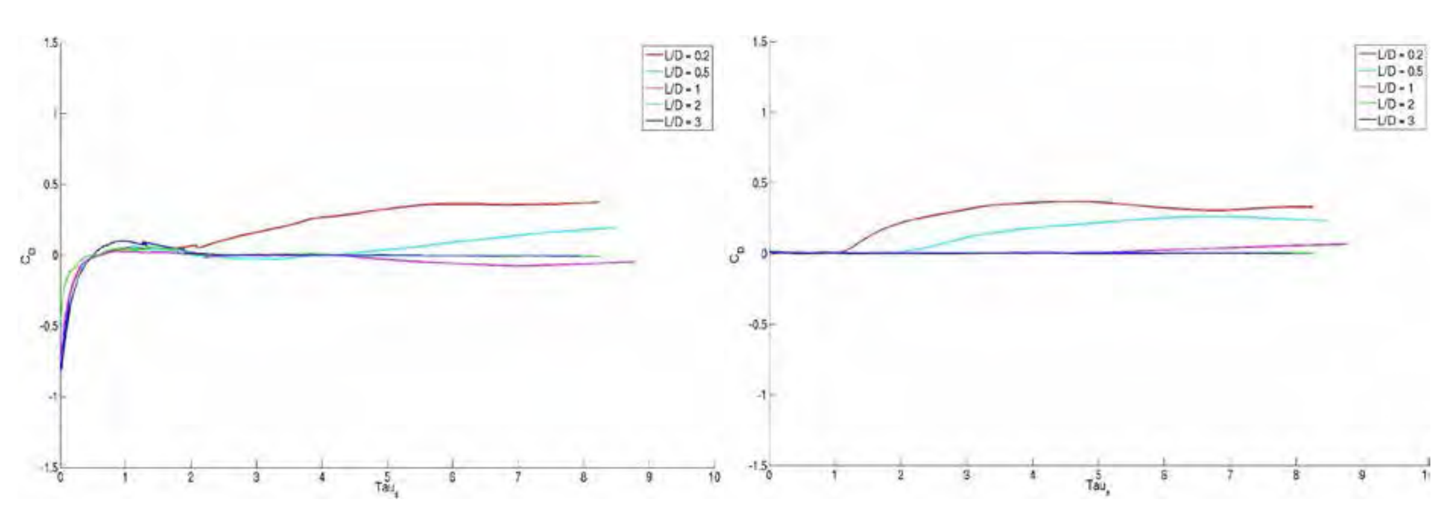
Shock Particle Interaction- Transverse Array
Mach 3.0 ; L/D = 0.2,0.5,1,2,3





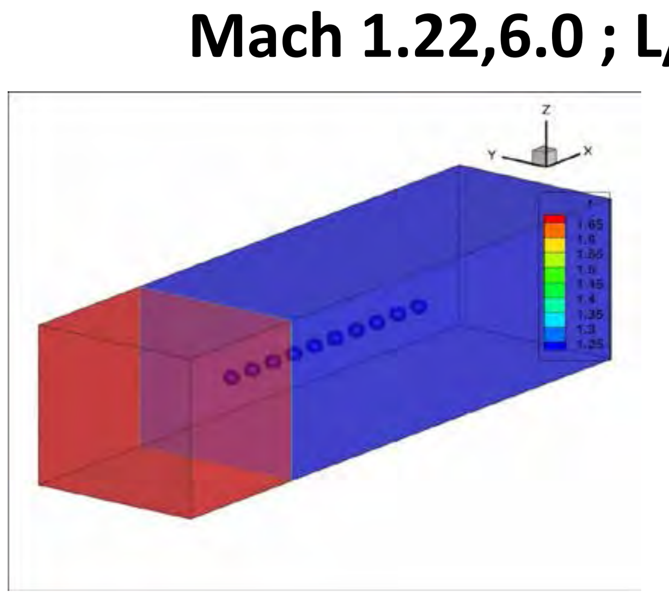
- These simulations mimic the effect of shock interaction with lead curtain of particles
- For different particle-particle spacing collected bow shock or regular reflections are observed in front of the particles

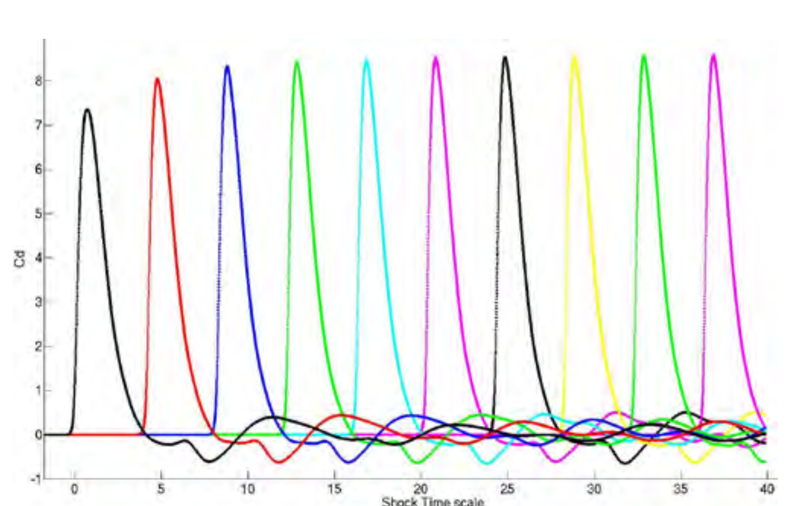
Shock Particle Interaction- Transverse Array
Mach 3.0 ; L/D = 0.2,0.5,1,2,3



- Force fluctuations on the edge particle
- These fluctuations will help in understanding behavior of edge of the particle curtain and will be used to model volume fraction effects

