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BE-Simulation Framework: Looking Under the Hood

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ECE Department, University of Florida

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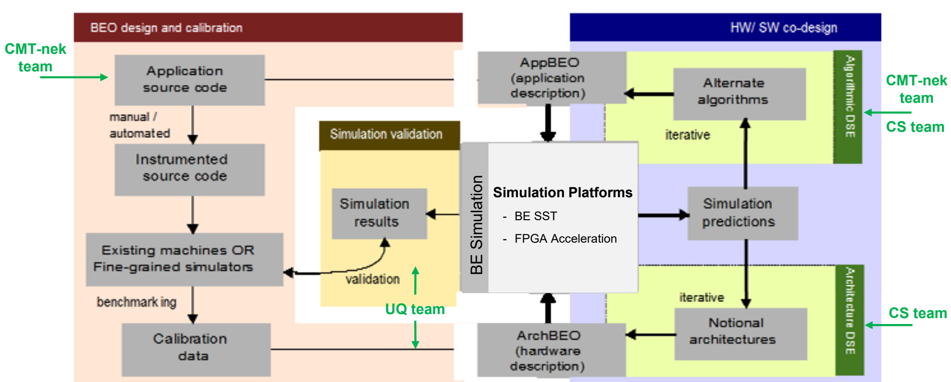
Co-Design Using *Behavioral Emulation*



* BEO – Behavioral Emulation Object

HW/SW co-design

- Algorithmic & architectural design-space exploration

Coarse-grained BE simulation

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

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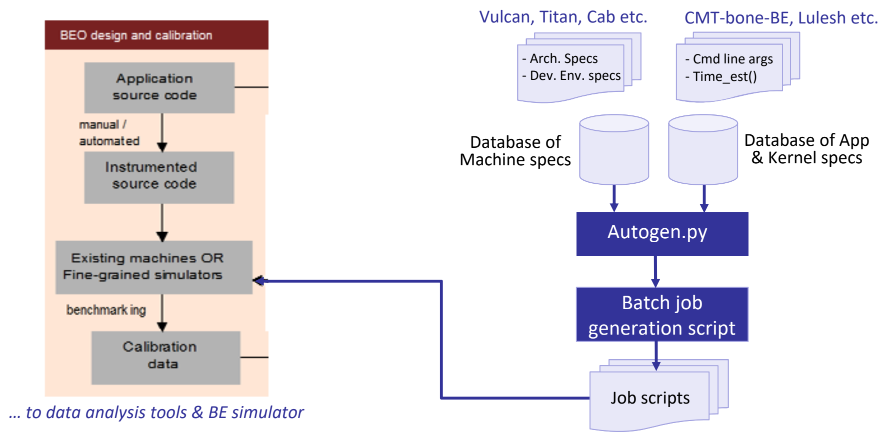
BE Framework Automation



- Designed a framework to simplify and automate benchmarking
  - Job scripts can be generated for different machine/app combinations
  - Easy to extend benchmarking to new applications & systems
- Leveraging similar framework for CMT-nek batch runs as well

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Application to AppBEO Conversion

Original Application → **Call Graph**

Instrumentation & Profiling

```
while((locDom->time() < locDom->stoptime())
  && (locDom->cycle() < opts.its)) {

  TimeIncrement(*locDom) ;
  LagrangeLeapFrog(*locDom) ;

  if ((opts.showProg != 0)
    && (opts.quiet == 0)
    && (myRank == 0)) {
    printf("cycle = %d, time = %e, dt=%e\n",
          locDom->cycle(),
          double(locDom->time()),
          double(locDom->deltatime()) ) ;
  }
}
```

Original Application   Call Graph

Computation Block
Communication Block
Computation and Communication Block

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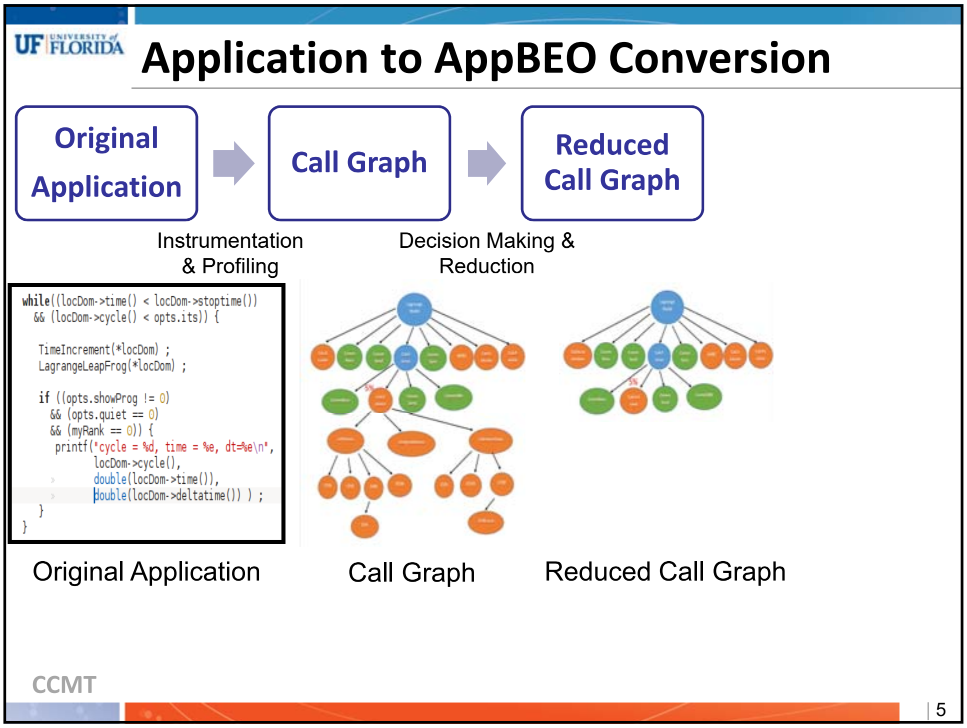
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Application to AppBEO Conversion
Original Application
Call Graph
Reduced Call Graph
Instrumentation & Profiling
Decision Making & Reduction
while((locDom->time() < locDom->stoptime())
&& (locDom->cycle() < opts.its)) {
TimeIncrement(*locDom) ;
LagrangeLeapFrog(*locDom) ;
if ((opts.showProg != 0)
&& (opts.quiet == 0)
&& (myRank == 0)) {
printf("cycle = %d, time = %e, dt=%e\n",
locDom->cycle(),
double(locDom->time()),
double(locDom->deltatime())) ;
}
}
Original Application
Call Graph
Reduced Call Graph
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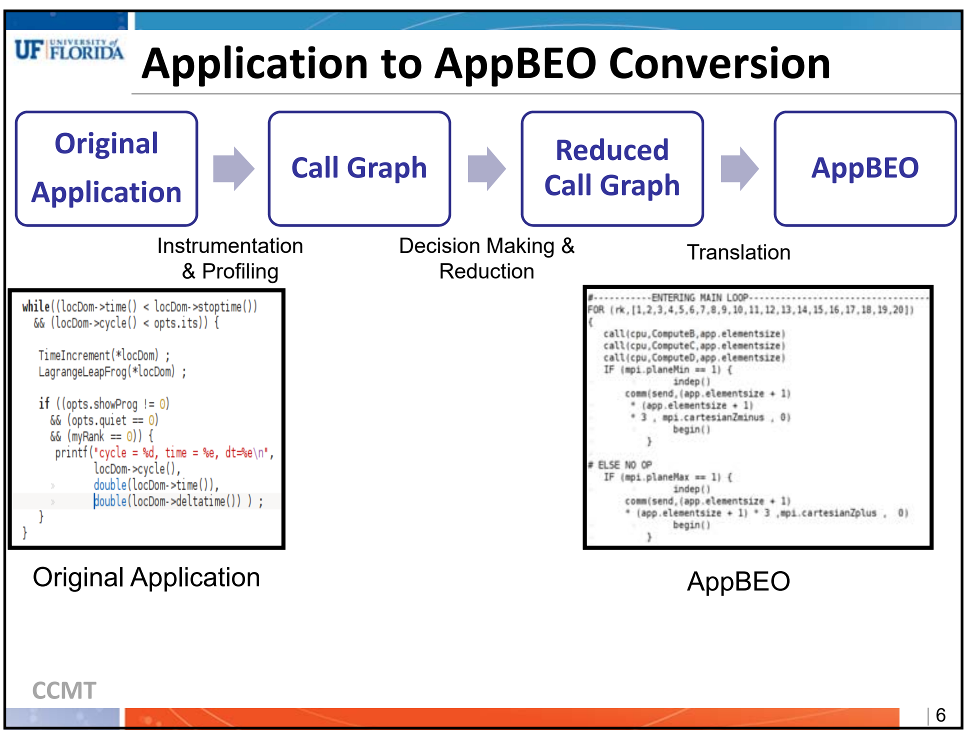
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Application to AppBEO Conversion
Original Application
Call Graph
Reduced Call Graph
AppBEO
Instrumentation & Profiling
Decision Making & Reduction
Translation
while((locDom->time() < locDom->stoptime())
&& (locDom->cycle() < opts.its)) {
TimeIncrement(*locDom) ;
LagrangeLeapFrog(*locDom) ;
if ((opts.showProg != 0)
&& (opts.quiet == 0)
&& (myRank == 0)) {
printf("cycle = %d, time = %e, dt=%e\n",
locDom->cycle(),
double(locDom->time()),
double(locDom->deltatime())) ;
}
}
#----------ENTERING MAIN LOOP----------
FOR (rk,[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20])
{
call(cpu,ComputeB,app.elementsize)
call(cpu,ComputeC,app.elementsize)
call(cpu,ComputeD,app.elementsize)
IF (mpi.planeMin == 1) {
indep()
comm(send,(app.elementsize + 1)
* (app.elementsize + 1)
* 3 , mpi.cartesianZminus , 0)
begin()
}
# ELSE NO OP
IF (mpi.planeMax == 1) {
indep()
comm(send,(app.elementsize + 1)
* (app.elementsize + 1) * 3 ,mpi.cartesianZplus , 0)
begin()
}
Original Application
AppBEO
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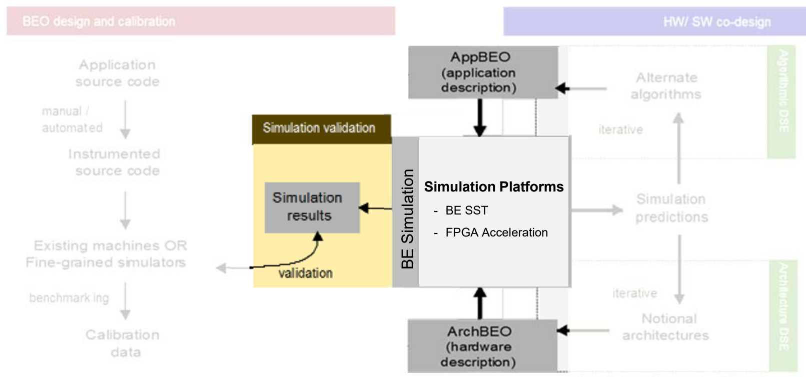
BE-SST Simulator



- SW Platform: **BE-SST** created by extending Sandia's SST
- HW Platform: Novo-G FPGA-based cluster

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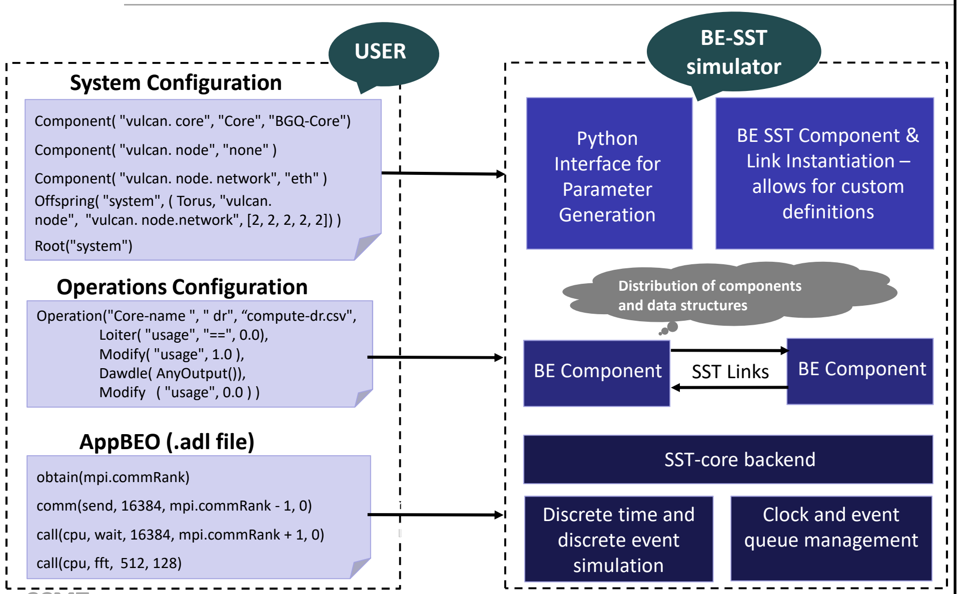
BE-SST v1.0 Features



