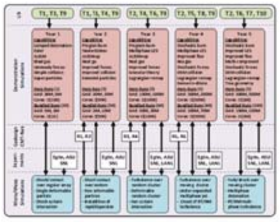
CCMT

Center for Compressible Multiphase Turbulence

DSE* of CMT-nek using BE**

Sai Prabhakar Rao Chenna
Advisor: Dr. Herman Lam, Dr. Greg Stitt
Department: ECE, UF



Simulation Roadmap

- Goals
  - Profile CMT-nek to identify candidates for DSE
  - Perform algorithmic DSE of CMT-nek using BE methods & tools
- Simulation roadmap
  - Early DSE to enhance CMT-nek performance on future exascale systems

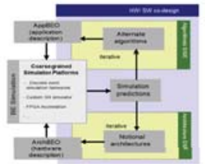
---

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

Motivation & Approach

- Motivation: Very large design space
  - CMT-nek provides various algorithmic and parametric options
  - Algorithmic DSE helps in rapid performance evaluation of these options on future exascale systems

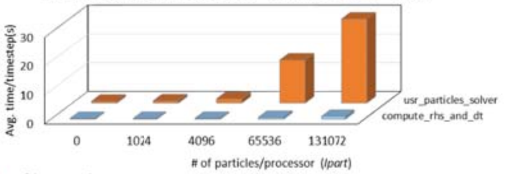
- Iterative DSE steps:
  - Identify DSE candidates - most expensive subroutines
  - Model algorithms for these subroutines
  - Use BE to predict performance



CMT-nek Profiling: Gas vs Particle Solver

- Input parameters:
  - *lpart* = # of particles/processor; *lx1* = Element size; *lelt* = # of elements/processor

Gas vs Particle Subroutines (lelt = 128; # processes = 256)

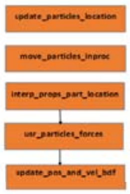


- Observations:
  - Particle solver (*usr_particles_solver*) - most expensive CMT-nek subroutine
  - Gas solver (compute_rhs_and_dt) depends on # of particles (*lpart*)

CMT-nek Alternate Algorithms

- Explore accuracy vs execution time trade-off of alternate algorithms for portions of CMT-nek (particles phase):
  1. **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
  2. **Particle Interpolation** - interpolates fluid properties acting on particles:
     - Current : Barycentric Interpolation
     - Alternate : Reduced Barycentric Interpolation

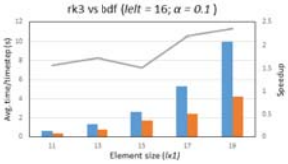
Control-flow graph of rk3 algorithm

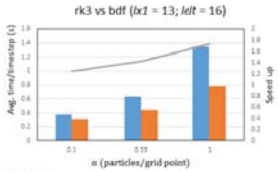


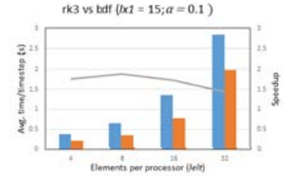
Control-flow graph of bdf algorithm

BE Simulation: rk3 vs bdf time integration

- Summary:
  - bdf is 1.5-2x faster than rk3
  - Both algorithms vary
    - non-linearly w.r.t. element size(*lx1*) and element count(*lelt*)
    - linearly w.r.t. α (particles/gridpoint)

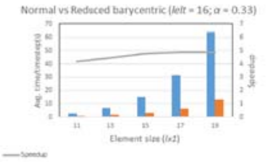


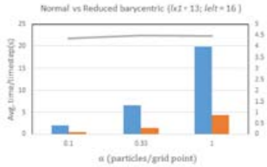


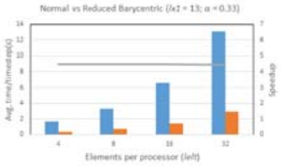


BE Simulation: Normal vs Reduced interpolation

- Summary:
  - Reduced Barycentric interpolation provides 4.5x speedup
  - Both algorithms vary
    - non-linearly w.r.t element size(*lx1*) and element count(*lelt*)
    - linearly w.r.t α(particles/gridpoint)







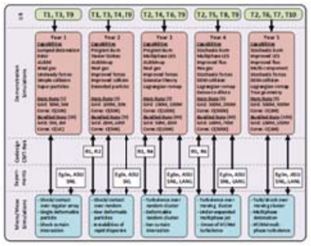
CCMT

Center for Compressible Multiphase Turbulence

Uncertainty Quantification of Shock Tubes

Brad Durant
Advisor: S. Balachandar
Department: Mechanical Engineering, UF

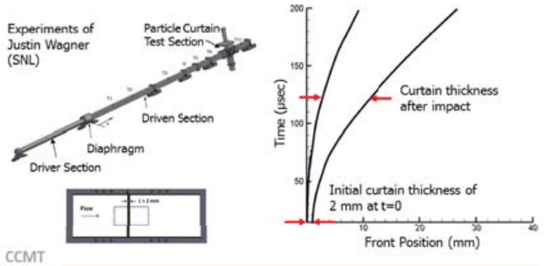
- Goals
  - Reproduce measurement processing from Sandia shock tube to identify sources of uncertainty
  - Propagate identified sources of uncertainty from experiments into simulations
- Simulation roadmap
  - T6: Force coupling and
  - T4: Particle-particle interaction



Simulation Roadmap

Motivation

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



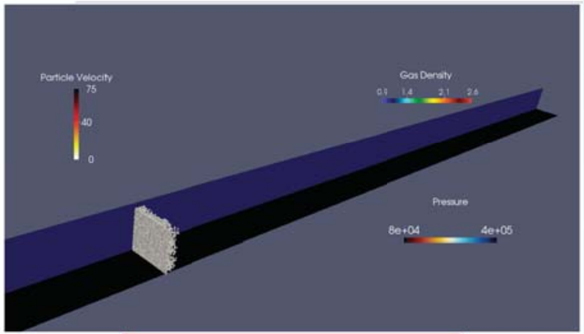
UB Workflow - Experiment Worksheet

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

UB Workflow Simulation Worksheet

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

Typical Particle Curtain Simulation



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

Summary and Future Work

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

CCMT

Center for Compressible Multiphase Turbulence

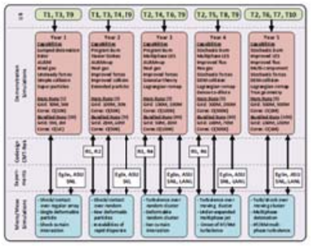
Particles Jet Formation Study

Student M. Giselle Fernandez

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

Department: Mechanical and Aerospace, UF

- Goals
  - Measurement of PM3 and PM4 in simulations
  - Optimization of initial PVF conditions that grow into jets
- Simulation roadmap
  - Validation of PM4 and PM4



Simulation Roadmap

Motivation

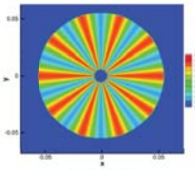
- Finding initial perturbations in PVF (non-uniformities) that are strongly amplified in simulations. This will be accomplished by a process of OPTIMIZATION
- Extracting data from simulations to QUANTIFY jet length and quantity. This would be needed at the initial stages of accomplishing goal 1

$$\boxed{\phi^p(\theta) = \phi_0^p\left[1 + A_1 cos(k_1\theta) + A_2 cos(k_2\theta + \Phi_{12}) + A_3 cos(k_3\theta + \Phi_{13})\right]}$$

PVF

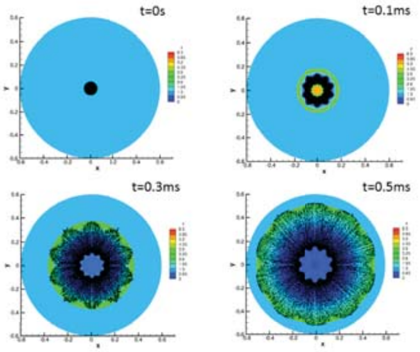
Base PVF

- The results presented here are calculated using $\varphi_0^p = 0.05, A_1 = 0.1\sqrt{2}, A_2 = A_3 = 0,$ $\Phi_{12} = 0, \Phi_{13} = 0,\ k_1 = 10, k_2 = 0$ and $k_3 = 0$



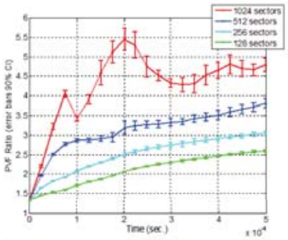
Initial PVF

Density Contours and Computational Particles



PVF Ratio as a Measure of Jet Formation

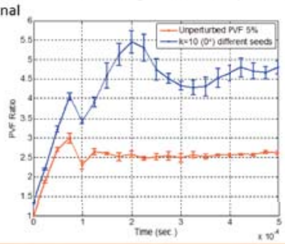
- PVF Ratio is the ratio of the highest PVF in any sector to the lowest one
- The figure shows that PVF Ratio is sensitive to the number of sectors chosen (1024 is the highest resolution possible for the current grid)
- Error bars represent 90 % CI calculated from 5 realizations, where particles were randomly distributed differently each time



Schematic of a sector

Noise Level

- The figure shows PVF Ratio as a function of time for the unperturbed case (uniform PVF) and the perturbed case (wavelength 10, amplitude $0.1\sqrt{2}$)
- Error bars represent 90 % CI calculated from 5 realizations where particles were randomly distributed differently each time
- With a 90% confidence we can distinguish between perturbed and unperturbed signal



Conclusions and Future Work

- Imposing a single mode perturbation in the PVF leads to an equivalent single mode rearrangement of particles at later times
- With a 90% CI we can clearly distinguish the PVF Ratio signal of the perturbed PVF case from the unperturbed PVF case
- Optimization will be carried out, where the design variables considered are the parameters of a three mode sinusoidal perturbation (amplitude, wavelength, and phase angle between modes)
- Initial experiments showed that we can start with an initial perturbation with a PVF Ratio of 1.3, and grow it to a PVF Ratio of 5
- The implementation of a multi-fidelity surrogate model will be considered to reduce the cost of the optimization process maintaining a desirable accuracy

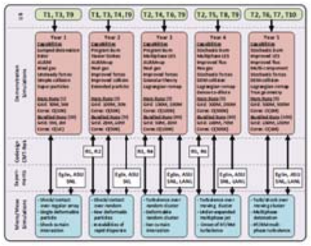
CCMT

Center for Compressible Multiphase Turbulence

Optimization of CMT-nek on CPUs/GPUs

Mohamed Gadou
Advisor: Prof. Sanjay Ranka
Department: CISE, UF

- Goals
  - Optimization of CMT-bone on hybrid architecture with multiple CPUs/GPUs
  - Performance/Energy modeling of CMT-bone on HMPs
  - Implementation of CMT-bone on Intel KNL
- Simulation roadmap
  - Our research roadmap is closely tied with CMT-nek development.

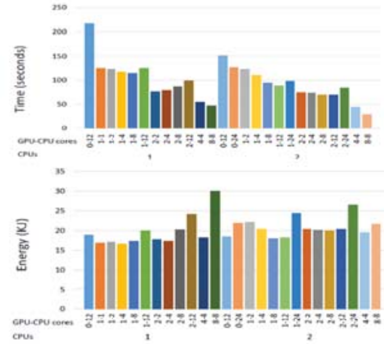


Simulation Roadmap

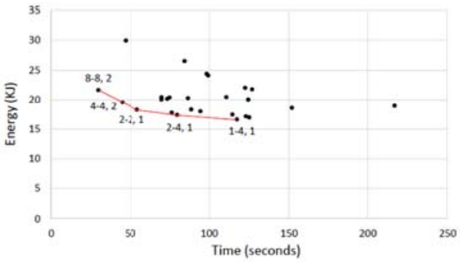
Motivation

- Implementation of load balancing techniques for dividing the work for multiple GPUs and a large number of CPU cores on multiple sockets
- Exploring a wide variety of architectural configurations consisting of a variable number of GPUs and CPU cores in terms of performance, energy and power requirements
- Create performance, power and energy models for CMT-bone on those architectures
- Implementation and Optimization of CMT-bone on Intel Knights Landing processors (KNL)

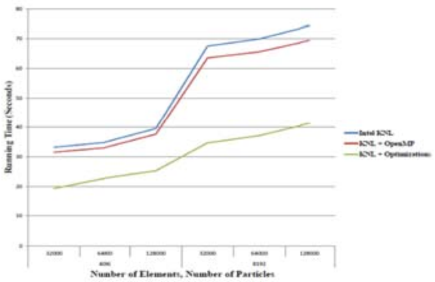
Energy and Performance on HMPs with GPUs



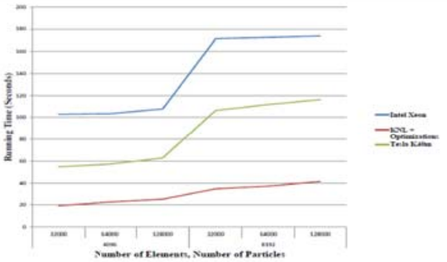
Performance Energy tradeoffs



CMT-bone performance on Intel KNL



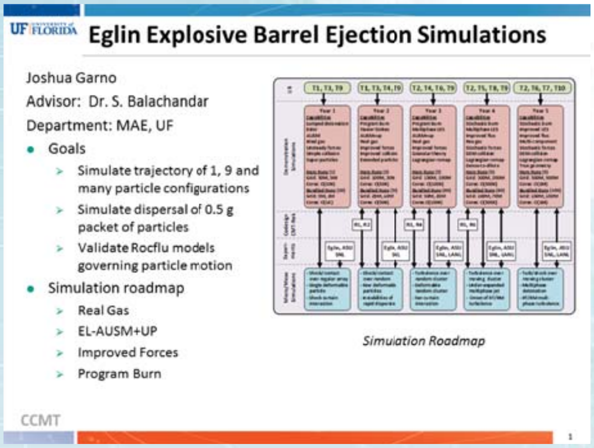
CMT-bone performance on Intel KNL



- Power Measurements for CMT-bone on Intel KNL
- Performance and Energy modeling on Intel KNL
- CMT-bone on Multiple Nodes for Intel KNL

CCMT

Center for Compressible Multiphase Turbulence



Eglin Explosive Barrel Ejection Simulations

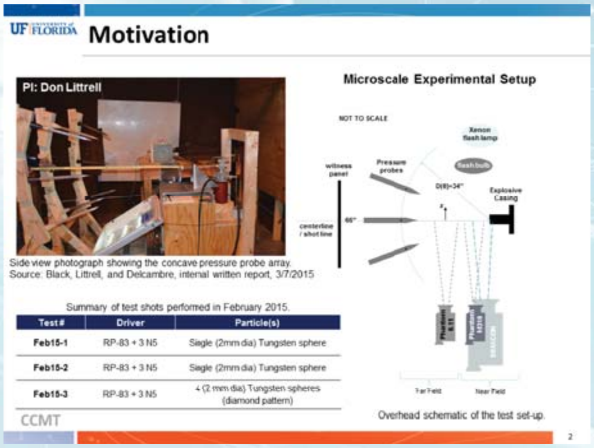
Joshua Garno

Advisor: Dr. S. Balachandar

Department: MAE, UF

- Goals
  - Simulate trajectory of 1, 9 and many particle configurations
  - Simulate dispersal of 0.5 g packet of particles
  - Validate Rocflu models governing particle motion
- Simulation roadmap
  - Real Gas
  - EL-AUSM+UP
  - Improved Forces
  - Program Burn

Simulation Roadmap



Motivation

PI: Don Littrell

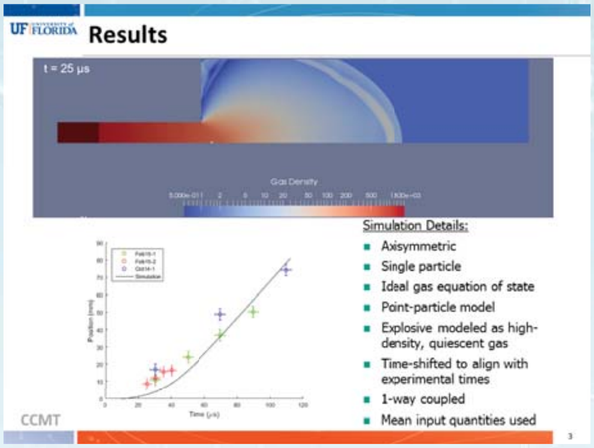
Side view photograph showing the concave pressure probe array.
Source: Black, Littrell, and Delcambre, internal written report, 3/7/2015

Summary of test shots performed in February 2015.

Test #	Driver	Particle(s)
Feb15-1	RP-83 + 3 N5	Single (2mm dia) Tungsten sphere
Feb15-2	RP-83 + 3 N5	Single (2mm dia) Tungsten sphere
Feb15-3	RP-83 + 3 N5	4 (2 mm dia) Tungsten spheres (diamond pattern)

Microscale Experimental Setup

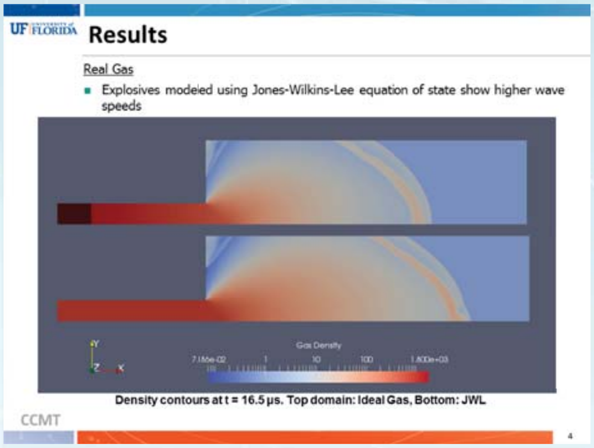
Overhead schematic of the test set-up.