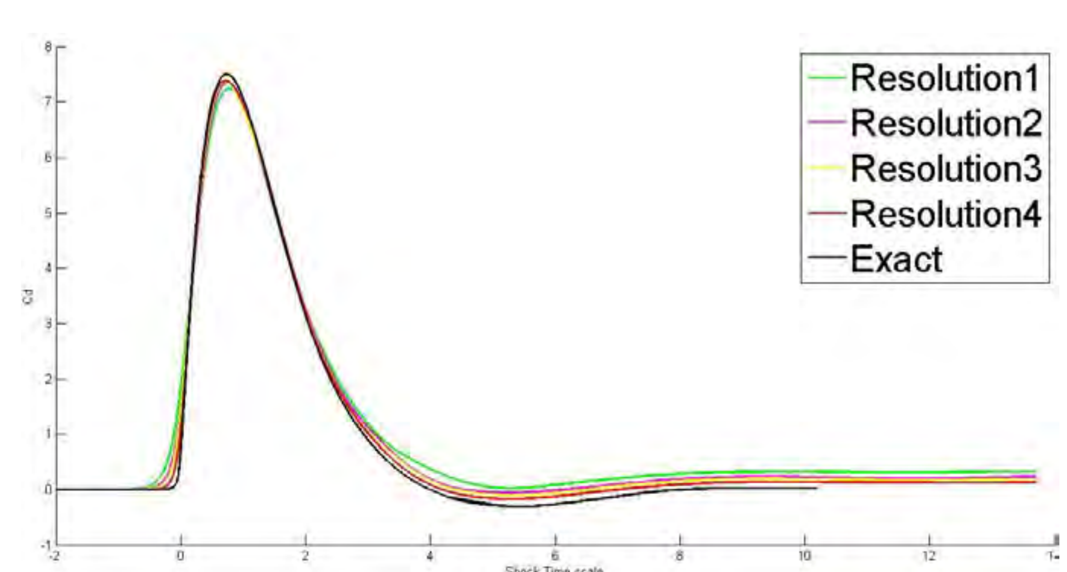
Shock Particle Interaction- Horizontal Array
Mach 1.22,6.0 ; L/D = 1.0





- These simulations help in understanding shock particle-bed interaction
- It can be concluded from these simulations that peak force asymptotes after about 5 layers deep in the particle bed

Grid Resolution Study
Single and Multiple particles



- Using Richardson Extrapolation technique to establish optimum grid resolution criteria for surface mesh and global mesh for shock-particle interaction

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Function Extrapolation using Surrogates

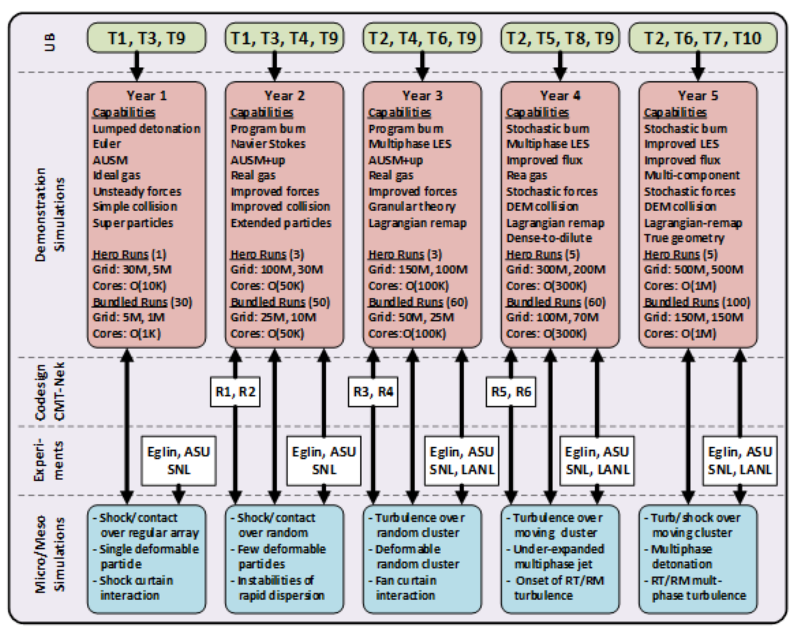
Student: Yiming Zhang

Advisors: Prof. Raphael T. Haftka

Prof. Nam-Ho Kim

Department: MAE, UF

- Goals
  - Characterization of functions
  - Developing data-fitting strategy for extrapolation
- Simulation roadmap
  - Extrapolation for computation performance
  - Extrapolation for challenging physical functions (T6,T7: Finite Re, Ma and volume fraction model)
  - Extrapolation for V&V of simulation near boundary (T4: Particle collision models)



