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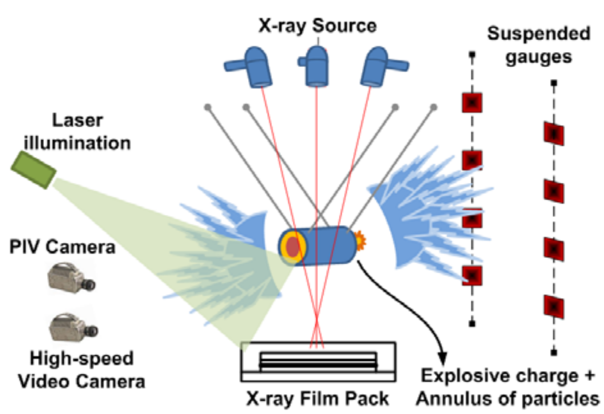
CENTER FOR COMPRESSIBLE MULTIPHASE TURBULENCE

TST Review

October 30-31, 2017



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Internship Presentations

Paul Crittenden
Mohamed Gadou
Trokon Johnson
Yash Mehta

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Contact Front Instability and Code Verification

Lawrence Livermore National Laboratory

Spring 2017

Paul Crittenden
PhD Student
Mechanical and Aerospace Engineering Department
University of Florida

Introduction

- Mentor Dr. Kambiz Salari (Sam Schofield, Tim Dunn)
- Worked on analytical stability results
- Ran shock tube test cases using ALE3D (Eulerian-Eulerian)
- ALE3D is a multi-physics numerical simulation software tool
- Main goal of the work was verification of my multiphase code

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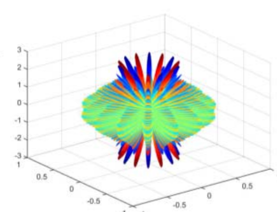
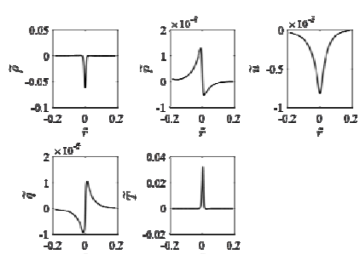
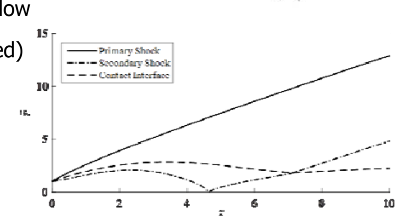
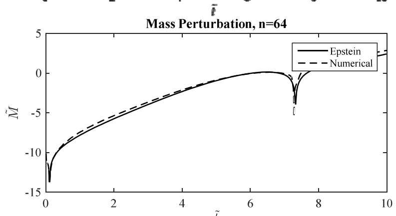
Single-phase Instability

- Assumptions about contact (Epstein)
  - Spherical Harmonics
  - Spatially constant density
  - Irrotational base and perturbed flow
  - Equal compression rates (removed)
  - Incompressible perturbations









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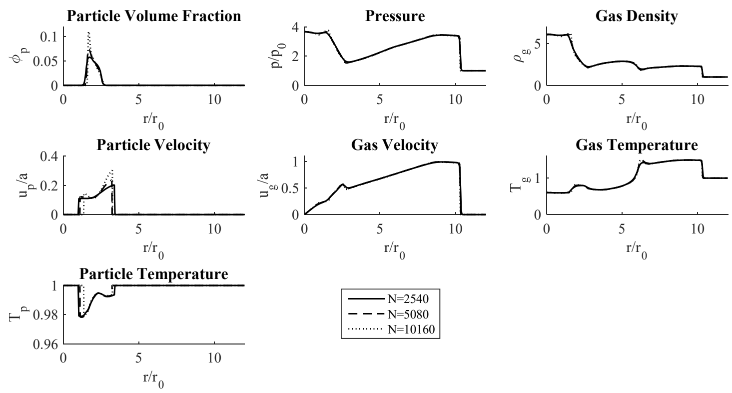
Two-Phase Verification-ALE3D



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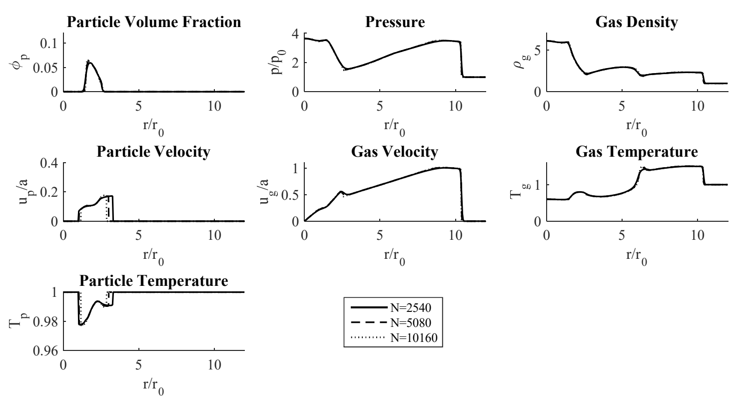
Two-Phase Verification-AUSM1D



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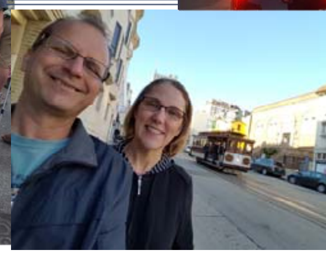
Activities at LLNL

- Seminars
- End of internship presentation







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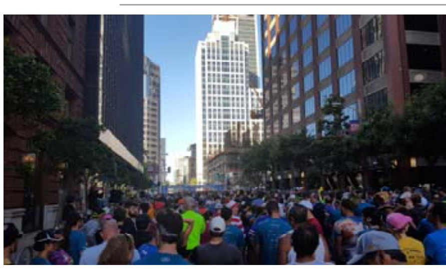
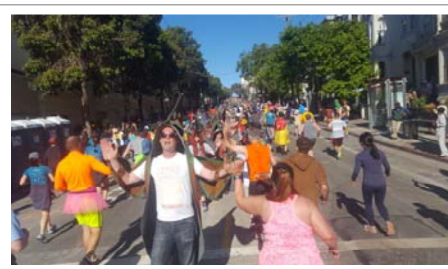
Bay to Breakers!

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My Internship at LANL

Mohamed Gadou
Computer and Information Science and Engineering
University of Florida

- Mentors:
- Galen Shipman
- David Daniel
- Ryan Braithwaite

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Interning at The Lab

- Amazing environment for learning
- Organized workspace and excellent mentorship
- Opportunity for interacting with best minds in various Science fields
- Great Friendly and Helpful coworkers
- Aligned Values to Personal Values (Integrity, Safety, Security, Respect, ..)

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Architecture Description

- Measuring Performance, Power, and Energy

Name	Description
IBM Power 8 + P100	- IBM power8 server with 2 sockets - Reported TDP of 190 watts per socket - NVLink to reduce data transfer overhead between CPUs/GPUs - 2 Nvidia Tesla P100 GPUs
Intel Broadwell – 2 sockets	- Intel Broadwell family E5 with 2 sockets - TDP of 135 watts per socket
Intel Haswell + K80	- Intel Haswell family E5 with 2 sockets - TDP of 120 watts per socket - 2 of ½ NVIDIA Tesla K80 GPUs
Intel KNL	- Intel Knights Landing with 72 cores - High Bandwidth memory is available (MCDRAM) - Multiple MCDRAM Configurations - MCDRAM size is 16 GB

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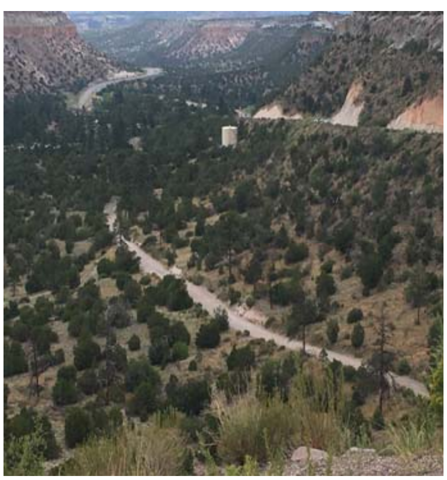
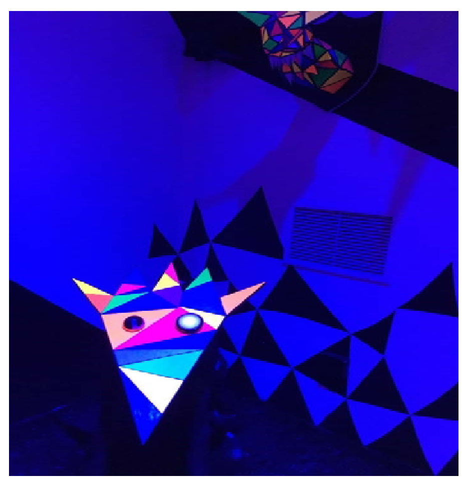
Life at Los Alamos





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LANL PCSRI: Toward Parallelized Dictionary Learning and Sparse Coding

Trokon Johnson, The University of Florida

Mentors:
Cristina Garcia Corona (CCS-3)
Brendt Wohlberg (T-5)

Overview: Parallel Computing Summer Research Institute

- 10 Week Program
  - Crash Course of HPC Topics
    - MPI
    - Vectorization
    - Scrum
    - Quantum Computing
  - Special Projects
    - Small group projects for the duration
  - Contacts
    - Experts in different HPC areas

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Project: SPORCO Acceleration

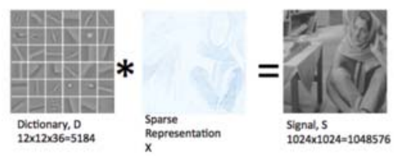
- Goal:
  - Sparse Coding: efficiently represent signals using dictionaries
    - can be used for denoising, feature identification, etc
  - Dictionary Learning: creates dictionary elements by training on signals
- Contribution
  - Parallelized existing convolutional dictionary learning library (SPORCO)
    - mpi4py
- Impact
  - Significant reduction in time to create trained dictionary elements
  - Allows for largest convolutional dictionary problem solved, to our knowledge

Sparse Coding

$$\arg\min_{\{\mathbf{x}_m\}} \frac{1}{2}\left\|\sum_m \mathbf{d}_m * \mathbf{x}_m - \mathbf{s}\right\|_2^2 + \lambda \sum_m \|\mathbf{x}_m\|_1$$

Dictionary Update

$$\arg\min_{\{\mathbf{d}_m\}} \frac{1}{2}\sum_k \left\|\sum_m \mathbf{d}_m * \mathbf{x}_{k,m} - \mathbf{s}_k\right\|_2^2$$



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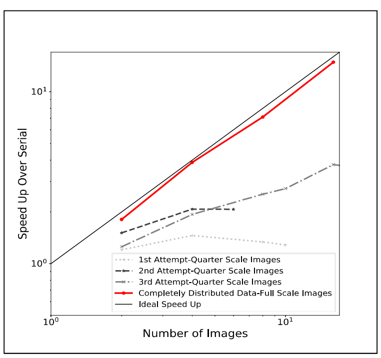
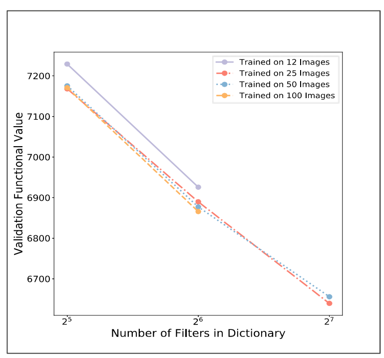
Results





- Great weak scaling results
- Allowed for much larger tests
  - 256x256 -> 1024x1024
  - 100 Images

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Excursions

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Excursions, pt. 2

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Shock Interaction with Moving Particles

Lawrence Livermore National Laboratory

Summer 2017

Yash Mehta
PhD Student
Mechanical and Aerospace Engineering Department
University of Florida

Introduction

- Mentor Dr. Kambiz Salari
- Worked on analyzing data from ALE3D simulations
- ALE3D is a multi-physics numerical simulation software tool using arbitrary Lagrangian-Eulerian (ALE) techniques
- Main goal of the work was to understand motion of multiple particles under detonation conditions

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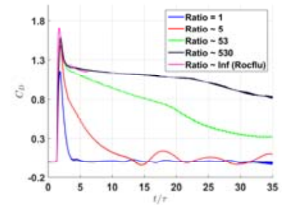
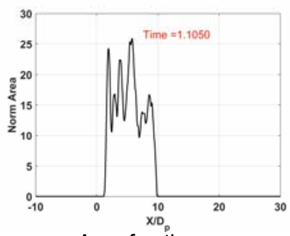
Shock Interacting with Moving Particle(s)

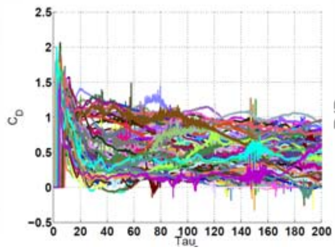
$M_s = 3.00$; $\varphi = 10\%$; $\rho_p/\rho_f = 530$



