CCMT

Center for Compressible Multiphase Turbulence (CCMT) Updates

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Demonstration Problem

Center for Compressible Multiphase Turbulence

Overarching Goals

- To radically advance the field of CMT
- To advance predictive simulation science on current and near-future platforms with uncertainty budget as backbone
- To advance a co-design strategy that combines behavioral emulation, exascale algorithms, exascale CS
- To educate students and postdocs in exascale simulation science and place them at NNSA laboratories

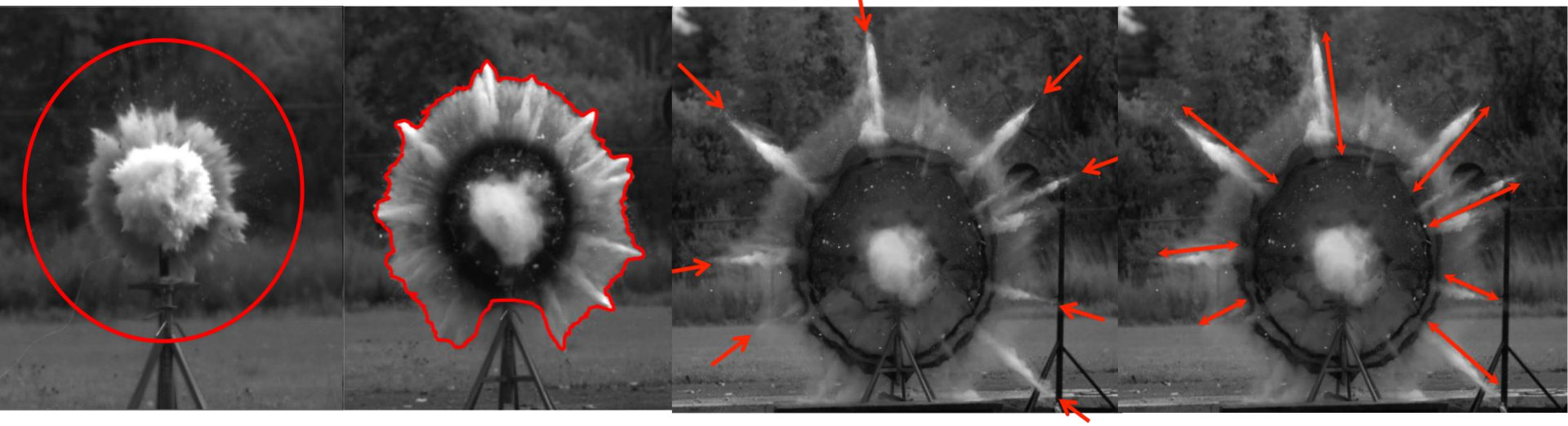
Prediction Metrics

PM-1: Blast Wave Location

PM-2: Particle Front Location

PM-3: Number of Instability Waves

PM-4: Amplitude of Instability Waves

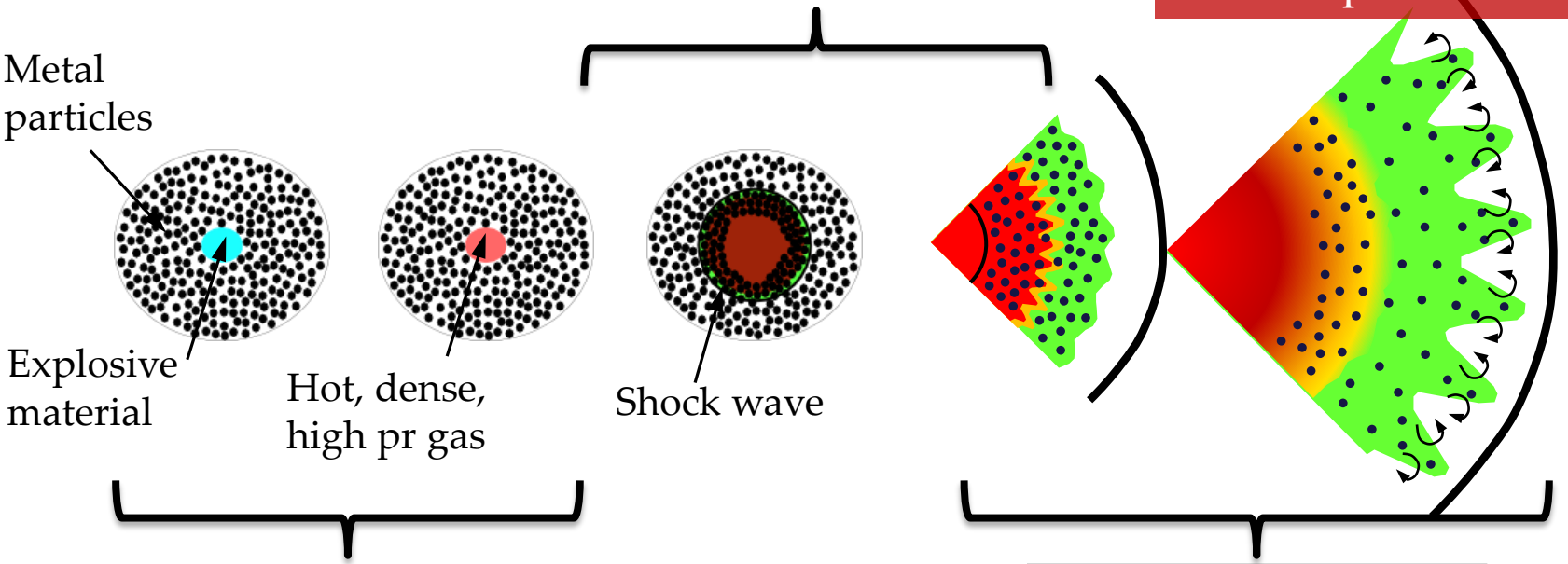


Physical Models – Sources of Error

T8:Deformation model

Compaction/collision phase

T4: Interaction model
T5:Compaction model



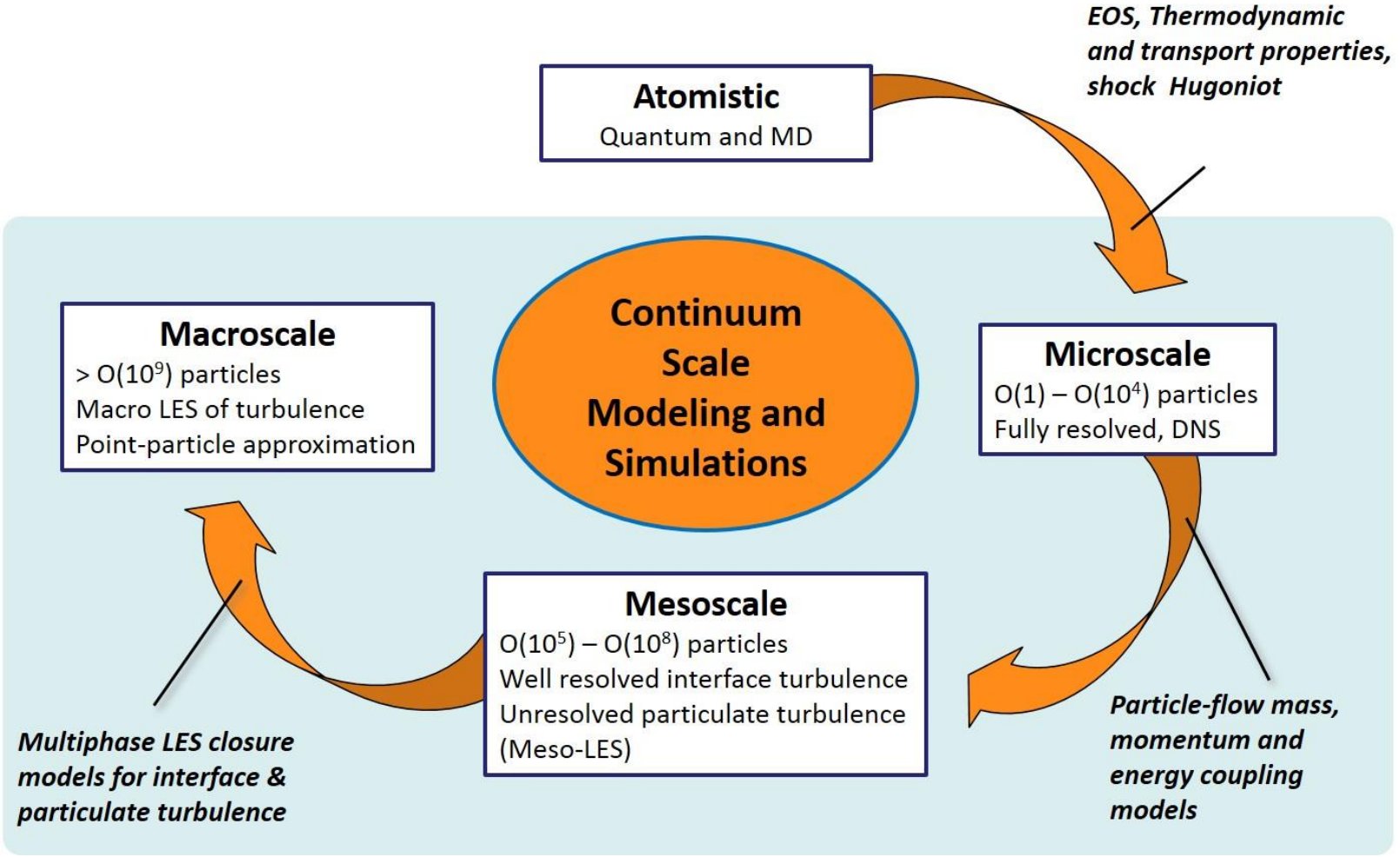
Detonation phase

Dispersion phase

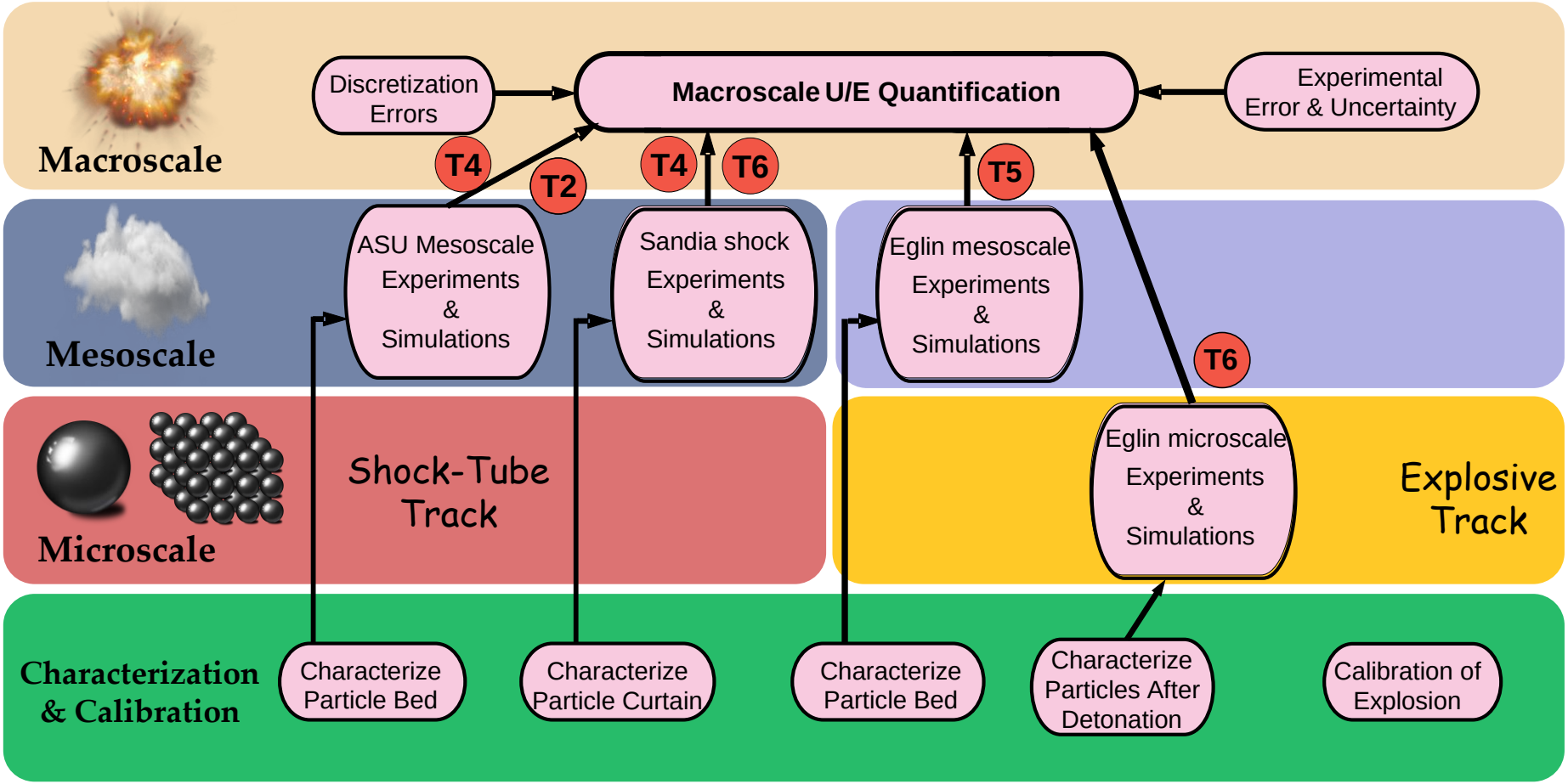
T1:Detonation model

T2: Multiphase turbulence model
T3:Thermodynamic & transport model