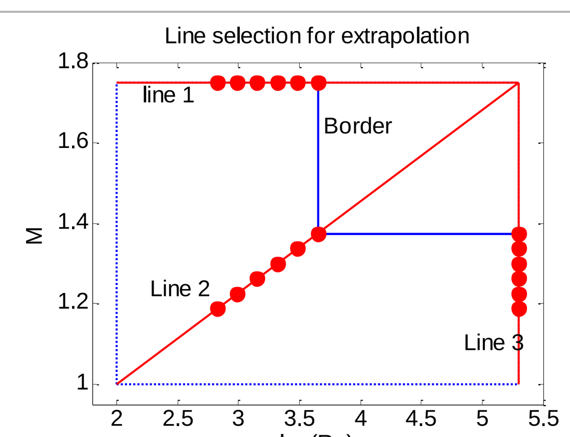
Simulation Roadmap

Motivation and Current Progress

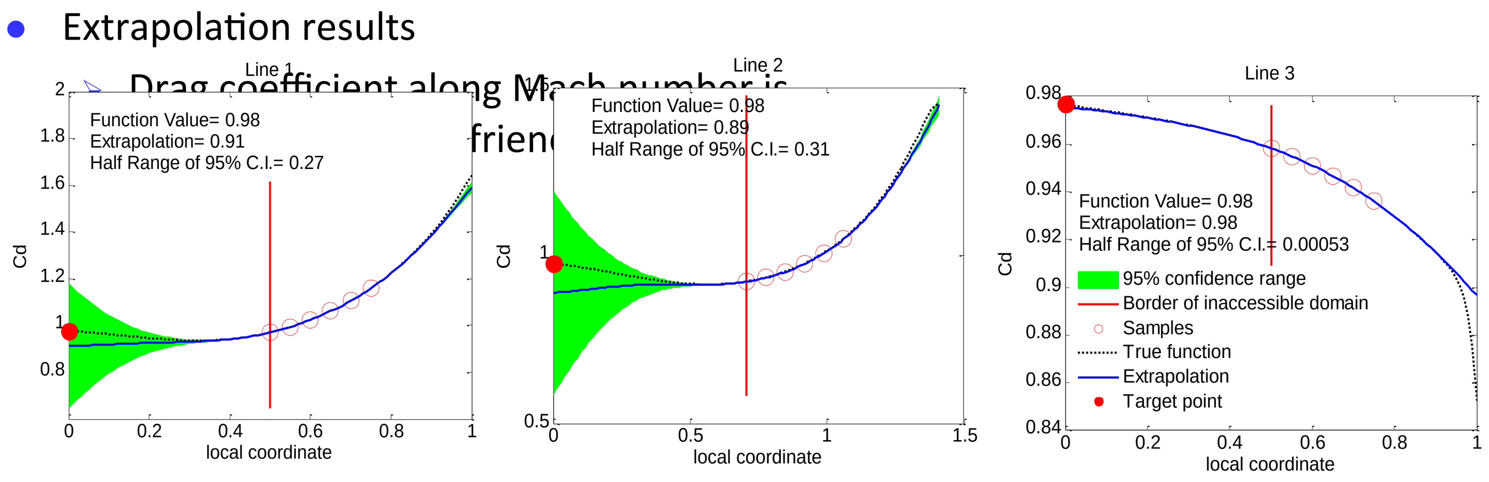
- Why extrapolation?
  - Predicting unknown events/domains (e.g. extreme condition, future event, system-level uncertainty, inavailability of samples)
- Current Research focus
  - Extrapolation towards one point using method of converging lines
  - Regularization method for extrapolation
- Publications
  - Y. Zhang, N. H. Kim, C. Park, R. T. Haftka, "Function Extrapolation at One Inaccessible Point Using Converging Lines," ASME 2015 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference
  - Y. Zhang, N. H. Kim, C. Park, R. T. Haftka, "One-dimensional Function Extrapolation Using Surrogates," 11th World Congress on Structural and Multidisciplinary Optimization

Extrapolation for A Physical Application

- Drag Coefficient function $f \downarrow Cd (M, Re)$
  - Extrapolation of Drag Coefficient in supersonic domain
  - Lines are selected to maximize angles between lines



- Extrapolation results
  - Drag coefficient along Mach number is
  frien

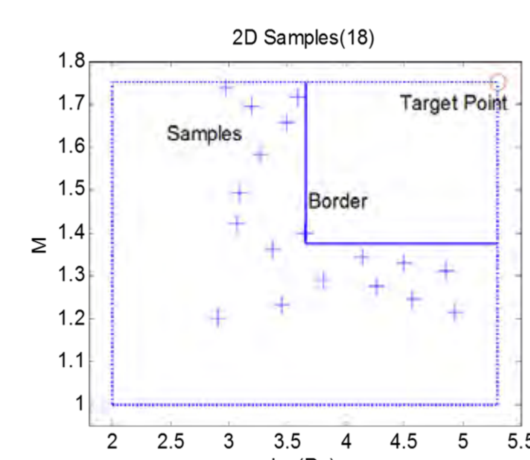


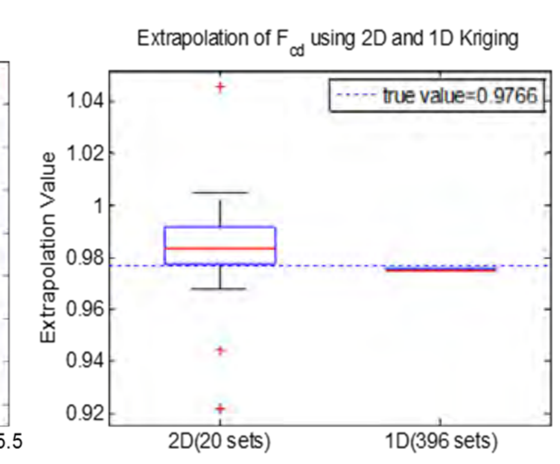
Extrapolation for A Physical Application

- Combination of lines
  - Combination using Bayesian theory

$$\frac{1}{\sigma_p^2} = \sum_{i=1}^{n} \frac{1}{\sigma_i^2} \qquad \frac{\mu_p}{\sigma_p^2} = \sum_{i=1}^{n} \frac{\mu_i}{\sigma_i^2}$$

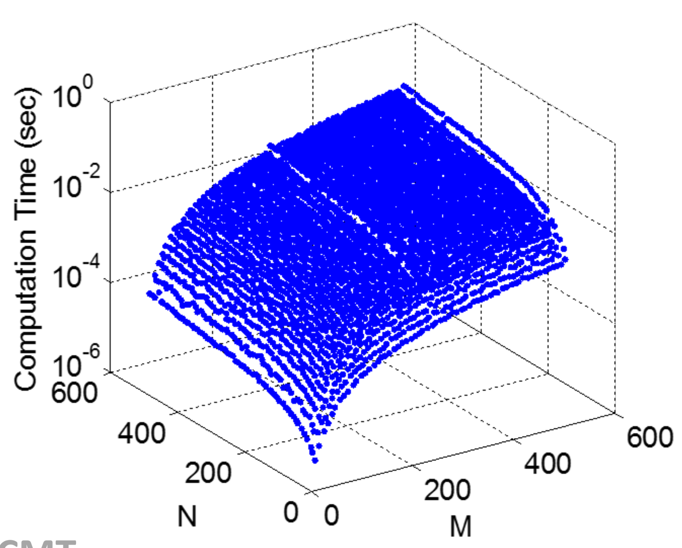
- Converging lines versus multi-dimensional surrogate extrapolation
  - 2D Kriging based on Latin Hypercube Sampling repeated 20 times
  - Point-extrapolation based on lines perturbed within ±5 degrees