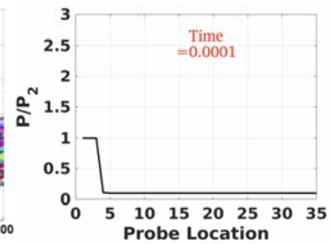
Drag single particle ; $M_s = 3.00$



Area fraction;
$M_s = 3.00$; $\varphi = 10\%$



Drag ;
$M_s = 3.00$; $\varphi = 10\%$



Pressure through domain;
$M_s = 3.00$; $\varphi = 10\%$

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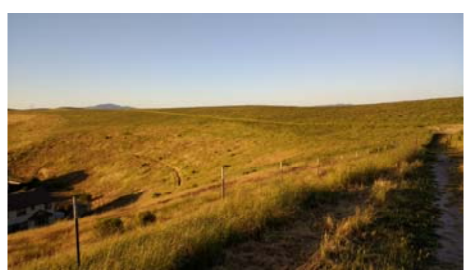
Activities at LLNL

- NIF tour
- Summer Interns barbecue
- Summer seminar series (various programs)
- Computation program – "Apple Time"
- Computation seminar – end of internship presentation



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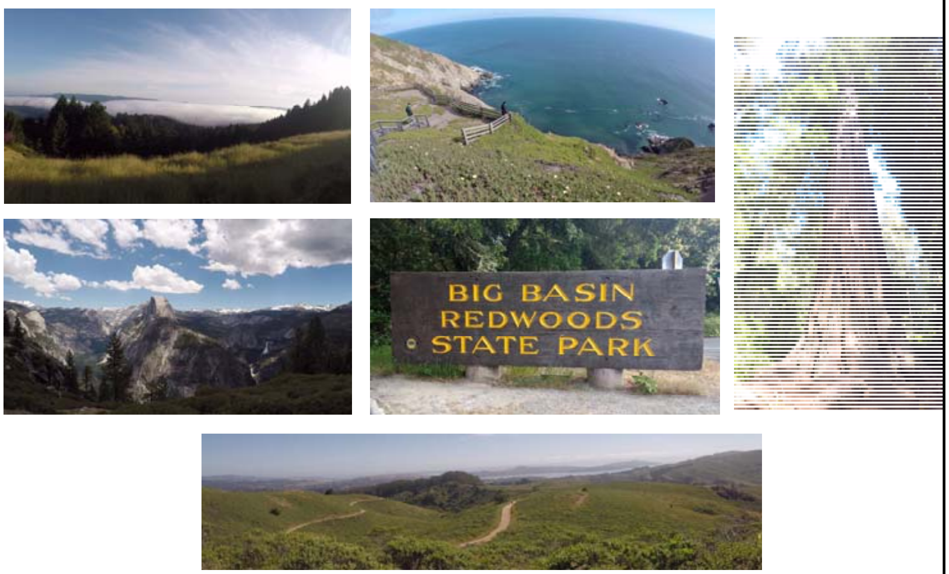
Life around Livermore



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Do you have any questions?

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Surrogate Modeling of the JWL Equation of State

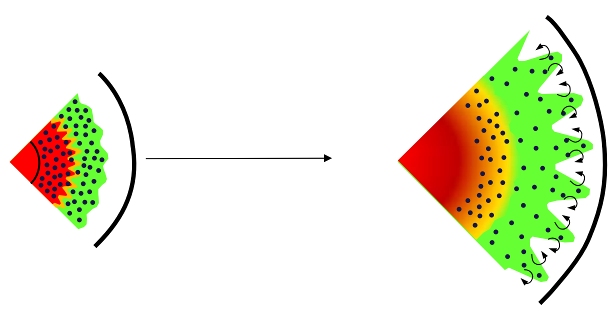
Frederick Ouellet

PhD Student

UF UNIVERSITY of FLORIDA

Goal – Handling Cells with Mixed E.O.S.

Initial State | Early Time



- A short time after detonation, there are both pure explosive products and pure air
- At later time, pure species still exist but a mixture region will form where two equations of state must be satisfied
- Goal is to find a way to simplify and speed up the gas computations in this zone

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Standard Approaches for Mixed Cells

Method of Tackling	Pros	Cons
Mass fraction weighted averaging	• Algebraic equations • Small data storage	• Does not place species equilibrium requirement
Tabulated data	• Interpolation is only operation • Can place species equilibrium requirement	• Must store the tabulated data • Interpolation error
Polynomial regressions/curve fits	• Algebraic equations • Small data storage • Can place species equilibrium requirement	• Curve fit errors
Iterative schemes	• Small data storage • Can place species equilibrium requirement	• Computationally expensive

- Rocflu uses a Broyden's method iterative solver to enforce pressure and temperature equilibrium between air and the explosive products

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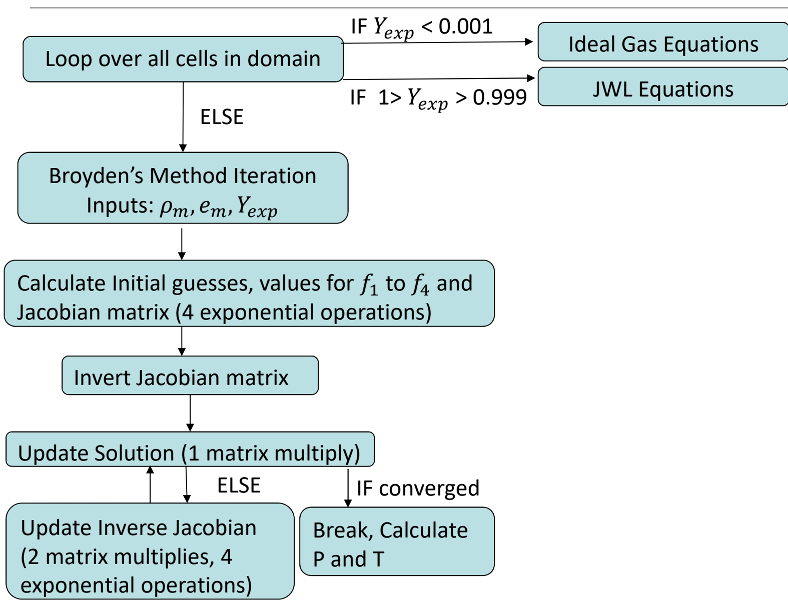
The Iterative Solver



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Looking at the Big Picture

- What is an iterative scheme really doing?

Inputs:
ρ_m, e_m, Y_{exp}

↓

Outputs:
1) Common pressure/temperature for both EoS
2) Internal energy attributed to the air and the products
3) Density attributed to the air and the products

- If we compute the common pressures and temperatures outside of the code, a curve fit can be applied

Models Implemented in Rocflu

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

$$\boxed{\begin{aligned} P_{JWL}(\rho, e) &= A\left(1-\frac{\omega}{R_1 V}\right)e^{-R_1 V} + B\left(1-\frac{\omega}{R_2 V}\right)e^{-R_2 V} + \omega\rho e \\ T_{JWL}(P,\rho) &= \left(\frac{1}{\rho\omega C_v}\right)\left(P - Ae^{-R_1 V} - Be^{-R_2 V}\right) \end{aligned}}$$

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

	Iterative Method	One Equation Model	Multi-Fidelity Surrogate
Advantages	- Accuracy - Problem independent	- Speed - Algebraic equation	- Speed - Accounts for species equation
Disadvantages	- May be slow to converge - Computationally expensive	- Uncertainty and error - JWL + ideal gas case only	- Uncertainty - Equation of State specific (problem specific)
Used In	HR 2	HR 3/4/5	Future HRs

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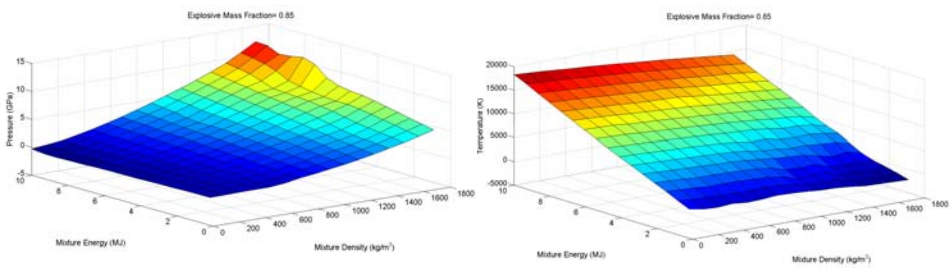
Surrogate Model - Development



- Kriging method used to generate two models for mixed cell pressure and temperature in terms of ρ_m, e_m and Y_{exp} using 50-800 sampling points

- Domain Space: $\rho_m \rightarrow (1, 1770)$
  $e_m \rightarrow (1.25e5, 1.5e7)$
  $Y_{exp} \rightarrow (0, 1)$

- Average relative errors (for 200 point model):
  - Pressure: 1.298%
  - Temperature: 0.132%

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Flowchart – Iterative vs. Surrogate

Loop over all cells in domain

IF $Y_{exp} < 0.001$ → Ideal Gas Equations

IF $1 > Y_{exp} > 0.999$ → JWL Equations

ELSE

Broyden's Method Iteration
Inputs: ρ_m, e_m, Y_{exp}

Calculate Initial guesses, values for f_1 to f_4 and Jacobian matrix (4 exponential operations)

Invert Jacobian matrix

Update Solution (1 matrix multiply)

ELSE

Update Inverse Jacobian (2 matrix multiplies, 4 exponential operations)

IF converged

Break, Calculate P and T

Surrogate Model
Inputs: ρ_m, e_m, Y_{exp}

Read in fit parameters

Call model operations twice (2 matrix multiplies, n_{pts} exp. operations each)

Output P and T

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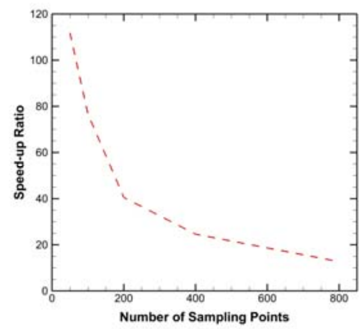
Surrogate Model Results –Timing

Standalone Surrogate

- Data taken from calculations of pressure/temperatures of 1000 mixture states

Model	Computing Time (s)	Speed-up
50 Pts.	0.0087	111.81
100 Pts	0.0127	76.61
200 Pts	0.0240	40.51
400 Pts	0.0396	24.60
800 Pts	0.0766	12.70
Iterative	0.9733	1.00

- Surrogate model with 200 points performed calculations 40.5 times faster than the iterative solver



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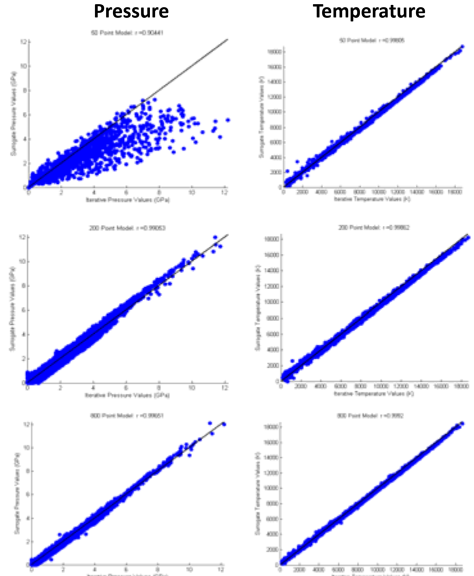
Surrogate Model Results – Accuracy

Pressure **Temperature**



Standalone Surrogate

- Data taken from same calculations of 1000 mixture pressure/temperatures
- The 200 point model is the smallest model with 99% correlation for both pressure and temperature

Sampling Pts	$R_{Pressure}$	$R_{Tempature}$
50	0.9044	0.9981
100	0.9247	0.9984
200	0.9905	0.9986
400	0.9952	0.9987
800	0.9965	0.9992

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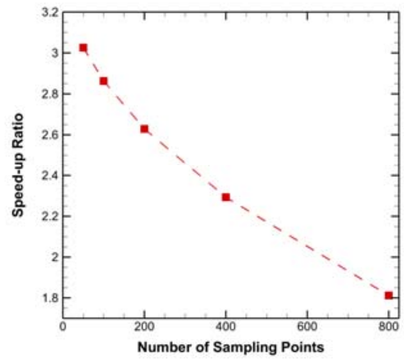
Simulation Results – Timing

- Simulation is run until first appearance of a species mixture cell
- 1000 time steps are run for each EoS model to gather timing data
- Process is repeated five times and averaged
- Notable code speed-up factor:
  - 200 points: 2.63

Simulation Description
- 2D, Cylindrical grid
- Outer radius = 0.3 m
- 400,000 cells
- Gas-Only



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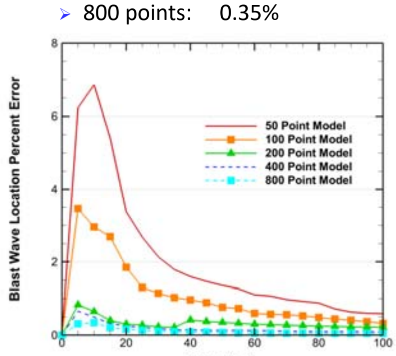
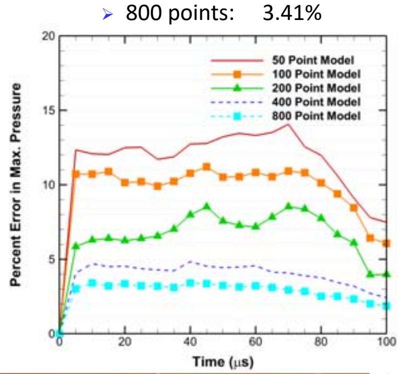
Simulation Results – Accuracy

Simulation Description
- 2D, Cylindrical grid
- Outer radius = 0.3 m
- 400,000 cells
- Gas-Only

- Maximum errors in blast wave location:
  - 50 points: 6.85%
  - 200 points: 0.83%
  - 800 points: 0.35%
- Maximum errors in peak pressure:
  - 50 points: 14.06%
  - 200 points: 8.52%
  - 800 points: 3.41%





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Conclusions and Future Work

Conclusions:

- Surrogate models allow for faster computations of the equation of state in mixture cells
- The models produce results that approach the iterative scheme given a sufficient number of sampling points in the input space

Future Work:

- **Multiple Species:**
  - Using an iterative solver, this means going from a 4×4 system of equations to an $2\mathrm{n} \times 2\mathrm{n}$ system of equations
  - As long as the same number of sampling points are used to create a new surrogate, the computation time would remain fixed
- **Multiphase Flows:**
  - Tests to verify that shifting to the surrogate models does not impact the particle metrics
- Paper in preparation with this work: F. Ouellet, C. Park, B. Rollin, R. T. Haftka and S. Balachandar: A Multi-Fidelity Surrogate Model for Handling Gas Mixture Equations of State

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Do you have any questions?