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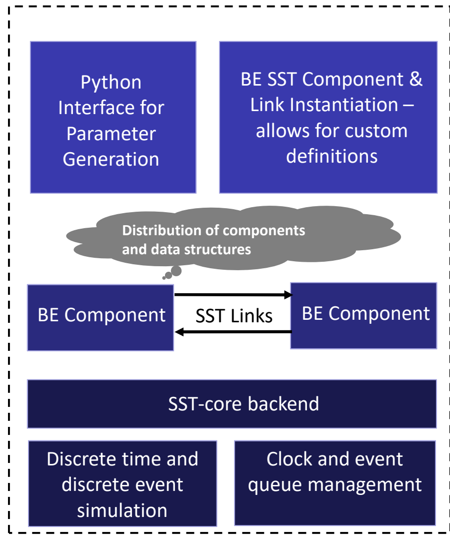
BE-SST model enhancements

- Communication model enhancements:
  - Dynamic generation of network routes provide better performance scaling and parallel performance
  - Overhead modeling at both sender/receiver endpoints
- Interpolation API allows easy switching between different interpolation methods for better accuracy
- Improved scalability and robustness of software product
  - Reduced storage by deleting handled events from queues
  - Switched from static routes to runtime routing



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Interpolation Interface

- Interpolation interface allows easy switching between different interpolation methods for better accuracy
  - Available schemes: linear, polynomial, lagrangian, kriging

1. Define default in operation configuration file

```
Operation( "BGQ-core", "computeConv", "vulcan-compute-conv.csv", "linear", "elementSize",
        Loiter( "usage", "==", 0.0),
        Modify( "usage", 1.0 ),
        Dawdle( Outputs(0) ),
        Modify( "usage", 0.0 ) )
Operation( "BGQ-core", "prepareFaces", "vulcan-compute-face-proper.csv", "polynomial-4", "elementSize", "elementsPerProcess",
        Loiter( "usage", "==", 0.0),
        Modify( "usage", 1.0 ),
        Dawdle( Outputs(0) ),
        Modify( "usage", 0.0 ) )
```

2. Overwrite with the AppBEO instructions

```
call(cpu, computeConv, lagrange, app.elementSize)
call(cpu, prepareFaces, linear, app.elementSize, app.elementsPerProcess)
```

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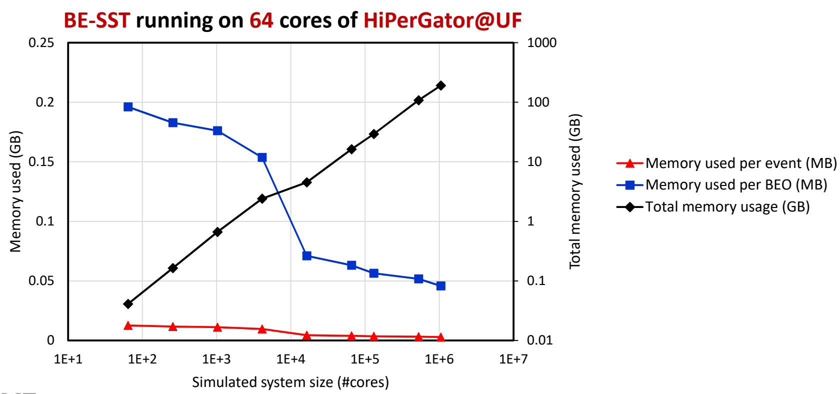
Memory Footprint of BE-SST

- BE simulations of different size systems with 3d-mesh topology running CMT-bone-BE
- Observations:
  - Memory used per BEO decreases because each core of HiPerGator is simulating more than one BEO
  - Memory usage has considerably reduced from previous version of BE-SST



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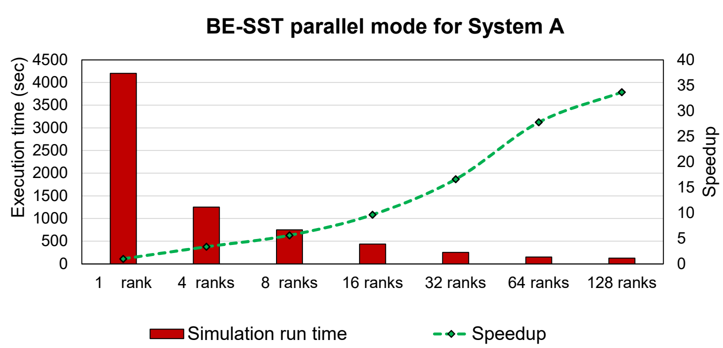
Results – Parallel Performance of BE-SST

- BE-SST demonstrates good performance scalability
  - Simulation of System A with 131,072 cores executing CMT-bone-BE
  - 385,025 network links in 3D Mesh topology [64, 64, 32]
  - Peak speedup of 33.7x was achieved on 128 MPI ranks



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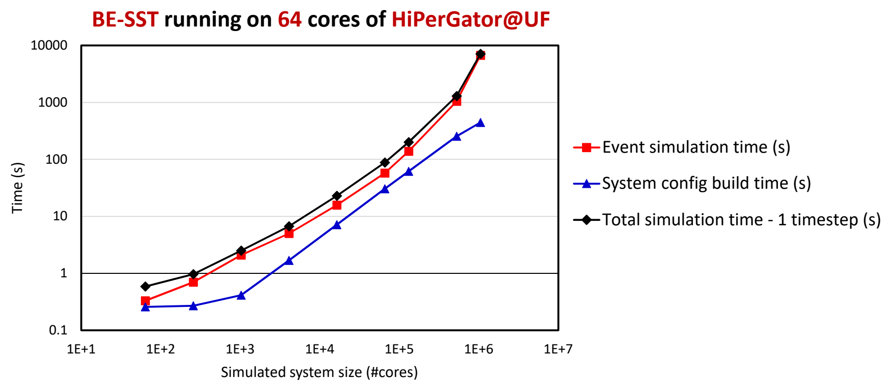
Parallel Performance of BE-SST

- BE simulations of 3d-mesh system running CMT-bone-BE
  - Simulations of machines with upto a million cores
  - With dynamic routing
- System config build time is not a bottleneck for large simulations



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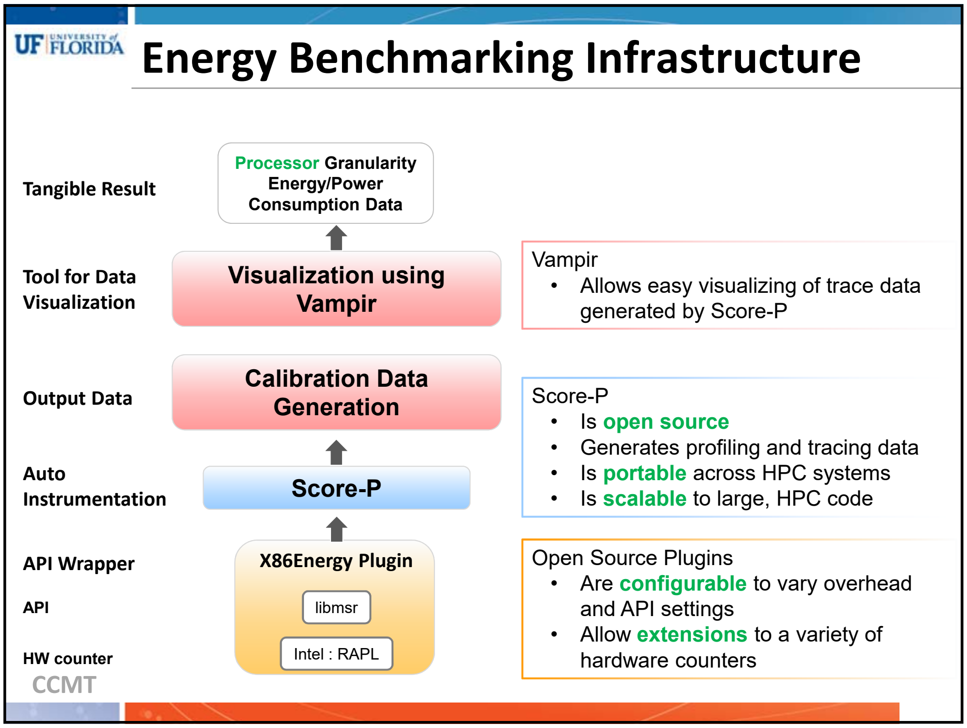
Do you have any questions?


Energy Benchmarking Infrastructure
Tangible Result
Processor Granularity Energy/Power Consumption Data
Tool for Data Visualization
Visualization using Vampir
Vampir
• Allows easy visualizing of trace data generated by Score-P
Output Data
Calibration Data Generation
Score-P
• Is open source
• Generates profiling and tracing data
• Is portable across HPC systems
• Is scalable to large, HPC code
Auto Instrumentation
Score-P
API Wrapper
X86Energy Plugin
API
libmsr
HW counter
Intel : RAPL
Open Source Plugins
• Are configurable to vary overhead and API settings
• Allow extensions to a variety of hardware counters
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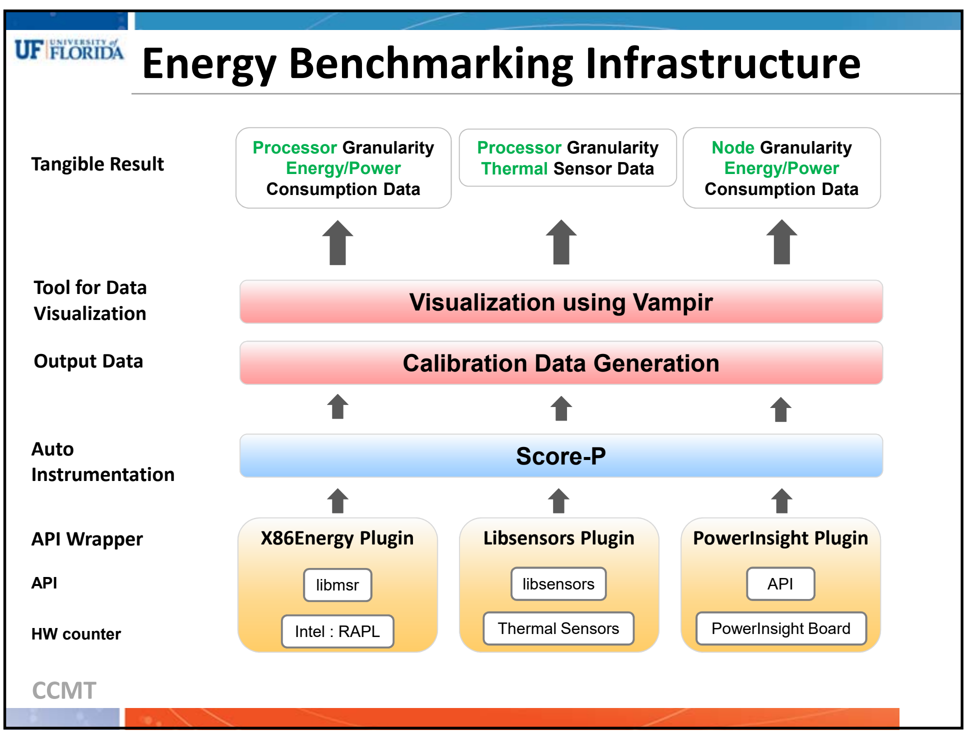
Energy Benchmarking Infrastructure
Tangible Result
Processor Granularity Energy/Power Consumption Data
Processor Granularity Thermal Sensor Data
Node Granularity Energy/Power Consumption Data
Tool for Data Visualization
Visualization using Vampir
Output Data
Calibration Data Generation
Auto Instrumentation
Score-P
API Wrapper
X86Energy Plugin
Libsensors Plugin
PowerInsight Plugin
API
libmsr
libsensors
API
HW counter
Intel : RAPL
Thermal Sensors
PowerInsight Board
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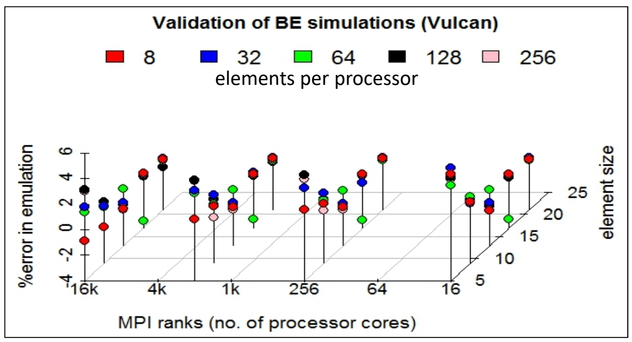
Validation of BE simulation on Vulcan