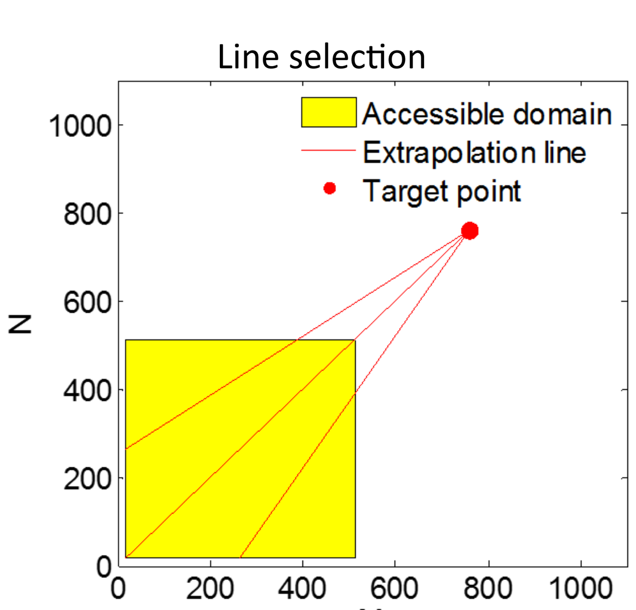




Extrapolation for A CS Application

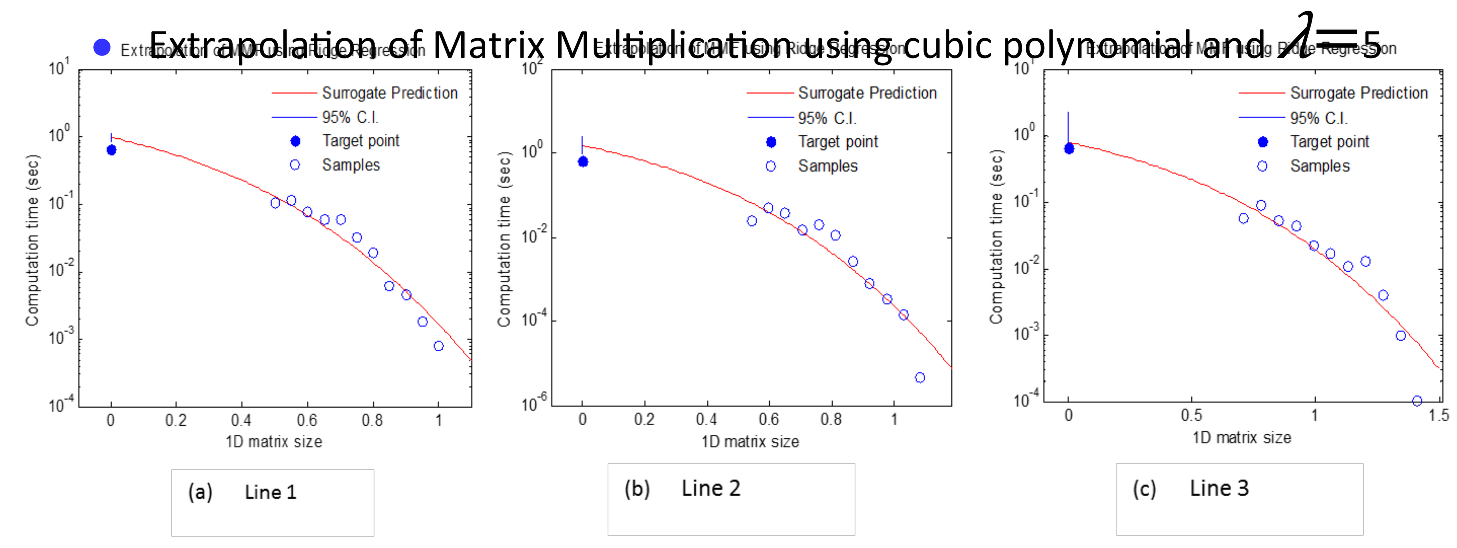
- Matrix Multiplication function (strong noise)
  - Extrapolation of computational time for matrix size out of the sampling domain
  - Initial attempt for predicting computational performance of a simulation platform





Extrapolation for CS Application

- Ridge Regression
  - Penalized polynomial regression surface as: $\sum_i (y_i - x_i^T \beta)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$
  - The shrinkage parameter λ will reduce over-fitting noise
  - Select λ by simulating extrapolation in the accessible domain
- Extrapolation of Matrix Multiplication using cubic polynomial and λ=5