This work was supported by the U.S. Department of Energy, National Nuclear Security Administration, Advanced Simulation and Computing Program, as a Cooperative Agreement under the Predictive Science Academic Alliance Program, under Contract No. DE-NA0002378.

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Surrogate-Based Optimization for Exploring the Physics in Explosive Dispersal of Particles

M. Giselle Fernández-Godino
PhD Student (UB-Physics)

UF UNIVERSITY of FLORIDA

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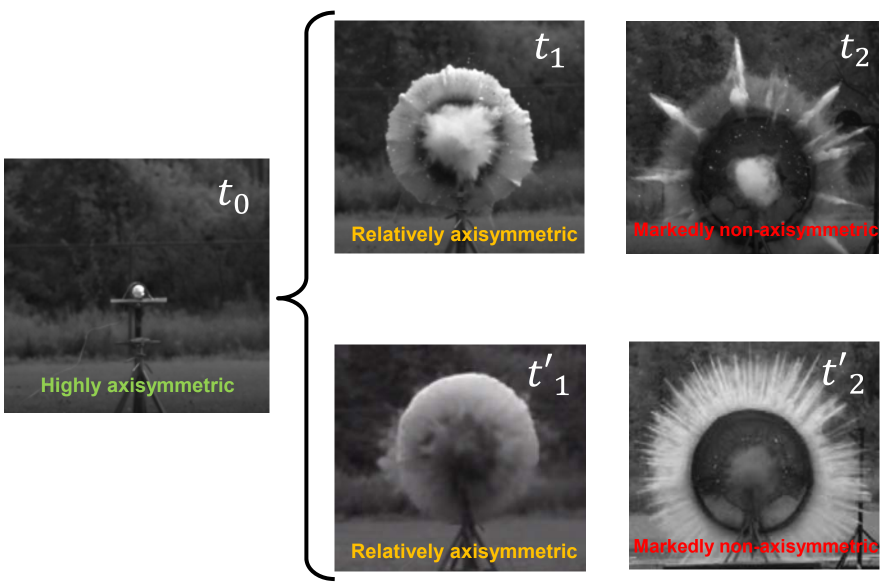
Departure from Axisymmetry



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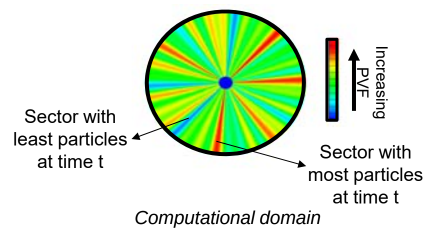
Questions

- What is a good metric of **departure** from **axisymmetry**?
  - Difference between the Particle Volume Fraction (PVF) of the sector with most particles and the one with least.



- Which **initial disturbances amplify most** the departure?
  - Multimodal initial PVF perturbations
  - Optimization
  - Surrogate models

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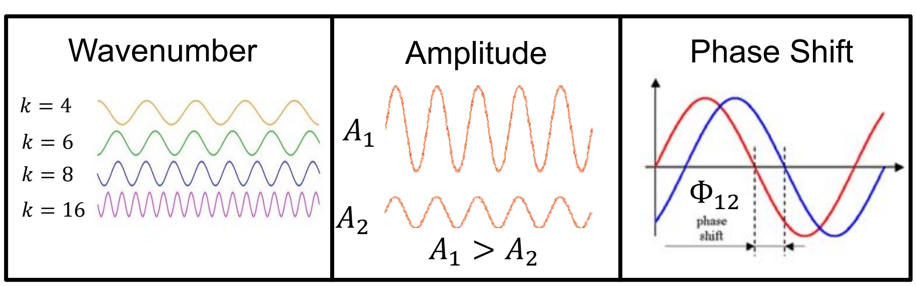
Parametrization of Initial PVF Perturbation

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

Particle Volume Fraction (PVF)

Base PVF

Design Variables



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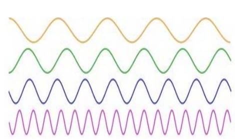
Parametrization of Initial PVF Perturbation

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

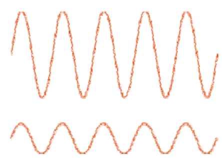
Single-modal Bi-modal Tri-modal

Effective $k = \frac{\sum_{i=1}^{n} k_i}{n}$ Effective $A = \sqrt{\sum_{i=1}^{n} A_i^2} = 0.1\sqrt{2}$

Wavenumber



Amplitude



Phase Shift

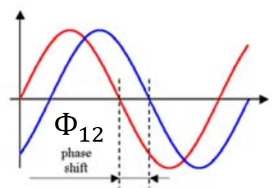


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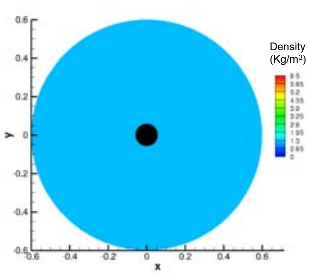
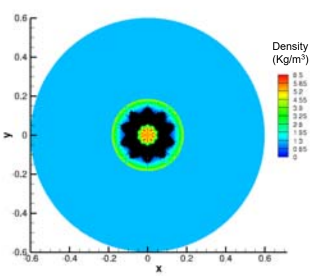
Illustration from Simulations

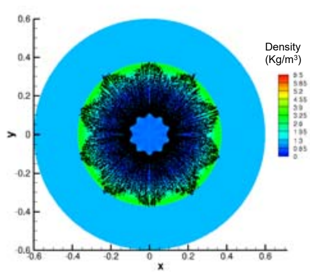
Single mode, $k = 10$, $A = 0.1\sqrt{2}$



t=0s



t=100μs



t=300μs

- Computational particles on top of density contours
  - Single mode, $k = 10$, $A = 0.1\sqrt{2}$
- Initial sinusoidal angular particle volume fraction (PVF) perturbations translate in finger like structures at later times
  - Particles travel faster in sectors where PVF is initially lower

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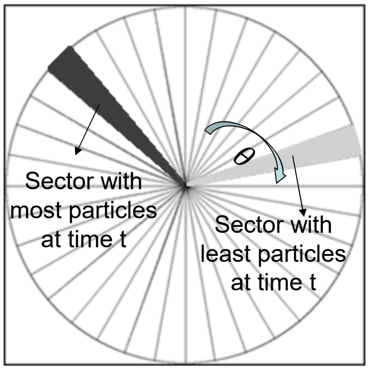
Departure from Axisymmetry



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

$$\zeta(t) = Norm.Max.PVF\ Diff(t) = \frac{[Max(PVF(\theta)) - Min(PVF(\theta)](t)}{[Max(PVF(\theta)) - Min(PVF(\theta))](t=0)}$$

- PVF per sector $= \frac{Volume\ of\ particles}{Volume\ of\ the\ sector}$
- PVF of sector with most particles minus PVF of sector with least particles, divided by this difference at t=0s
- This metric does not take into account radial variations

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Runs: Summary

	# Runs LF/HF	Machine	Case	Individual Time LF/HF
	14/6	HPG	1 parameter	15h/24h
	40/40	HPG	2 parameters	6h/24h
	80/20	Quartz	3 parameters	6h/24h
	100/0	Quartz	5 parameters	6h
	1600/800	Quartz	7 parameters	6h/24h
TOTAL	**1834/866**			**11,130h/20,784h**

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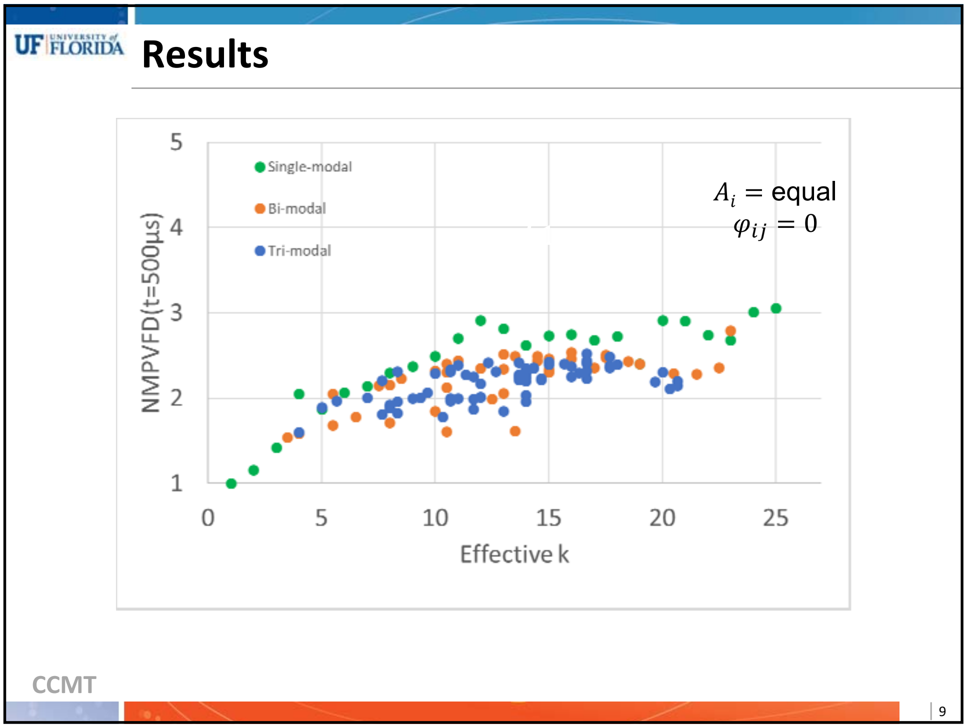
Results
Single-modal
Bi-modal
Tri-modal
A_i = equal
$\varphi_{ij} = 0$
NMPVFD(t=500μs)
Effective k
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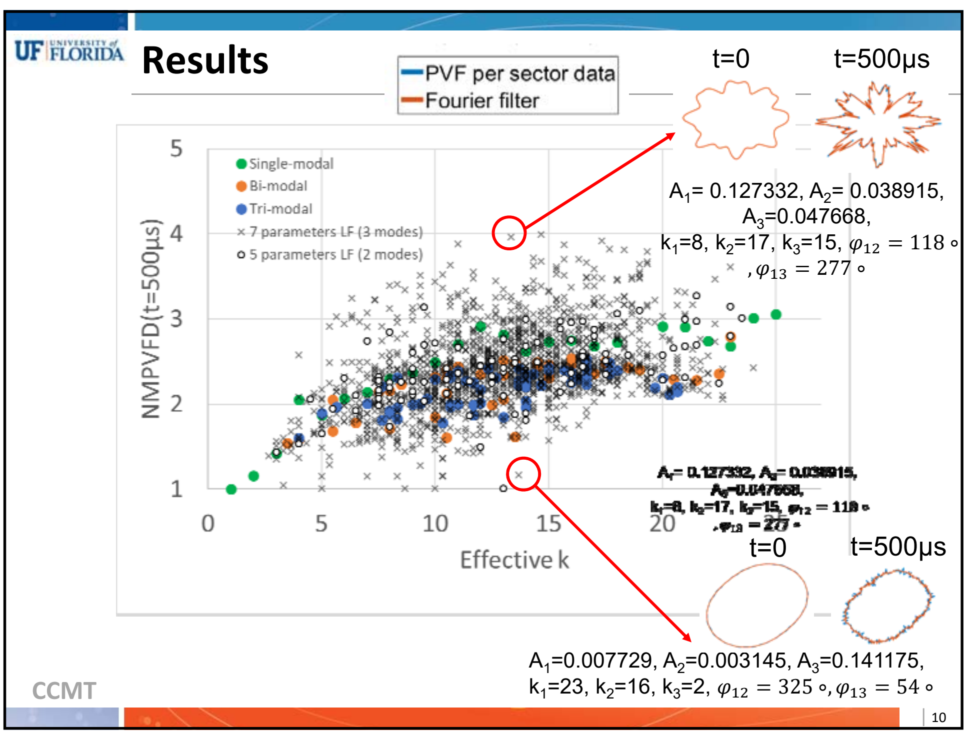
Results
PVF per sector data
Fourier filter
t=0
t=500μs
Single-modal
Bi-modal
Tri-modal
7 parameters LF (3 modes)
5 parameters LF (2 modes)
A_1= 0.127332, A_2= 0.038915, A_3=0.047668,
k_1=8, k_2=17, k_3=15, $\varphi_{12} = 118\circ$, $\varphi_{13} = 277\circ$
NMPVFD(t=500μs)
Effective k
t=0
t=500μs
A_1=0.007729, A_2=0.003145, A_3=0.141175,
k_1=23, k_2=16, k_3=2, $\varphi_{12} = 325\circ$, $\varphi_{13} = 54\circ$
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Surrogate based Optimization