- Design of experiment
  - Element size (ES) = 5,9,13,17,21
  - Elements per processor (EPP) = 8,32,64,128,256
  - Number of processors (NP) = 16,256,2048,16384
- Calibration data obtained through in situ benchmarking
- Observation: % error in emulation varies between -3% to 5%



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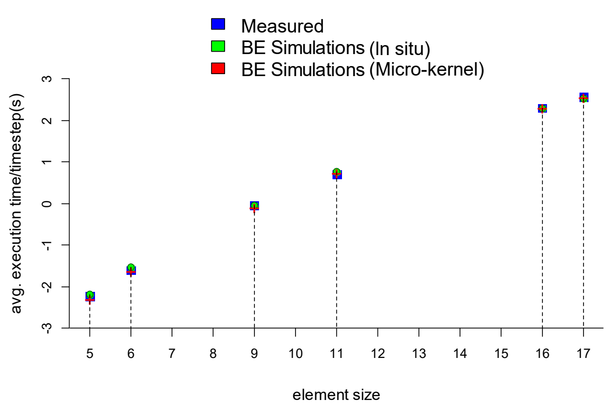
In situ vs. Micro-kernel Benchmarking

- Micro-kernel benchmarking for calibration to support notional exploration
  - E.g., no source available
- Simulation of 5d torus system with 2048 cores
  - Error is comparable with in situ benchmarking methods for this initial study



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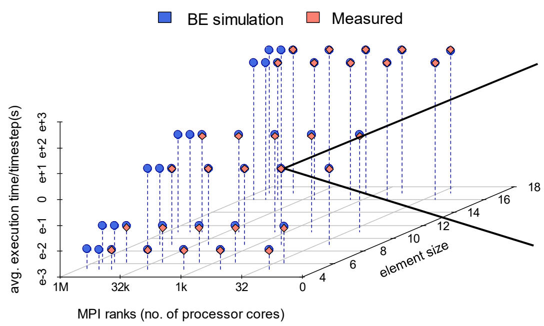
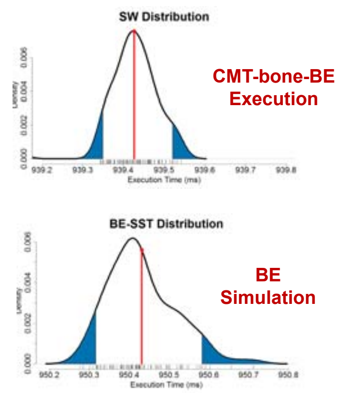
BE Simulations of CMT-bone-BE on Vulcan





- Average % error between CMT-bone-BE simulation and execution time is 4% and max. error is 9%

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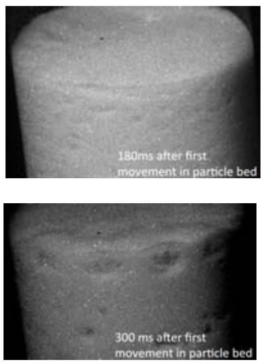
Particle Laden Simulations in CMT-nek

David Zwick

PhD student

Motivation & Setup

- While not fully resolved, Eulerian-Lagrangian simulations can simulate a realistic number (billions) of particles
- ASU experiment has $O(10^9)$ particles



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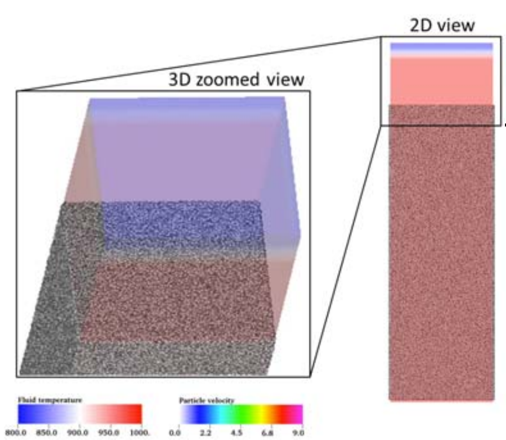
One-Way Coupled Results (ASU)



Largest one-way simulations CMT-nek:

Year	Ranks	Elements	Grid pts.	Particles
3	8k	60k	20 million	50 million
4	131k	131k	250 million	20 billion
4	131k	524k	905 million	905 million

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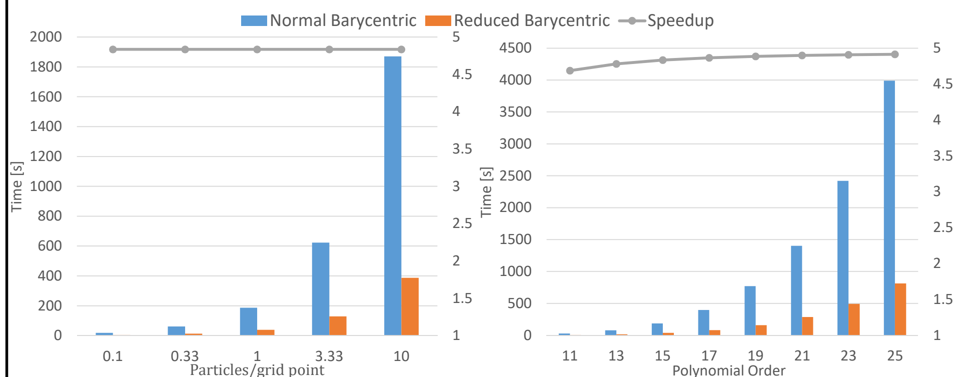
Collaboration with BE Team

- Full spectral interpolation is costly (normal barycentric algorithm)
- Reduced barycentric interpolation is cheaper
  - 5x speedup on average over full barycentric approach
  - 8x speedup for higher polynomial orders



Ranks	Elements/rank	Polynomial
4096	64	15

Ranks	Elements/rank	Particles/grid pt.
4096	64	1

*Times are total time per time step

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Governing Equations

Fluid Momentum

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{h} = \mathbf{f}$$

Particle Momentum

$$M_p \frac{d\mathbf{V}}{dt} = \mathbf{F}_{hyd}$$

Particle Forces

$$\mathbf{F}_{hyd} = \mathbf{F}_{qs} + \mathbf{F}_{un} + \mathbf{F}_{iu}$$

$$\mathbf{F}_{qs} = \frac{Re_p M_p}{24\tau_p}(\mathbf{u} - \mathbf{V})C_D$$

$$\mathbf{F}_{un} = M_g \frac{D\mathbf{u}}{Dt}$$

$$\mathbf{F}_{iu} = \frac{1}{2} V_p \left(\rho_g \frac{D\mathbf{u}}{Dt} - \frac{d(\rho_g \mathbf{V})}{dt} \right) C_M$$

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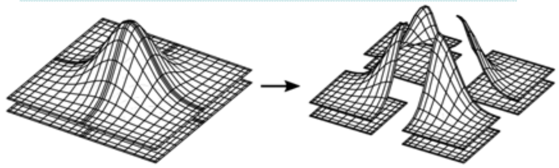
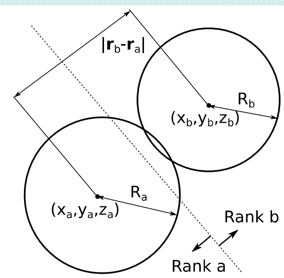
Computational Hurdles in Coupling

Each particle's influence extends beyond its element/rank

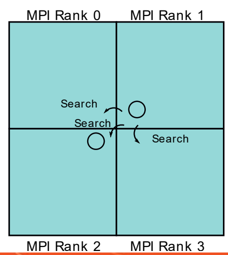
Back coupling with gas for two-way coupling



Particle-particle interaction



Nearest-neighbor search



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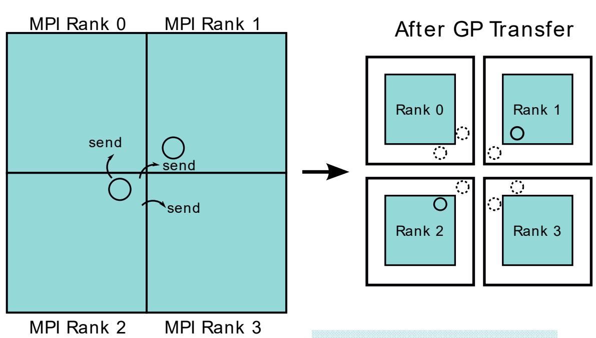
Ghost Particle Algorithm

Idea:

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



GP steps:

1. Create GP
2. Send GP

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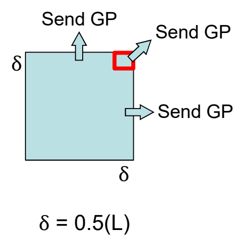
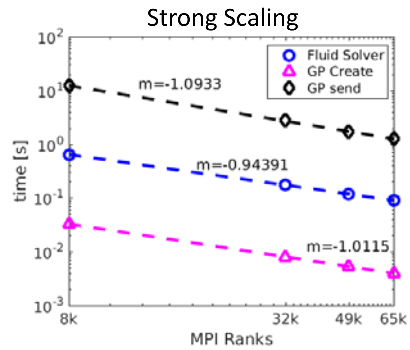
Scaling of Ghost Particle Algorithm

Scalability of algorithm:

- We consider a test case of an expansion wave over a bed of particles
- Particles are randomly distributed and advected by the wave

MPI Ranks	Elements	Polynomial	Grid points	Particles	Time steps
8k–65k	432,000	5	54 million	27 million	2000





*Times are total time per time step per MPI rank

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Back Coupling with Gas

- Accomplished through the use of a filtering kernel g_m for mollification
- Gaussian kernel is used for g_m
- For example, to transfer particle property A to the grid as a:

$$a(\mathbf{x}) = \sum_{i=1}^{N_p} A(\mathbf{X}^{(i)}) g_m(|\mathbf{x} - \mathbf{X}^{(i)}|) V_p^{(i)}$$

A	a
1	particle volume fraction
$\mathbf{F}_{hyd}/V_p^{(i)}$	particle hydrodynamic force

Fluid Momentum

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{h} = \mathbf{f}$$

For an element in weak form

$$\int_{V_\Omega} v_k f_k dV_\Omega \rightarrow v_k^T B f_k$$

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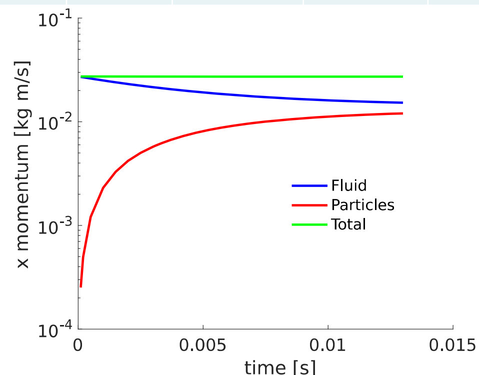
Momentum Conservation

Particles are placed at rest in a uniform flow and subjected to Stokes drag

- Particles speed up and fluid slows down
- Total momentum remains constant

Domain	Elements	Polynomial	Particles	MPI Ranks
x,y,z = [-1,1]	64	11	200,000	64



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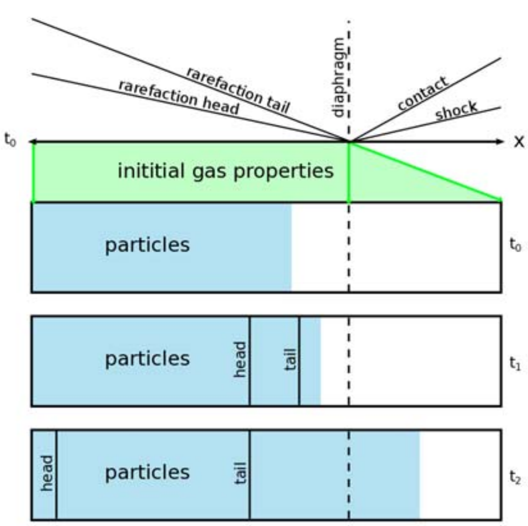
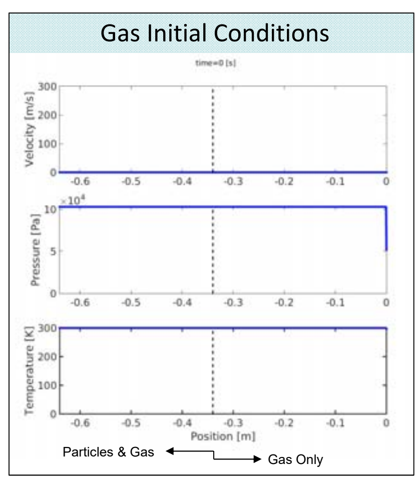
Application to ASU Experiment