Results

Simulation Details:

- Axisymmetric
- Single particle
- Ideal gas equation of state
- Point-particle model
- Explosive modeled as high-density, quiescent gas
- Time-shifted to align with experimental times
- 1-way coupled
- Mean input quantities used

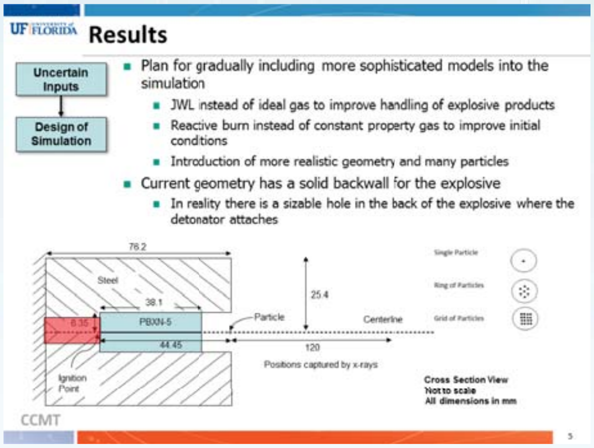


Results

Real Gas

- Explosives modeled using Jones-Wilkins-Lee equation of state show higher wave speeds

Density contours at t = 16.5 µs. Top domain: Ideal Gas, Bottom: JWL



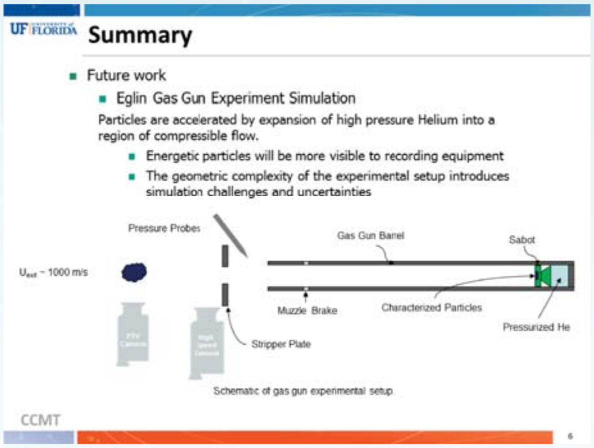
Results

Uncertain Inputs → **Design of Simulation**

- Plan for gradually including more sophisticated models into the simulation
  - JWL instead of ideal gas to improve handling of explosive products
  - Reactive burn instead of constant property gas to improve initial conditions
  - Introduction of more realistic geometry and many particles
- Current geometry has a solid backwall for the explosive
  - In reality there is a sizable hole in the back of the explosive where the detonator attaches

Positions captured by x-rays

Cross Section View
Not to scale
All dimensions in mm



Summary

- Future work
  - Eglin Gas Gun Experiment Simulation

  Particles are accelerated by expansion of high pressure Helium into a region of compressible flow.
    - Energetic particles will be more visible to recording equipment
    - The geometric complexity of the experimental setup introduces simulation challenges and uncertainties

Schematic of gas gun experimental setup.

CCMT

Center for Compressible Multiphase Turbulence

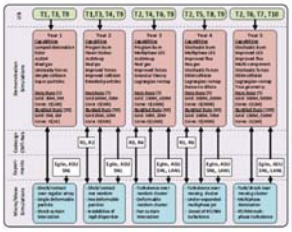
Support for Benchmarking & AppBEO Creation

Trokon Johnson

Advisors: Dr. Herman Lam, Dr. Greg Stitt

Department: ECE, UF

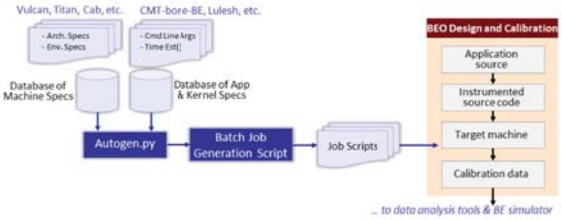
- Goals
  - Benchmarking automation
  - Benchmarking for CMT-nek DSE*
  - Formalize AppBEO creation process
- Simulation roadmap
  - Support for BE* in early DSE of CMT-nek code development
  - Automate & formalize process for BE



Simulation roadmap

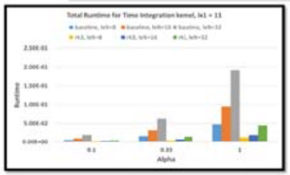
*DSE – Design Space Exploration
*BE – Behavioral Emulation

Benchmarking Automation

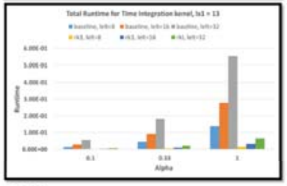


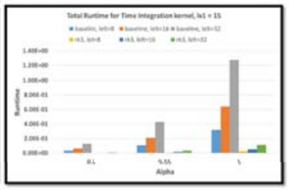
- Extended framework to simplify and automate benchmarking
  - Required for both calibration and validation data collection
  - Job scripts can be generated for different machine/app combinations
  - Easy to extend benchmarking to new applications & systems

Benchmarking for Interpolation DSE: Time Integration



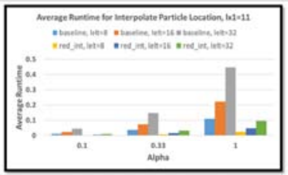
- Goal: Benchmark CMT-nek particle kernels to enable BE simulations for Algorithm DSE
  - Titan:
    - Cray XK7 architecture
    - Cray Gemini interconnect
    - 16-core AMD opterons; 18k nodes;
    - 1 K20X Kepler GPUs/Node (not used)
    - 32GB + 6GB memory/node

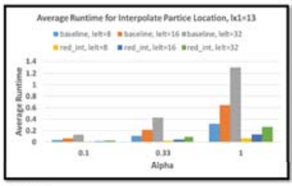


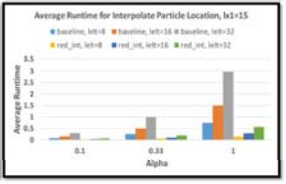


Benchmarking for Interpolation DSE: Interpolation

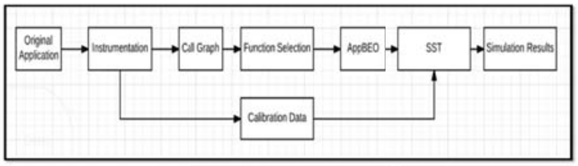
- Application parameters:
  - lx1: element size
  - lelt: elements per processor
  - alpha: # of particles/gridpoint
  - Average Runtime: average runtime for kernel across 100 timesteps







AppBEO Process Documentation



- Streamline process for creating AppBEO from existing programs
  - More easily add additional applications
  - Expedite process BEO generation for BE-SST
  - Facilitates DSE

```
subroutine usr_particles_init

...

call rzero(rpart,lr*lpart)
call izero(ipart,li*lpart)
call set_part_pointers
call init_interpolation(red_interp)
call place_particles
call move_particles_inproc
if (two_way.eq.1) then
   call compute_neighbor_el_proc
   call particles_solver_nearest_neighbor(bc_part)
endif

return
end
```

Original Application

```
#usr_particles_init()(
    call(cpu,rzero,lpart)
    call(cpu,izero,lpart)
    call(cpu,set_bounds_box,nelt,lx1)
    call(cpu,set_part_pointers)
    call(cpu,init_interpolation,lx1)
    call(cpu,place_particles,n)

    #move_particles_inproc routine starts(
        icalld1 = 0

        IF (icalld1 == 0)
        {
                call(?,intpts_setup,?)
                call(?,crystal_setup,?)
                icalld1 = icalld1 + 1
        }

        call(cpu,particles_in_nid,n,nelt)
        call(cpu,findpts,n)
        call(cpu,update_findpts_info)
        call(cpu,ComputeC,n)
        call(comm,crystal_tuple_transfer)
        call(cpu,crystal_tuple_sort,n)
    )#End move_particles_inproc
)#End usr_particles_init
```

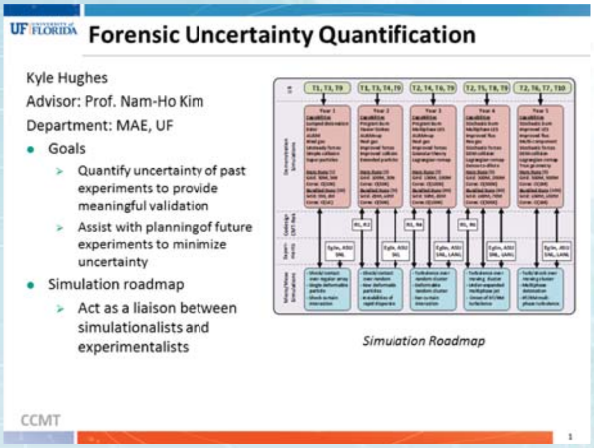
AppBEO

Future Work

- Translation from application to AppBEO
  - Auto-translate using intermediate representation
  - Further improve process of making AppBEO
- Expand DSE with additional alternative algorithms
  - Using automated tools to profile applications
    - E. g. ScoreP, Allinea, ...
  - Identify potential bottlenecks using multi-parameter modeling
  - Explore on other metrics, in addition to runtime
    - Complexity, accuracy

CCMT

Center for Compressible Multiphase Turbulence

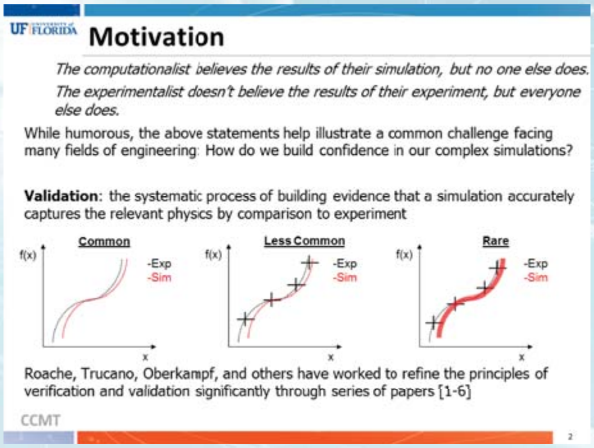


Forensic Uncertainty Quantification

Kyle Hughes
Advisor: Prof. Nam-Ho Kim
Department: MAE, UF

- Goals
  - Quantify uncertainty of past experiments to provide meaningful validation
  - Assist with planningof future experiments to minimize uncertainty
- Simulation roadmap
  - Act as a liaison between simulationalists and experimentalists

Simulation Roadmap



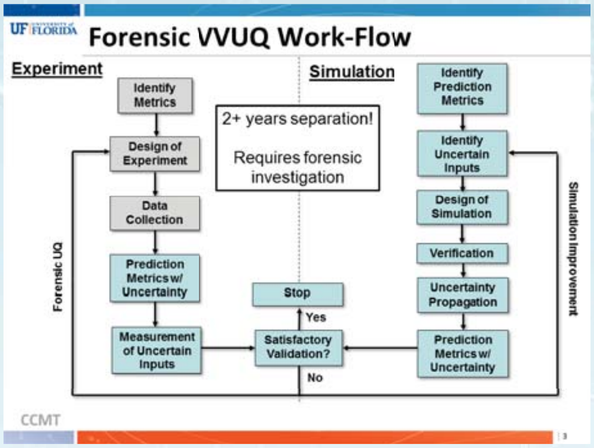
Motivation

The computationalist believes the results of their simulation, but no one else does. The experimentalist doesn't believe the results of their experiment, but everyone else does.

While humorous, the above statements help illustrate a common challenge facing many fields of engineering: How do we build confidence in our complex simulations?

Validation: the systematic process of building evidence that a simulation accurately captures the relevant physics by comparison to experiment

Roache, Trucano, Oberkampf, and others have worked to refine the principles of verification and validation significantly through series of papers [1-6]



Forensic VVUQ Work-Flow

Experiment

Identify Metrics
Design of Experiment
Data Collection
Prediction Metrics w/ Uncertainty
Measurement of Uncertain Inputs

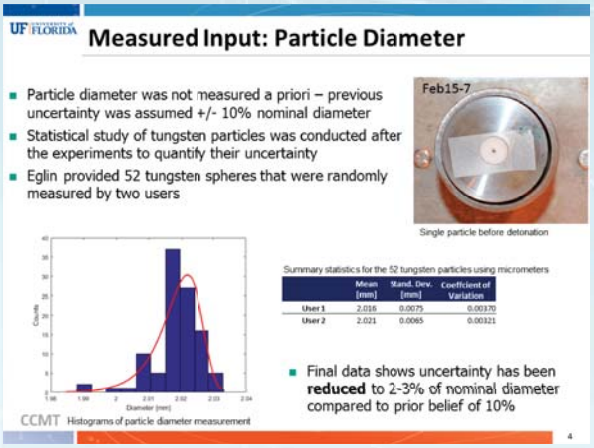
Simulation

Identify Prediction Metrics
Identify Uncertain Inputs
Design of Simulation
Verification
Uncertainty Propagation
Prediction Metrics w/ Uncertainty

2+ years separation!

Requires forensic investigation

Satisfactory Validation?
Yes
Stop
No



Measured Input: Particle Diameter

- Particle diameter was not measured a priori – previous 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

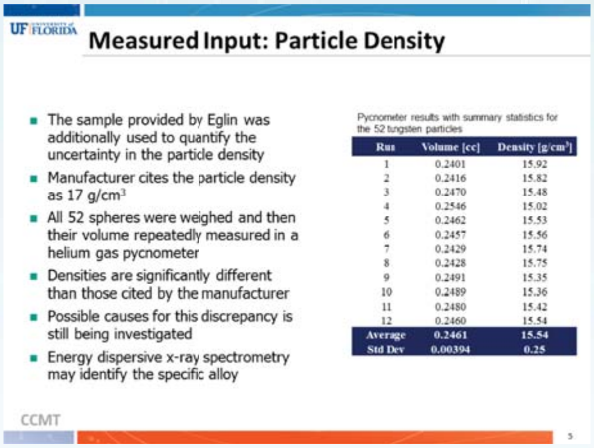
Single particle before detonation

Histograms of particle diameter measurement

Summary statistics for the 52 tungsten particles using micrometers

	Mean [mm]	Stand. Dev. [mm]	Coefficient of Variation
User 1	2.016	0.0075	0.00370
User 2	2.021	0.0065	0.00321

- Final data shows uncertainty has been **reduced** to 2-3% of nominal diameter compared to prior belief of 10%

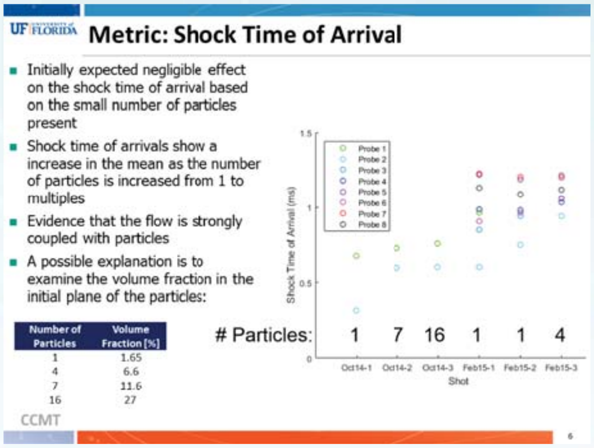


Measured Input: Particle Density

- 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 is 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 [cc]	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



Metric: 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

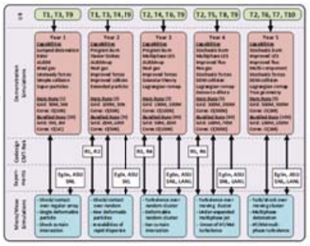
CCMT

Center for Compressible Multiphase Turbulence

Compressible Multiphase Turbulence Modeling

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

- Goals
  - Develop multiphase compressible LES model
  - Improved force modeling
  - Validation and integration into Rocflu and CMT-nek
- Simulation roadmap
  - Implement single phase LES and extend it to multiphase flows
  - Validate existing force-models and develop new models in collaboration with microscale team
  - Perform mesoscale simulations

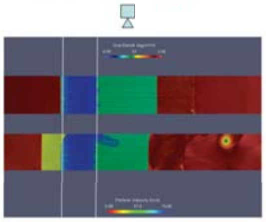


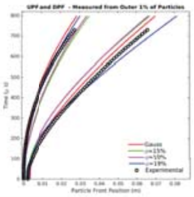
Simulation Roadmap

Point-Particle Model Validation

- Validation against experiments (Sandia MST)
- Effect of gap and initial particle curtain profile has been studied

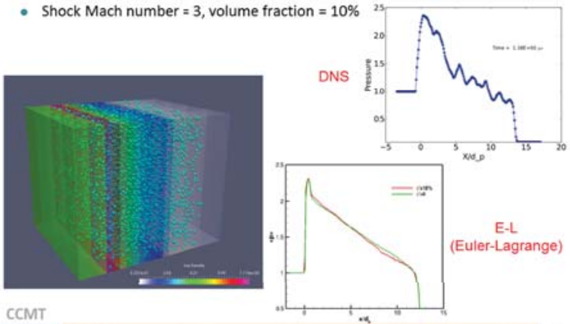
Simulations (M = 1.66)	Particle Volume Fraction (%)	Curtain thickness (mm)
Run 1	10	3.1
Run 2	15	2
Run 3	Distribution	3.4
Run 4	19	2





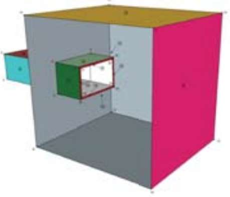
Point-Particle Model Validation

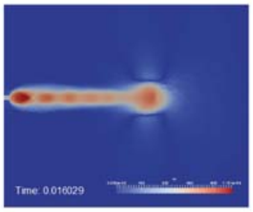
- Validation against numerical simulations (Random bed of particles)
- Mean flow quantities from E-L simulations are compared against DNS data
- Shock Mach number = 3, volume fraction = 10%



Multiphase LES

- Performed simulations of single phase open-ended shocktube[1]
- Integrated single-phase *LES* models in Rocflu
- Code verification and validation is in progress

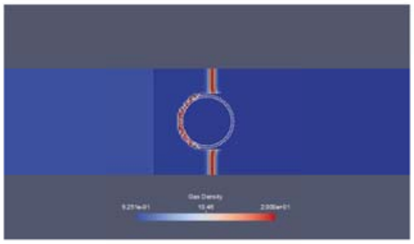




[1] *'Open-Ended Shock Tube Flows: Influence of Pressure Ratio and Diaphragm Position'*, A.Haselbacher, S. Balachandar and S. W. Keifer, AIAA Journal

Immersed Boundary

- Immersed boundary capability is being implemented in Rocflu
- A snapshot from the test simulation at shock Mach number = 3 is shown below



1. Uhlmann, Markus. "An immersed boundary method with direct forcing for the simulation of particulate flows." Journal of Computational Physics 209.2 (2005): 448-476.