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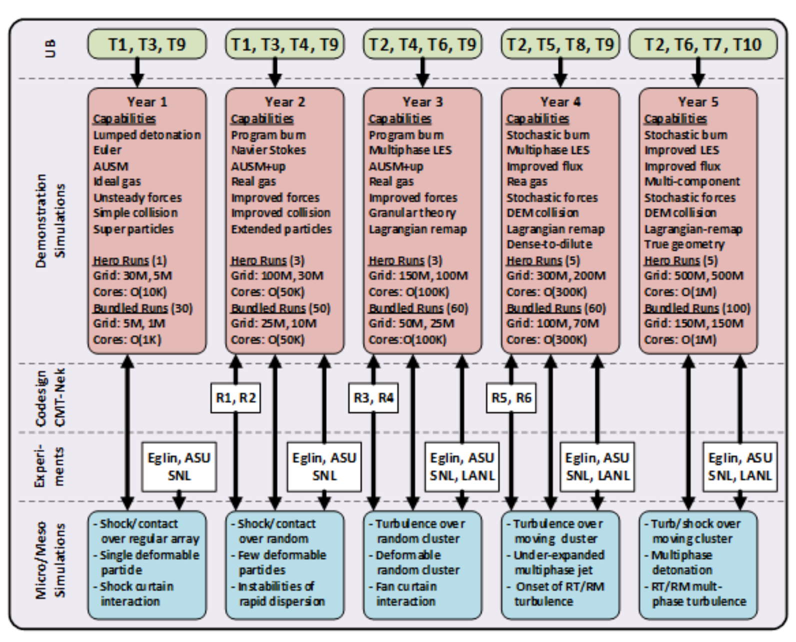
Shock Tube Experiments at ASU

Student: Heather Zunino
Advisor: Professor Ron Adrian
Department: MAE, ASU

- Goals
  - Perform experiments on an existing shock tube
    - 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
    - Instabilities within the bed may excite the RT and RM instabilities at the surface
- Simulation roadmap
  - Provide data for early-stage validation of computational codes developed by PSAAP Center

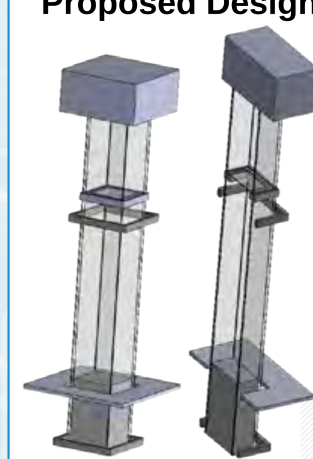


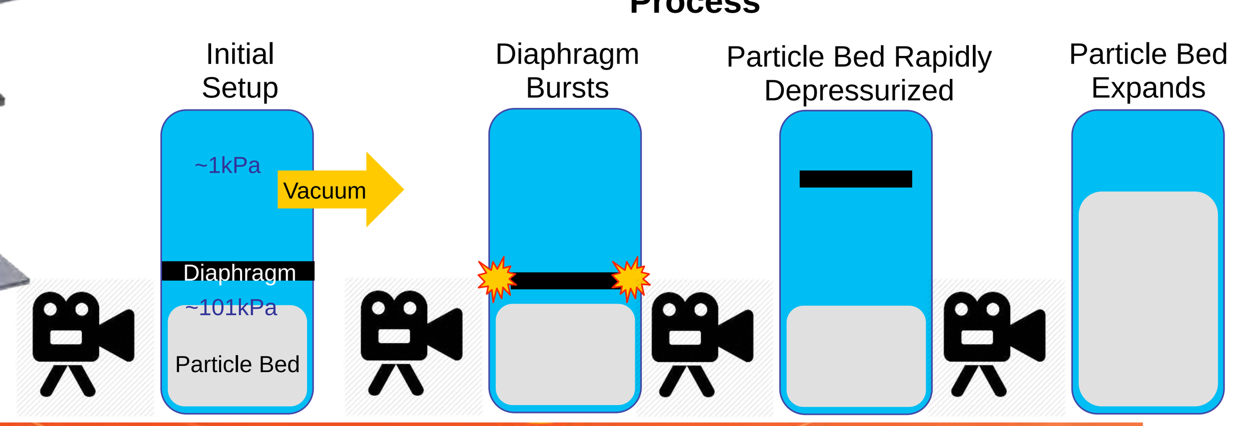
Simulation Roadmap

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
  - Flat sidewalls instead of round tube
  - Large footprint for better analyses of bed expansion, interface, and instabilities
  - Reduce the scatter and uncertainty in current data
  - Simpler physics involved than in the PSAAP capstone experiment