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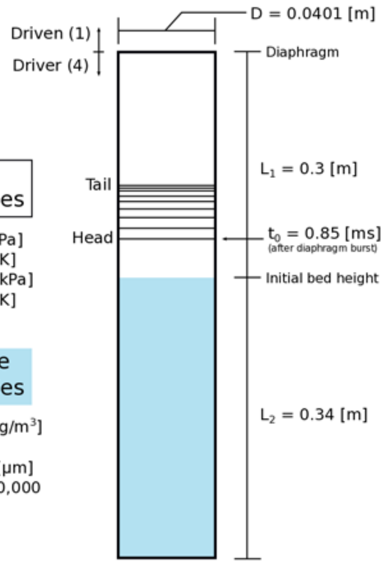
Simulation Setup

fluid properties

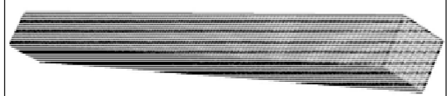
P_1 = 10 [kPa]
T_1 = 294 [K]
P_4 = 101 [kPa]
T_4 = 294 [K]

particle properties

ρ_p = 25 [kg/m^3]
Φ_p = 60%
D_p = 100 [μm]
N_p = 8,000,000



Fluid Grid Setup



Elements	Grid points	MPI Ranks	SPL
8,192	1,000,000	8,192	76

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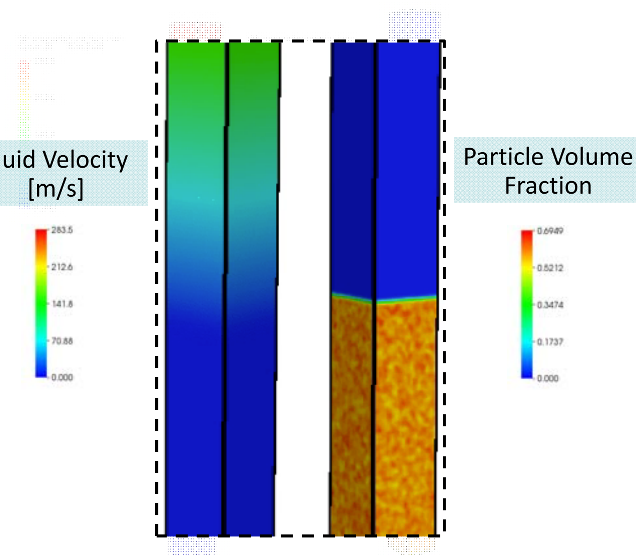
Simulation Results



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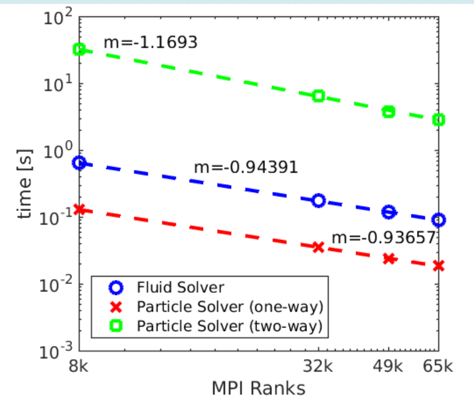
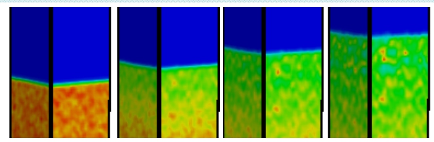
Simulation Results

Strong Scaling



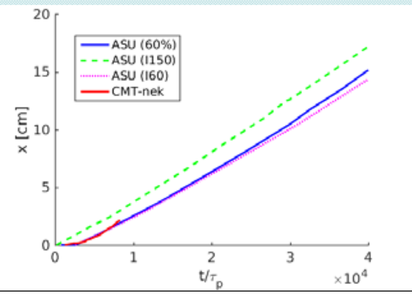
*Times are total time per time step per MPI rank for the same setup as the ghost particle scaling

Void Formation



t = 850.0 [μs] t = 876.3 [μs] t = 884.8 [μs] t = 892.4 [μs]

Bed Height



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Future work

- Larger simulations on Mira
- Improved force modeling
  - PIEP
  - Volume filtering correction
  - Effects on validation metrics
- Load balancing
  - Conference paper in preparation with Computer Science group
- UQ and V&V

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Do you have any questions?

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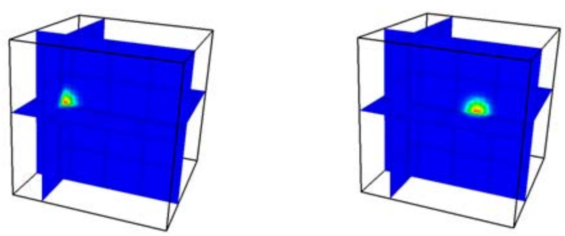
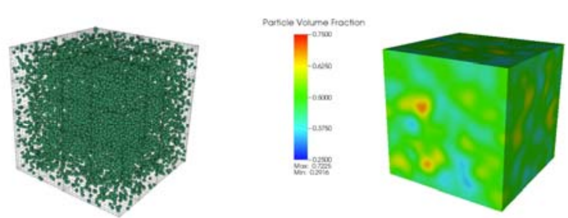
Filtering Examples

- Using ghost particle approach, a mollification kernel is used to spread properties to the Eulerian grid

Force from a single particle



Volume from a cloud of particles



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Surrogate Modeling of the JWL Equation of State

Frederick Ouellet
PhD Student

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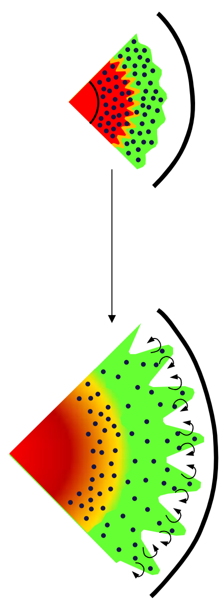
The Mixed-Cell Problem with Real Gas E.O.S.



- A short time after detonation, there is pure explosive product (red) and pure air (green)
- At this point, use real gas equations in red cells and ideal gas equations in green cells
- At later time, there are still red and green cells but also a mixing layer shown by the orange cells
- Here, both equations of state must be used

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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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Looking at the Big Picture

- What is the 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

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Models Implemented in Rocflu

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

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

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

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

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

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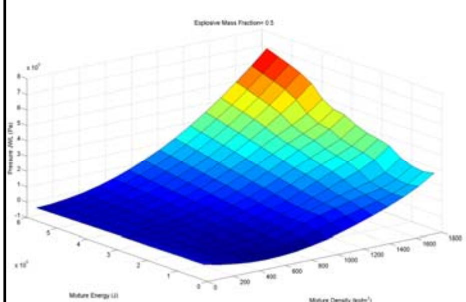
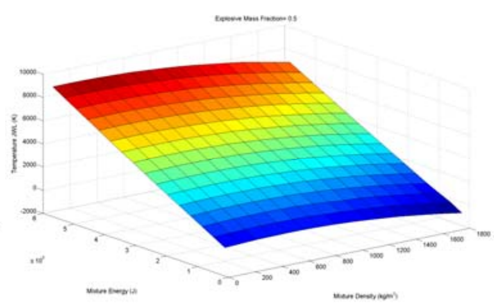
Surrogate Model - Development





- Models for mixed cell pressure and temperature generated by Kriging with 200 sampling points by UQ team
- Domain Space: $\rho_m \rightarrow (1, 1770)$
  $e_m \rightarrow (1.25e5, 1.5e7)$
  $Y_{exp} \rightarrow (0, 1)$
- Average relative errors:
  - Pressure: 1.298%
  - Temperature: 0.132%

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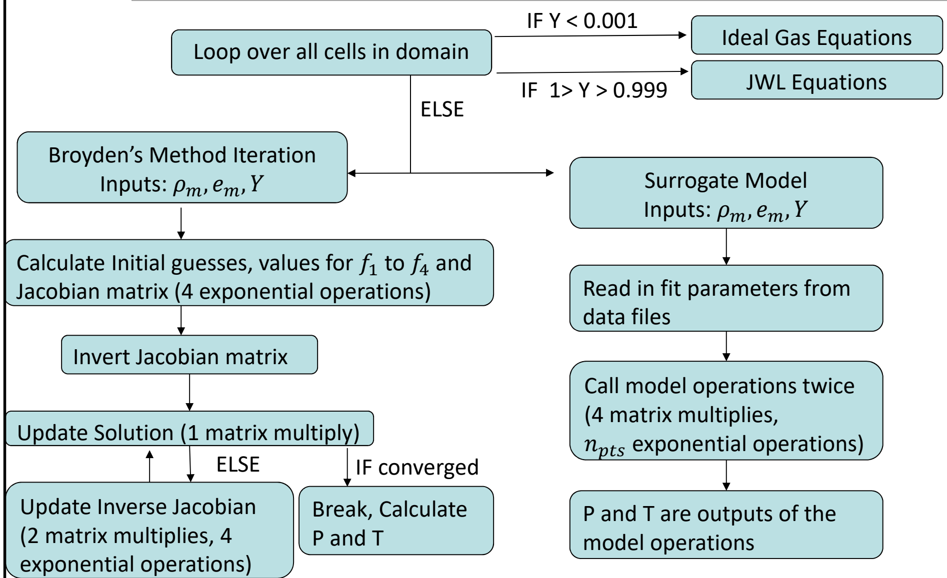
Flowchart – Iterative vs. Surrogate



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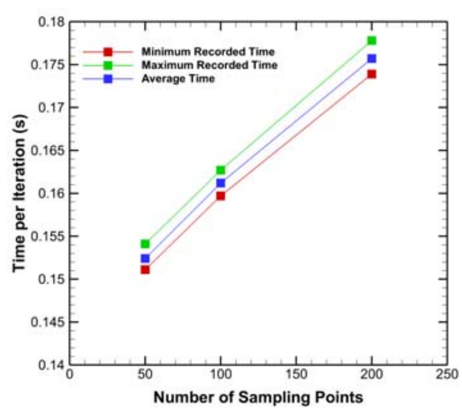
Surrogate Model Results – Computation Time

Run	seconds/Time step (Iterative)	seconds/Time Step (Surrogate)	Ratio	Previous Model
1	0.4636	0.1739	2.6662	-
2	0.4314	0.1778	2.4262	-
3	0.4766	0.1754	2.7178	-
Avg.	0.4572	0.1757	2.6024	2.6313

- Average time per iteration in computing 1000 time steps in Rocflu
- Results averaged over three runs
- Speed up ratio for 200 point model is about 2.60



- Preliminary results from study on differing numbers of sampling points
- Adding more points increases computation time

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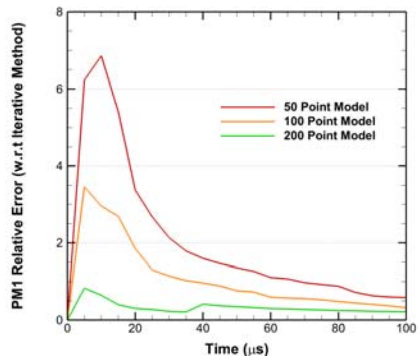
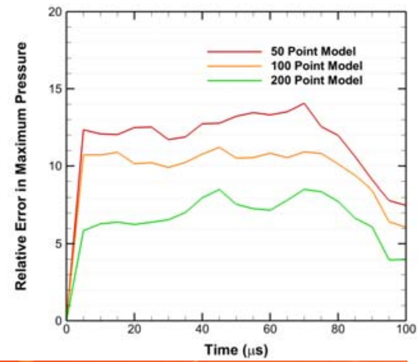
Surrogate Model Results – Simulation



- Maximum error in blast wave location for the 200 point model is 0.83%
- Maximum error in peak pressure for 200 point model is 8.51%
- Increasing number of sampling points reduces errors obtained using the surrogate



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

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Future Work

Effect of Sampling Points
- Study of the effect that altering the number of sampling points has to the model error
- Goal is to verify that 200 sampling points hits ideal midpoint of accuracy and computing time

Multiple Species
- Suppose an experiment dealt with a detonation process that contained n species
- If using Rocflu's iterative solver, this means going from a 4×4 system of equations to an $2n \times 2n$ system
- As long as the same number of test points are used to create a new surrogate, its computation time would remain roughly the same

Implementation with Multiphase flows
- Implement the model into simulations of flows with particles.
- Goal is to ensure the surrogate and the iterative scheme have minimal differences in particle trajectories, allowing for confident use in simulating experiments

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Microscale Simulations and Modeling

Yash Mehta

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Outline

- Fully resolved simulations of shock interaction with randomly distributed bed of particles :
  - Varying volume fraction
  - Varying shock Mach number
  - 1-D Riemann model for interpreting/analyzing results from numerical simulations
- Pair-wise Interaction Extended Point Particle (PIEP) model