Summary & Future Work

Summary

- Numerical simulations have been performed to validate point-particle models against experimental and numerical (DNS) data
- Work is in progress to validate single-phase *LES* models implemented in the code
- Preliminary immersed boundary (IB) capability has been added to Rocflu

Future Work

- Extend the single phase *LES* models to simulate multiphase flows
- Study influence of grid-refinement and volume fraction fluctuations on flow statistics in Euler-Lagrange simulations
- Validate and fine-tune IB implementation

CCMT

Center for Compressible Multiphase Turbulence

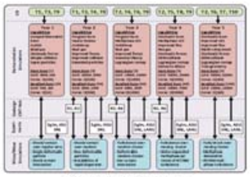
Improving Accuracy and Scalability of Behavioral Emulation (BE) Methodology

Student: Nalini Kumar

Advisors: Dr. Herman Lam, Dr. Greg Stitt

Department: ECE, UF

- Goals
  - Apply BE methodology, demonstrated for device and system simulations, to simulation of large-scale systems
  - Design & validate simulation models of existing machine architectures
  - Improve communication modeling in BE



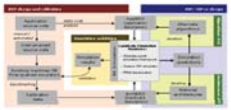
Simulation Roadmap

- Simulation roadmap
  - Design and evaluate BE simulation framework which will enable early design-space exploration to aid and assist CMT-nek code developers

Motivation and Guiding Principles of BE

- Allow performance analysis at different levels of system organization (device, node, rack, machine) – *Multi-scale simulation*
- Allow use of performance models agnostic of how they were developed (testbed, fine-grained simulations, analytical models etc.) – *Component-based simulation*
- Allow arch DSE by providing ability to build notional archs by plugging different components in the simulation – *Component-based simulation*
- Allow fast algorithm DSE by simulation from high-level scripts, and not requiring working code – *Coarse-grained simulation*
- Allow reasonably accurate performance analysis within a reasonable time – *Coarse-grained simulation*

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



Improved AppBEO and ProcBEO Models

- CMT-bone-BE captures computation- & communication-intensive portions of CMT-nek workflow in C & MPI
  - Derivative computation, volume-to-surface data extraction, face data exchange (with neighbors)
- Improved CMT-bone-BE model by adding additional instructions to AppBEO for the following functions:
  - Communication initialization for neighbor face-data exchange
  - Buffer creation with face data that needs to be transported
  - Buffer cleanup
- Improved calibration of ProcBEO models for existing machines by replacing microkernel benchmarking with in-situ benchmarking
  - In-situ methods are more accurate but microkernel benchmarking is important for algorithmic design-space exploration

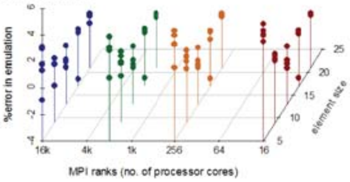
Improved Network Models

- Earlier version (TST 2016) of BE simulator supported only static routing
  - Reduces simulator scalability
  - Poor network modeling (can't model adaptive routing techniques)
- Improved network model to dynamically generate communication information for each communication event
  - Calculate path of packet at each intermediate node of the network
  - Can be used to model network congestion
  - Also improves scalability of the BE-SST simulator
- Also updated network modeling with
  - Cable delay model,
  - Separate software and hardware latency models,
  - Network setup overhead model, and
  - Utilizable bandwidth as a function of message size model

Validating BE Simulations of Vulcan

- Application case study: CMT-bone-BE (gas solver)
  - Element size: 5, 8,13,17, 21
  - Elements/core: 8, 32, 64, 128, 256
  - MPI ranks: 16, 256, 2k, 16k
- Vulcan @ LLNL
  - IBM BG/Q with 16 cores/node and 16GB memory/node
  - 24k nodes, and 390k cores in a 5d-torus

- With application of in-situ methods and improved ProcBEO and CommBEO models, ~5% error is observed in BE simulations



Summary

Conclusions

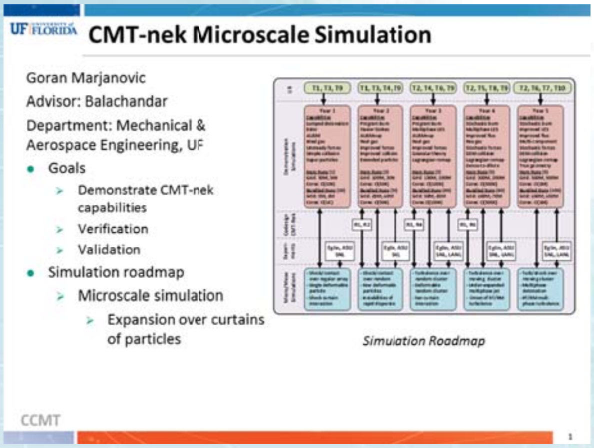
- Improved CMT-bone-BE application models by adding more parts of application to simulation models
- Improved BE ProcBEO and CommBEO models to greatly improve simulation accuracy (~5% error) and simulator scalability
- Validated simulations of system with ~20k nodes

Future Work

- Evaluate feasibility of using together models calibrated with data obtained from microkernel and in-situ instrumentation
- Add models for adaptive routing to further improve network modeling

CCMT

Center for Compressible Multiphase Turbulence



CMT-nek Microscale Simulation

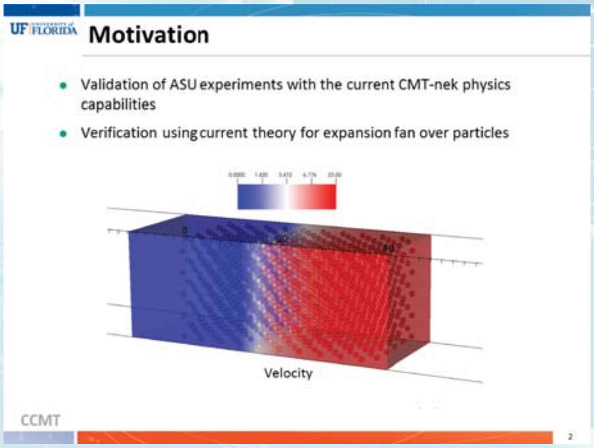
Goran Marjanovic

Advisor: Balachandar

Department: Mechanical & Aerospace Engineering, UF

- Goals
  - Demonstrate CMT-nek capabilities
  - Verification
  - Validation
- Simulation roadmap
  - Microscale simulation
    - Expansion over curtains of particles

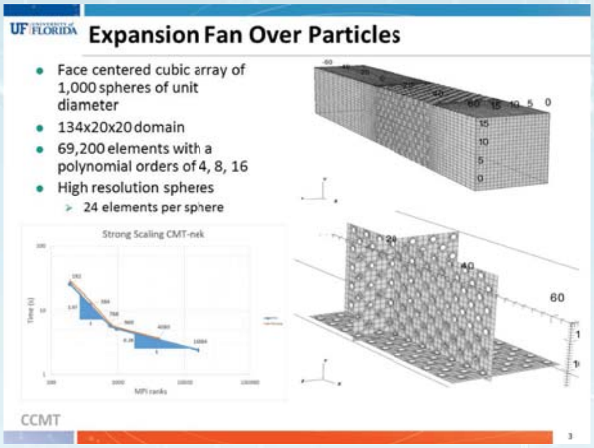
Simulation Roadmap



Motivation

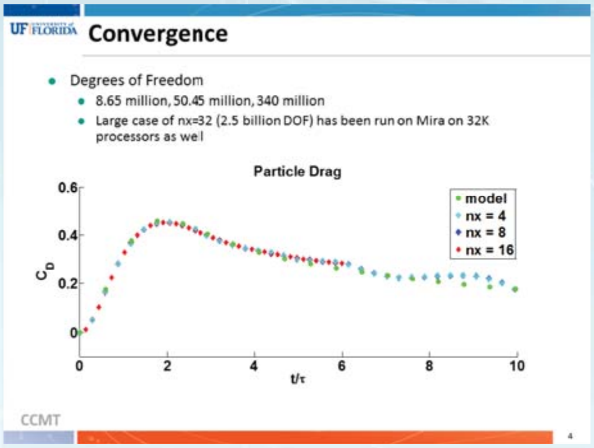
- Validation of ASU experiments with the current CMT-nek physics capabilities
- Verification using current theory for expansion fan over particles

Velocity



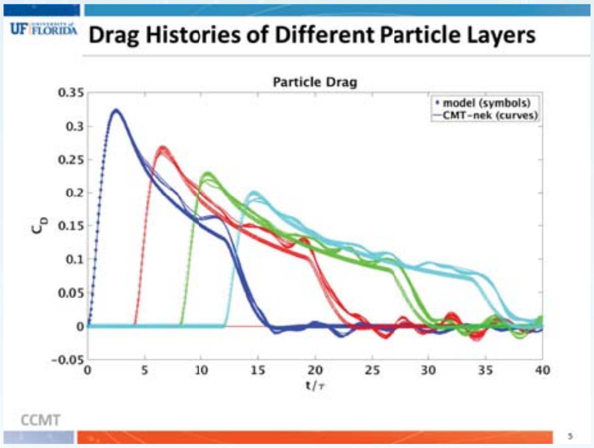
Expansion Fan Over Particles

- Face centered cubic array of 1,000 spheres of unit diameter
- 134x20x20 domain
- 69,200 elements with a polynomial orders of 4, 8, 16
- High resolution spheres
  - 24 elements per sphere



Convergence

- Degrees of Freedom
  - 8.65 million, 50.45 million, 340 million
  - Large case of nx=32 (2.5 billion DOF) has been run on Mira on 32K processors as well



Drag Histories of Different Particle Layers

Future Goals

- Extend microscale runs to upcoming CMT-nek code
  - Navier-Stokes solver
  - Shock capturing capabilities
- Validate SNL shock tube particle curtain experiments
- Verify analytical results of shock waves over particles

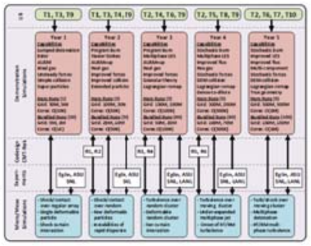
CCMT

Center for Compressible Multiphase Turbulence

Uncertainty Quantification of Shock Tubes

Justin Mathew
Advisor: Prof. Kim and Prof. Haftka
Department: Mechanical Engineering, UF

- Goals
  - Reproduce measurement processing from Sandia and ASU shock tubes to identify sources of uncertainty
  - Propagate identified sources of uncertainty from experiments into simulations
- Simulation roadmap
  - T2: Multiphase turbulence modeling and uncertainty
  - T4: Validation, UQ and UR of the shock tube simulation

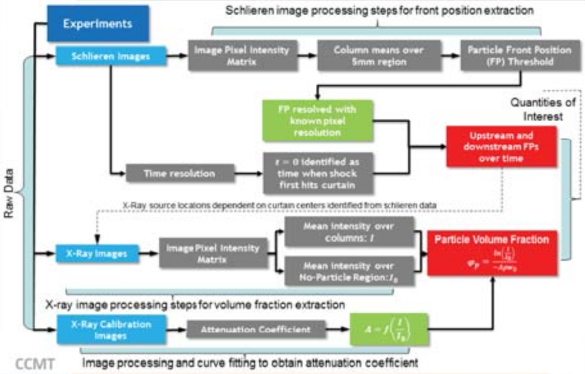


Simulation Roadmap

Motivation

- The study of measurement processes in shock tube experiments allows for uncertainty analysis of quantities of interest to be used in validating simulation code.
- Two experiments have predominantly been studied:
  - Vertical shock tube experiments at ASU conducted by Heather Zunino are studied to characterize input and output parameters used to validate turbulence models developed by the simulation team.
  - Horizontal shock tube experiments conducted by Justin Wagner with the multiphase shock tube (MST) at Sandia National Laboratory are studied to identify and understand uncertainty sources in the experiments and their effects on simulation results.
- Understanding measurement process uncertainties and relaying information to simulation tests provides a two-fold benefit:
  - Identification of which experimental uncertainties are significant for simulation purposes in terms of matching measured quantities of interests.
  - Further uncertainty quantification to reduce measurement processing uncertainties which lead to smaller simulation uncertainties

Sandia MST - Image Processing



Schlieren image processing steps for front position extraction

Experiments

Raw Data

Schlieren Images → Image Pixel Intensity Matrix → Column means over 5mm region → Particle Front Position (FP) Threshold

FP resolved with known pixel resolution

Time resolution → $t = 0$ identified as time when shock first hits curtain

Upstream and downstream FPs over time

Quantities of Interest

X-Ray source locations dependent on curtain centers identified from schlieren data

X-Ray Images → Image Pixel Intensity Matrix → Mean intensity over columns: I; Mean intensity over No-Particle Region: I_0

Particle Volume Fraction $\varphi_p = \frac{\ln\left(\frac{I}{I_0}\right)}{-A\rho w_3}$

X-ray image processing steps for volume fraction extraction

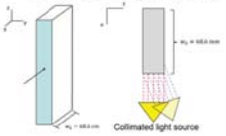
X-Ray Calibration Images → Attenuation Coefficient → $A = f\left(\frac{I}{I_0}\right)$

Image processing and curve fitting to obtain attenuation coefficient

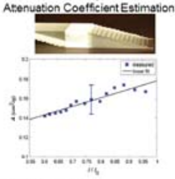
Experimental Uncertainties from Sandia MST

- Measurement processing uncertainties are the major source of uncertainty in extracting front positions and particle volume fractions from schlieren and X-ray experiments.
- Variation in schlieren imaging set up is identified as the key source of uncertainty affecting the front positions
  - A one degree misalignment is estimated to cause up to 1.2 mm of error in edge position.
- Uncertainty associated with estimation of attenuation coefficient from calibration experiments is found to be the major source of uncertainty in calculation of particle volume fraction

Particle Curtain Edge Uncertainty



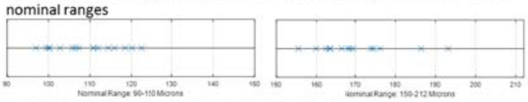
Calibration Experiment for Attenuation Coefficient Estimation*

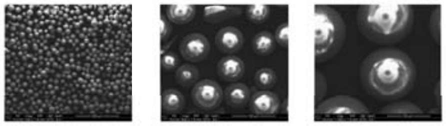


* Wagner JL, Kearney SP, Beresh SJ, DeMauro, EP, Pruett BO (2015) Flash X-ray measurements on the shock-induced dispersal of a dense particle curtain. Exp Fluids 52:213

ASU Shock Tube Particle Characterization

- 4 samples of particles with nominal diameter ranges: 45-90 microns, 90-150 microns, 150-212 microns, 211-297 microns
- Pycnometer estimates of particle density averaged $2.46\frac{g}{cm^3}$ for all particles with very low uncertainty. This is slightly lower than nominal $2.5\frac{g}{cm^3}$ for glass.
- SEM image processing shows particle diameters tending to the lower end of nominal ranges





Summary and Future Work

Sandia

- The study of the MST characterized image processing methods for quantities of interest and identified major contributing sources of uncertainty.
- Future work:
  - Additional 1D simulation runs to determine response to identified uncertainties
  - Consideration for 2D simulations by accounting for variation of quantities of interest through the vertical direction

ASU

- Preliminary particle characterization of ASU experiments have supplemented early simulation development.
- Future work:
  - Expansion of ASU particle characterization to consider volume fraction uncertainties using a CT scan of mock particle bed
  - Preliminary uncertainty analysis will begin for proposed image processing techniques to obtain quantities of interest from new experiments.