Proposed Design

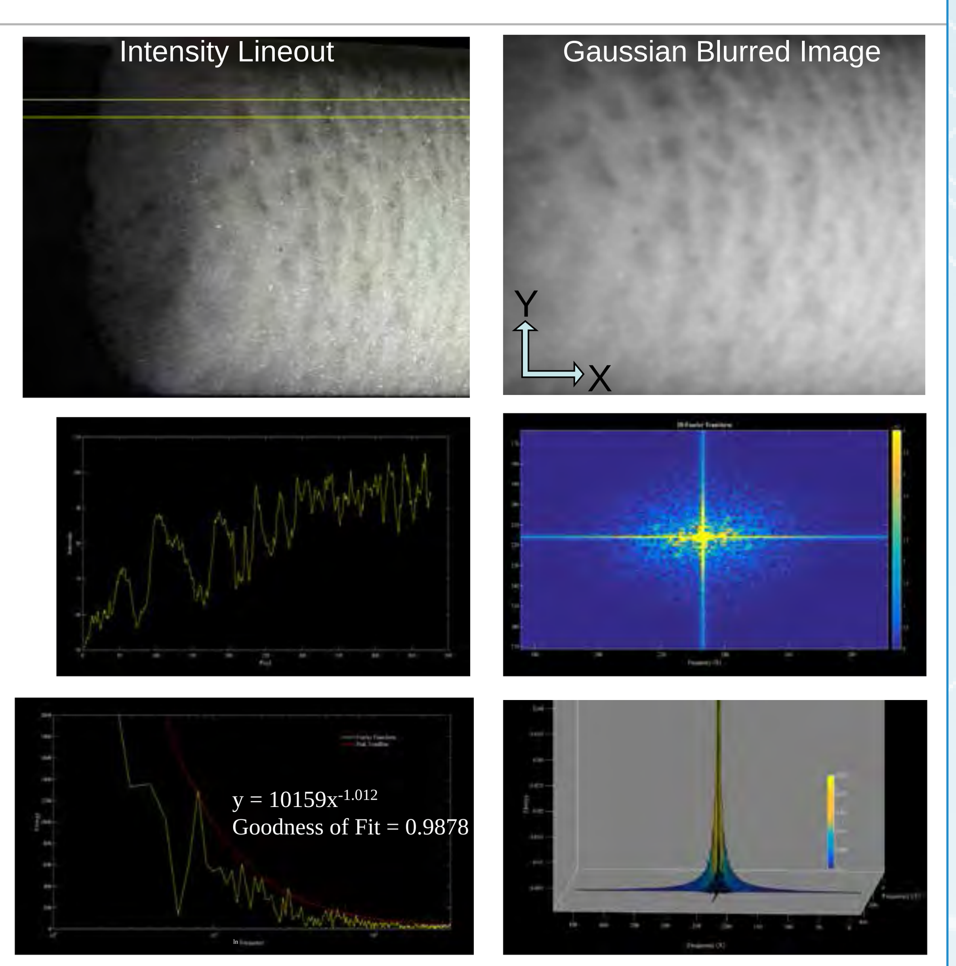




Results

Rapid Decompression

- Particle void regions form in particle bed
  - First appearance is near particle bed surface
  - Voids appear deeper in particle bed as time progresses
- Disturbances in the particle bed at incipient expansion may cause the void pattern seen at later times
- Periodic
  - 1D and 2D Fourier Transform
- Voids grow in time
  - Frequency peak fitting measures void growth



Results

- Interface instabilities develop and grow in time
- Flow structures resulting from rapid decompression may be directly related to the spikes seen during an explosion
  - Amplification
  - Provide initial perturbations for RM and RT instabilities

PSAAP

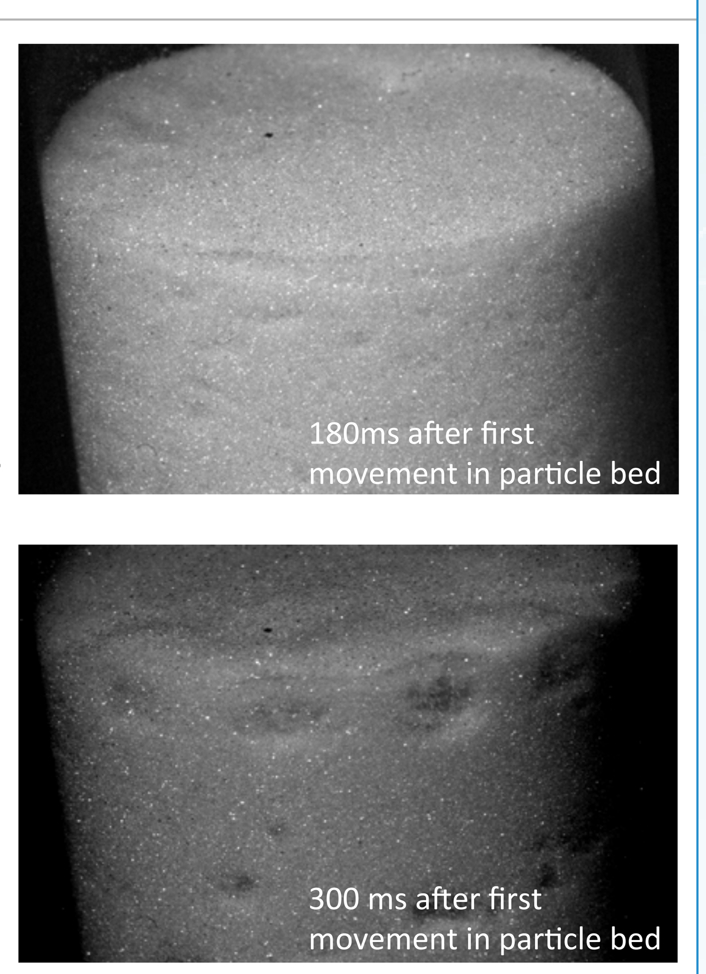
- Edge of interface develops wave-like features
  - ~ 2.5 ms*
- Sharp structures develop along perimeter of particle bed
  - ~ 3.5 ms *
- Sharp structures develop in the center of particle bed
  - ~ 5ms *

*times are relative to the first sign of movement at the top of the particle bed

Results

Slow Leak Experiment

- Particle bed depressurized at two rates
- Particle void regions appear during both stages of depressurization
- Rapid decompression may cause more regular particle void patterns
- Larger voids rise and overtake smaller voids
- Cells appear throughout depth of particle bed during slower decompression
  - Voids are not limited to the upper region of the particle bed during early times, as is seen in the experiments with a more rapid decompression
- RMI and RTI may appear in voids



Summary

- Experiments completed on existing cylindrical shock tube at ASU
- Designs nearly-complete for new large shock tube with square footprint
- Fourier investigation
  - Revealed regularity in patterns of particle void regions
  - Examined growth rate of particle void regions
- Interface instabilities
  - Structures appear near wall region first
    - Rounded, wave-like structures
    - Sharp spikes
  - Similar structures appear further from the wall in later times
  - Potential initiation and amplification of Rayleigh-Taylor and Richtmyer-Meshkov instabilities
- Slow leak experiment
  - Larger voids rise and overtake smaller voids
  - Faster decompression shows more regular particle void patterns

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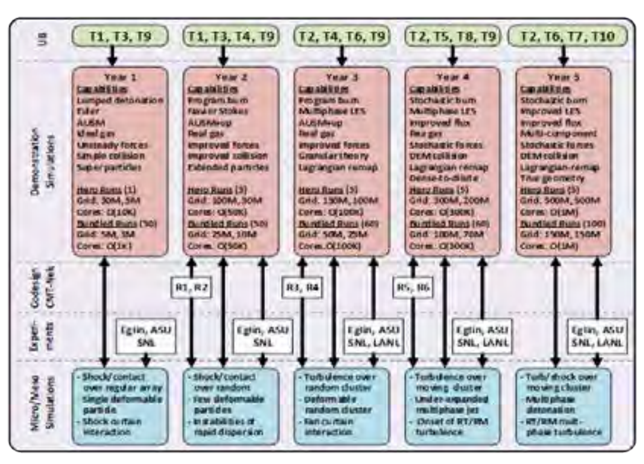
Behavioral Emulation Methodology for Fast Design Space Exploration