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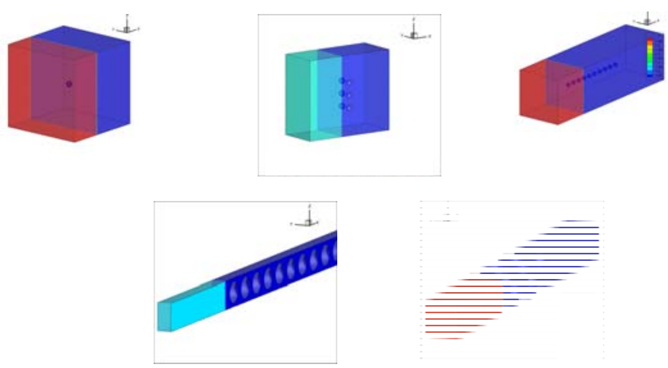
Fully Resolved Simulations

- We have performed multiple fully resolved simulations of shock interaction with particles
- Particle arrangement, particle volume fraction and, shock Mach number was varied
- Different physical mechanisms occurring during shock particle interaction were identified



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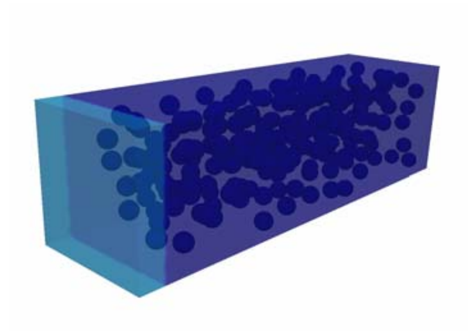
Shock Interaction with Random Bed of Particles



- We have performed multiple simulations by varying the volume fraction and the shock Mach number : $M_s = 1.22, 1.66$ and, 3.00 ; $\varphi = 1.25, 10, 15, 20$ and, 25%
- Number of particles in the computational domain varied from 200 to 500
- Effect of viscosity and particle motion was neglected in these simulations

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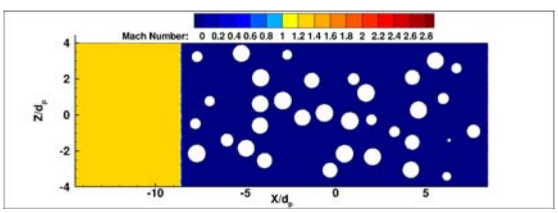
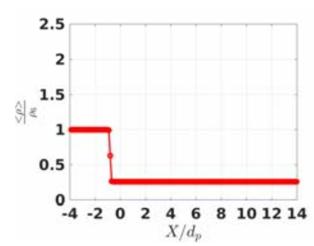
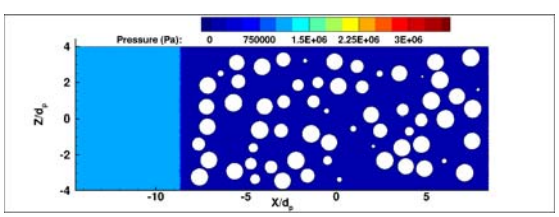
Flow Properties



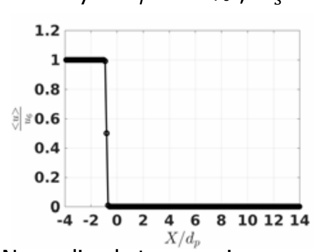
Mach number contour plot for $\varphi = 10\%$; $M_s = 3.0$



Normalized stream-wise averaged density for $\varphi = 10\%$; $M_s = 3.0$



Pressure contour plot for $\varphi = 25\%$; $M_s = 3.0$



Normalized stream-wise averaged velocity for $\varphi = 25\%$; $M_s = 3.0$

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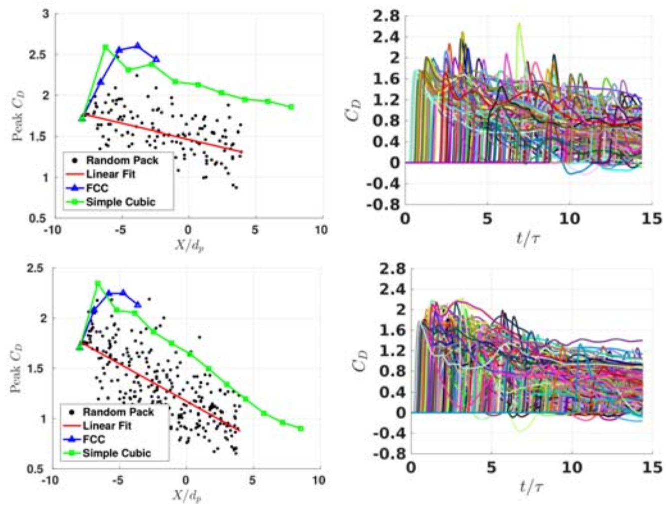
Forces on particles ; $M_s = 3.0$

$\varphi = 10\%$ $\varphi = 15\%$

$\varphi = 20\%$ $\varphi = 25\%$



- There is a high variability for the peak drag and a clear downward trend

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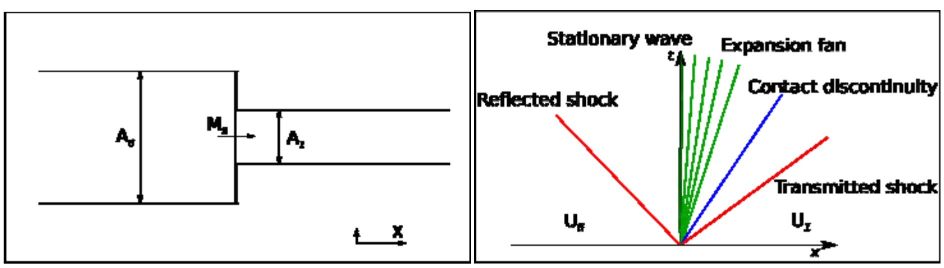
1-D Riemann Model



- Shock interaction with bed of particles can be modeled as shock interaction with an area change in a 1-D context
- This is a standard Riemann problem with an additional parameter - area change

$$\frac{\partial \phi}{\partial t} = 0$$

Han etal 2012 "Exact Riemann solutions to compressible Euler equations in ducts with discontinuous cross-section". *Journal of Hyperbolic Differential Equations*, 09(03), pp. 403-449

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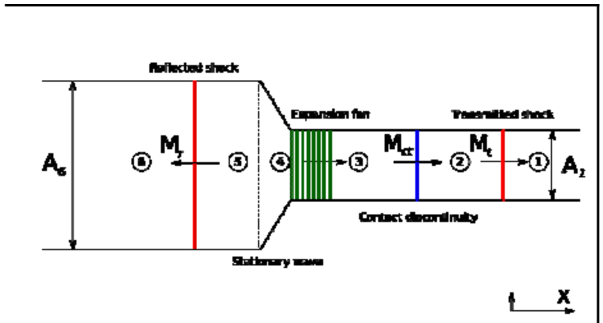
1-D Riemann Model



- We obtain a "steady" state solution for different volume fractions
- Reflected shock travels upstream of the area change, there is a resonant expansion fan at the location of area change, contact discontinuity and, transmitted shock travel downstream
- For a given shock Mach number and volume fraction there exists a unique solution

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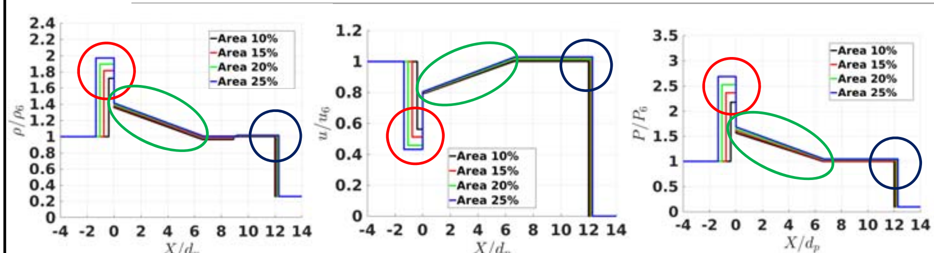
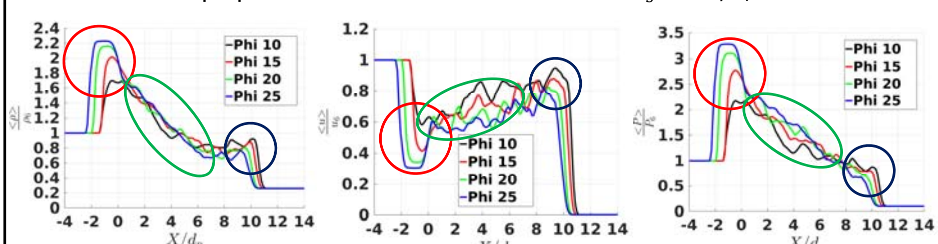
1-D Riemann Model Vs Numerical Simulation



Flow properties obtained from 1-D model for $M_s = 3.0;\ t/\tau = 12$



Averaged flow properties obtained from numerical simulations for $M_s = 3.0;\ t/\tau = 12$

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1-D Riemann Model Vs Numerical Simulation

φ_1	M_r	M_t	P_5/P_6
10%	1.41	3.00	1.000
15%	1.47	3.03	1.020
20%	1.52	3.05	1.035
25%	1.56	3.07	1.047

Flow properties obtained from 1-D model for $M_s = 3.0$; $t/\tau = 12$

φ_1	M_r	M_t	P_5/P_6
10%	1.41	2.75	0.874
15%	1.59	2.64	0.799
20%	1.67	2.43	0.718
25%	1.72	2.34	0.678

Averaged flow properties obtained from numerical simulations for $M_s = 3.0$; $t/\tau = 12$

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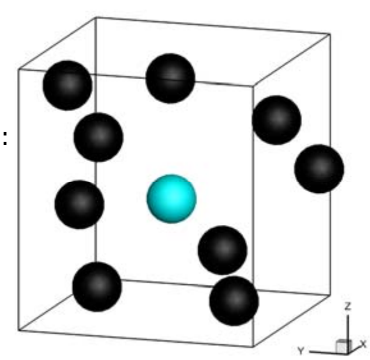
Pairwise Interaction Extended Point Particle Model (PIEP)

- Force on a single sphere is given by the Generalized Faxen's Theorem (F_{flow})
- Force on a single sphere in a bed of particles is :

$$F = F_{flow} + F_{diff}$$

- Force due to presence of other particles (F_{diff}):

$$F_{diff} = \sum_{j=1}^{N-1} F_{j \to i}$$



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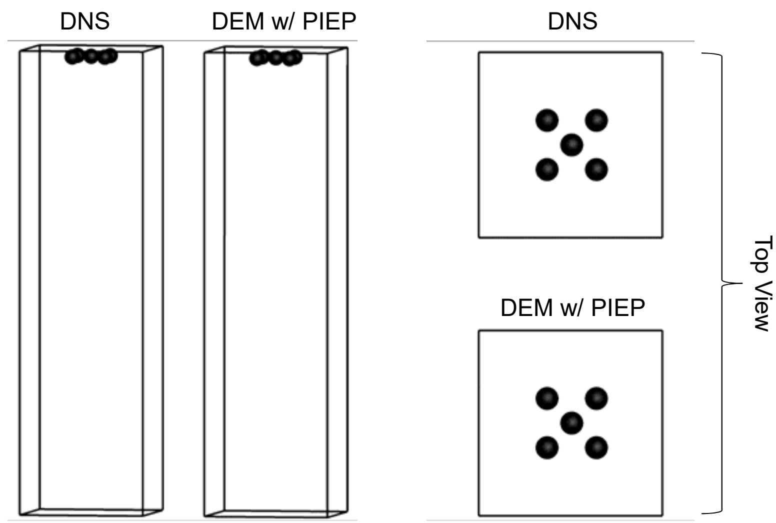
PIEP – Incompressible Flow



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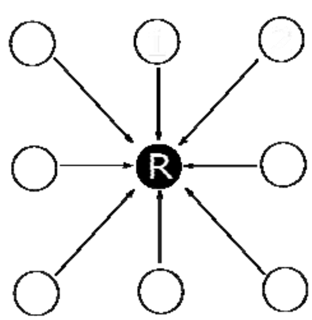
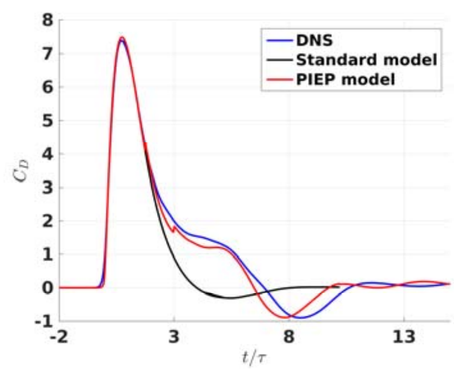
PIEP – Compressible Flow