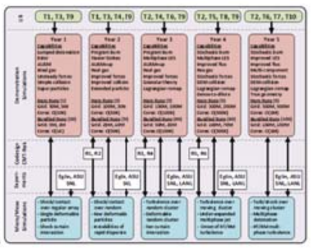
CCMT

Center for Compressible Multiphase Turbulence

Microscale – Shock Particle Interaction

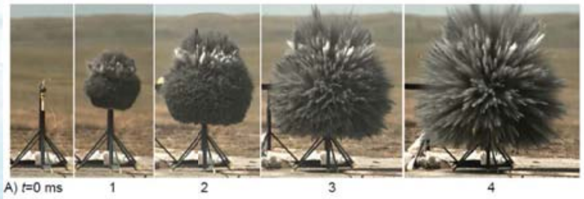
Yash Mehta
Advisor: Prof. S. Balachandar
Department: MAE, UF

- Goals
  - Fully resolved DNS of shock interaction with particles
  - Developing models for predicting particle motion and force history
- Simulation roadmap
  - Simulating shock interaction with random bed of particles (Inviscid and Viscous)
  - Integration of force models in Meso-Macro scale simulations



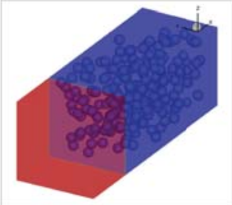
Simulation Roadmap

Motivation



- There is a need for understanding the interaction of high energy post detonation products with the particles
- Fully resolved Direct Numerical Simulations are used to obtain force history on particles and understanding the underlying physical phenomena during shock particle interaction
- Results from DNS are used to develop models for predicting the motion of particles in complex flows

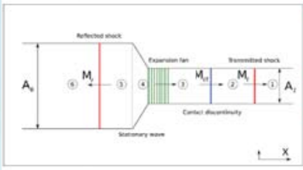
Shock Interaction with Random Bed of Particles



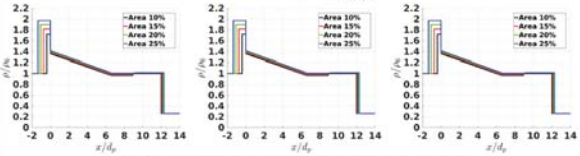
	$M_s = 1.22$	$M_s = 1.66$	$M_s = 3.00$
$\varphi = 1.25\%$	RUN1	RUN2	RUN3
$\varphi = 10\%$	RUN4	RUN5	RUN6
$\varphi = 15\%$			RUN7
$\varphi = 20\%$	RUN8	RUN9	RUN10
$\varphi = 25\%$			RUN11

- Matrix of simulations were performed to understand the effect of shock Mach number and volume fraction
- Number of particles in the computational domain varied from 200 to 500
- Effect of viscosity and particle motion was neglected in these simulations

1-D Riemann Model

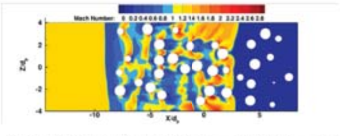


- Shock interaction with bed of particles can be modeled as shock interaction with an area change
- This is a standard Riemann problem with an area change
- Shock interaction with an area change leads to a unique solution with multiple different family of waves

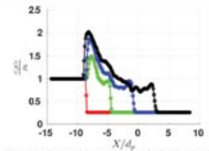


Flow properties predicted using 1-D Riemann model

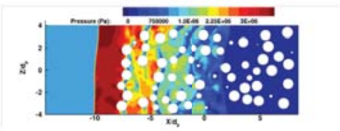
Flow Properties



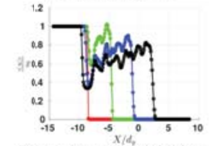
Mach number contour plot for $\varphi = 10\%$; $M_s = 3.0$; $t/\tau = 12$



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



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



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

Comparing 1-D Theory and Averaged Numerical Simulation Results

ϕ_1	M_r	$u_r(m/s)$	M_t	P_5/P_6	ρ_5/ρ_6	u_5/u_6	P_4/P_6	ρ_4/ρ_6	u_4/u_6	P_2/P_6	ρ_2/ρ_6	u_2/u_6	ρ_2/ρ_3
10%	1.41	-33	3.00	2.178	1.721	0.562	1.567	1.359	0.791	1.000	1.000	1.000	1.014
15%	1.47	-64	3.03	2.365	1.816	0.513	1.606	1.377	0.795	1.020	1.007	1.012	1.019
20%	1.52	-91	3.05	2.529	1.896	0.471	1.645	1.395	0.799	1.035	1.012	1.021	1.009
25%	1.56	-115	3.07	2.687	1.971	0.432	1.687	1.414	0.805	1.047	1.016	1.029	1.011

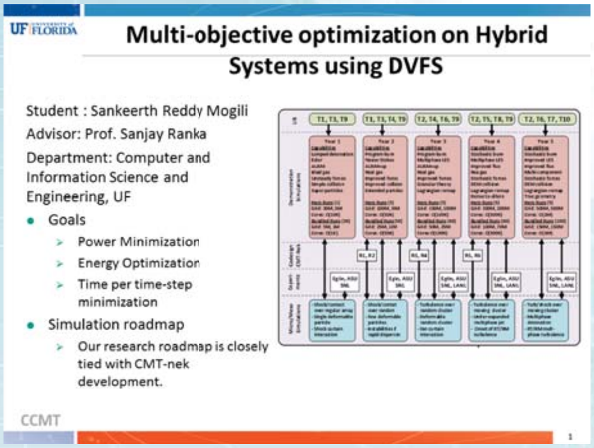
Table summarizing flow properties obtained from 1-D model for $M_s = 3.0$; $t/\tau = 12$

ϕ_1	M_r	M_t	P_5/P_6	ρ_5/ρ_6	u_5/u_6	P_4/P_6	ρ_4/ρ_6	u_4/u_6	P_2/P_6	ρ_2/ρ_6	u_2/u_6
10%	1.41	2.75	2.174	1.699	0.582	1.879	1.473	0.646	0.874	0.921	0.881
15%	1.59	2.64	2.778	2.016	0.412	1.811	1.379	0.659	0.799	0.880	0.822
20%	1.67	2.43	3.101	2.160	0.339	2.186	1.665	0.633	0.718	0.805	0.789
25%	1.72	2.34	3.277	2.229	0.304	2.216	1.606	0.562	0.678	0.761	0.751

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

CCMT

Center for Compressible Multiphase Turbulence



Multi-objective optimization on Hybrid Systems using DVFS

Student : Sankeerth Reddy Mogili

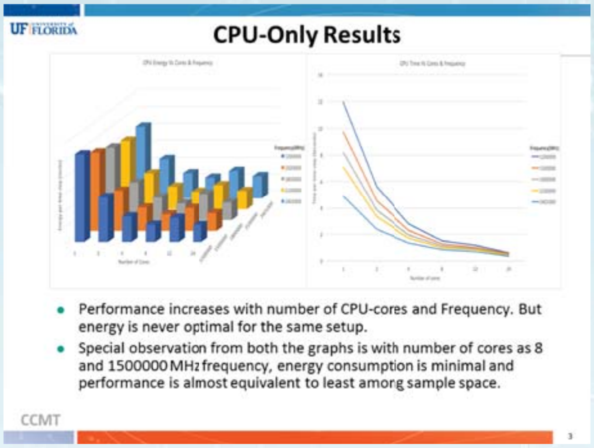
Advisor: Prof. Sanjay Ranka

Department: Computer and Information Science and Engineering, UF

- Goals
  - Power Minimization
  - Energy Optimization
  - Time per time-step minimization
- Simulation roadmap
  - Our research roadmap is closely tied with CMT-nek development.

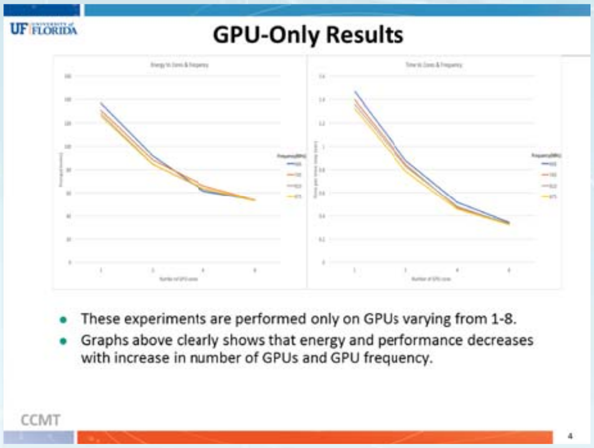
Motivation

- Experimental Setup :
  - Dual 12-core Intel© Xeon© CPU E5-2695 v2 @ 2.40GHz (2 threads per core) processors.
  - 8 NVIDIA© Tesla© K40m, 2880 cores each, providing a total of 23040 GPU cores.
  - Operating System: CentOS 6
  - Software: CUDA, MATLAB, AMPL, and other mathematical modeling packages.
- To cope with the growing concern for minimizing power consumption in HPC systems, most modern processors and co-processors are equipped with DVFS mechanisms.
- We present power-performance and energy-performance trade-off on hybrid(CPU + GPU) systems using proxy application.
- Our study can be used to find the optimal experimental configuration which includes number of CPU cores, number of GPU cores, CPU frequency, GPU frequency and GPU load distribution to minimize power, energy and execution time.



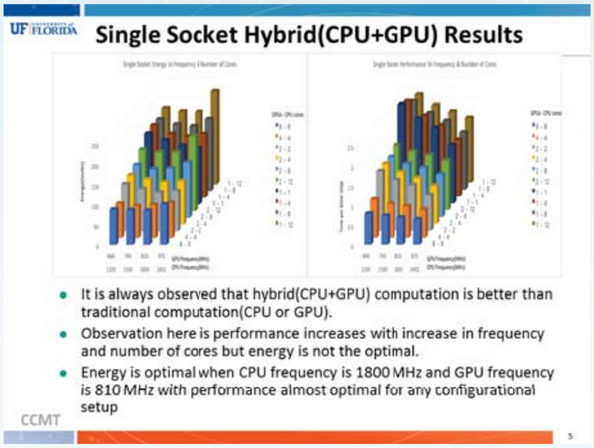
CPU-Only Results

- Performance increases with number of CPU-cores and Frequency. But energy is never optimal for the same setup.
- Special observation from both the graphs is with number of cores as 8 and 1500000 MHz frequency, energy consumption is minimal and performance is almost equivalent to least among sample space.



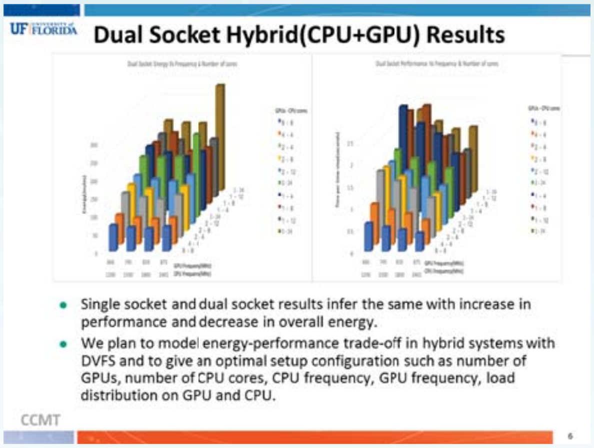
GPU-Only Results

- These experiments are performed only on GPUs varying from 1-8.
- Graphs above clearly shows that energy and performance decreases with increase in number of GPUs and GPU frequency.



Single Socket Hybrid(CPU+GPU) Results

- It is always observed that hybrid(CPU+GPU) computation is better than traditional computation(CPU or GPU).
- Observation here is performance increases with increase in frequency and number of cores but energy is not the optimal.
- Energy is optimal when CPU frequency is 1800 MHz and GPU frequency is 810 MHz with performance almost optimal for any configurational setup



Dual Socket Hybrid(CPU+GPU) Results

- Single socket and dual socket results infer the same with increase in performance and decrease in overall energy.
- We plan to model energy-performance trade-off in hybrid systems with DVFS and to give an optimal setup configuration such as number of GPUs, number of CPU cores, CPU frequency, GPU frequency, load distribution on GPU and CPU.

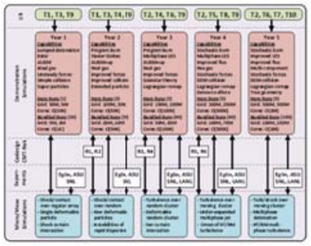
CCMT

Center for Compressible Multiphase Turbulence

Behavioral Emulation (BE) Models

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

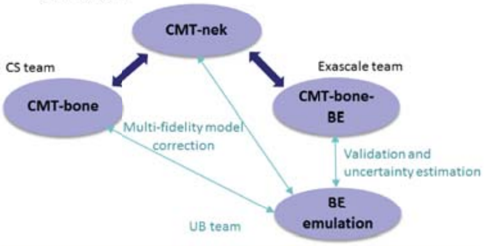
- Goals
  - Validation and uncertainty estimation of BE
  - Reduce computation budget of CMT-nek (with UB team)
  - Verify trend among CMT-nek, CMT-bone, and CMT-bone-BE
- Simulation roadmap
  - BE helps in simulating CMT-nek on exascale systems (notional architectures)



Simulation Roadmap

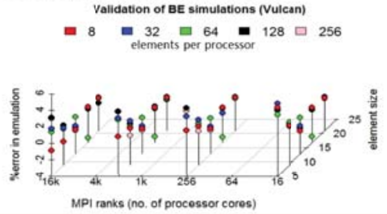
Assessing Behavioral Emulation

- Motivation
  - Improve BE models via validation and uncertainty estimation
  - Reduce computational budget by fitting BE emulation to CMT-nek using Multi-Fidelity Surrogate (MFS)
  - Compare and verify trends among CMT-nek, CMT-bone, and CMT-bone-BE



Validation of BE simulation on Vulcan

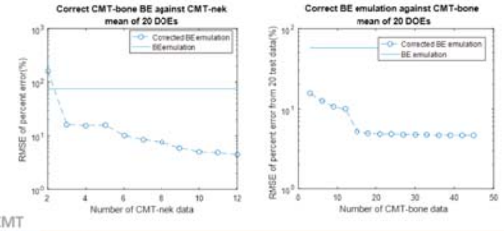
- Design of experiment
  - Element size (ES) = 5,9,13,17,21
  - Elements per processor (EPP) = 8,32,64,128,256
  - Number of processors (NP) = 16,256,2048,16384
- Calibration data obtained through in-situ benchmarking
- Observation
  - % error in emulation varies between -3% to 5%



Corrected BE against CMT-nek & CMT-bone

w/ UB

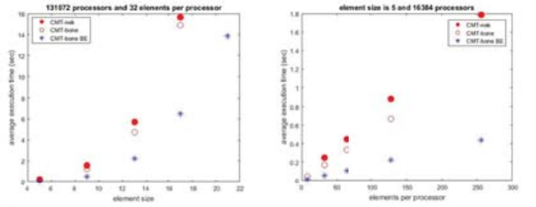
- Accuracy of corrected BE emulation at 10 left-out nek test points (left figure)
  - Overall error (RMSE) is less than 10% with 7 or more nek data
  - Max error is less than 20% (at the 10 test points) with 9 or more nek data
- Accuracy of corrected BE emulation at 20 left-out bone test points (right figure)
  - Overall error (RMSE) is less than 5% with 15 or more bone data
  - Max error is less than 10% (at the 20 test points) with 17 or more bone data



Trends of CMT-nek, bone and bone-BE

w/ UB

- Experimental setup
  - Varying ES with fixed EPP=32 and NP=131072 (left figure)
  - Varying EPP with fixed ES=5 and NP=16384 (right figure)
- Observation
  - Similar trends across three applications – polynomial (left) and linear (right)
  - CMT-bone-BE has different slope – captures only spectral element solver kernel of nek/bone



Summary

- Validation of BE simulation
  - Less than 5% error between CMT-bone-BE and BE emulation – good models
- Multi-fidelity surrogate
  - MFS can be used to fit BE emulation data to CMT-nek and CMT-bone with very few points, thus saving computational budget
- Similarity in trend line
  - Trend lines among CMT-nek, CMT-bone and CMT-bone-BE have been verified to be similar

FUTURE WORK

- Compare and analyze in-situ and micro-kernel benchmarking
- Memory modeling using SST
  - Multi-Level Memory (MLM)
  - Simulate CMT-bone on KNL using SST for performance measure of MLM

CCMT

Center for Compressible Multiphase Turbulence

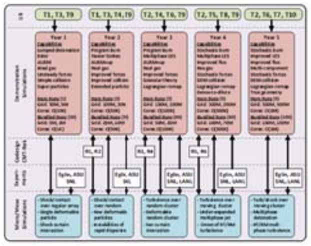
Eulerian-Lagrangian Interphase Coupling UQ and UR

Student: Sam Nili

Advisor: Prof. Kim, Haftka & Balachandar

Department: MAE, UF

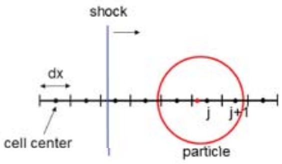
- Goals
  - Identify and quantify potential errors for numerical force models of Eulerian-Lagrangian multi-phase dispersed
  - Reduce the errors by model improvement
- Simulation roadmap
  - T4: Verification and validation of the shock tube simulation
  - Uncertainty reduction via model improvement



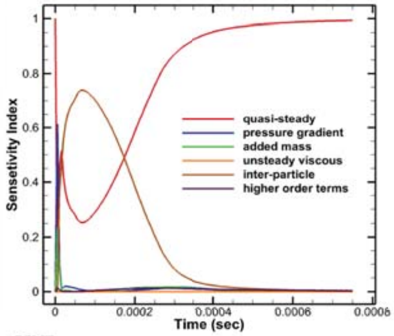
Simulation Roadmap

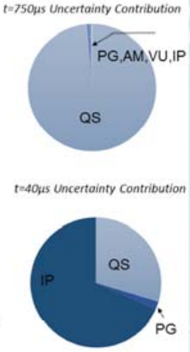
Motivation

- Particle force models are candidates for model improvement.
- Uncertainty Quantification (UQ): Separate and rank the contribution of individual potential model error using global sensitivity analysis (GSA)
- Uncertainty Reduction (UR): Allocate the resources to reduce a known error contributor that prevents convergence by improving the models and their numerical implementation
- Challenge: The main assumption of point particle model is smaller particle size compared to grid size
- Finite particle size prevents force convergence
- Solution: Compute the average gas quantities at the particle location to obtain the forces



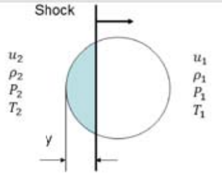
GSA of Upstream Front Particle Position (Shock Tube Simulation)

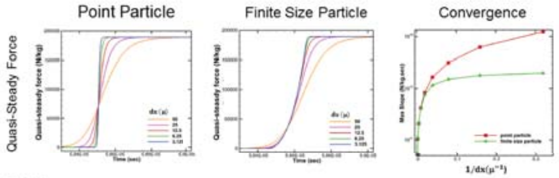




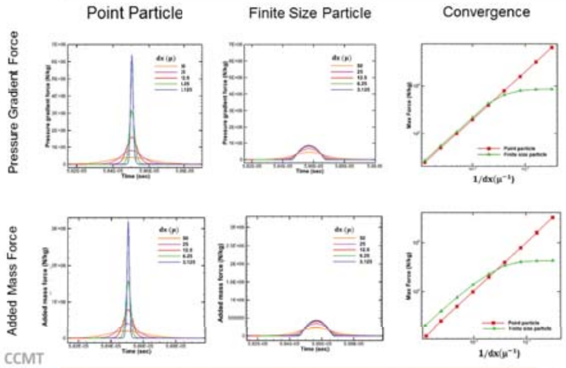
Computing Forces Using Averaged Gas Quantities

- Single particle shock interaction
- 1-Way coupling
- Stationary particle
- Particle diameter = 115 μ
- Grid size range : 800 μ to 3.125 μ





Computing Forces Using Averaged Gas Quantities



Summary

Global Sensitivity Analysis

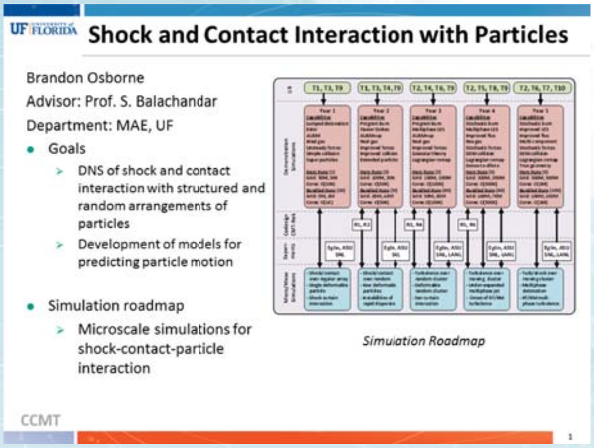
- Error in quasi-steady force likely dominates error at later time
- Effect of inter-particle force decreases as shock develops
- Coupling between errors is negligible

Interphase Convergence

- For the quasi-steady force, the slope was converged to a finite value with the finite particle method
- For the pressure gradient and added mass force, the maximum force was converged by grid refinement
- Upgrading point particle to finite size particle and grid refinement do not change the impulse of pressure gradient and added mass force. Hence, we *cannot* characterize the finite particle size as the largest contributor to error.