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

Design Variables

$$\left.\begin{array}{c} \underset{A_1,A_2,A_3,k_1,k_2,k_3,\Phi_{12},\Phi_{13}}{maximize} \quad Norm.Max.\ PVF\ Diff. \end{array}\right\} \text{Objective Function}$$

$$\left. Subject\ to \sqrt{A_1^2 + A_2^2 + A_3^2} = constant \right\} \text{Energy Constraint}$$

- ✓ LF (low-fidelity) is a reduced grid of about 0.25HF (high-fidelity) cost
- ✓ HFS (high-fidelity surrogate) fits HF alone, MFS (multi-fidelity surrogate) fits both together

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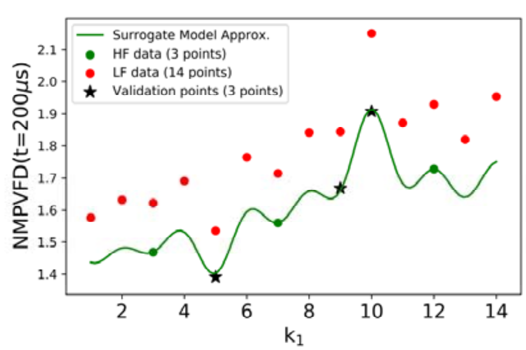
Single Parameter Study (tri-modal pert.)

- Tri-modal perturbation
- One variable, k_1
- k_2=15, k_3=25, A_1=A_2=A_3=0.1633, Φ_{12}=Φ_{13}=0 remain constant



- Surrogate model obtained using 14 LF points, 3 HF points and 3 validation points
- The model is able to predict the validation points quite well just with a few HF points
- General trend : NMPVFD increases as k increases
- k_1=5 show a lower growth while k_1=10 a higher one. Important triadic interaction between modes!

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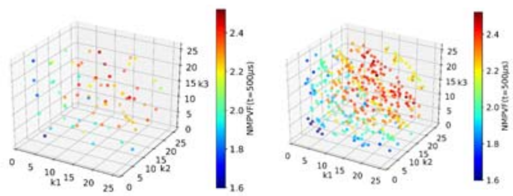
3 Parameters Study (tri-modal pert.)

- Simplified problem: Three variables, k_1 , k_2, and k_3
- $A_1=A_2=A_3=0.1\sqrt{2/3}$, Φ_{12}, $\Phi_{13}=0$ remain constant
- General trend: NMPVFD increases with the effective k
- Preliminary Bayesian MFS is use to fit the MFS
- Mirror points reduce the CV error a 77%
- Mirror points are points with the same output. i.e. In this case wave numbers (2,4,3) has mirror points (2,3,4) (3,2,4) (3,4,2) (4,2,3) (4,3,2)



Left. LF data without mirror points (70 points). Right. LF data including mirror points (420=70x6).

CV not including mirror points	CV error including mirror points
0.186147	0.042238

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Conclusions and Future Work

- 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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Thank you!
Do you have any questions?

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Pairwise Interaction Extended Point-Particle (PIEP) Modeling

W. Chandler Moore

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NNSA

Outline

- Neighbors matter due to fluid-mediated Particle-Particle interactions
- Previously formulated PIEP model provides a rational approach to accounting for this fluid-mediated Particle-Particle interaction at low volume fractions
- The addition of a data-driven term greatly enhances the PIEP model at high volume fractions

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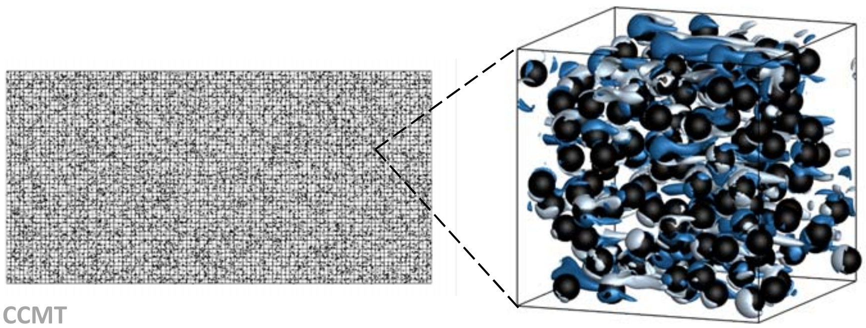
Euler-Lagrange Approach

- Orders of magnitude faster than fully resolved simulations
  - EL & EE only viable approaches for practical problems
  - Point-particle models are needed for EL



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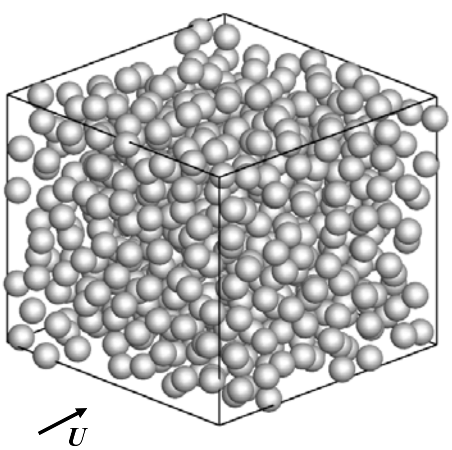
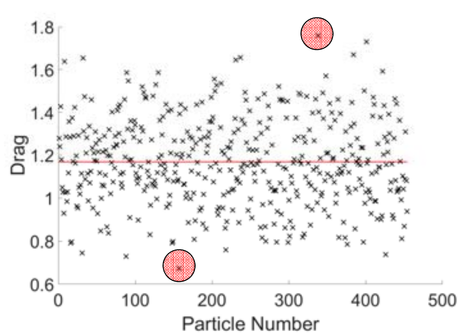
Fully Resolved Simulations

- Immersed boundary method, Grid = $(490)^3$, $d/\Delta x$ = 60





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

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

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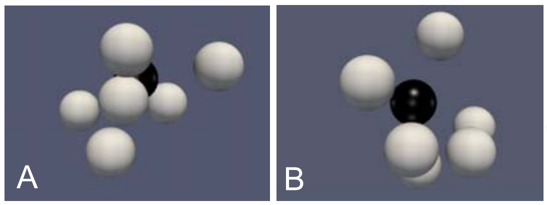
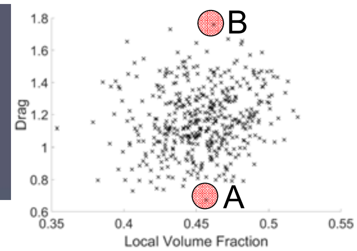
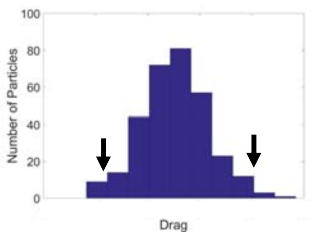
Exact Location of Neighbors

View as seen by Incoming Flow





Similar Local Volume Fraction



- Local volume fraction cannot explain the variations
- Upstream, downstream, lateral neighbors have different influence

Akiki, Balachandar, JCP, *307*, 34-59 (2016)
Akiki, Jackson, Balachandar, Phys Rev Fluids, 1, 044202 (2016)

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Current PIEP Model

$$\boldsymbol{F}_{PIEP} = \boldsymbol{F}_{qs} + \boldsymbol{F}_{un} + \boldsymbol{F}_{am} + \boldsymbol{F}_{vu} + \boldsymbol{F}_{L} + \boldsymbol{F}_{c}$$

$$T_{PIEP} = \boldsymbol{T}_{qs} + \boldsymbol{T}_{un} + \boldsymbol{T}_{c}$$

where, using perturbation maps resulting from direct numerical simulations (DNS),

$$\boldsymbol{F}_{PIEP} \equiv \boldsymbol{F}_{PIEP}(Re, \phi, \mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_N, \mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_N)$$

$$\boldsymbol{T}_{PIEP} \equiv \boldsymbol{T}_{PIEP}(Re, \phi, \mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_N, \mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_N)$$

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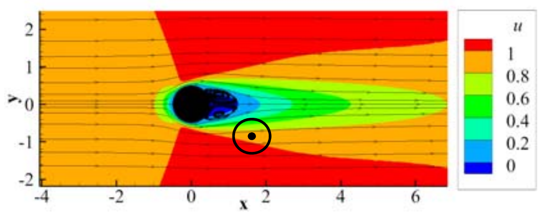
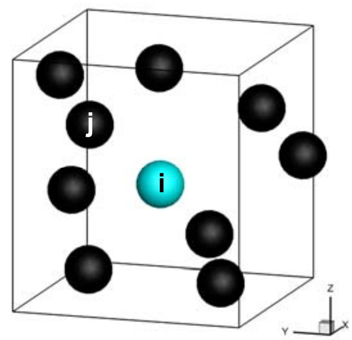
Example: Quasi-Steady Force

$$\boldsymbol{F}_{qs,i} = \boldsymbol{F}_{ra}(\phi_i, Re_i) + \left\{ 3\pi \propto d_i \left(\sum_{\substack{j=1 \\ j\neq i}}^{N} \overline{\boldsymbol{u}_{j\to i}}^{S} \right) \left[1 + 0.15 \left(Re_i \right)^{0.687} \right] \right\}$$



Akiki, Jackson, Balachandar, JFM, 813, 882-928 (2017)
Akiki, Moore, Balachandar, JCP, 351, 329-357 (2017)



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Data-Driven Volume Fraction Correction

$$R^2 = 1 - \frac{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - F_{PI}(n) \right]^2}{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - \langle F_{DNS} \rangle \right]^2}$$

Case	Lateral Force R^2 (DNS vs PIEP)
$\phi = 0.1$, $Re = 40$	0.68
$\phi = 0.2$, $Re = 16$	0.34
$\phi = 0.45$, $Re = 21$	0.09

$$\boldsymbol{F}_{PIEP,Data-Driven} = \boldsymbol{F}_{PIEP} + \boldsymbol{F}_{\phi,C}$$

$$\boldsymbol{T}_{PIEP,Data-Driven} = \boldsymbol{T}_{PIEP} + \boldsymbol{T}_{\phi,C}$$

where

$$\boldsymbol{F}_{\phi,C} \equiv \boldsymbol{F}_{\phi,C}(Re, \phi, \mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_N)$$

$$\boldsymbol{T}_{\phi,C} \equiv \boldsymbol{T}_{\phi,C}(Re, \phi, \mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_N)$$

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Nonlinear Regression Modeling

For a given Re and volume fraction:

Response Variable (output)

$$\boldsymbol{F}_{\phi,C} \equiv \text{function of } \{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\}$$
$$\boldsymbol{T}_{\phi,C} \equiv \text{function of } \{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\}$$

Predictor Variables (inputs)

Function Form and Parameters

Let us define a set of scalar invariants (*I*) that fully define the configuration formed by the *N* neighbors.

$$\begin{aligned} x-\text{Separation} &: \; r_{x,1}, r_{x,2}, \cdots, r_{x,N} \\ y-\text{Separation} &: \; r_{y,1}, r_{y,2}, \cdots, r_{y,N} \\ z-\text{Separation} &: \; r_{z,1}, r_{z,2}, \cdots, r_{z,N} \end{aligned}$$

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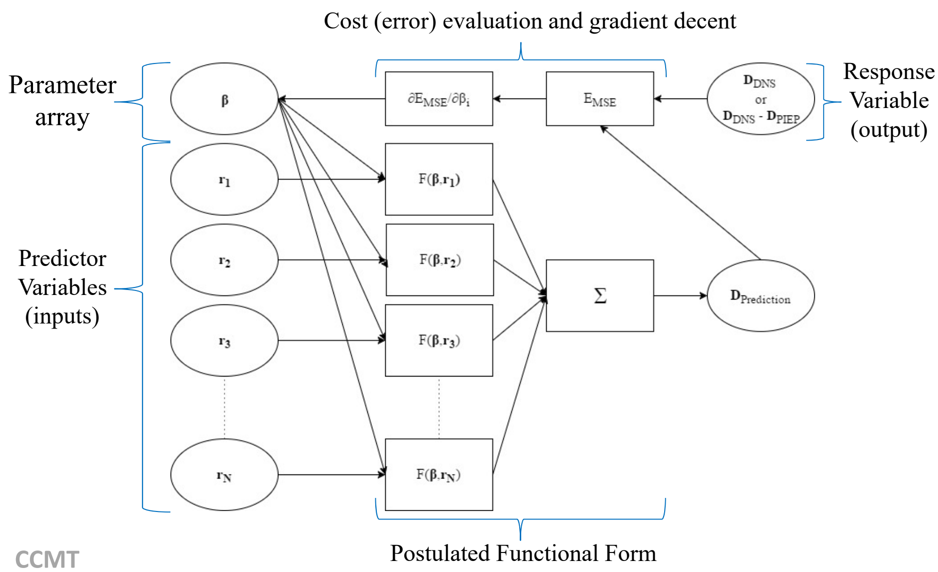
Regression Modeling (drag)