- Shock interaction with transverse array of particles





- $F_R = F_{shock} + 4 * F_{1-R} + 4 * F_{2-R}$
- Drag force on the center particle

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Future Work

- Post processing the simulation data
- Viscous simulations for shock interaction with particles
- Developing PIEP model for compressible flows

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Predicting Execution Times of CMT-nek using Multi-fidelity Surrogate

Yiming Zhang

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Accomplishments

- **Coordinated the multi-fidelity error reduction for CMT codes at large-scale runs**
  - Designed the experiments for comparing CMT-nek (Jason Hackl), CMT-bone (Tania Banerjee) , CMT-bone BE (Aravind Neelakantan) and BE emulation (Aravind Neelakantan)
- **Predicted execution times of CMT-nek using multi-fidelity surrogate**
  - Proposed a multi-fidelity surrogate to fit a few CMT-nek runs together with BE emulations. The multi-fidelity prediction had 4% root-mean-square difference (RMSD) with CMT-nek
  - Submitted to IEEE Cluster 2017 titled as "Using Multi-fidelity Surrogates of Skeleton Apps for Predicting Application Performance"

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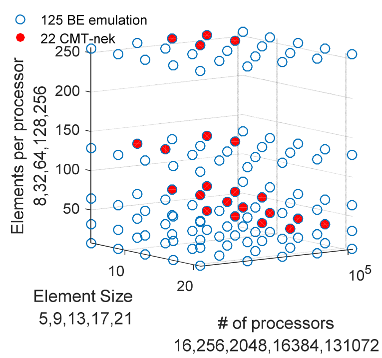
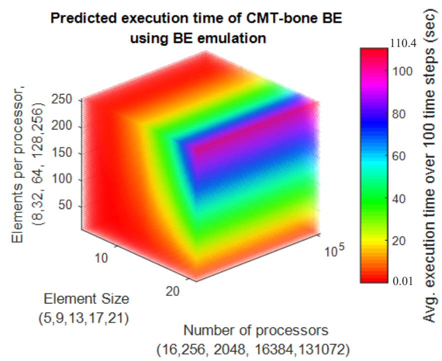
Design of Experiments at Large-Scale Runs

- Execution times of a typical no-particle test (on Vulcan) using up to 130k processors, 34 million (131072 × 256) elements and 311 billion (21^3 × 131072 × 256) computational grid points
- 125 (5^3) runs for BE emulation & CMT-bone BE, with subsets for CMT-nek & CMT-bone





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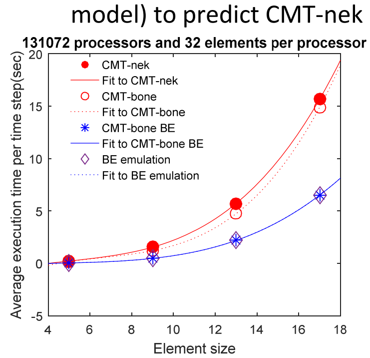
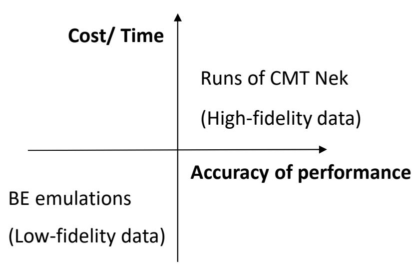
CMT codes vs. BE emulation

- Similar trend, but large difference
  - Effective emulation (low-fidelity model) could predict the overall trend well of CMT-nek runs (high-fidelity model)
  - Emulations of CMT-bone BE simplify the calculations, which were much smaller than the execution times of CMT-nek
  - Using multi-fidelity surrogate translates emulations (low-fidelity model) to predict CMT-nek runs (high-fidelity model)





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Predictions using Multi-fidelity Surrogate

Translate BE emulation against a few CMT-nek runs by polynomial function

Form of translation function

Selected a popular form with a scale factor and a discrepancy surrogate

$$\hat{f}_{nek}(x) = \rho \hat{f}_{BE}(x) + \delta(x)$$

Schemes to determine surrogate parameters

Developed a multi-fidelity surrogate for improved robustness and accuracy

- Bayesian vs. Deterministic
- Spatial distribution vs. Residual error
- Sequential vs. Simultaneous

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Test Plan To Evaluate Multi-fidelity Predictions

- Selected 10 runs (out of 22) of CMT-nek as validation runs to examine the accuracy of emulation
- The overall difference (root-mean-square) between original BE emulation and CMT-nek was 74% at the 10 validation points
- Adopted 2 to 12 remaining runs of CMT-nek as samples to translate BE emulations using the multi-fidelity surrogate
- For each number of samples, repeated random selection 20 times to account for the effect of sampling plan

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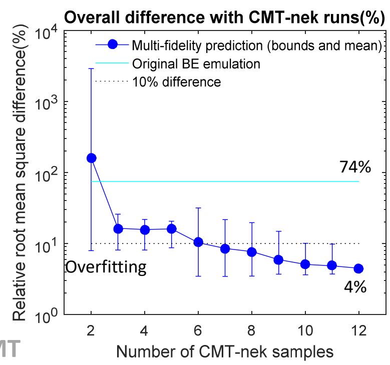
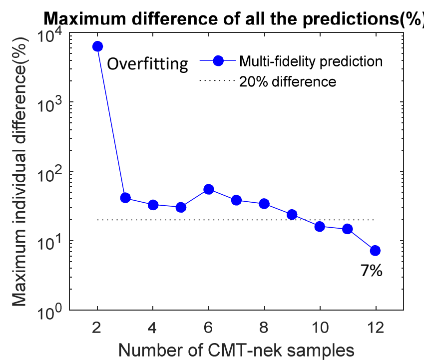
Multi-fidelity Predictions of CMT-nek Runs

- Overall difference (root-mean-square) is less than 10% with 6 or more CMT-nek samples for correction
- Max error is less than 20% (at the 10 validation runs) with 9 or more CMT-nek samples for correction
- The proposed multi-fidelity surrogate was more accurate than other approaches





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Ongoing Work

- Investigating the capability of corrected BE emulation to extrapolate the execution time of CMT-nek runs towards exascale computing
- Sampling strategy for extrapolating the execution time of CMT-nek runs while incorporating varying cost of runs

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Deeper look into Collapsed Pipeline Approach

Carlo Pascoe

Center for Compressible Multiphase Turbulence (CCMT)

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

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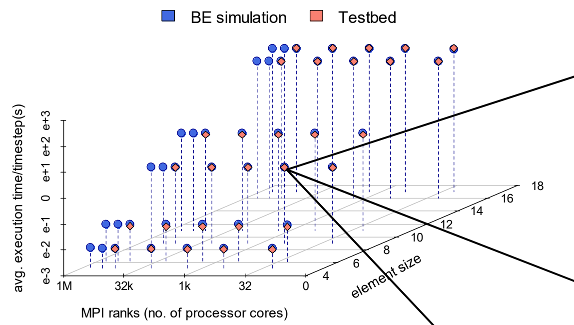
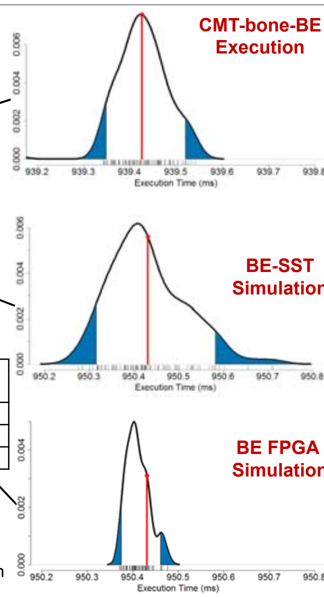
Simulations of CMT-bone-BE on Vulcan





Simulation Method	Num. of MPI Ranks	Num. of Timesteps	Num. of Events	Num. of FPGAs	% Logic Utilization	FPGA Clk Frequency	Latency to First Output	Mega Sims/Sec
BE-SST	128	1	5,952	NA	NA	NA	NA	0.00000152
FEP	128	1	5,952	1	66 %	280 - 320 MHz	66	280 – 320
CP	128	1	5,952	1	2 %	315 - 355 MHz	458	1.68 – 1.99

- BE software and BE FPGA simulations produce similar results
- Fully-expanded approach provides greatest performance at cost of more resources
- Collapsed approach allows for greatly reduced resource utilization and increased scalability at cost of slightly reduced performance

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Outline

- Motivation
  - Fully-expanded v Collapsed Pipeline Approach
  - Simple Motivating Example
- Collapsed Pipeline Single-FPGA Performance/Scalability
- Collapsed Pipeline Multi-FPGA Performance/Scalability
- Moving Forward
  - Validation of multi-FPGA predictions
  - Increased performance with Stratix 10
  - Partially-collapsed pipeline approach

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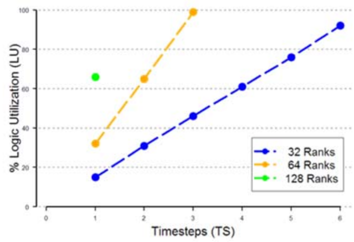
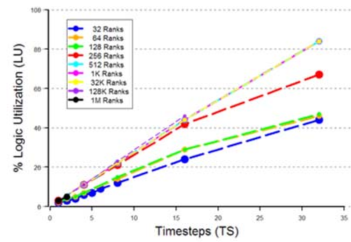
Fully-Expanded v Collapsed Approach





Fully-Expanded Pipeline

Advantages:

- Superior performance in terms of simulation throughput and latency

Limitations:

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

Collapsed Pipeline

Advantages:

- Resources scale linearly with timesteps, but sublinearly with MPI Ranks
- Better scaling on single and multiple FPGAs

Limitations:

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

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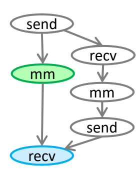
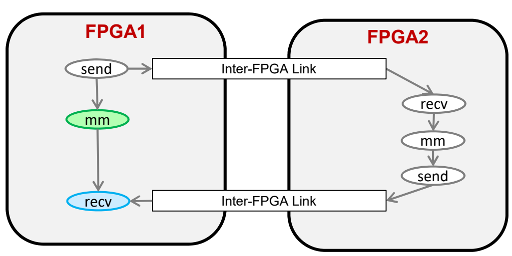
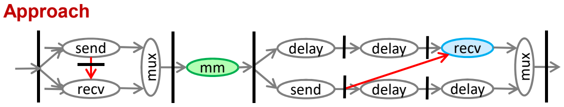
Simple Motivating Example

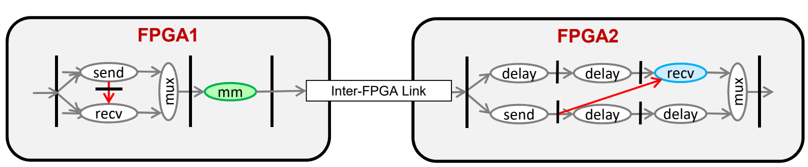
Fully-expanded Approach





Collapsed Approach





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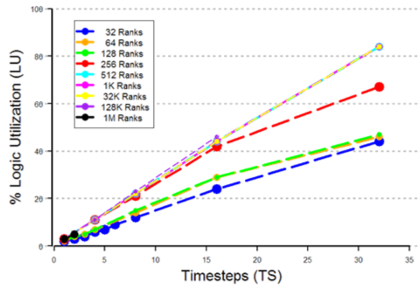
Collapsed Pipeline Single-FPGA Performance/Scalability



Ranks	TS	% LU	Num. of Events	Lat to First Out (cycles)	Mega Sims /second*	Giga Events /second*
32	32	44	43,008	7,532	10.5	450
64	32	46	92,160	10,252	5.23	482
128	32	47	190,464	10,316	2.62	498
256	32	67	393,216	13,516	1.31	515
512	**32**	**84**	**811,008**	**20,684**	**0.65**	**531**
1K	32	84	1,646,592	21,196	0.33	539
32K	**32**	**84**	**55,443,456**	**241,868**	**1.02E^{-2}**	**567**
128K	16	46	111,673,344	333,932	2.56E^{-3}	285
1M	2	5	112,459,776	1,148,056	3.19E^{-4}	36

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

Pipelines scale linearly with length of simulation, however blockram eventually becomes limiting resource
- e.g., only fit 2 TS for 1 million ranks on Stratix V
- Motivation to explore partially-collapsed pipeline approach

Increased performance expected with Stratix 10
- Collapsed hardware specifically designed to exploit new Stratix 10 architecture

CCMT *Collapsed performance of CMT-Bone-BE with varied MPI ranks and simulation timesteps on a single Stratix V S5GSMD8K1F40C2 @ 335MHz

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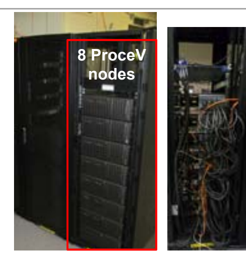
Collapsed Pipeline Multi-FPGA Performance/Scalability

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

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

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

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



Novo-G#
- 64 GiDEL ProceV (Stratix V)
- 4x4x2 3D torus or 5D hypercube
- 6 Rx-Tx links per FPGA
- Measured 32 Gbps per link
- 150 ns latency across links

- Require 64bits/cycle between FPGAs
- 335MHz, 21.4 Gbps, 51 additional lat
- 450MHz, 28.8 Gbps, 68 additional lat
- 500 MHz before link BW saturation

* See poster from Carlo Pascoe

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

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Moving Forward

- Validation of multi-FPGA predictions
- Increased performance with Stratix 10
- Partially-collapsed pipeline approach

Do you have any questions?