CCMT

Center for Compressible Multiphase Turbulence

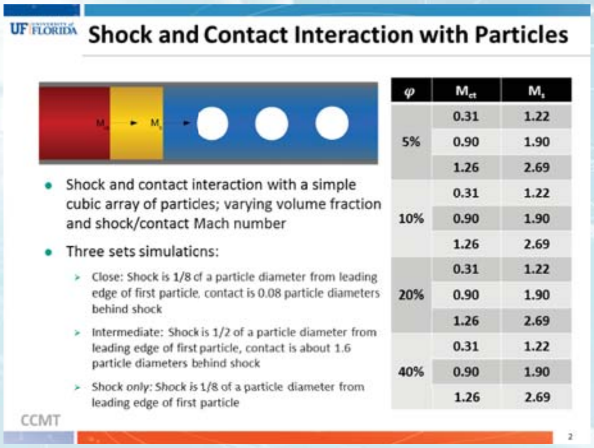


Shock and Contact Interaction with Particles

Brandon Osborne
Advisor: Prof. S. Balachandar
Department: MAE, UF

- Goals
  - DNS of shock and contact interaction with structured and random arrangements of particles
  - Development of models for predicting particle motion
- Simulation roadmap
  - Microscale simulations for shock-contact-particle interaction

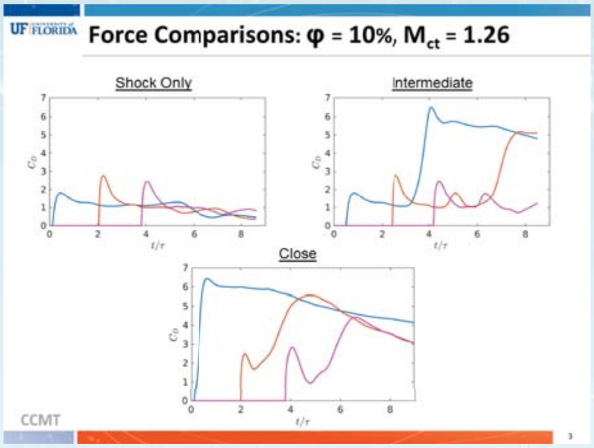
Simulation Roadmap



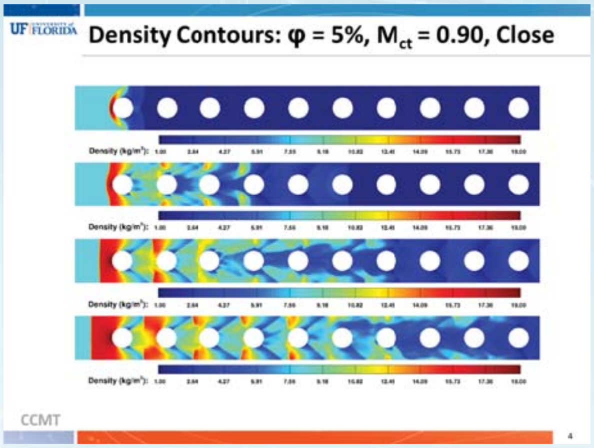
Shock and Contact Interaction with Particles

- Shock and contact interaction with a simple cubic array of particles; varying volume fraction and shock/contact Mach number
- Three sets simulations:
  - Close: Shock is 1/8 of a particle diameter from leading edge of first particle, contact is 0.08 particle diameters behind shock
  - Intermediate: Shock is 1/2 of a particle diameter from leading edge of first particle, contact is about 1.6 particle diameters behind shock
  - Shock only: Shock is 1/8 of a particle diameter from leading edge of first particle

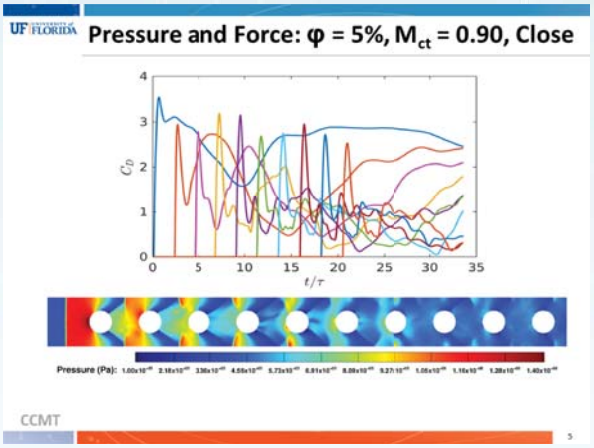
φ	M_{ct}	M_s
5%	0.31	1.22
	0.90	1.90
	1.26	2.69
10%	0.31	1.22
	0.90	1.90
	1.26	2.69
20%	0.31	1.22
	0.90	1.90
	1.26	2.69
40%	0.31	1.22
	0.90	1.90
	1.26	2.69



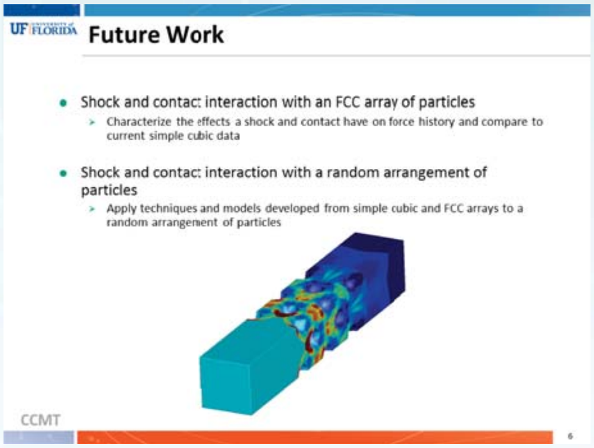
Force Comparisons: φ = 10%, M_{ct} = 1.26



Density Contours: φ = 5%, M_{ct} = 0.90, Close



Pressure and Force: φ = 5%, M_{ct} = 0.90, Close



Future Work

- Shock and contact interaction with an FCC array of particles
  - Characterize the effects a shock and contact have on force history and compare to current simple cubic data
- Shock and contact interaction with a random arrangement of particles
  - Apply techniques and models developed from simple cubic and FCC arrays to a random arrangement of particles

CCMT

Center for Compressible Multiphase Turbulence

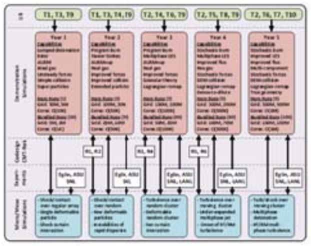
Surrogate Modeling of the Equation of State

Frederick Ouellet

Advisor: Dr. S. Balachandar

Department: MAE, UF

- Goals
  - Develop a surrogate model for use in evaluating the equation of state in mixed air/product cells.
  - Perform and analyze simulations of the Eglin blastpad experiments.
- Simulation roadmap
  - Real gas equation of state capabilities in code.
  - Analysis of instabilities of rapid dispersion.



Simulation Roadmap

Motivation

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

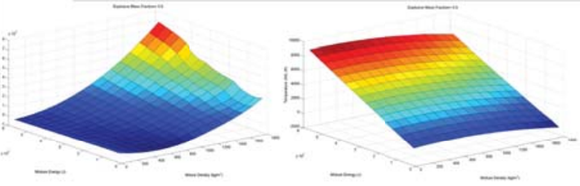
- Real gas equations of state are needed for explosive products
- Iterative methods for handling mixed product-air cells are computationally expensive
- A surrogate model would provide a faster alternative

Explosive dispersal of a packed bed of sand particles

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

- The pictures taken by Frost et al. during their detonation experiments show the formation of coherent jets at late time. We believe that initial detonation conditions and/or particle distribution may play a role in their formation

Surrogate Model – Development



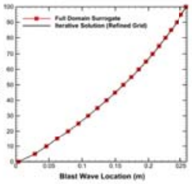
Surfaces of surrogate model for pressure (left) and temperature (right) at explosive mass fractions of 0.5

- New Kriging surrogate model for pressure and temperature in mixed cells generated over full density domain using absolute error as the main criteria for selecting the 200 sampling points
- Model replaces iterative Broyden's Method solver with matrix multiplication
- Note that not all inputs to the surrogate will produce physically possible pressures and temperatures

Test Simulation Description

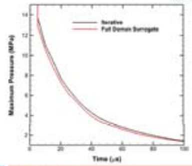
- 2D, Quarter-Cylinder grid
- Outer radius = 0.3 m
- 400,000 cells
- Gas-Only

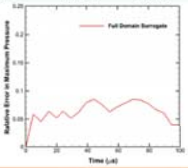
Surrogate Model – Preliminary Results



- Runs with the newest model show good agreement in the blast wave radius compared to the iterative method
- There is an undershoot in the maximum pressure recorded at each time which is capped at 8%
- Timing of runs shows comparable results to tests of prior models

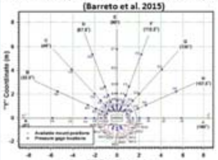
Run	s/Time step (Iterative)	s/Time Step (Surrogate)	Ratio	Previous Model
1	0.4636	0.1739	2.6662	-
2	0.4314	0.1778	2.4262	-
3	0.4766	0.1754	2.7178	-
Avg.	0.4572	0.1757	2.6024	2.6313



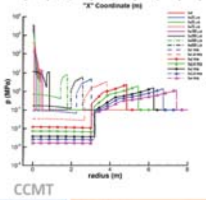


Eglin Blastpad

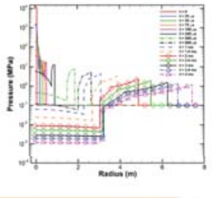
Locations of experimental pressure transduces (54 total)
(Barreto et al. 2015)



- Based on parameters given to the center by Eglin, a 1D, bare charge simulation was performed in order to provide predictive data before experiments are performed
- Simulations used a one-equation JWL model to account for the Comp-B and air mixture that occurs during the detonation process
- Pressure profiles were extracted for times up to 6 ms. Those up to 4ms are shown below.



Pressure profiles of gas-only simulations of the Eglin blastpad experiment (Left – Ideal Gas, Right – JWL)



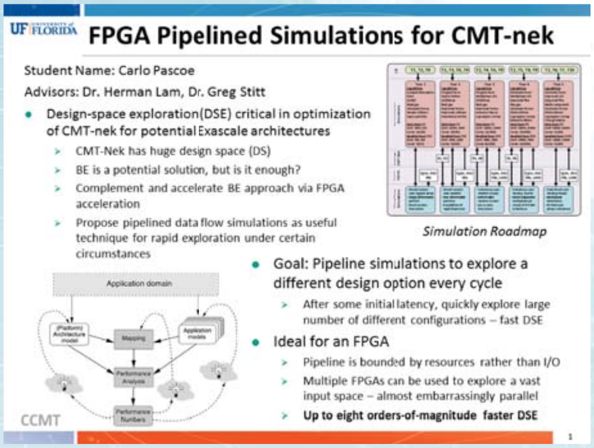
Summary & Future Work

- Summary
  - Developed improved surrogate models to handle real gas calculations in mixed air-product cells.
  - Surrogate model shows good agreement in the location of the blast wave compared to the iterative method and speeds up the code when used instead of the iterative method.
  - Preliminary simulations of the bare charge blastpad experiment to be performed by Eglin were performed in one dimension. Pressure profiles were extracted for predictive use.
- Future Work
  - Improve surrogate model to reduce error in capturing the peak pressure in simulations at later times. In addition, test different numbers of sampling points for a sensitivity analysis.
  - Create models for different mixtures of species, including possibly more than two
  - Perform simulations of the Eglin blastpad experiment in higher dimensions with tungsten particles and a reactive burn initial condition.
  - Work on improved compaction models for more accurate and realistic simulations at higher particle volume fractions. This work will focus on finding alternatives or additions to the currently used *Harris-Crighton* [2] model.

[2] Harris, S., and Crighton, D., 1994, "Solitons, Solitary Waves, and Voidage Disturbances in Gas-Fluidized Beds," J. Fluid Mech., 266, pp.243-276.

CCMT

Center for Compressible Multiphase Turbulence



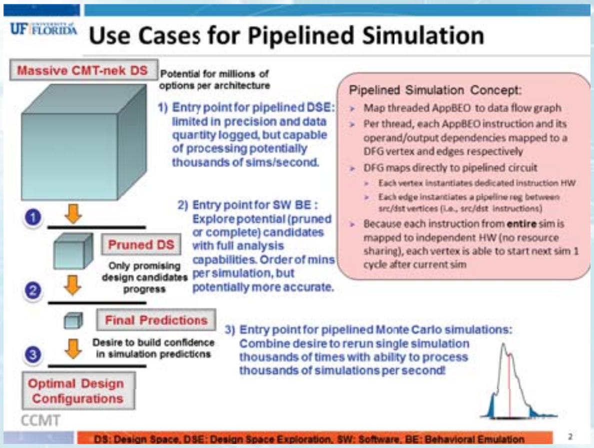
FPGA Pipelined Simulations for CMT-nek

Student Name: Carlo Pascoe

Advisors: Dr. Herman Lam, Dr. Greg Stitt

- Design-space exploration(DSE) critical in optimization of CMT-nek for potential Exascale architectures
  - CMT-Nek has huge design space (DS)
  - BE is a potential solution, but is it enough?
  - Complement and accelerate BE approach via FPGA acceleration
  - Propose pipelined data flow simulations as useful technique for rapid exploration under certain circumstances
- Goal: Pipeline simulations to explore a different design option every cycle
  - After some initial latency, quickly explore large number of different configurations – fast DSE
- Ideal for an FPGA
  - Pipeline is bounded by resources rather than I/O
  - Multiple FPGAs can be used to explore a vast input space – almost embarrassingly parallel
  - **Up to eight orders-of-magnitude faster DSE**

Simulation Roadmap



Use Cases for Pipelined Simulation

Massive CMT-nek DS

Potential for millions of options per architecture

1) Entry point for pipelined DSE: limited in precision and data quantity logged, but capable of processing potentially thousands of sims/second.

Pruned DS

Only promising design candidates progress

2) Entry point for SW BE : Explore potential (pruned or complete) candidates with full analysis capabilities. Order of mins per simulation, but potentially more accurate.

Final Predictions

Desire to build confidence in simulation predictions

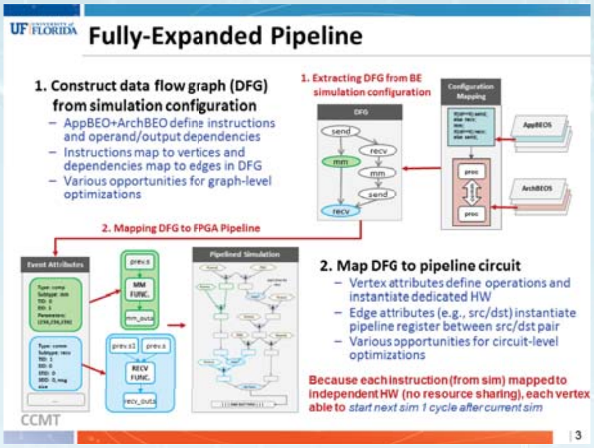
3) Entry point for pipelined Monte Carlo simulations: Combine desire to rerun single simulation thousands of times with ability to process thousands of simulations per second!