For a given Re and volume fraction:



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Postulating the Functional Form

$$D(I) = \sum_{i=1}^{N} \left[\left(\sum_{m=1}^{M} \sum_{l=0}^{L} a_{l,m} j_l(k_{j,l,m}\, r_i) Y_{l,0}(\theta_i) + \sum_{m=1}^{M} \sum_{l=0}^{L} b_{l,m} n_l(k_{n,l,m}\, r_i) Y_{l,0}(\theta_i) \right) H(r_i) \right]$$

$$L_y(I) = \sum_{i=1}^{N} \left[\left(\sum_{m=1}^{M} \sum_{l=0}^{L} a_{l,m} j_l(k_{j,l,m}\, r_i) Y_{l,0}(\theta_i) + \sum_{m=1}^{M} \sum_{l=0}^{L} b_{l,m} n_l(k_{n,l,m}\, r_i) Y_{l,0}(\theta_i) \right) \hat{\mathbf{r}}_i \cdot \mathbf{e}_y\, H(r_i) \right]$$

$$T_z(I) = \sum_{i=1}^{N} \left[\left(\sum_{m=1}^{M} \sum_{l=0}^{L} a_{l,m} j_l(k_{j,l,m}\, r_i) Y_{l,0}(\theta_i) + \sum_{m=1}^{M} \sum_{l=0}^{L} b_{l,m} n_l(k_{n,l,m}\, r_i) Y_{l,0}(\theta_i) \right) \hat{\mathbf{r}}_i \cdot \mathbf{e}_y\, H(r_i) \right]$$

where

$$Y_{l,0}(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \qquad \frac{dj_l(k_{j,l,m}\, r_{min})}{dr} = 0 \quad \text{and} \quad \frac{dn_l(k_{n,l,m}\, r_{min})}{dr} = 0\,.$$

$a_{l,m}$ and $b_{l,m}$ make up the array of parameters, β, to be determined by regression

N, M, and L are the hyper parameters that must be optimized using a second data set

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Coefficient of Determination (R^2) Results

R^2 Values:		Current PIEP Model			Data-Driven		
ϕ	*Re*	Drag	Lift	Torque	Drag	Lift	Torque
0.1	**40**	0.70	0.68	0.75	0.72	0.75	0.79
0.1	**70**	0.65	0.68	0.65	0.67	0.72	0.72
0.1	**173**	0.35	0.59	0.45	0.44	0.60	0.58
0.2	**16**	0.38	0.34	0.48	0.66	0.74	0.71
0.2	**89**	0.50	0.48	0.72	0.62	0.63	0.77
0.45	**21**	0.01	0.09	0.47	0.55	0.59	0.76
0.45	**115**	0.21	0.19	0.51	0.63	0.57	0.65

$$R^2 = 1 - \frac{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - F_{PI}(n) \right]^2}{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - \langle F_{DNS} \rangle \right]^2}$$

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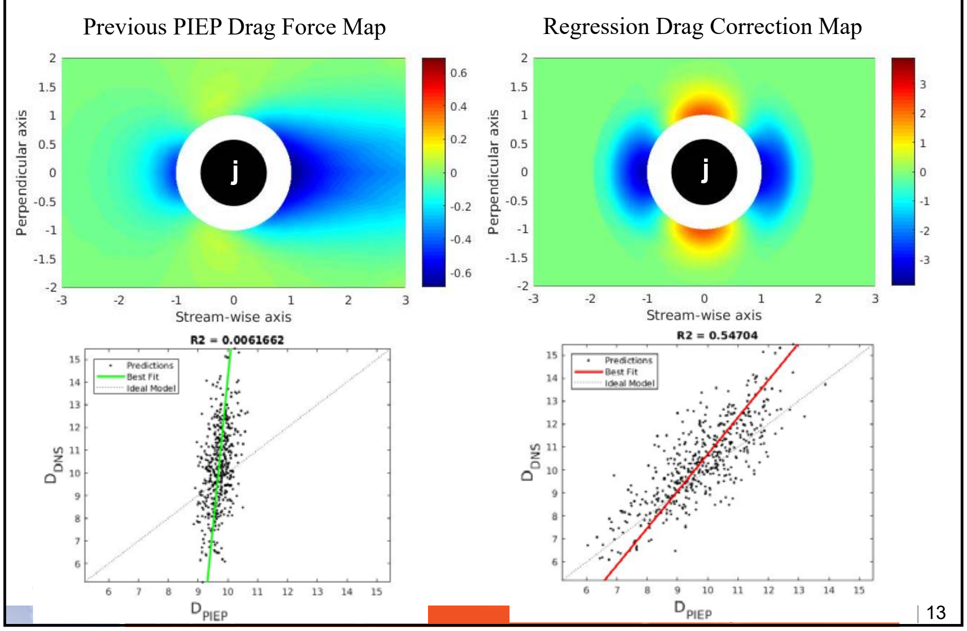
Drag Regression Results (ϕ = 0.45 & Re = 21)



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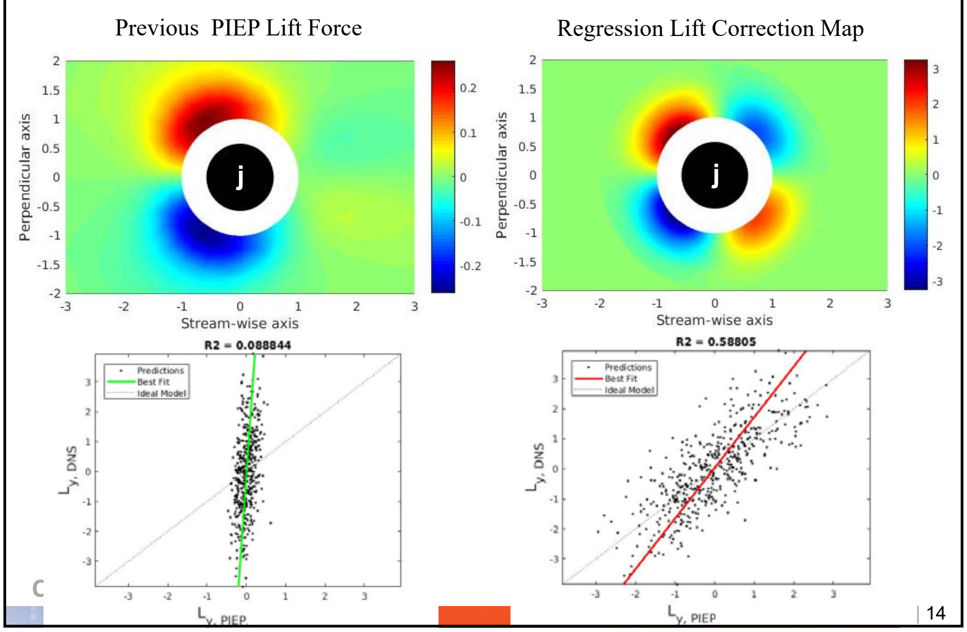
Lift Regression Results (ϕ = 0.45 & Re = 21)



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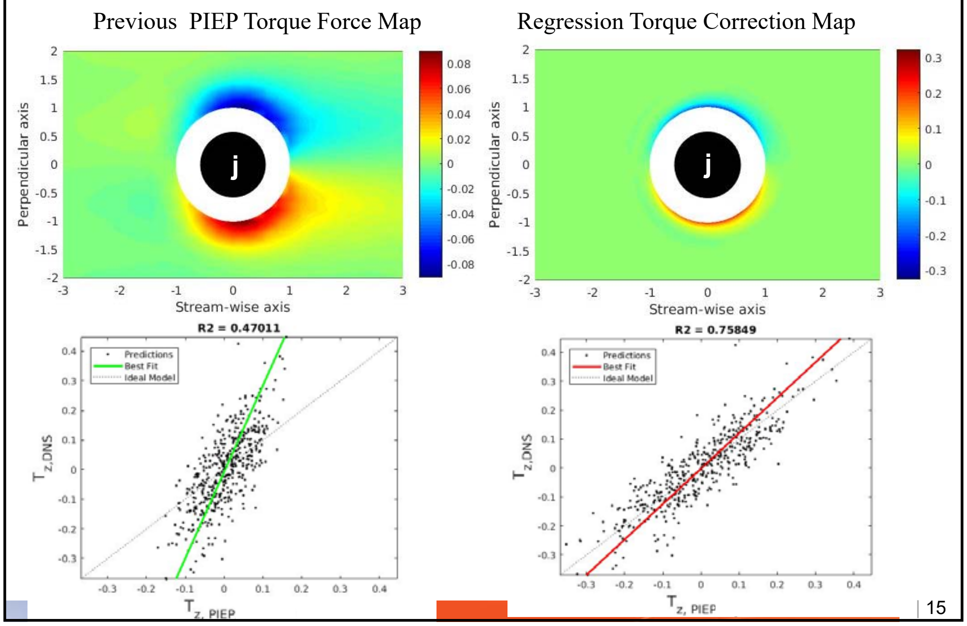
Torque Regression Results (ϕ = 0.45 & *Re* = 21)



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Main Message

- Neighboring particle locations matter
  - Local volume fractions is not sufficient for force modeling
- Fluid-mediated Particle-Particle interactions are strong
- Previously formulated PIEP model provides accurate forces/torque predictions at low volume fractions
- Implementing a data driven approach allows the PIEP model to predict forces/torques at high volume fractions

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Thank you!
Questions?

Acknowledgment:
This material is based upon work supported in part by National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-1315138 and in part by the the U.S. Department of Energy, National Nuclear Security Administration, Advanced Simulation and Computing Program, as a Cooperative Agreement under the Predictive Science Academic Alliance Program, under Contract No. DE-NA0002378.

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Extra Slides:

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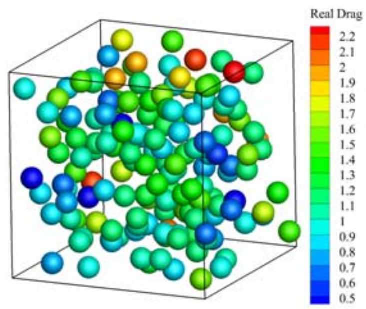
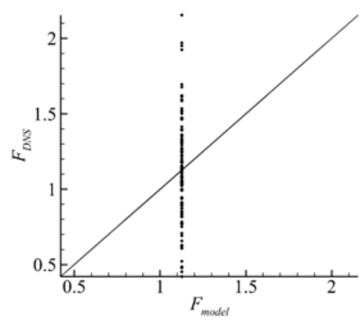
Ideal Point Particle Model



$$R^2 = 1 - \frac{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - F_{PI}(n) \right]^2}{\sum_{n=1}^{N_p} \left[F_{DNS}(n) - \langle F_{DNS} \rangle \right]^2}$$

R^2 = 0.00



If the model is EXACT

Recovers Fully-Resolved physics

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Postulating the Functional Form

Substitute a general functions for neighbor specific functions ($F_{x,i}$, F_i, *and* T_i) ,

$$\mathbf{F}_{\mathrm{VF}} = \sum_{i=1}^{N} \left(F_{x,P}(I_i)\, \mathbf{e}_x + F_P(I_i)\, \hat{\mathbf{r}}_i \right) \qquad \mathbf{T}_{\mathrm{VF}} = \sum_{i=1}^{N} \left(T_P(I_i)\, \mathbf{e}_x \times \hat{\mathbf{r}}_i \right)$$

Individual component functions:

$$\mathbf{F}_{\mathrm{VF}} = D(I)\mathbf{e}_x + L_y(I)\mathbf{e}_y + L_z(I)\mathbf{e}_z \qquad \mathbf{T}_{\mathrm{VF}} = T_x(I)\mathbf{e}_x + T_y(I)\mathbf{e}_y + T_z(I)\mathbf{e}_z$$

Combine the above formulations:

$$\boxed{\begin{aligned} D(I) &= \sum_{i=1}^{N} \left(F_{x,P}(I_i) + F_P(I_i)\, \hat{\mathbf{r}}_i \cdot \mathbf{e}_x \right) , \\ L_y(I) &= \sum_{i=1}^{N} \left(F_P(I_i)\, \hat{\mathbf{r}}_i \cdot \mathbf{e}_y \right) , \end{aligned}}$$

$$L_z(I) = \sum_{i=1}^{N} \left(F_P(I_i)\, \hat{\mathbf{r}}_i \cdot \mathbf{e}_z \right) .$$

$$T_x(I) = 0 ,$$

$$T_y(I) = \sum_{i=1}^{N} \left(T_P(I_i)\, \hat{\mathbf{r}}_i \cdot \mathbf{e}_z \right) ,$$

$$\boxed{T_z(I) = \sum_{i=1}^{N} \left(T_P(I_i)\, \hat{\mathbf{r}}_i \cdot \mathbf{e}_y \right) .}$$

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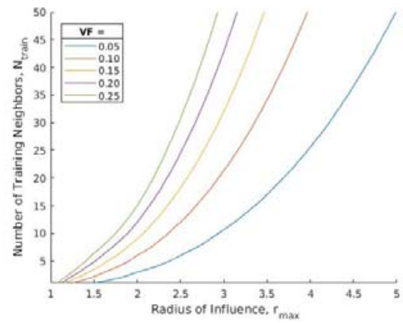
Postulating the Functional Form