T6: Point particle force model
T7: Point particle heat transfer model

Multiscale Integration Strategy



Uncertainty Budget – Overall Plan



- T2 – Turbulence modeling
- T4 – Particle interaction modeling
- T5 – Compaction modeling
- T6 – Force coupling modeling

Y1-Y4 Accomplishments

1. Uncertainty quantified experiments (Forensic UQ)
2. Co-design of CMT-nek – An Exascale code
3. Dynamic load balancing – A must for multiphase flow
4. Physics-driven & data-driven modeling
5. Design space exploration with Behavioral Emulation (BE)

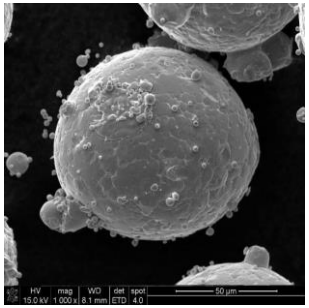
Lab Interactions

Validation Blastpad Experiments (@Eglin AFB)

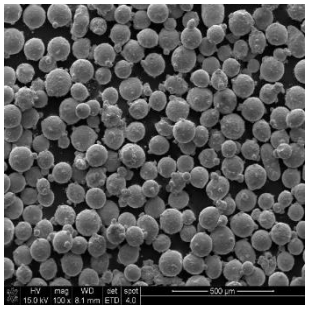
Input Parameter	Source
Explosive length [mm]	AFRL measurement
Explosive diameter [mm]	AFRL measurement at 5 locations
Explosive density [kg/m^3]	AFRL calculation
Explosive quality	AFRL X-ray
Particle diameter [mm]	CCMT measurement
Particle density [kg/m^3]	CCMT measurement
Particle volume fraction	AFRL calculation
Ambient pressure [kPa]	AFRL weather station
Ambient temperature [C]	AFRL weather station
Probe locations [m]	CCMT measurement