Student: Nalini Kumar
Advisor: Prof. Alan George
Department: ECE, UF

- Goals
  - Develop concepts for a platform independent, fast & scalable simulation methodology
  - Design & validate simulation models of existing architectures
  - Enable modeling & performance prediction on notional architectures



Simulation Roadmap

- Simulation roadmap
  - Enable early algorithm design space exploration to aid and assist CMT-nek code developers at different stages in the simulation roadmap

Motivation and Guiding Principles

– Allow performance analysis at different levels of system organization (device, node, rack, machine) – *Multi-scale simulation*

– Allow use of performance models agnostic of how they were developed (testbed experiments, fine-grained simulation, analytical models etc.) – *Component-based simulation*

– Allow arch DSE by providing ability to build notional archs by plugging different components in the simulation – *Component-based simulation*

– Allow fast algorithm DSE by simulation from high-level scripts, and not requiring working code – *Coarse-grained simulation*

– Allow reasonably accurate performance analysis within a reasonable time – *Coarse-Grained Simulation*

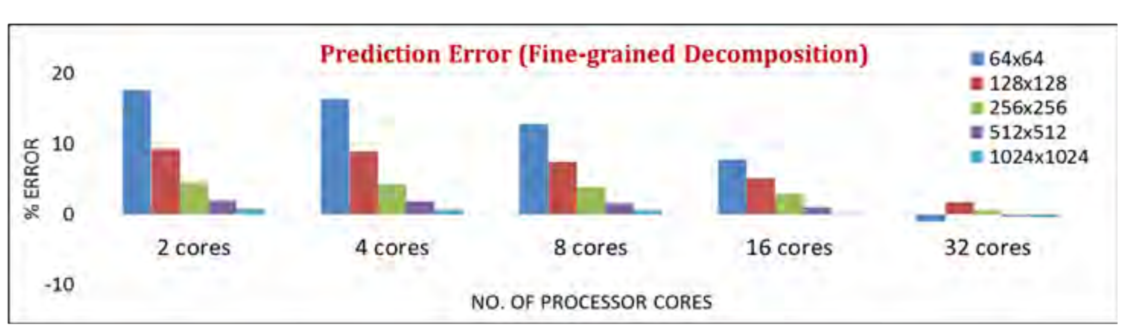
– Finally, ensure simulation approach is portable to any PDES framework

CMT-Nek code developers will be able to use BE simulation capabilities to analyze performance on future systems, understand potential bottlenecks, and revise code development plan accordingly

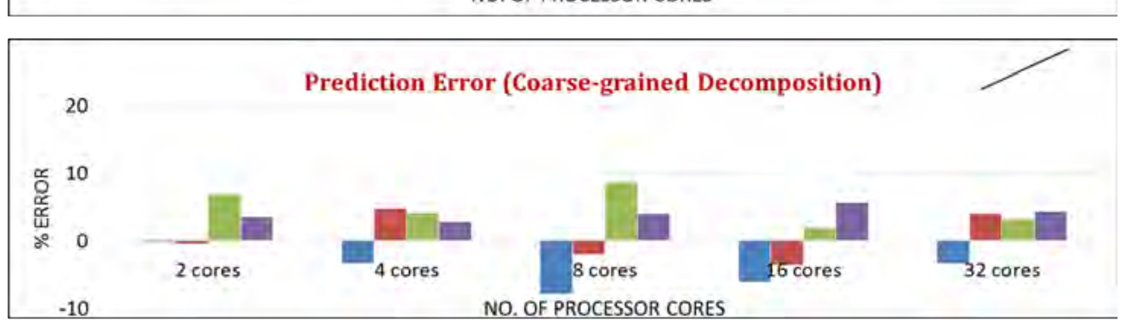
Simulation Validation

It is important to evaluate accuracy of coarse-grained BE approach

– Evaluate use of fine vs. coarse-grained app decomposition
– **Device:** Many-core device with user accessible mesh network (Tile-Gx36)
– **Application:** Parallel 2D matrix multiply