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Simulation-Motivated Forensic Uncertainty Quantification of Eglin Microscale Experiments

Kyle Hughes
Graduate Student

April 21, 2017

Forensic UQ Perspective

- Significant time lag is present between the microscale experiments and the simulations
  - Not unusual in validation exercises
- As time grows, it becomes steadily more difficult to decrease the epistemic (or lack of knowledge) uncertainty of the experiments
  - Experimental setup or samples are often unavailable for analysis and must be recreated
- Uncertainty may be recognized and reduced through **forensic uncertainty quantification** (UQ) by an independent investigator
- Forensic UQ of the past experiments can be analogous to performing forensics at a crime scene
  - Document all the experimental details (crime scene)
  - Clarify details with experimentalists (witnesses)
  - Quantify uncertain inputs and prediction metrics (forensics lab)
  - Compare to simulation to identify inconsistencies (culprits)
- **Goal:** Apply forensic UQ to the Eglin microscale explosive experiments

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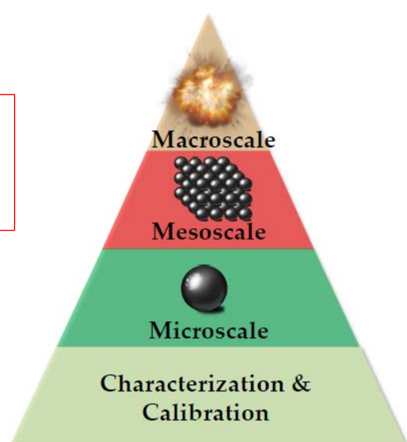
Validation Hierarchy

- CCMT employs a physics-based validation hierarchy
- Eglin conducts experiments at all three scales of interest to CCMT
- **Microscale** (O(1-10^4) particles)
  - Validation of microscale drag models
  - Explosive tests conducted October 2014 and February 2015
- **Mesoscale** (O(10^6) particles)
  - Examination of instabilities, volume fraction effects
  - Explosive tests conducted November 2015
  - Gas gun tests in planning stages
- **Macroscale** (O(10^9) particles)
  - Validation of full simulation
  - Explosive tests (AFRL blastpad) in planning stages



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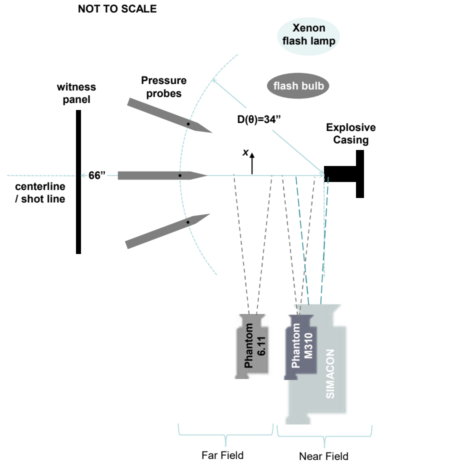
Microscale Experiments

Side view photograph showing the concave pressure probe array.

Summary of test shots performed in October 2014 and February 2015.

Test #	Particle(s)
Oct14-1	Single (2 mm dia) Tungsten sphere
Oct14-2	Ring of 7 (2 mm dia) Tungsten spheres
Oct14-3	Grid of 16 (2 mm dia) Tungsten spheres
Feb15-1	Single (2mm dia) Tungsten sphere
Feb15-2	Single (2mm dia) Tungsten sphere
Feb15-3	Diamond of 4 (2 mm dia) Tungsten spheres



Overhead schematic of the test set-up.

Sources: Myles Delcambre, Internal CCMT Fall 2014 presentation
Black, Littrell, and Delcambre, Eglin internal written report, 3/7/2015

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Validation and UQ Framework - Microscale

- Experiments
  - Measured Input → Explosive length, Explosive diameter, Explosive density, Casing outer diameter, Casing inner diameter, Particle diameter, Particle density, Particle initial location(s), Ambient pressure, Ambient temperature
    - Measurement Uncertainty
  - Measured Prediction Metrics → Particle trajectory, Contact line location
    - Sampling Uncertainty → Limited # of x-ray exposures, Limited framerates
    - Measurement Uncertainty → User error, Instrument resolution
    - Systematic Uncertainty → Apparatus misalignment, T_0

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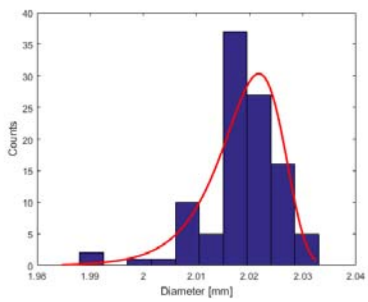
Measured Input: Particle Diameter

- Particle diameter was not measured a priori – initial uncertainty was assumed +/- 10% nominal diameter
- Statistical study of tungsten particles was conducted after the experiments to quantify their uncertainty
- Eglin provided 52 tungsten spheres that were randomly measured by two users

Single particle before detonation (Source: Don Littrell, 2/26/2015)



Histograms of particle diameter measurement

- Final data shows uncertainty has been **reduced** to 2-3% of nominal diameter compared to prior belief of 10%
- Smaller range of diameters will also decrease number of runs necessary to construct the surrogate

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Measured Input: Particle Density

- The sample provided by Eglin was additionally used to quantify the uncertainty in the particle density
- Manufacturer cites the particle density as 17 g/cm^3
- All 52 spheres were weighed and then their volume repeatedly measured in a helium gas pycnometer
- Densities are significantly different than those cited by the manufacturer
- Possible causes for this discrepancy are still being investigated
- Energy dispersive x-ray spectrometry may identify the specific alloy

Pycnometer results with summary statistics for the 52 tungsten particles

Run	Volume [cm^3]	Density [g/cm^3]
1	0.2401	15.92
2	0.2416	15.82
3	0.2470	15.48
4	0.2546	15.02
5	0.2462	15.53
6	0.2457	15.56
7	0.2429	15.74
8	0.2428	15.75
9	0.2491	15.35
10	0.2489	15.36
11	0.2480	15.42
12	0.2460	15.54
Average	0.2461	15.54
Std Dev	0.00394	0.25

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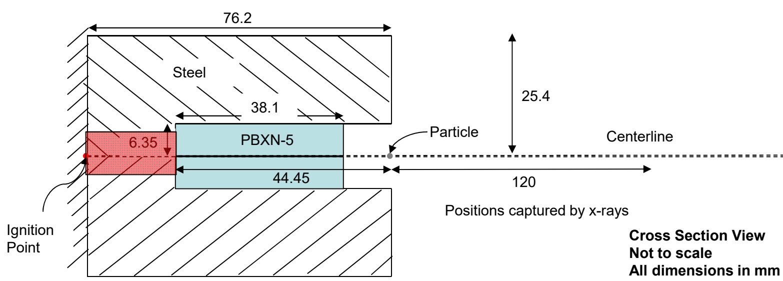
Microscale Simulations T_0

- Large assumptions currently made in the simulations
  - High density quiescent gas is representative of the explosive after reaction
  - Requires time shift to align the experiment and simulation
- To align with experiments need to account for both time of detonator to act and the time for the explosive to burn
  - Manufacturer reported detonator function time: 5.38 ± 0.125 μs
  - Assuming constant detonation velocity through the explosive: 4.31 μs
  - Total delay: ~9.7 μs



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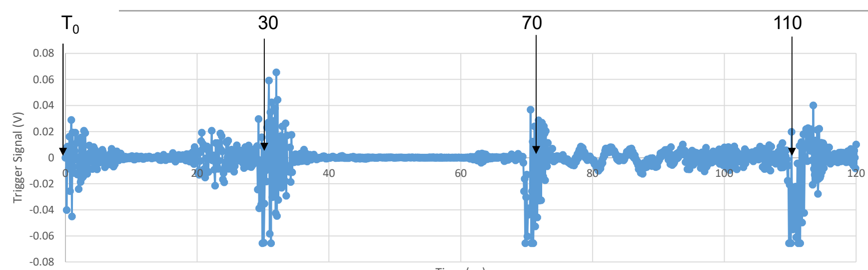
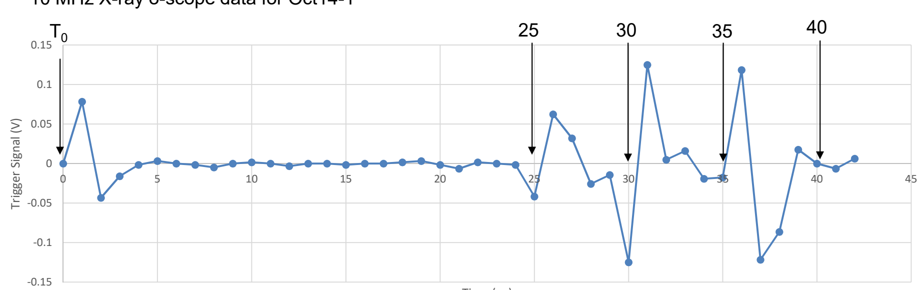
Timing Uncertainty



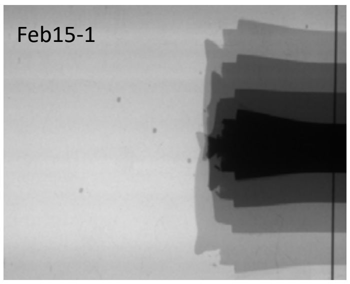
10 MHz X-ray o-scope data for Oct14-1



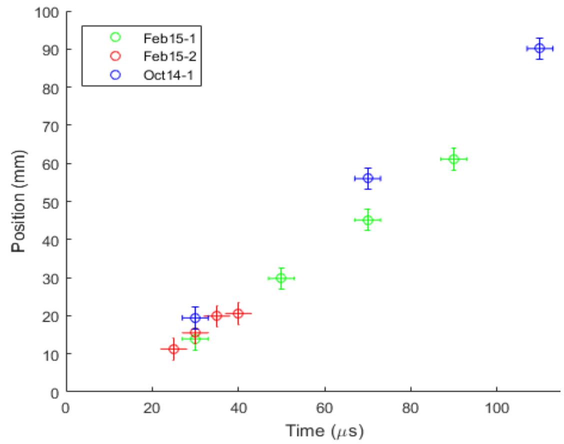
1 MHz X-ray o-scope data for Feb15-2

Metric: Single Particle Position

- Horizontal error bars are determined from oscilloscope records
- Vertical error bars are determined based on spread in data at repeated times



Multiple exposure x-ray of single particle



Single particle position from x-ray data

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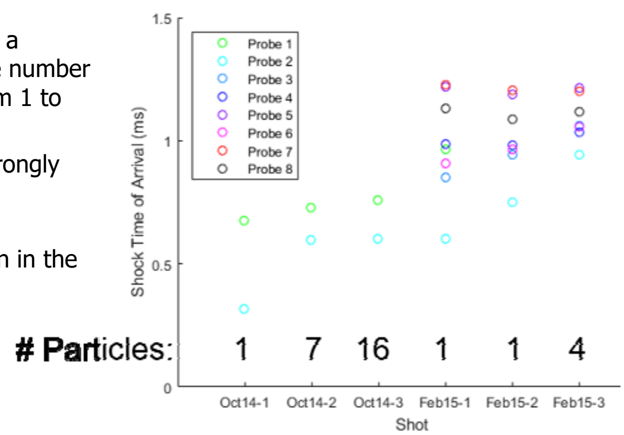
Shock Time of Arrival

- Initially expected negligible effect on the shock time of arrival based on the small number of particles present
- Shock time of arrivals show a increase in the mean as the number of particles is increased from 1 to multiples
- Evidence that the flow is strongly coupled with particles
- A possible explanation is to examine the volume fraction in the initial plane of the particles:

Number of Particles	Volume Fraction [%]
1	1.65
4	6.6
7	11.6
16	27



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Conclusions and Future Work

Conclusions

- Uncertainty quantification effort for even this "simplified" problem requires extensive back and forth between UQ, simulation, and experimental teams (5+ months)
- Understanding of the simulation assumptions and inputs can help drive forensic investigation
  - Difficulty of determining T_0 resulted in significant investigation into oscilloscope records
- Forensic UQ found a surprise that neither experimentalist or simulationist expected: The small number of particles show significant coupling with the flow

Future Work

- Completion of the uncertainty quantification of remaining microscale uncertain inputs
  - The explosive parameters are especially critical but also challenging
- Construction of surrogates to propagate input uncertainties through simulation
- Comparison of the experimental prediction metrics with simulation results for validation of the drag force models for a single particle

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Do you have any questions?