Optimal Design Configurations

Pipelined Simulation Concept:

- Map threaded AppBEO to data flow graph
- Per thread, each AppBEO instruction and its operand/output dependencies mapped to a DFG vertex and edges respectively
- DFG maps directly to pipelined circuit
  - Each vertex instantiates dedicated instruction HW
  - Each edge instantiates a pipeline reg between src/dst vertices (i.e., src/dst instructions)
- Because each instruction from **entire** sim is mapped to independent HW (no resource sharing), each vertex is able to start next sim 1 cycle after current sim

DS: Design Space, DSE: Design Space Exploration, SW: Software, BE: Behavioral Emulation

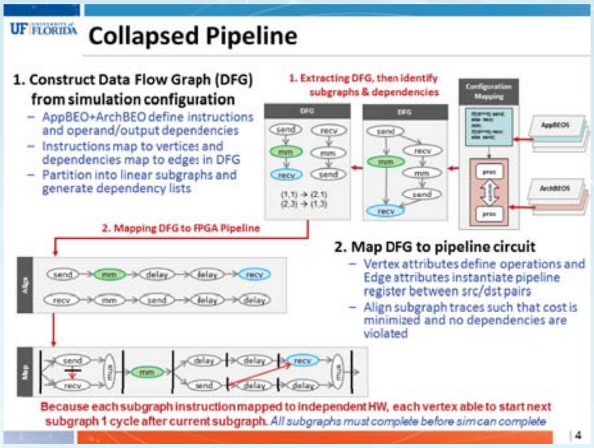


Fully-Expanded Pipeline

1. Construct data flow graph (DFG) from simulation configuration
   - AppBEO+ArchBEO define instructions and operand/output dependencies
   - Instructions map to vertices and dependencies map to edges in DFG
   - Various opportunities for graph-level optimizations

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

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



Collapsed Pipeline

1. Construct Data Flow Graph (DFG) from simulation configuration
   - AppBEO+ArchBEO define instructions and operand/output dependencies
   - Instructions map to vertices and dependencies map to edges in DFG
   - Partition into linear subgraphs and generate dependency lists

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

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

Fully-Expanded & Collapsed Pipeline Tradeoffs

Performance of fully-expanded (left) & collapsed (right) dataflow pipelines for CMT-Bone-BE with varied MPI ranks and simulation timesteps on a single Stratix V 5SGSMD8K1F40C2. ('-' indicates configuration unable to fit on a single FPGA)

	Num. of MPI Ranks	Num. of Timesteps	Num. of Events	% Logic Utilization	Clk Rate (MHz)	Latency to First Output (cycles)	Mega Sims perSecond
1.	32	1	1,344	15 / 2	325 / 340	64 / 278	325 / 10.63
2.	32	2	2,688	31 / 3	290 / 340	118 / 512	290 / 10.63
3.	32	3	4,032	46 / 4	285 / 330	172 / 746	285 / 10.31
4.	32	4	5,376	61 / 6	280 / 330	226 / 980	280 / 10.31
5.	32	5	6,720	76 / 7	305 / 335	280 / 1,214	305 / 10.47
6.	32	6	8,064	92 / 9	270 / 330	334 / 1,488	270 / 10.31
7.	32	8	10,752	- / 12	- / 325	- / 1,916	- / 10.16
8.	32	16	21,504	- / 24	- / 320	- / 3,788	- / 10.00
9.	32	32	43,008	- / 44	- / 320	- / 7,532	- / 10.00
10.	64	1	2,880	32 / 2	295 / 340	65 / 394	295 / 5.31
11.	64	2	5,760	65 / 4	310 / 365	119 / 712	310 / 5.70
12.	64	3	8,640	99 / 5	295 / 340	173 / 1,030	295 / 5.31
13.	64	4	11,520	- / 7	- / 365	- / 1,348	- / 5.70
14.	64	8	23,040	- / 14	- / 330	- / 2,620	- / 5.16
15.	64	16	46,080	- / 29	- / 320	- / 5,164	- / 5.00
16.	64	32	92,160	- / 46	- / 335	- / 10,252	- / 5.23
17.	128	1	5,952	66 / 2	280 / 340	66 / 458	280 / 2.66
18.	128	2	11,904	- / 4	- / 375	- / 776	- / 2.93
19.	128	3	17,856	- / 5	- / 365	- / 1,094	- / 2.85
20.	128	4	23,808	- / 7	- / 355	- / 1,412	- / 2.77
21.	128	8	47,616	- / 15	- / 320	- / 2,684	- / 2.50
22.	128	16	95,232	- / 30	- / 320	- / 5,228	- / 2.50
23.	128	32	190,464	- / 47	- / 335	- / 10,316	- / 2.62

Fully-Expanded Pipeline

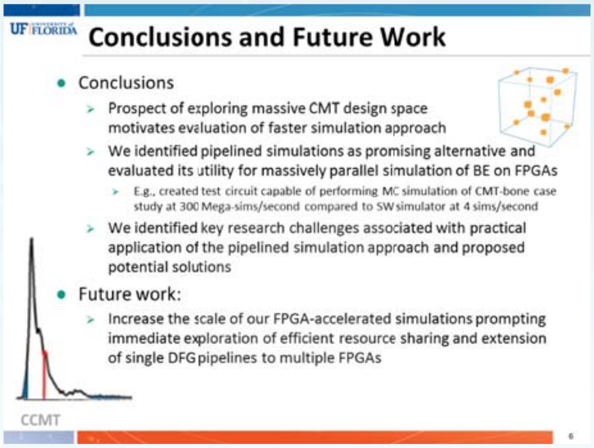
Advantages:
- Orders of magnitude higher simulation throughput

Limitations:
- Resources scale linearly with both MPI Ranks and number of timesteps
- Scaling across multiple FPGAs expected to be ineffective

Collapsed Pipeline

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

Limitations:
- Lower simulation throughput, but still more than sufficient for rapid design-space exploration



Conclusions and Future Work

- Conclusions
  - Prospect of exploring massive CMT design space motivates evaluation of faster simulation approach
  - We identified pipelined simulations as promising alternative and evaluated its utility for massively parallel simulation of BE on FPGAs
    - E.g., created test circuit capable of performing MC simulation of CMT-bone case study at 300 Mega-sims/second compared to SW simulator at 4 sims/second
  - We identified key research challenges associated with practical application of the pipelined simulation approach and proposed potential solutions
- Future work:
  - Increase the scale of our FPGA-accelerated simulations prompting immediate exploration of efficient resource sharing and extension of single DFG pipelines to multiple FPGAs

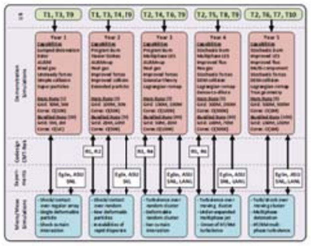
CCMT

Center for Compressible Multiphase Turbulence

BE-SST* Simulator

Ajay Ramaswamy
Advisor: Dr. Lam, Dr. Stitt
Department: ECE, UF

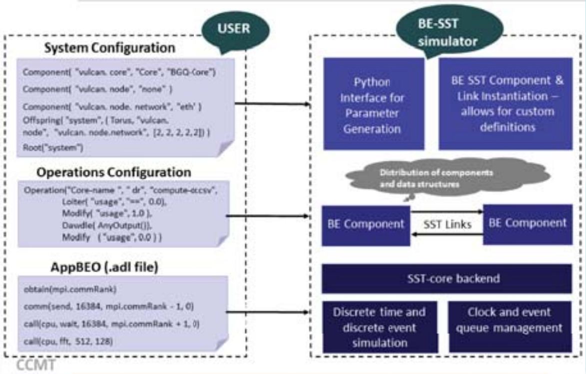
- Goals
  - Use SST framework to develop BE methods and run parallel, scalable simulations
  - Run simulations of large HPC systems
  - Improve communication models and interpolation API
- Simulation roadmap
  - BE-SST simulator enables scalable design space exploration on exascale systems



Simulation Roadmap

*SST: Structural Simulation Toolkit from Sandia National Laboratory

BE-SST Features



System Configuration

```
Component( "vulcan. core", "Core", "BGQ-Core")
Component( "vulcan. node", "none" )
Component( "vulcan. node. network", "eth' )
Offspring( "system", ( Torus, "vulcan.
node", "vulcan. node.network", [2, 2, 2, 2,2]) )
Root("system")
```

Operations Configuration

```
Operation("Core-name ", " dr", "compute-dr.csv",
          Loiter( "usage", "==", 0.0),
          Modify( "usage", 1.0 ),
          Dawdle( AnyOutput()),
          Modify   ( "usage", 0.0 ) )
```

AppBEO (.adl file)

```
obtain(mpi.commRank)
comm(send, 16384, mpi.commRank - 1, 0)
call(cpu, wait, 16384, mpi.commRank + 1, 0)
call(cpu, fft, 512, 128)
```

Python Interface for Parameter Generation

BE SST Component & Link Instantiation – allows for custom definitions

Distribution of components and data structures

BE Component ⇄ SST Links ⇄ BE Component

SST-core backend

Discrete time and discrete event simulation

Clock and event queue management

Results - Scaling Simulations with BE-SST

- Simulations of different machine sizes with 3D mesh system topology, running CMT-bone-BE with **static routing**
- Simulations run on 64 MPI ranks on HiPerGator @ University of Florida

No. of cores	Total No. of BEOs	System config build time (s)	Routing info build time (s)	Event simulation time (s)	No. of events	Memory usage
64	209	0.24	0.015	0.339	3809	40.85 M
256	897	0.13	0.037	1.524	16672	552.91 M
1k	3777	0.41	0.161	2.153	70816	664.68 M
4k	15617	1.58	1.830	5.510	294464	2.38 G
16k	63489	6.45	27.450	17.334	1200192	4.45 G
64k	257025	26.92	209.550	72.840	4868224	15.82 G
128k	516097	54.83	871.380	186.700	9781376	28.29 G
512k	2076673	219.29	14666.740	1814.600	39395456	103.71 G

- Building routing tables at simulation start is very time consuming
- Dynamic info generation should significantly improve total simulation time

Results - Scaling Simulations with BE-SST

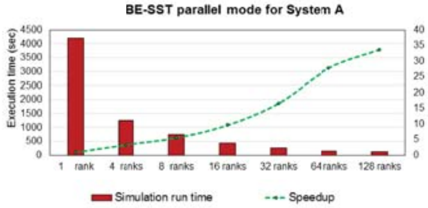
- Simulations of different machine sizes with 3D mesh system topology, running CMT-bone-BE with **dynamic routing**
- Simulations run on 64 MPI ranks on HiPerGator @ University of Florida

No. of cores	Total No. of BEOs	System config build time (s)	Event simulation time (s)	No. of events	Memory usage
64	209	0.257	0.328	3233	41.32 M
256	897	0.268	0.697	14088	164.16 M
1k	3777	0.412	2.087	59808	665.47 M
4k	15617	1.676	4.994	248384	2.3992 G
16k	63489	7.128	15.684	1011776	4.51101 G
64k	257025	30.499	57.390	4102272	16.2123 G
128k	516097	61.644	138.500	8241280	29.1278 G
512k	2076673	255.090	1041.050	33185920	107.4360 G

- Time to build network topology info is included in system config build time
- No separate time for building routing info
- Improvement in overall simulation time!

Results – Parallel Performance of BE-SST

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



Summary

- BE-SST communication models
  - Dynamic routing methods improved total simulation time for large runs when compared to static routing tables
  - Static routing is limited by large routing information at build times
  - Dynamic routing can become expensive when source and destination components are separated by several hops
- Parallel simulation runs
  - BE-SST shows good parallel performance scalability showing a max speedup of 33.7x
- Future work
  - Build memory and cache models in BE-SST
  - Optimize memory usage of BE-SST to improve performance scaling

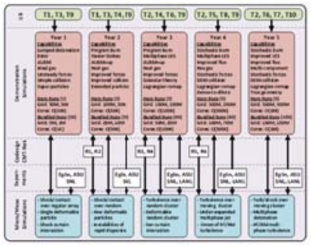
CCMT

Center for Compressible Multiphase Turbulence

Energy and Thermal Modeling

Mason Rawson
Advisor: Dr. Lam, Dr. Stitt
Department: ECE, UF

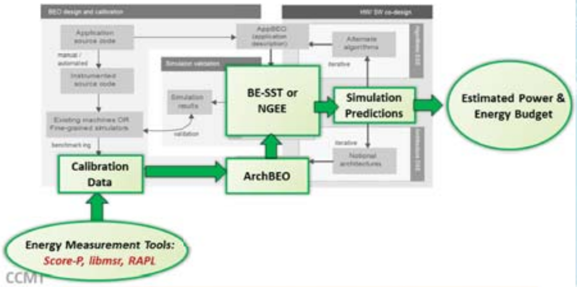
- Goals
  - Design and implement a framework for assessing performance and energy consumption tradeoffs across entire HPC systems
  - Understand processor level thermal effects on performance and energy consumption
- Simulation roadmap
  - Explore design space of future HPC systems to incorporate power and energy



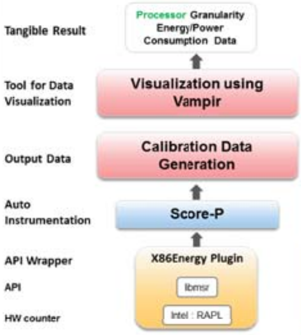
Simulation Roadmap

Energy and Thermal Modeling

Goal: Create an extendable, configurable, portable, and scalable benchmarking methodology for generating energy models to be integrated into ArchBEOs for scaling studies



Energy Benchmarking Infrastructure



Tangible Result — Processor 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

API — libmsr

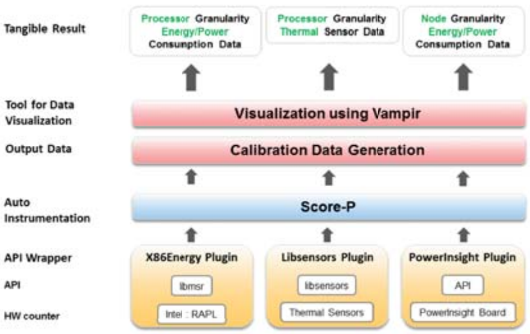
HW counter — Intel : RAPL

Vampir
- Allows easy visualizing of trace data generated by Score-P

Score-P
- Is open source
- Generates profiling and tracing data
- Is portable across HPC systems
- Is scalable to large, HPC code

Open Source Plugins
- Are configurable to vary overhead and API settings
- Allow extensions to a variety of hardware counters

Energy Benchmarking Infrastructure

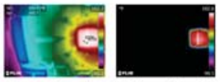


Tangible Result	Processor Granularity Energy/Power Consumption Data	Processor Granularity Thermal Sensor Data	Node Granularity Energy/Power Consumption Data
Tool for Data Visualization	Visualization using Vampir		
Output Data	Calibration Data Generation		
Auto Instrumentation	Score-P		
API Wrapper	X86Energy Plugin	Libsensors Plugin	PowerInsight Plugin
API	libmsr	libsensors	API
HW counter	Intel : RAPL	Thermal Sensors	PowerInsight Board

Thermal Aware Computing Lab (TACL)

- Purpose
  - Develop detailed understanding of processor level thermal effects on performance and energy consumption
  - Develop thermal and energy aware optimizations for multicore processors
  - The Intel Knights Landing is an ideal use case since it is a large multicore processor likely to be utilized in future HPCs
- Equipment
  - Flir A35c IR Camera
    - 320x256, 60Hz, 7.5 to 13.0μm spectral range, Uncooled VOX microbolometer detector
  - Knights Landing (KNL)
    - A newly released 72-core, each hyperthreaded, processor created for parallel computing and HPC systems

Flir A35c IR Camera



Thermal Imaging on Zedboard Zynq Dual Arm-FPGA System-on-Chip

KNL server node

Energy and Thermal Modeling

SUMMARY

- Energy and Thermal Modeling
  - Energy and thermal benchmarking will allow the simulator to predict a energy and power budget
  - Open source auto-benchmarking tools such as ScoreP has potential to extended to reading hardware counter such as RAPL
- Thermal Aware Computing Lab (TACL)
  - TACL will search for processor level thermal and energy consumption optimizations

FUTURE WORK

- Continue to develop energy benchmarking system
- Solve problems of RT processor thermography such as heat syncs, update frequency of IR camera, environmental control, etc…
- Analyze thermography on the KNL server processor under various loads

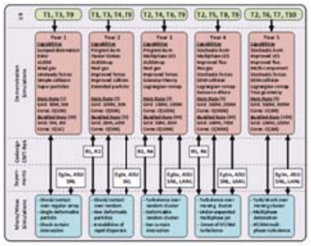
CCMT

Center for Compressible Multiphase Turbulence

RocSDT: Shock-Particle Interaction

Prashanth Sridharan
Advisor: Dr. Thomas L. Jackson
Department: ME, UF

- Goals
  - Investigate aluminum spherical particles under various shock loading conditions
  - Implement modelling technology to create robust level-set algorithms that handle mixture of deforming and rigid particles
- Simulation roadmap
  - Preliminary research conducted to produce transient force/drag histories



Simulation Roadmap

Motivation/Background

- **Purpose:** quantify momentum exchange of a particle under shock loading through the imparted transient drag coefficient curve, which can be used to create correlations, for point-particle force models, and kernels for larger scale simulations
- The particle and medium are governed by:
  level-set advection and compressible Euler equations

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

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

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

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

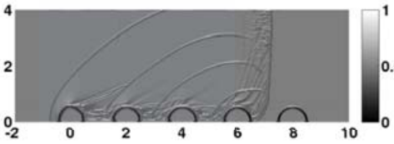
closed with a stiffened gas equation of state

$$p = (\gamma-1)\rho e - \gamma P^{\infty}$$

Motivation/Background

- **Level-Set Background:** This method is advantageous due to its ease in handling time-dependent complex topological changes, including dynamic creation of interfaces
- Level-set methods utilize the gradients in velocity to simulate the interface's topological changes, without taking into account particle's elasticity
- At moderate resolutions, this method is prone to unphysical mass/volume loss as well as particle "shrinking"/"disappearance"

1-D array of aluminum particles interacting with M=6 shock



Results – Mass/Shape Loss

- Simulation of a Aluminum particle loaded by shock
  - When run to large final times the particle eventually "disappears"
  - Coarser grids show more pronounced mass loss

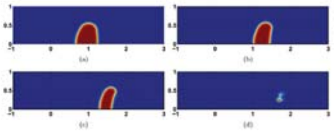


Figure 1: ϕ_1 contours of shock-particle interaction at nondimensional times of $t/\tau = 10$ (a), 12.6 (b), 14.6 (c), and 17 (d).
Post-shock pressure $p_s = 1$ GPa; resolution $d_p/30$.