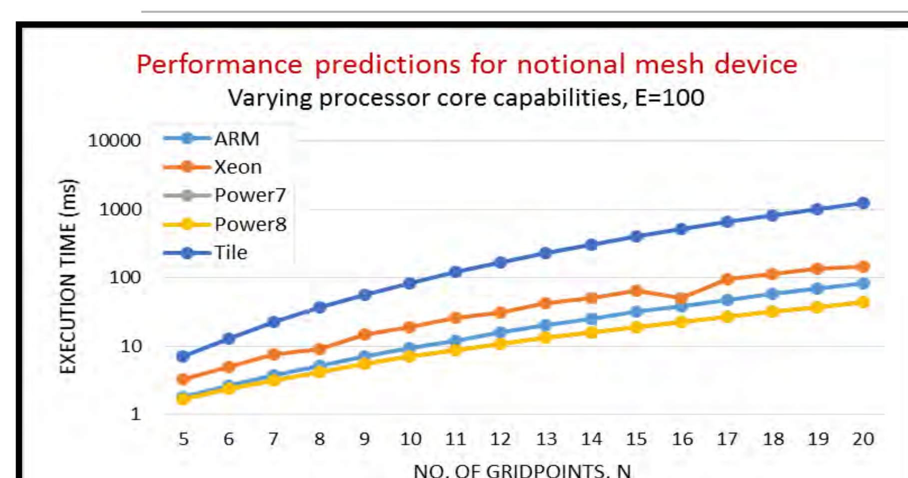


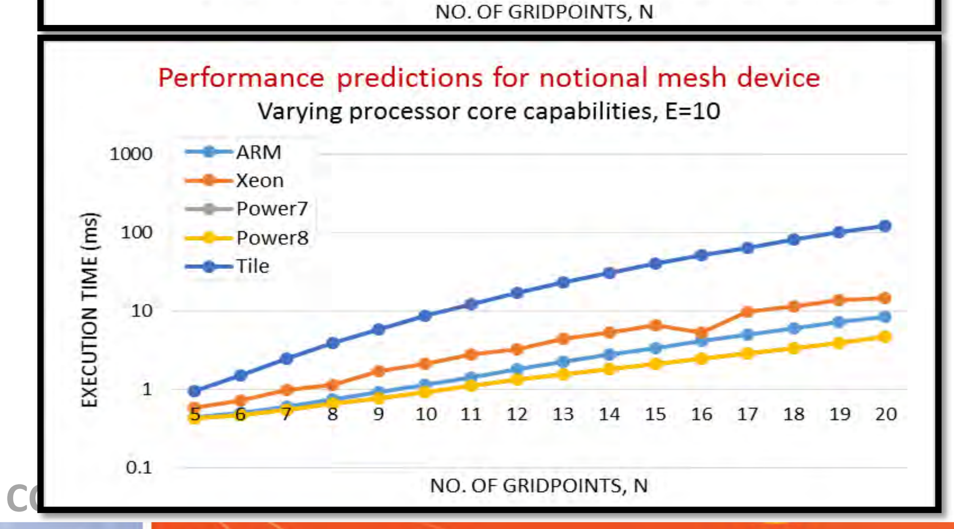
– Fine-grained decomposition into dot products



– Coarse-grained decomposition into small matrix multiplies

Performance Prediction (1)





Architecture design space exploration with spectral element solver

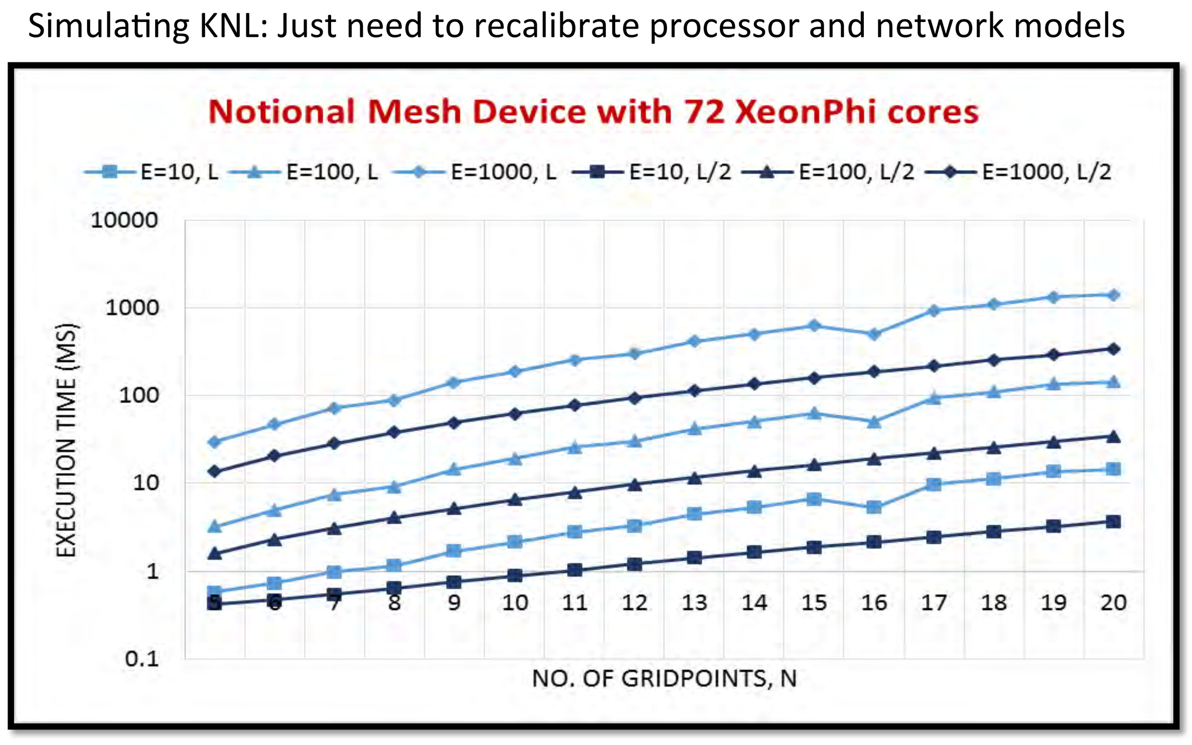
– Mesh network with different processor cores
– Mesh network remains the same between experiments
– Two graphs show the performance for two problem sizes

IBM Power8 and APM X-Gene ARM64 calibration was performed on ASC testbeds at Sandia National Laboratories, Albuquerque, New Mexico. All other experiments were performed on CHREC, UF testbeds.

Performance Prediction (2)

Architecture design space exploration with spectral element solver

– Mesh device with 72 Intel XeonPhi core models
– Mesh networks with two different latencies
– Simulating KNL: Just need to recalibrate processor and network models



Summary

Conclusions

– Behavioral Emulation allows co-design from early stages of app development and machine design
– Reasonable simulation accuracy gives some confidence in use of BE for architecture design space exploration

Future Work

– Extend BE framework for modeling nodes and systems
– Develop and evaluate methods for modeling network behavior of an app (network congestion) at different scales
– Integrate with an existing scalable PDES (eg. SST) and explore knowledge-based optimizations to the simulation framework

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