The function is only defined within radius of influence (r_{max})

$$H(r) = \begin{cases} 0 & r < d \\ 1 & d \leq r \leq r_{max} \\ 0 & r > r_{max} \end{cases}$$

where r_{max} can be found by root finding the following:

$$\int_{V_d}^{V_{r_{max}}} g(r)\rho dV - N_{train} = 0$$



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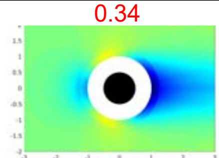
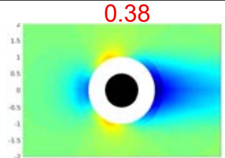
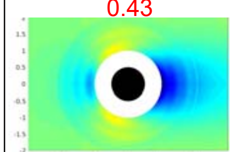
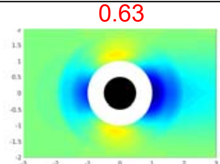
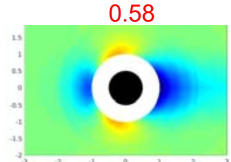
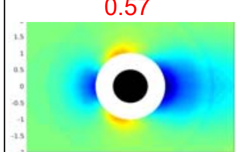
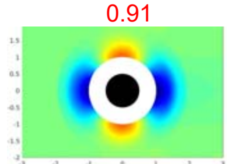
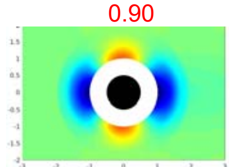
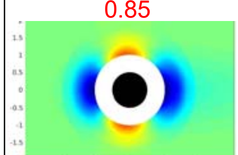
Re & VF vs. Symmetry for Drag

VF	Low Re	Medium Re	High Re
0.10	0.34 	0.38 	0.43 
0.20	0.63 	0.58 	0.57 
0.45	0.91 	0.90 	0.85 

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$[||M_{symmetric}|| - ||M_{asymmetric}||] / ||M||$

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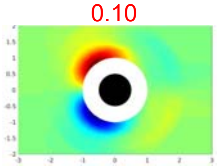
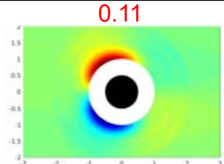
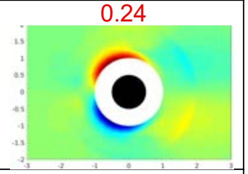
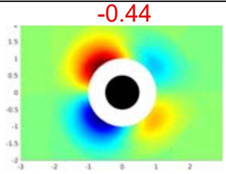
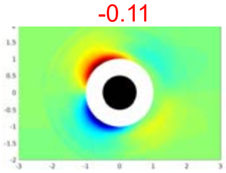
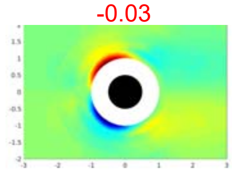
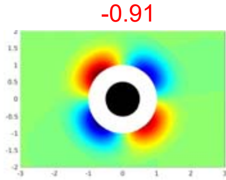
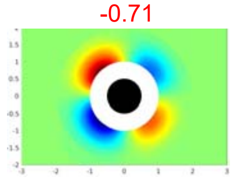
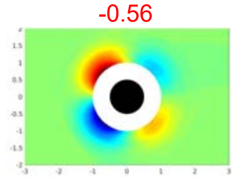
Re & VF vs. Symmetry for Lift

VF	Low Re	Medium Re	High Re
0.10	0.10 	0.11 	0.24 
0.20	-0.44 	-0.11 	-0.03 
0.45	-0.91 	-0.71 	-0.56 

CCMT $[||M_{symmetric}|| - ||M_{asymmetric}||] / ||M||$

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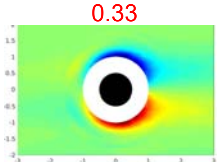
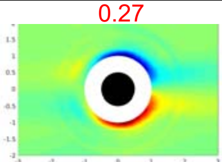
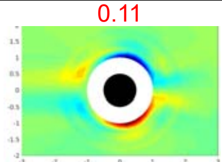
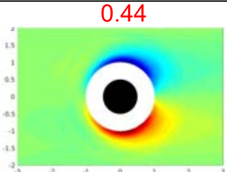
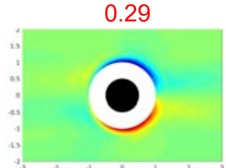
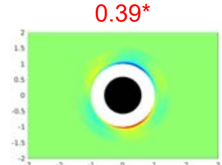
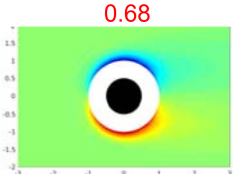
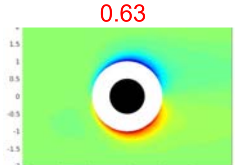
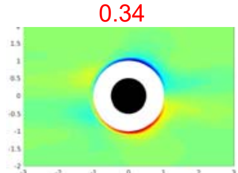
Re & VF vs. Symmetry for Torque

VF	Low Re	Medium Re	High Re
0.10	0.33 	0.27 	0.11 
0.20	0.44 	0.29 	0.39* 
0.45	0.68 	0.63 	0.34 

CCMT $[||M_{symmetric}|| - ||M_{asymmetric}||] / ||M||$ *Purely Statistical Model

CCMT

Microscale Shock and Contact Simulations

Brandon Osborne

CCMT

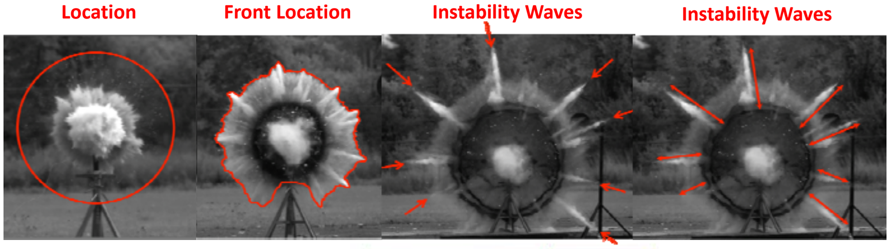
Motivation

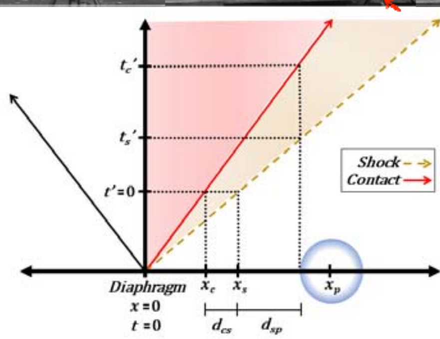
PM-1: Blast Wave Location

PM-2: Particle Front Location

PM-3: Number of Instability Waves

PM-4: Amplitude of Instability Waves





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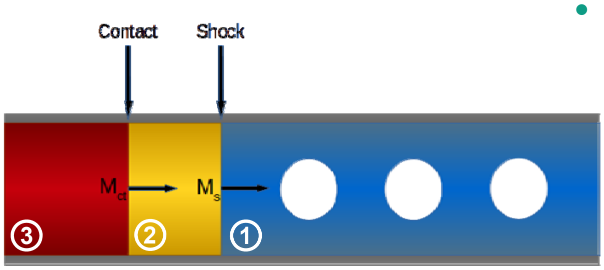
2

Simulation Overview



- Three sets simulations:
  - Close: Shock and contact reach first particle nearly simultaneously
  - Intermediate: Shock is 2 particle diameters downstream of first particle before the contact reaches its leading edge
  - Shock only: The simulation is absent a contact discontinuity

φ	M_{ct}	M_s	ρ_1 (kg/m³)	ρ_2 (kg/m³)	ρ_3 (kg/m³)	ρ_2/ρ_1	ρ_3/ρ_1
5-40%	0.31	1.22	1.20	1.65	2.15	1.37	1.78
	0.90	1.90	1.20	3.03	8.20	2.52	6.81
	1.26	2.69	1.20	4.27	26.35	3.54	21.87

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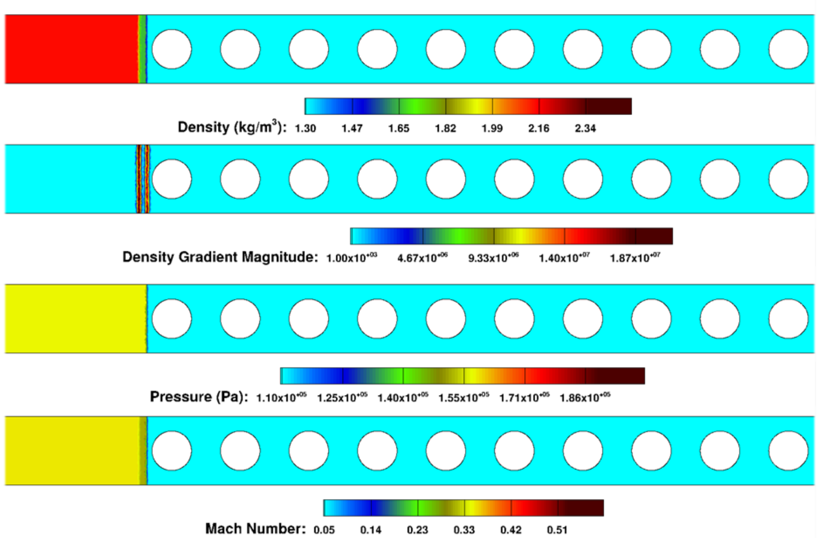
3

Contours: $\varphi = 10\%, M_{ct} = 0.31$, Close



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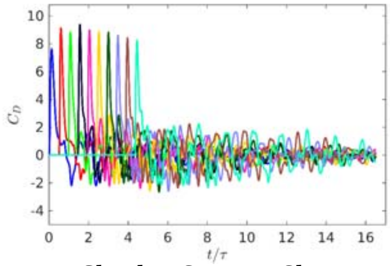
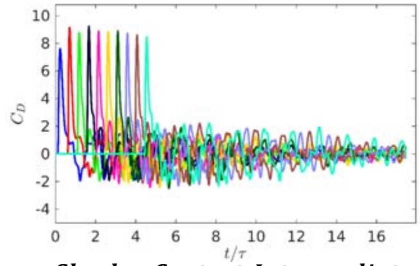
4

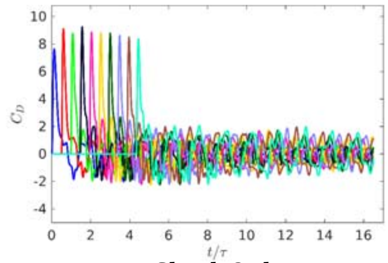
Case Comparison: $\varphi = 10\%,\ M_{ct} = 0.31$



$Shock + Contact, Close$

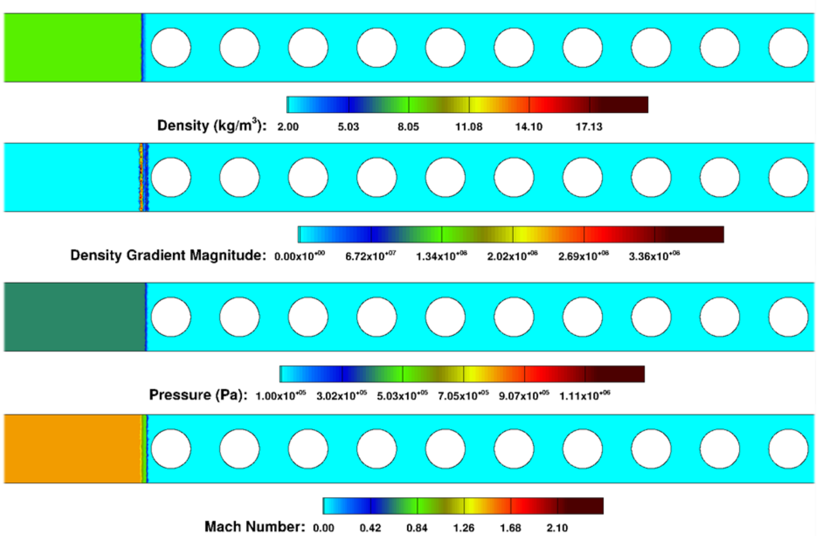


$Shock + Contact, Intermediate$



$Shock\ Only$

Contours: $\varphi = 10\%,\ M_{ct} = 0.90$, Close



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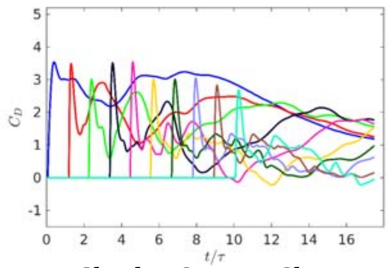
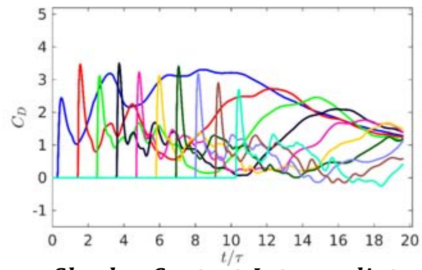
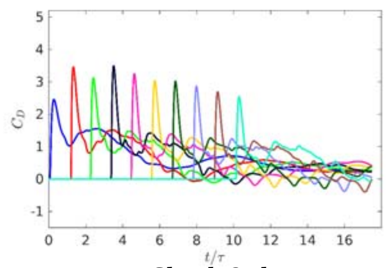
Case Comparison: $\varphi = 10\%$, $M_{ct} = 0.90$