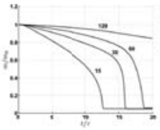


Figure 2: Time history of the mass of the aluminum particle at different grid resolutions d_p/N, with N labelled in the figure. Post-shock pressure $p_s = 1$ GPa.

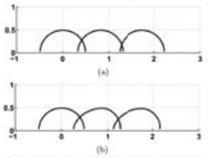
Results – Mass/Shape Correction

- Lagrange multipliers added to level-set reinitialization equations to preserve mass/volume

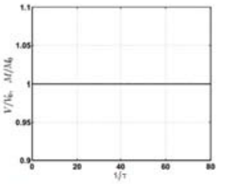
$$\frac{\partial(\rho_1\phi_1)}{\partial\tilde{t}} = H(\phi_1)\hat{n}\cdot(\nabla(\epsilon_h\hat{n}\cdot\nabla(\rho_1\phi_1)) - (1-2\phi_1)\nabla(\rho_1\phi_1)) + H(\phi_1)\lambda_{\rho_1}$$

- Preserve particle shape by adding a logistics source term (Fisher's population dynamics equation) to level-set reinitialization equation

$$\frac{\partial\phi_1}{\partial\tilde{t}} = \hat{n}\cdot\nabla\left(\epsilon_h|\nabla\phi_1| - \phi_1(1-\phi_1)\right) + H(\phi_1)\lambda_v + H(Y-p_s)\,k_s\,max(\phi_1,\phi_{1,0})(\phi_{1,0}-\phi_1)$$



Plot of $\phi_1 = 0.5$ showing particle boundary at various times with (a) and without (b) shape correction.



Plot of normalized particle volume and mass

Future Work

- The following is a non-comprehensive list of recommended numerical investigations for future work:
  - Initial particle shape's effect on transient drag coefficient curves
    - Quantification of errors with and without shape preservation
  - Investigation of particle medium combinations on transient drag coefficient curves
  - Validate shape preservation in 3D simulations with multiple rigid particles
  - Simulate Eglin Barrel Ejection Experiment after validation in 3D

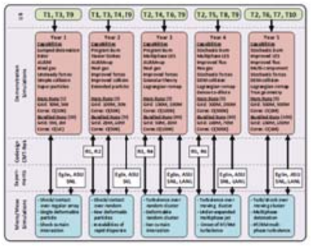
CCMT

Center for Compressible Multiphase Turbulence

Dynamic Load Balancing for CMT-nek

Student Name: Keke Zhai
Advisor: Prof. Sanjay Ranka
Department: CISE, UF

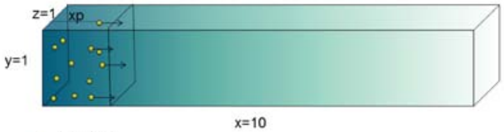
- Goals
  - To reduce simulation time and decrease power consumption on CMT-bone and CMT-nek by utilizing dynamic load balancing
- Simulation roadmap
  - This simulation includes moving particles and gas to simulate the actual particle movement within a fixed box



Simulation Roadmap

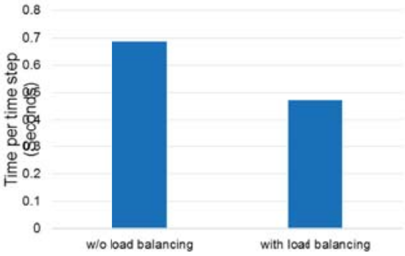
Background

- Simulation Testcase
  - A number of particles are in the leftmost part (1x1x1) of a rectangle box (10x1x1). And they all move along the x-axis of the box with the speed of 1/3*xp.
  - Gas also move along the x-axis.



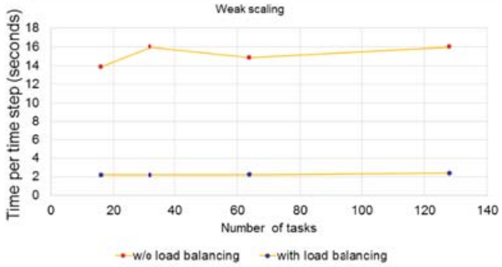
- Platform
  - CMT-bone on BG/Q (Vulcan, Mira)
  - CMT-bone hybrid on Titan
  - CMT-nek on BQ/Q (Vulcan, Mira)

Load Balancing Results on Titan



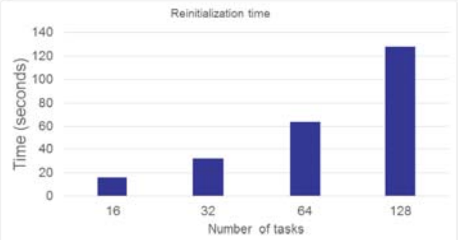
- We executed CMT-bone with 4096 elements and 256000 particles on 15 CPU cores and 1 GPU on a single Titan node. The average time taken to process one simulation time step was about 50% higher without load balancing compared to the time taken to process one simulation time step with load balancing.

Load Balancing Results on BG/Q



- With load balancing the processing time improved by 7 to 8 times on a BG/Q system. In this weak scaling study, loading was increased proportionately, with 16 ranks processing 4096 elements and 512000 particles.

Load Balancing Results on BG/Q



- With load balancing, the reinitialization time increases with the number of tasks. The time taken by reinitialization is about linear with number of tasks. For this experiment, each task was run on a separate BG/Q node.

Summary

- The load balancing results on CMT-bone and CMT-nek has been presented. It shows that it can effectively reduce the time taken by original CMT-bone and CMT-nek.
- Future Work:
  - Continuous improvement to the load balancing algorithm will be explored to reduce the unnecessary overheads taken by reinitialization.
  - Power consumption will be explored taken by load balancing algorithm and without load balancing to reduce power consumption.
  - More test cases will be added to make this algorithm more robust.

UF UNIVERSITY of FLORIDA
NNSA

CCMT

Center for Compressible Multiphase Turbulence

Correction of Performance Emulation

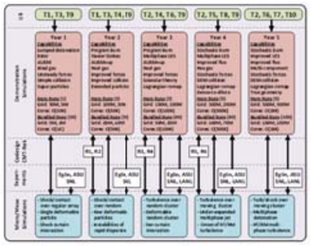
Student: Yiming Zhang

Advisor: Prof. Raphael T. Haftka

& Prof. Nam H. Kim

Department: Mechanical Engr. /UF

- Goals
  - Quantify similarity and difference between run times of CMT codes
  - Develop correction schemes for BE emulation to predict performance of CMT codes
- Simulation roadmap
  - Using advanced data analytics to assist performance emulation at different stages in the simulation roadmap



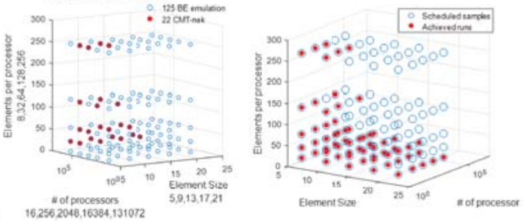
Simulation Roadmap

Motivation and Progress

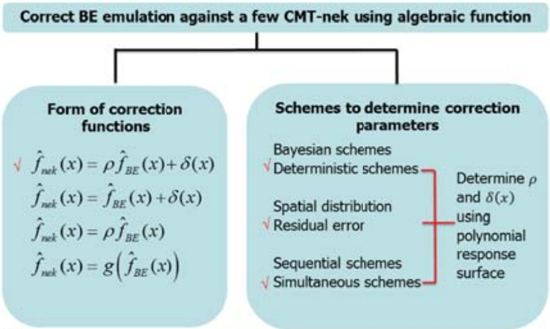
- **Coordinated multi-fidelity error reduction for CMT codes at large-scale runs**
  - Designed the experiments for comparing CMT-nek, CMT-bone, CMT-bone BE and BE emulation
  - Interacted with Nek team, CS team and Exascale team for data acquisition
- **Predicted performance of CMT codes using corrected BE emulation**
  - Proposed Simultaneous Deterministic Framework to correct BE emulation against CMT-nek. The corrected BE emulation had less-than-5% root-mean-square difference comparing with CMT-nek
  - Helped identify interpolation error in BE emulation and measurement error in CMT-bone through data visualization

Design of Experiments for Large-Scale Runs

- Quantity of interest
  - Execution time of a typical no-particle test (on Vulcan) using up to 34 million (131072×256) elements and 311 billion ($21^3 \times 131072 \times 256$) computational grid points
  - 125 (5^3) grid for BE emulation & CMT-bone BE, with subset for CMT-nek and CMT-bone



Multi-fidelity Correction



Correct BE emulation against a few CMT-nek using algebraic function

Form of correction functions

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

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

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

$\hat{f}_{nek}(x) = g\left(\hat{f}_{BE}(x)\right)$

Schemes to determine correction parameters

Bayesian schemes

√ Deterministic schemes

Spatial distribution

√ Residual error

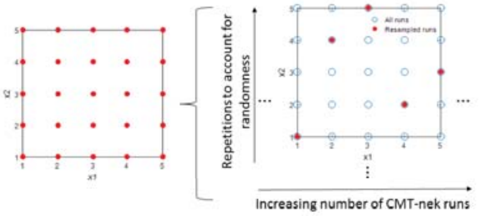
Sequential schemes

√ Simultaneous schemes

Determine ρ and $\delta(x)$ using polynomial response surface

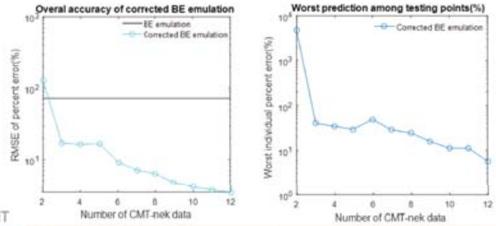
Robust Tests based on Resampling

- Testing plan to evaluate correction schemes
  - For given number of samples, resampled from 12 CMT nek runs (out of 22) without replacement. n (number of samples) × 50 (replicated sets) sets of data, n=1~12
  - Overall percentage accuracy was calculated at 10 left-out runs



Predicting CMT-nek from Corrected Emulation

- Performance of corrected BE emulation
  - Overall accuracy(root-mean-square error) is less than 10% with 6 or more CMT-nek samples. The proposed Simultaneous Deterministic Framework dominates tested approaches.
  - Max error is less than 20% (at the 10 test points) with 9 or more CMT-nek samples



UF UNIVERSITY of FLORIDA

NNSA

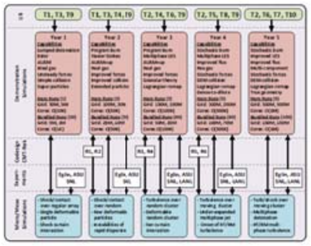
CCMT

Center for Compressible Multiphase Turbulence

Gas-Particle Mixtures Under Sudden Expansion

Heather Zunino
Advisor: Prof. Ronald Adrian
Department: SEMTE, ASU

- Goals
  - Perform repeatable experiments on a vertical shocktube at ASU
  - Examine expansion fan, flow structures, and instabilities
  - Provide data for validation of computational codes
- Simulation roadmap
  - The shocktube experiment at ASU will provide data for validating the codes being developed at UF.

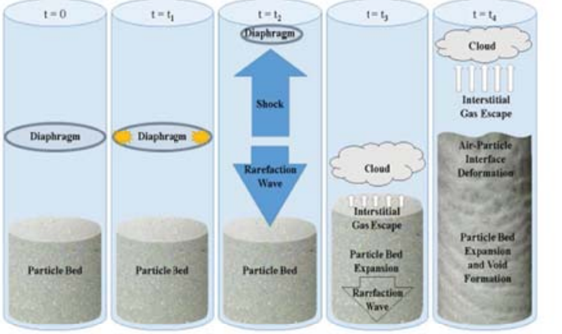


Simulation Roadmap

Motivation

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

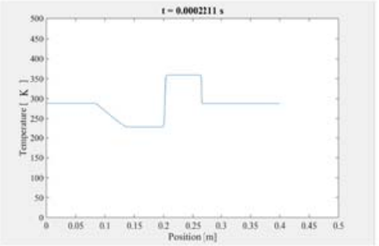
Results



Stages of Experiment

Results

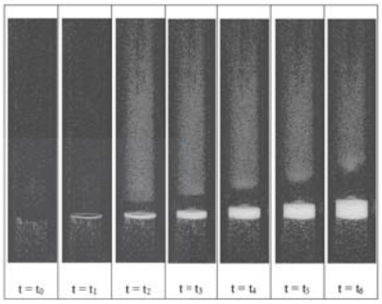
- Simulations suggest that 50K temperature drop can be expected to occur as the gas behind the shockwave expands.
- From a temperature drop between 298.15K and 233.15K, air is able to contain about 200x's less water vapor.



Simulated temperature profile of air in the shocktube 2.211E-4 s after the diaphragm bursts. This simulation was performed by Dr. Bertrand Rollin at UF.

Results

- Because low temperatures cause air's specific humidity to drop dramatically, a cloud forms in the shocktube.
- The cloud may actually be useful, as it is pushed upward by the air escaping the particle bed.
- In this experiment, the cloud is receding at 18-25 m/s.



Cloud formation and evolution: Each subsequent frame after t = t2, shows the cloud is pushed away from the particle bed by the air escaping the interstices.

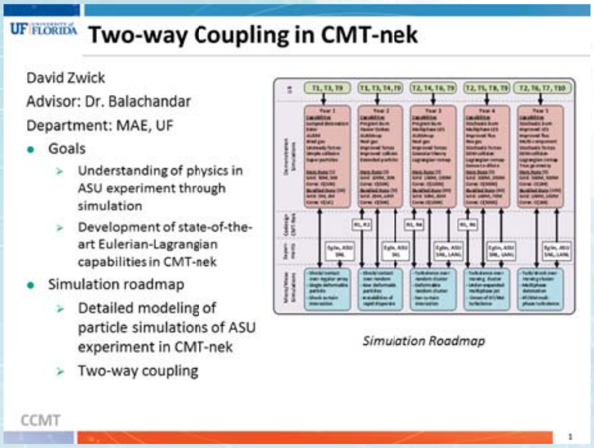
Looking Forward

- In 2017, the experimental team at ASU purchased new equipment to better measure the pressure fluctuations that occur over time. The addition of more pressure sensors will allow for multiple measurements at the same location along the length of the shocktube. By examining multiple pressure traces from the same location along the tube, it will be possible to determine whether the one-dimensional pressure equations are appropriate to describe the flow.
- A special type of data acquisition device (DAQ) was chosen to digitize the pressure measurements. The new DAQ can take over a million samples per second, which allows each of the eight new pressure sensors to be sampled at frequency of 150,000Hz. Also, the DAQ can take truly simultaneous samples. This will eliminate some distortions which are caused by only reading one channel at a time.
- Additionally, with the new computer, it will be possible to synchronize the data from the pressure sensors and the high-speed camera. This is very important for better understanding gas-particle interactions.
- With this new equipment, Dr. Blair Johnson will also be setting up a particle image velocimetry system. This system will be used to measure gas and particle velocities in the region above the dense particle bed.

UF UNIVERSITY of FLORIDA
NNSA

CCMT

Center for Compressible Multiphase Turbulence

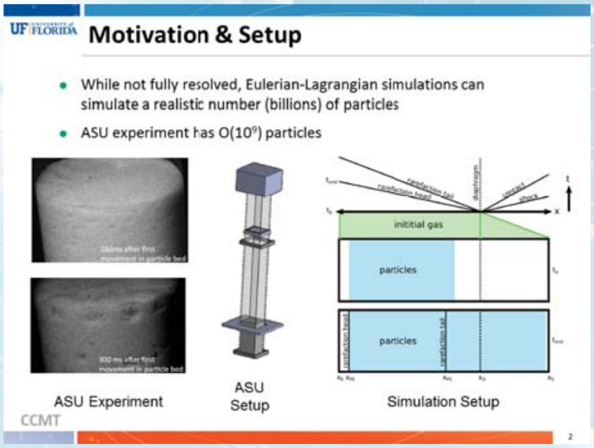


Two-way Coupling in CMT-nek

David Zwick
Advisor: Dr. Balachandar
Department: MAE, UF

- Goals
  - Understanding of physics in ASU experiment through simulation
  - Development of state-of-the-art Eulerian-Lagrangian capabilities in CMT-nek
- Simulation roadmap
  - Detailed modeling of particle simulations of ASU experiment in CMT-nek
  - Two-way coupling

Simulation Roadmap



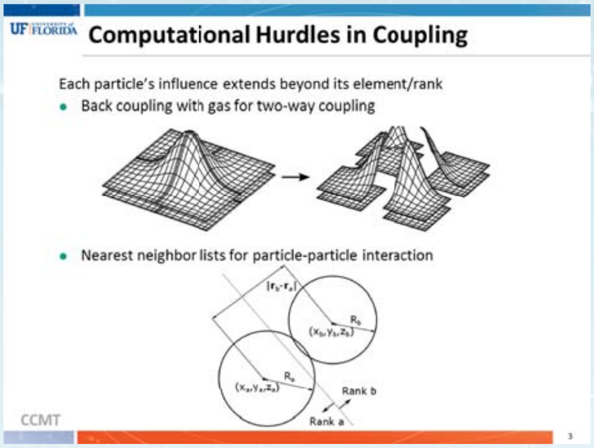
Motivation & Setup

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

ASU Experiment

ASU Setup

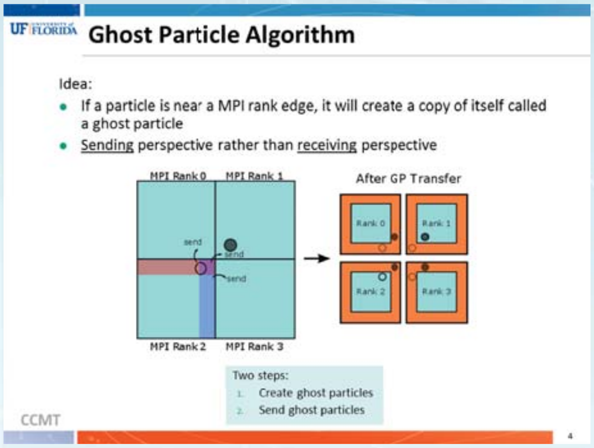
Simulation Setup



Computational Hurdles in Coupling

Each particle's influence extends beyond its element/rank

- Back coupling with gas for two-way coupling
- Nearest neighbor lists for particle-particle interaction