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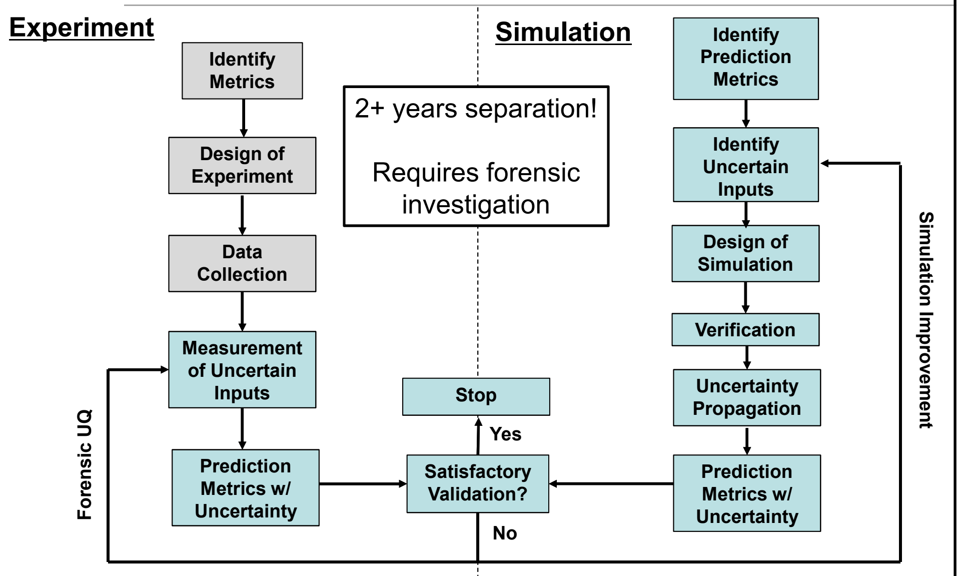
Forensic UQ Work-Flow



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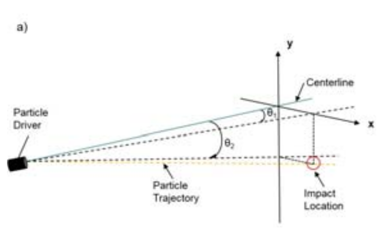
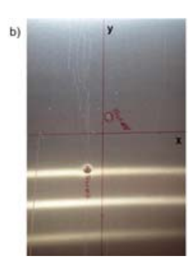
Out-of-Plane Motion: Witness Panel

- Witness panel results provides some indication of out-of-plane movement of the particles by providing final position
- Single particle shots show very small angles of the particles
- Repeated particles show significant spread such that two of the particles did not impact the panel while the other two impacted fairly close to the shot line
- The small angles of the single shot results allows elimination of out-of-plane movement as a large possible source of uncertainty





Angles obtained for February 2015 shots

	θ_1 (deg)	θ_2 (deg)
Feb15-1	-0.6494	-1.5718
Feb15-2	0.2392	0.7177
Feb15-3	2.8685	6.1961
	-6.5337	-5.0452

a) Angle conventions used for the witness panel results b) Raw witness panel results

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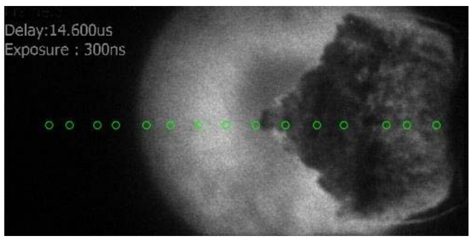
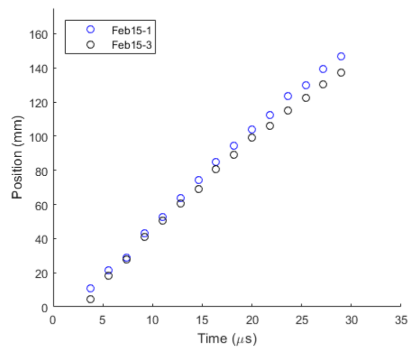
Metric: Contact Line

- Obtained from the high speed Simacon images (maximum 16 frames)
- Contact line results are obtained by the selection of the furthest location from explosive casing
- Contact line is only visible in a couple of frames in October 2014 shots (excluded)
- Uncertainty quantification of the results is on-going



Sample Image



Contact Line Results

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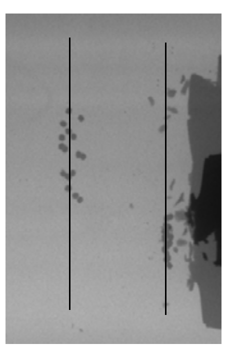
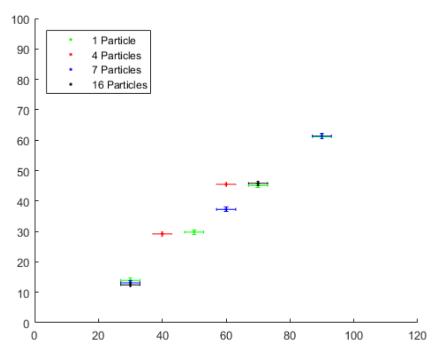
Metric: Average Particle Position

- Can be difficult to track each particle for the multiple particle shots
- An average of the particle packet is selected here to begin looking at the multiple particles
- Variance seems reduced by this choice of an average, very similar trends observed with respect to a single particle



Choice of average position for 16 particle shot (Oct14-3)



Average of multiple particles

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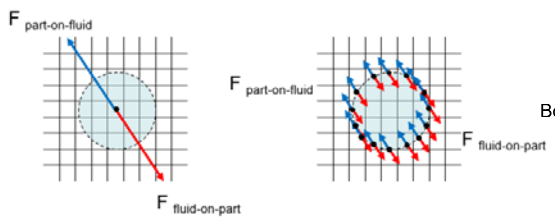
Simulation Capability

- Clear discussion of simulation capabilities is necessary for design of a validation experiment and forensic UQ
- Current simulation is missing a variety of physics
  - For instance, it does not include effects from particle non-sphericity and deformability
  - Experimentalists did an excellent job in minimizing this effect by using high-density, spherical tungsten particles
- Experimental evidence for significant particle-fluid interaction was surprising for both experimentalists and simulationists
  - Challenging to implement 2-way coupling for such large particles

Point Particle (Current)



Immersed Boundary Method (Future)

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Experimental Studies of Gas-Particle Mixtures Under Sudden Expansion at ASU

Heather Zunino
PhD Student
Dr. Ronald Adrian
Advisor

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Problem Statement and Goals

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

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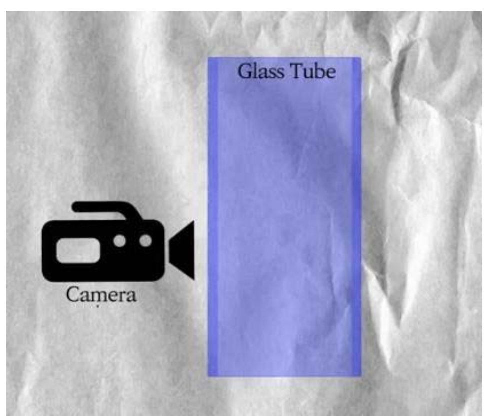
Experiment Description

- 1 meter glass tube
  - Cylindrical footprint
  - Inner diameter: 2”
- Particle bed
- Diaphragm
  - Tape
- High-speed camera
- Measurements
  - Contact line velocity
  - Gas velocity
  - Particle volume concentration
  - Particle interface
- Parameters: particle size and pressure ratio



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Experiment Description

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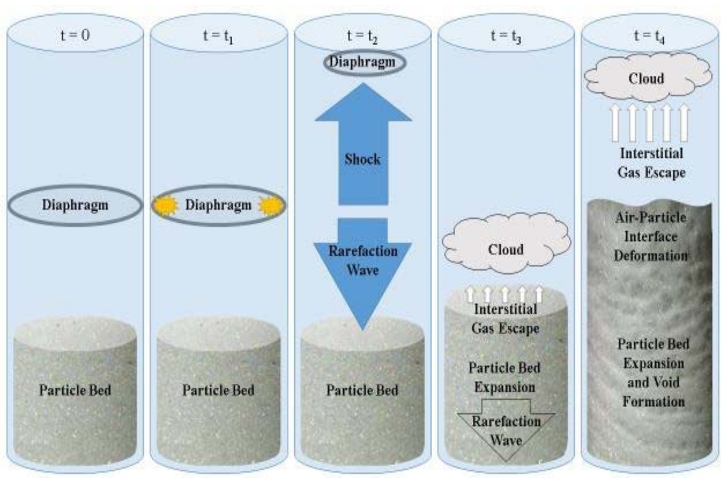
Stages of Experiment



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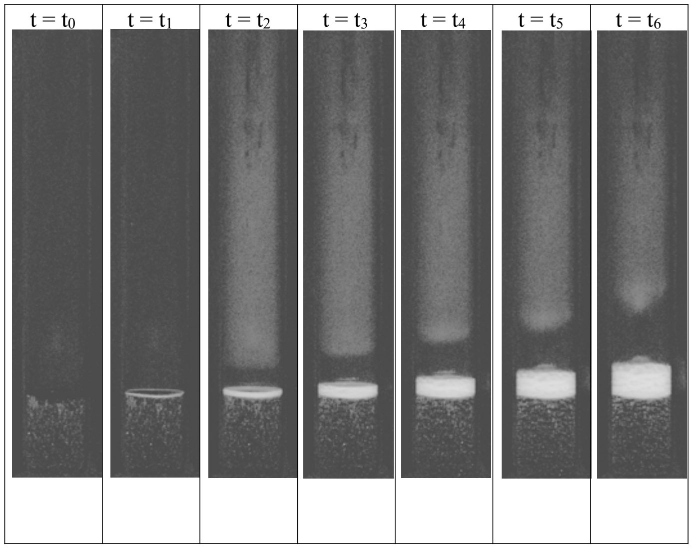
Cloud Evolution



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Reflected Shock Wave

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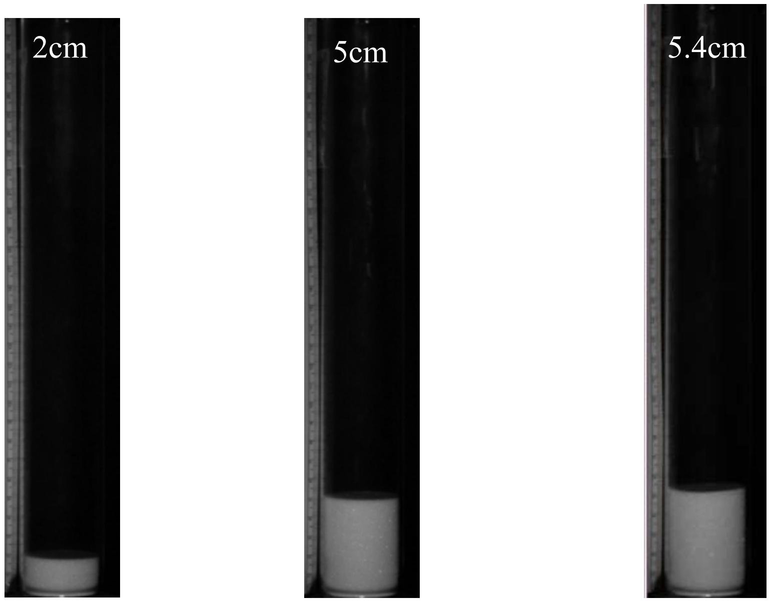
Interface Rise



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Hardware Additions

- 8 pressure sensors
  - 4 locations
  - 90º or 180º apart
- Data Acquisition
  - 8 simultaneous channels
  - Over 150kHz each channel
- Synchronization
  - Camera
  - Pressure sensors
  - Laser light sheet

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Summary

- Cloud evolution
  - Interframe appearance
  - Measure gas velocity escape
  - Gas escapes from edges of particle bed first
- Reflected shock wave
  - Use cloud droplets as gas tracer
  - Particles seem unaffected
- Interface rise
  - Different bed heights
  - Different initial volume fraction
- Hardware additions
  - Upgraded pressure sensors
  - Better temporal resolution
  - Synchronized data acquisition

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Do you have any questions?