$Shock + Contact, Close$



$Shock + Contact, Intermediate$



$Shock\ Only$

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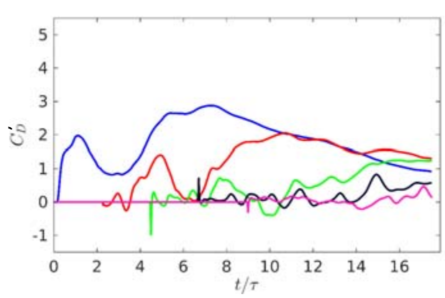
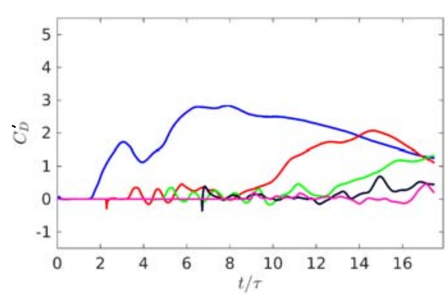
Difference Plots: $\varphi = 10\%$, $M_{ct} = 0.90$



$Shock + Contact, Close$



$Shock + Contact, Intermediate$

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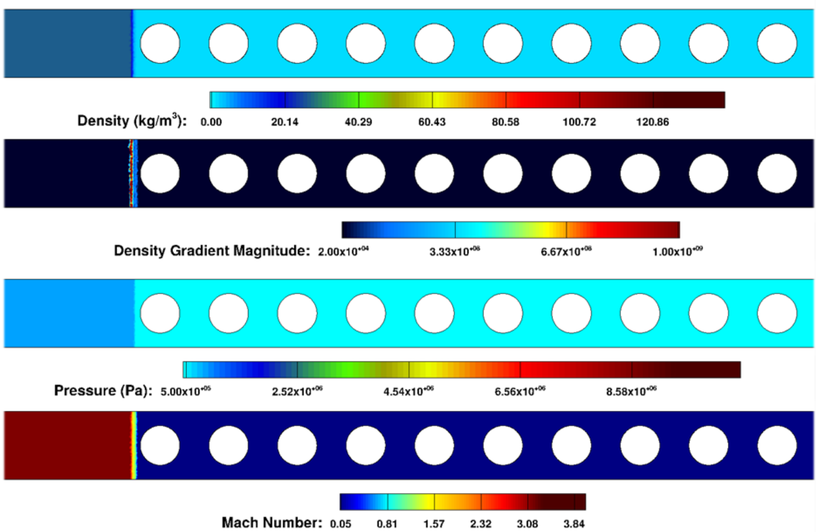
Contours: $\varphi = 10\%$, $M_{ct} = 1.26$, Close



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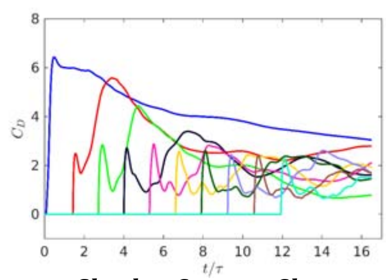
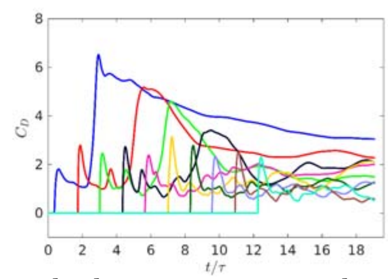
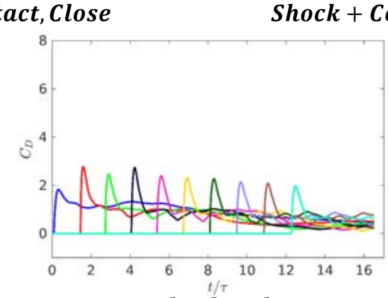
Case Comparison: $\varphi = 10\%$, $M_{ct} = 1.26$



$Shock + Contact, Close$



$Shock + Contact, Intermediate$



$Shock\ Only$

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10

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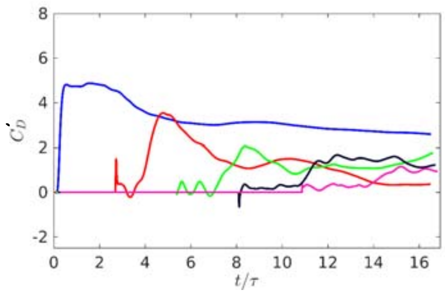
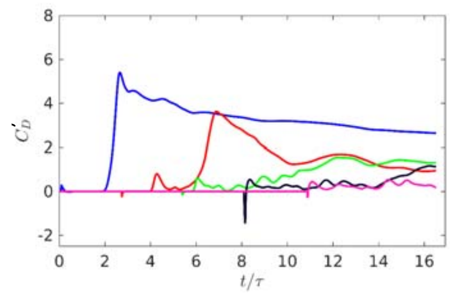
Difference Plots: $\varphi = 10\%$, $M_{ct} = 1.26$



$\boldsymbol{Shock + Contact, Close}$



$\boldsymbol{Shock + Contact, Intermediate}$

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11

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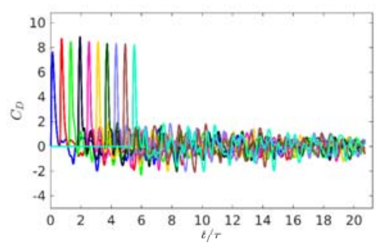
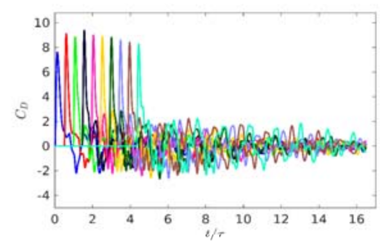
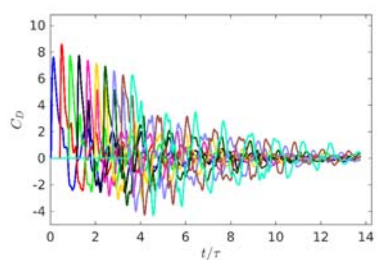
φ Comparison: $M_{ct} = 0.31$, Close



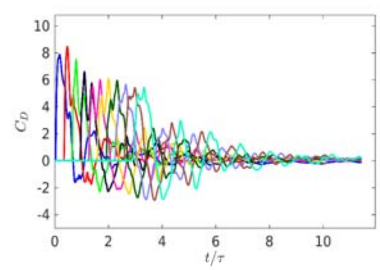
φ = 5%



φ = 10%



φ = 20%



φ = 40%

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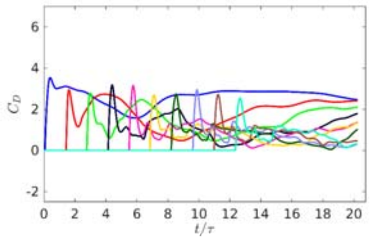
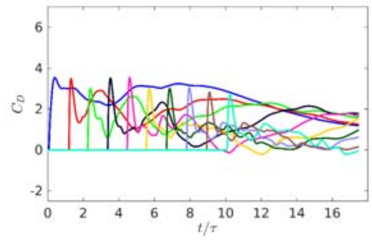
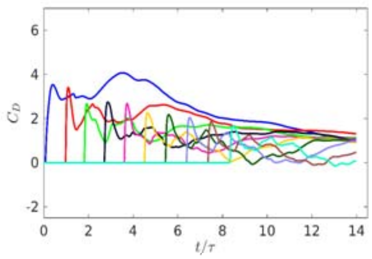
φ Comparison: $M_{ct} = 0.90$, Close



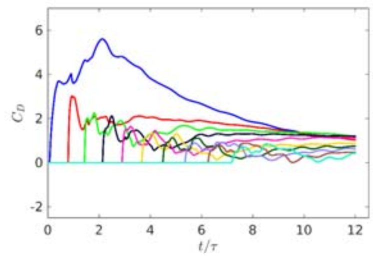
φ = 5%



φ = 10%



φ = 20%



φ = 40%

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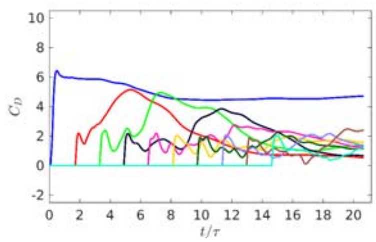
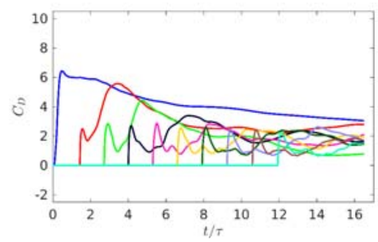
13

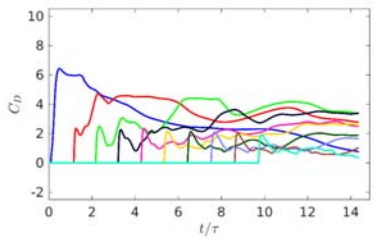
φ Comparison: $M_{ct} = 1.26$, Close



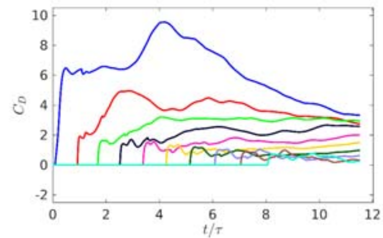
φ = 5%



φ = 10%



φ = 20%



φ = 40%

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Summary

- Subsonic post-shock Mach number
  - Formation of a wake as the contact passes the particles that results in a "stretching" of the contact interface
  - Force oscillations created by reflected waves are dampened by the contact
  - Oscillations of greater magnitude as volume fraction increases and a decrease in peak force for subsequent particles for higher volume fractions
- Near sonic post-shock Mach number
  - Rapid mixing of the contact interface
  - Formation of compression waves traveling upstream and shocks extending from particle surface to wall after sonic flow is reached
  - Increasing force on the first particle and decreasing force on subsequent particles as volume fraction increases
- Supersonic post-shock Mach number
  - Rapid mixing of the contact interface
  - Formation of bow shocks and shocklets
  - High particle forces and the formation of a compression wave traveling upstream for φ = 40%

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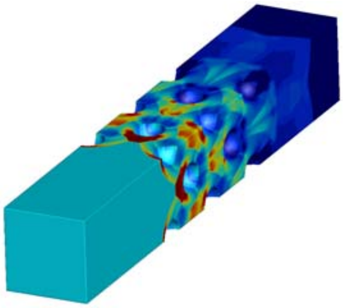
Future Work

- Shock and contact interaction with an FCC array of particles
  - Characterize the effects a shock and contact have on force history and flow field compare to current 1D array data
- Shock and contact interaction with a random arrangement of particles
  - Apply techniques and models developed from 1D and FCC arrays to a random arrangement of particles
- PIEP model application to shock-contact-particle interaction



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Thank you!
Do you have any questions?

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NNSA

CCMT

BE Simulations of CMT-nek

Sai Chenna (BE)

UF UNIVERSITY of FLORIDA

Outline: BE-simulation of CMT-nek

- Particle-solver
- Modelling approach
- Particle-distribution tool
- DSE of CMT-nek using BE

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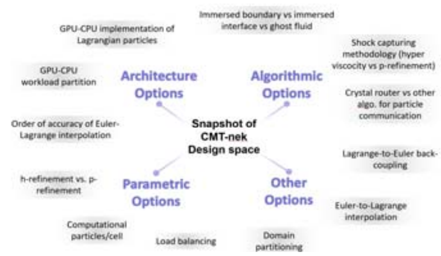
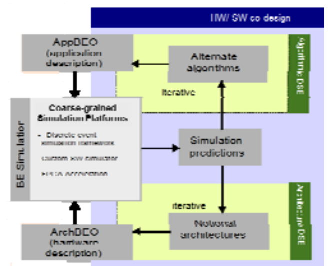
2

CMT-nek DSE: Motivation & Approach

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





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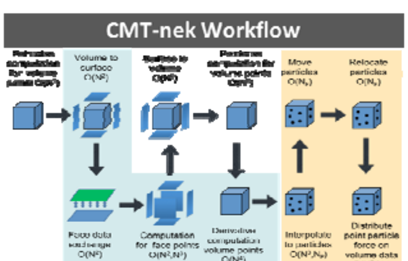
CMT-nek: Particle Solver subroutine

- **Particle solver** – *expensive kernel in CMT-nek*
  - Calculates the particle properties at each time-step
  - Assumptions
    - No particle to particle interaction
    - No two-way coupling
  - Parameters
    - *N – element size*
    - *nelt – elements-per-processor*
    - *α – particles/gridpoint*
    - *N_p - # particles = α*N^3*nelt*



update_particle_location	Check if particle moved outside the box and update its location
move_particles_inproc	Move particles to processor which owns it
interp_props_part_location	Interpolate fluid properties at particle location
usr_particles_forces	Calculate fluid forces acting on the particle
update_vel_and_pos	Update particle position and velocity