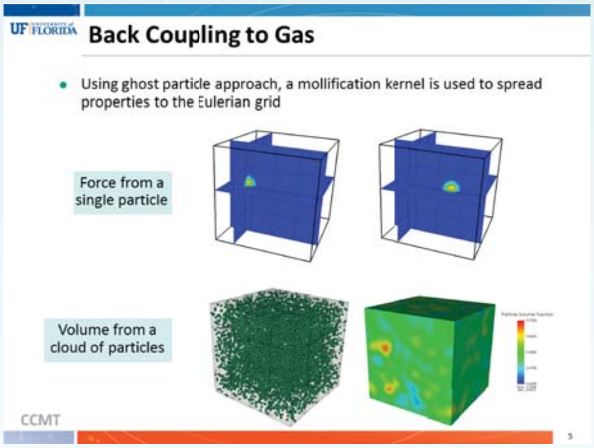
Ghost Particle Algorithm

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

Two steps:

1. Create ghost particles
2. Send ghost particles

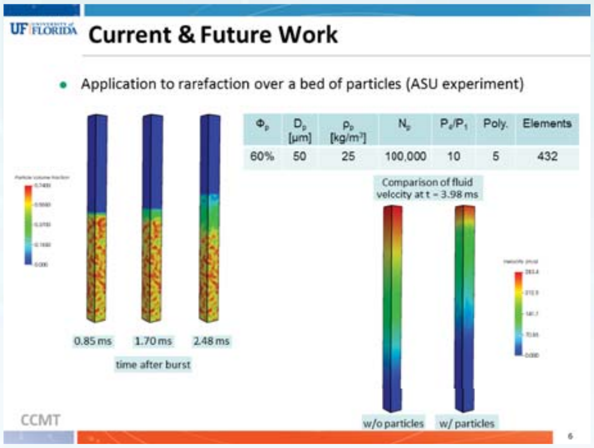


Back Coupling to Gas

- 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



Current & Future Work

- Application to rarefaction over a bed of particles (ASU experiment)

Φ_p	D_p [μm]	ρ_p [kg/m^3]	N_p	P_4/P_1	Poly.	Elements
60%	50	25	100,000	10	5	432

time after burst

Comparison of fluid velocity at t = 3.98 ms

CCMT

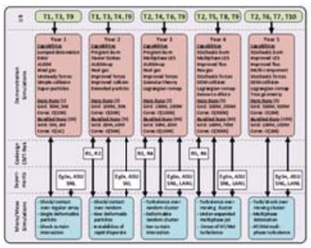
Center for Compressible Multiphase Turbulence

Uncertainty Budget for CMT Simulation

Dr. Chanyoung Park

Department: CCMT, UF

- Goals
  - V&V, UQ, UR and ER
  - Identify model errors
  - Reduce uncertainty for more accurate model error estimation
  - Develop UQ and function approximation tools
  - Multidisciplinary team interaction



Simulation Roadmap

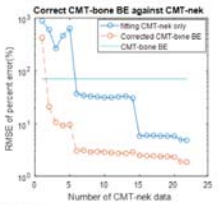
- Simulation roadmap
  - T3: JWL-EOS based on surrogate model
  - T4: Validation, UQ, UR and ER of the particle force model

Exploring Parameter Space of Hero Runs

- Parameter space exploration and UQ of hero runs are challenging because of its computational intensity
  - Even runninghero runs for acquiring sufficient number samples for building a surrogate is not feasible
  - Solution: Correct lower fidelity response with few high fidelity runs
- As a strategy to tackle the challenge, Multi-fidelity surrogate (MFS) has been applied and previous study revealed that
  - Mostly useful for saving computational cost for building an equivalently accurate surrogate
    MFS predictions are mostly extrapolative because of its correction based on a few high fidelity samples
- Various correction approaches are available for building an MFS
  - Discrepancy function based correction: $\hat{y}_H(\mathbf{x}) = \rho\hat{y}_L(\mathbf{x}) + \hat{\delta}(\mathbf{x})$
  - Calibration: $\hat{y}_H(\mathbf{x}) = \rho\hat{y}_L(\mathbf{x},\boldsymbol{\theta}) + \hat{\delta}(\mathbf{x})$
  - Different methods to build using Bayesian/deterministic frameworks

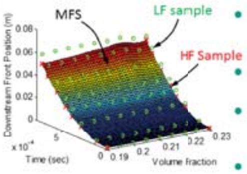
Cost Saving via Multi-Fidelity Surrogate

- The MFS frameworks were applied for predicting physical/mathematical functions: Borehole function and Hartmann 6 function.
- 99% (Borehole function) to 86% (Hartmann 6 function) cost savings were realized with the same accuracy with high fidelity only
- Bayesian frameworks often outperformed their deterministic counterparts

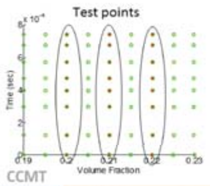


- Predicting CMT-nek execution time as function of processors, number of elements per processor and element size
- CMT-nek is at least 1.5 times more expensive than CMT-bone
- Low fidelity: 125 CMT-bone BE samples
- High fidelity: Variable number of CMT-nek samples
- With 6 CMT-nek samples, get 2% RMS error

Predicting 2D Meso Shocktube Sim with MFS



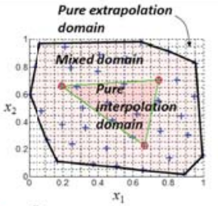
- The effectiveness of MFS was demonstrated with 1D (low-fidelity) and 2D (high-fidelity) mesoscale shock tube simulations
- One 1D simulation requires 1 hour while one 2D simulation requires 12 hours
- Run 1D simulations for 9 different volume fractions and run 2D simulations for 2 different volume fractions (19% and 23%)
- Evaluated the accuracy of the MFS using additional 2D runs for 3 volume fractions

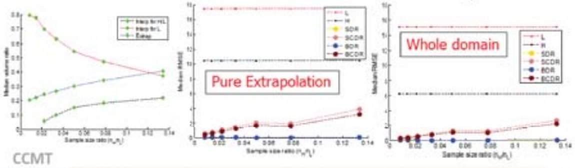


VF for HF samples	Max abs. error (Max % error)	Mean abs. error (Mean % error)
19% 23%	0.0031 (5.7%)	0.0006 (2.1%)
19% 21% 23%	0.0018 (3.3%)	0.0003 (0.9%)

MFS Works for Extrapolation

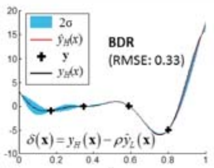
- Whole domain of interest (or sampling domain) is composed of 1) pure interpolation domain, 2) mixed domain and 3) pure extrapolation domain
- Since MFS often depends on a few high fidelity samples, correction is mostly extrapolation in terms of HF samples
- Accuracies of MFS for the three domains tell how successful is the extrapolation correction

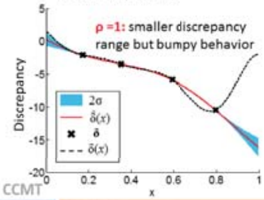


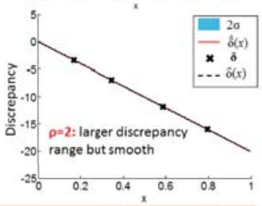


MFS Succeeds by Simplifying Correction

- Extrapolative correction becomes successful even with a few high fidelity samples when correction is a simple function
- Based on high dimensional problems, one 1D example is reproduced
- Selection of lower fidelity model is also important

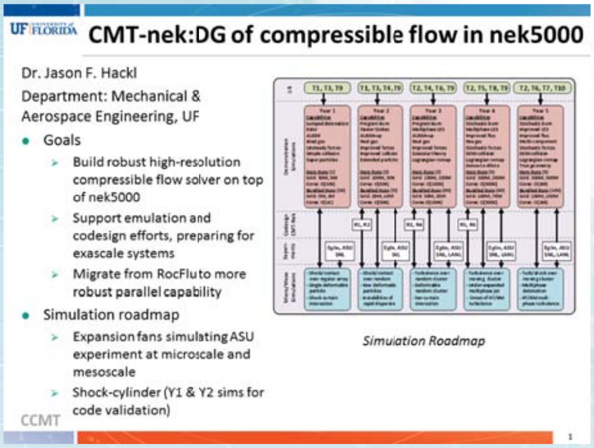






CCMT

Center for Compressible Multiphase Turbulence

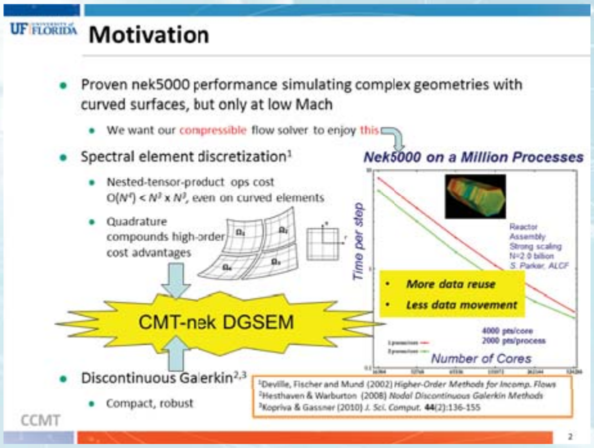


CMT-nek:DG of compressible flow in nek5000

Dr. Jason F. Hackl
Department: Mechanical & Aerospace Engineering, UF

- Goals
  - Build robust high-resolution compressible flow solver on top of nek5000
  - Support emulation and codesign efforts, preparing for exascale systems
  - Migrate from RocFlu to more robust parallel capability
- Simulation roadmap
  - Expansion fans simulating ASU experiment at microscale and mesoscale
  - Shock-cylinder (Y1 & Y2 sims for code validation)

Simulation Roadmap



Motivation

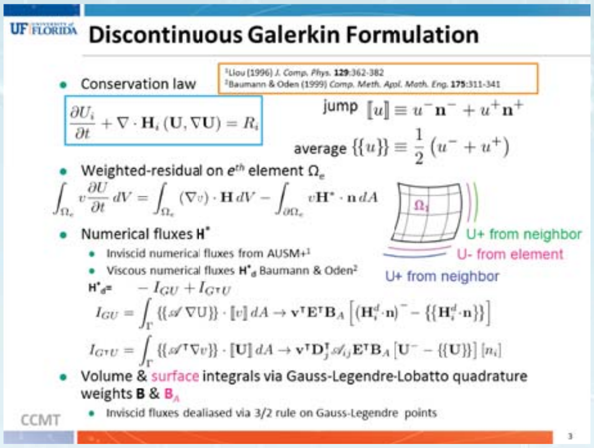
- Proven nek5000 performance simulating complex geometries with curved surfaces, but only at low Mach
  - We want our compressible flow solver to enjoy this
- Spectral element discretization[1]
  - Nested-tensor-product ops cost $O(N^4) < N^3 \times N^3$, even on curved elements
  - Quadrature compounds high-order cost advantages
- Discontinuous Galerkin[2,3]
  - Compact, robust

CMT-nek DGSEM

Nek5000 on a Million Processes

- *More data reuse*
- *Less data movement*

[1] Deville, Fischer and Mund (2002) *Higher-Order Methods for Incomp. Flows*
[2] Hesthaven & Warburton (2008) *Nodal Discontinuous Galerkin Methods*
[3] Kopriva & Gassner (2010) *J. Sci. Comput.* **44**(2):136-155



Discontinuous Galerkin Formulation

- Conservation law

$$\boxed{\frac{\partial U_i}{\partial t} + \nabla \cdot \mathbf{H}_i(\mathbf{U}, \nabla \mathbf{U}) = R_i}$$

jump $[\![u]\!] \equiv u^- \mathbf{n}^- + u^+ \mathbf{n}^+$

average $\{\{u\}\} \equiv \frac{1}{2}(u^- + u^+)$

- Weighted-residual on e^{th} element Ω_e

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

- Numerical fluxes $\mathbf{H}^*$
  - Inviscid numerical fluxes from AUSM+[1]
  - Viscous numerical fluxes $\mathbf{H}^*_d$ Baumann & Oden[2]

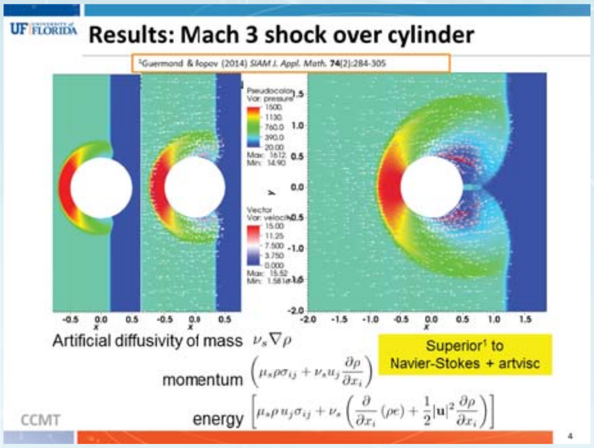
$$\mathbf{H}^*_d = -I_{GU} + I_{G^TU}$$

$$I_{GU} = \int_\Gamma \{\{\mathscr{A} \nabla \mathrm{U}\}\} \cdot [\![v]\!]\, dA \rightarrow \mathbf{v}^T \mathbf{E}^T \mathbf{B}_A \left[(\mathbf{H}_i^d \cdot \mathbf{n})^- - \{\{\mathbf{H}_i^d \cdot \mathbf{n}\}\}\right]$$

$$I_{G^TU} = \int_\Gamma \{\{\mathscr{A}^T \nabla v\}\} \cdot [\![\mathbf{U}]\!]\, dA \rightarrow \mathbf{v}^T \mathbf{D}_j^T \mathscr{A}_{ij} \mathbf{E}^T \mathbf{B}_A \left[\mathbf{U}^- - \{\{\mathbf{U}\}\}\right][n_i]$$

- Volume & surface integrals via Gauss-Legendre-Lobatto quadrature weights **B** & $\mathbf{B}_A$
  - Inviscid fluxes dealiased via 3/2 rule on Gauss-Legendre points

[1] Liou (1996) *J. Comp. Phys.* **129**:362-382
[2] Baumann & Oden (1999) *Comp. Meth. Appl. Math. Eng.* **175**:311-341



Results: Mach 3 shock over cylinder

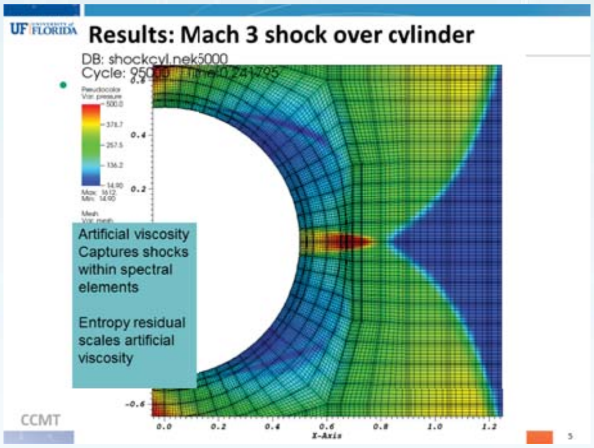
[1] Guermond & Popov (2014) *SIAM J. Appl. Math.* **74**(2):284-305

Artificial diffusivity of mass $\nu_s \nabla\rho$

momentum $\left(\mu_s \rho \sigma_{ij} + \nu_s u_j \frac{\partial \rho}{\partial x_i}\right)$

energy $\left[\mu_s \rho u_j \sigma_{ij} + \nu_s \left(\frac{\partial}{\partial x_i}(\rho e) + \frac{1}{2}|\mathbf{u}|^2 \frac{\partial \rho}{\partial x_i}\right)\right]$

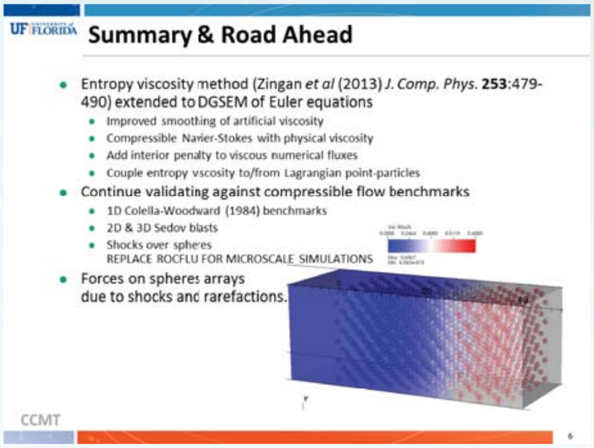
Superior[1] to Navier-Stokes + artvisc



Results: Mach 3 shock over cvlinder

Artificial viscosity Captures shocks within spectral elements

Entropy residual scales artificial viscosity



Summary & Road Ahead

- Entropy viscosity method (Zingan *et al* (2013) *J. Comp. Phys.* **253**:479-490) extended to DGSEM of Euler equations
  - Improved smoothing of artificial viscosity
  - Compressible Navier-Stokes with physical viscosity
  - Add interior penalty to viscous numerical fluxes
  - Couple entropy viscosity to/from Lagrangian point-particles
- Continue validating against compressible flow benchmarks
  - 1D Colella-Woodward (1984) benchmarks
  - 2D & 3D Sedov blasts
  - Shocks over spheres
    REPLACE ROCFLU FOR MICROSCALE SIMULATIONS
- Forces on spheres arrays due to shocks and rarefactions.