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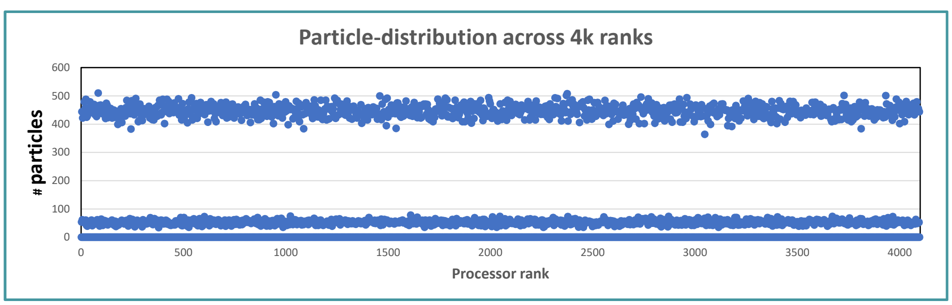
Modelling Approach

- Symbolic Regression
  - Tool to generate multi-parameter performance models for computation kernels
  - No prior knowledge of kernel required
  - Captures machine-specific performance behaviours
- Trace-driven simulation
  - Building a tool which determines particle distribution from a trace file based on user-specified parameters
  - Determines # particles residing and moving in each processor at given time-step
  - Improves accuracy of BE-simulation

CCMT 5

Modelling Approach: Trace-driven simulation

- Particle solver kernel
  - Workload per processor depends on # particles
  - # particles/processor is dynamic
    - varies among processors – *depends on total # of processors*
    - varies at each timestep – *based on fluid forces on particles*
  - Need a trace to perform simulations



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Modelling Approach: Trace-driven simulation

- Particle-distribution tool
  - Input: trace data containing particle location at each time-step
  - Output
    - # particles residing in each rank @ every timestep
    - # particles moving across each rank @ every timestep
  - Particle movement doesn't depend on # processors
    - Single trace for a given problem size is sufficient to predict particle movement for any # of processors

0	1
2	3

0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15

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7

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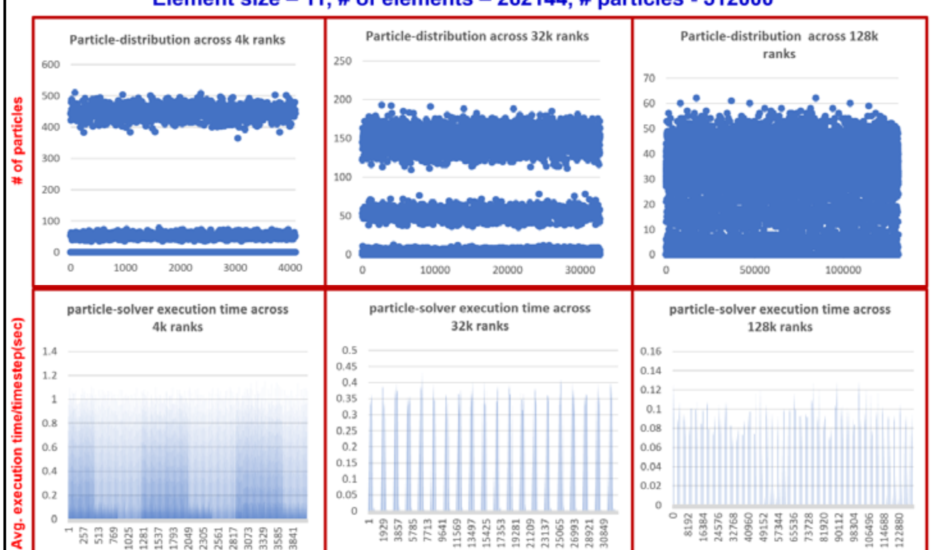
Particle-distribution tool: Results

Element size – 11, # of elements – 262144, # particles - 512000



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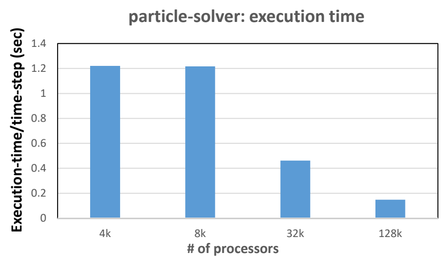
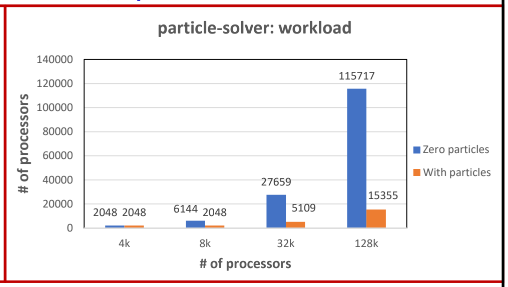
8

Particle solver: Strong Scaling

Element size – 11, # of elements – 262144, # particles – 512000





- No speedup obtained by increasing # of cores from 4k to 8k
- Increase in processor-count results in
  - Huge load imbalance
  - Poor resource utilization
- Need for better mapping algorithm – ***load-balancing algorithm***
- Trace-driven simulation provides optimal configuration by identifying
  - Computation cost
  - Communication cost
  - Resource utilization

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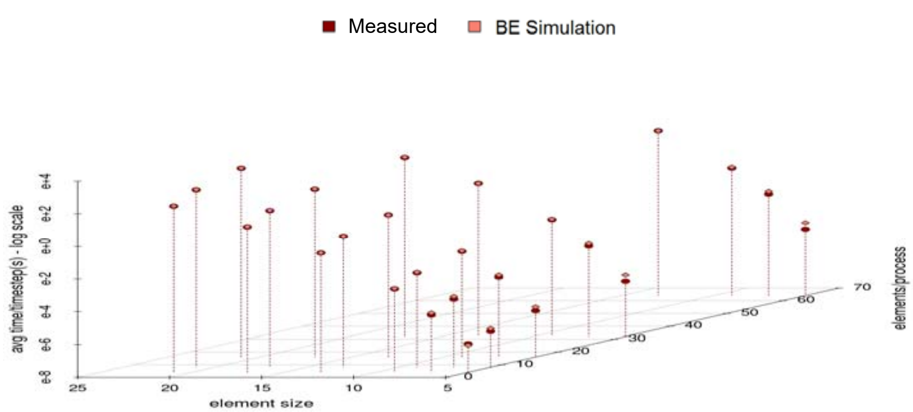
Validation of Particle Solver Model

CMT-nek particle solver (baseline version) - Validation results on Vulcan



- Observed an average error of **4%** in simulations

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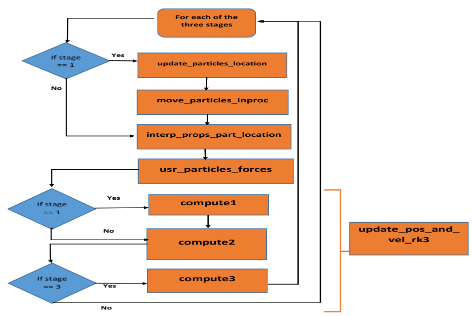
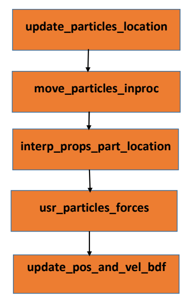
Particle Solver: Algorithmic options

- Evaluate performance of various algorithmic options available for particle-solver kernel
- **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**



Control-flow graph of rk3 algorithm



Control-flow graph of bdf algorithm

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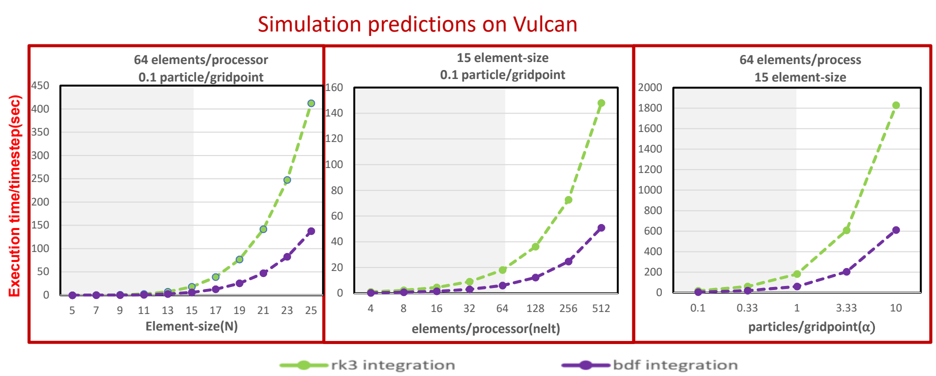
Simulator Predictions: Time Integration



- Both algorithms vary
  - ***non-linearly*** w.r.t ***element-size(N)*** and ***elements-per-processor(nelt)***
  - ***linearly*** w.r.t ***particles/gridpoint(α)***
- bdf time integration provides **3x** speedup over rk3

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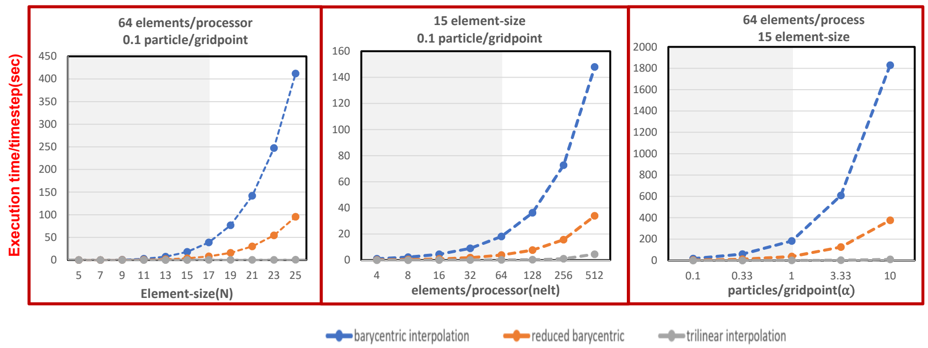
Simulator Predictions: Interpolation

Simulation predictions on Vulcan



- Algorithms vary
  - ***non-linearly*** w.r.t ***element-size(N)*** and ***elements-per-processor(nelt)***
  - ***linearly*** w.r.t ***particles/gridpoint(α)***
- Reduced barycentric interpolation provides **5x** speedup
- Tri-linear interpolation provides **164x** speedup

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Conclusions & Future work

- Conclusions
  - BE Methods
    - **Symbolic Regression**
      - accurate, doesn't require prior knowledge of kernel
    - **Trace-driven simulation**
      - improves BE-simulation accuracy
      - provides optimal configuration for a given problem
  - BE Simulations of particle-solver:
    - **Validation** – average error of **4%**
    - **DSE**
      - bdf time-integration algorithm provides **3x** speedup
      - Reduced barycentric interpolation provides **5x** speedup
      - Tri-linear provides **164x** speedup
- Future work
  - **BE Simulations of CMT-nek**
    - modelling Gas-solver kernel
    - Adding two-way coupling into particle-solver AppBEO
  - **CMT-nek DSE**
    - BE Simulations of CMT-nek on ***Notional Architectures***

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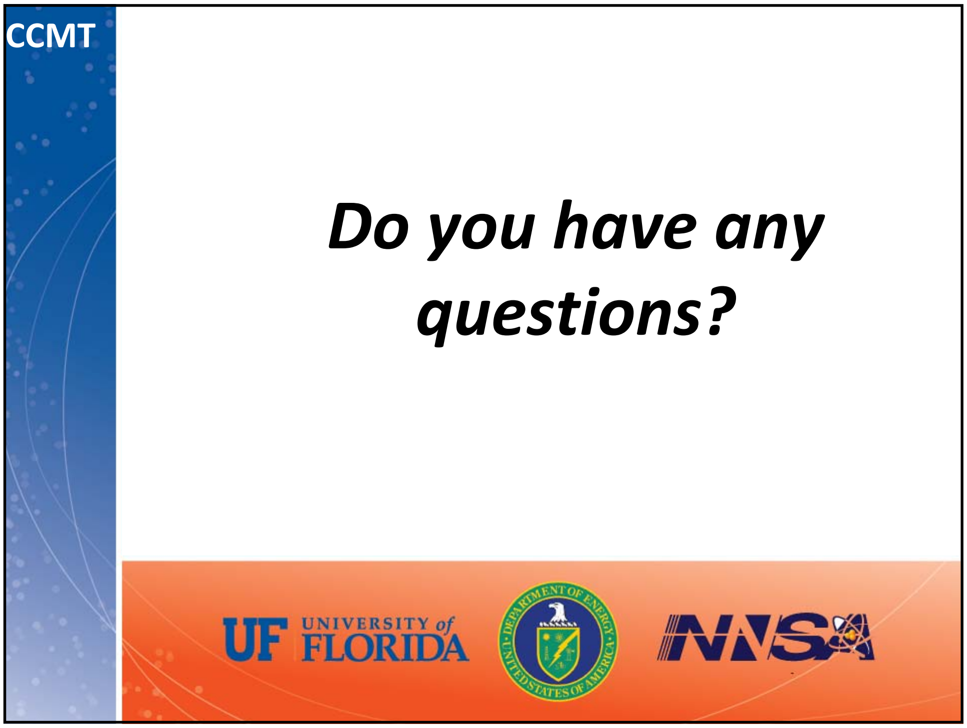
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Do you have any questions?
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NNSA