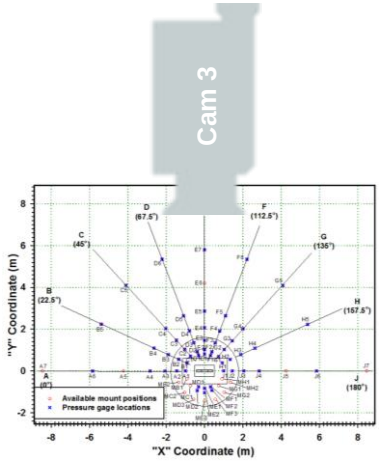
Poster: Kyle Hughes, UF

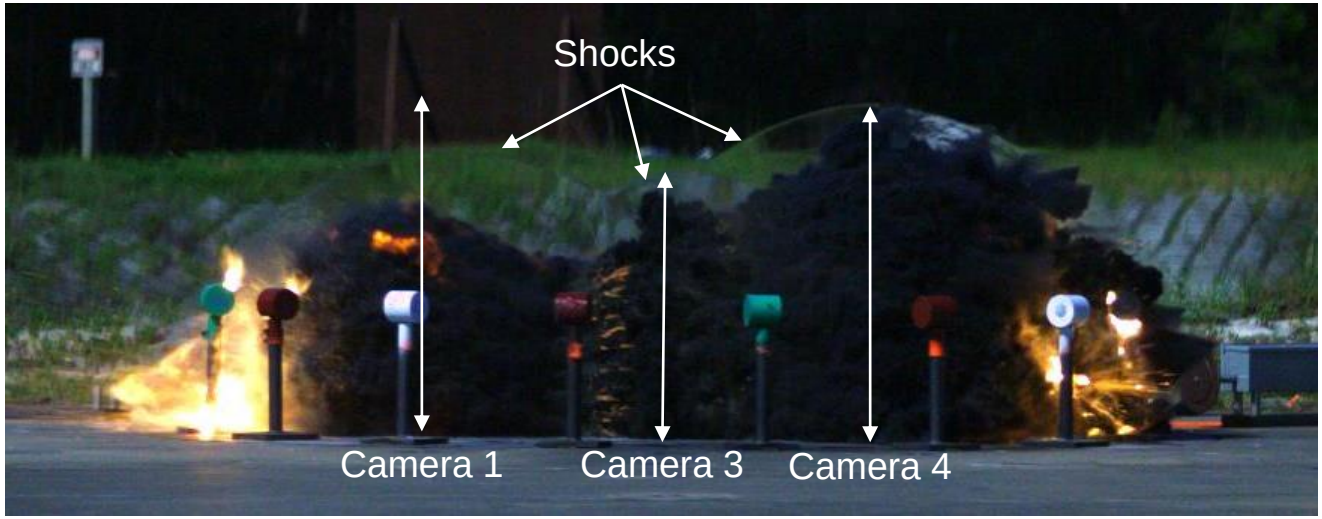
SEM of single steel particle at 1000x zoom.



SEM of several steel particles at 100x zoom.







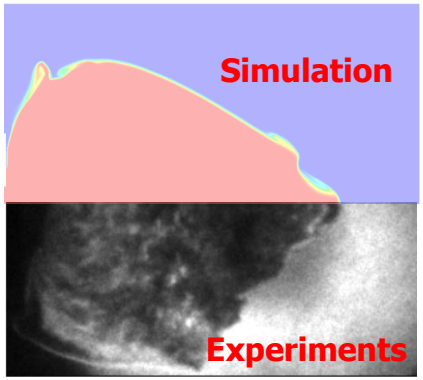
Cam 1

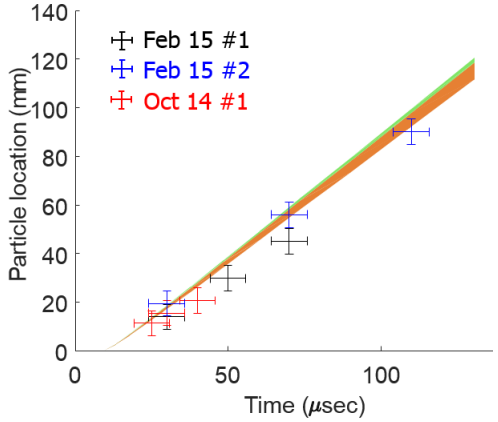
Cam 4

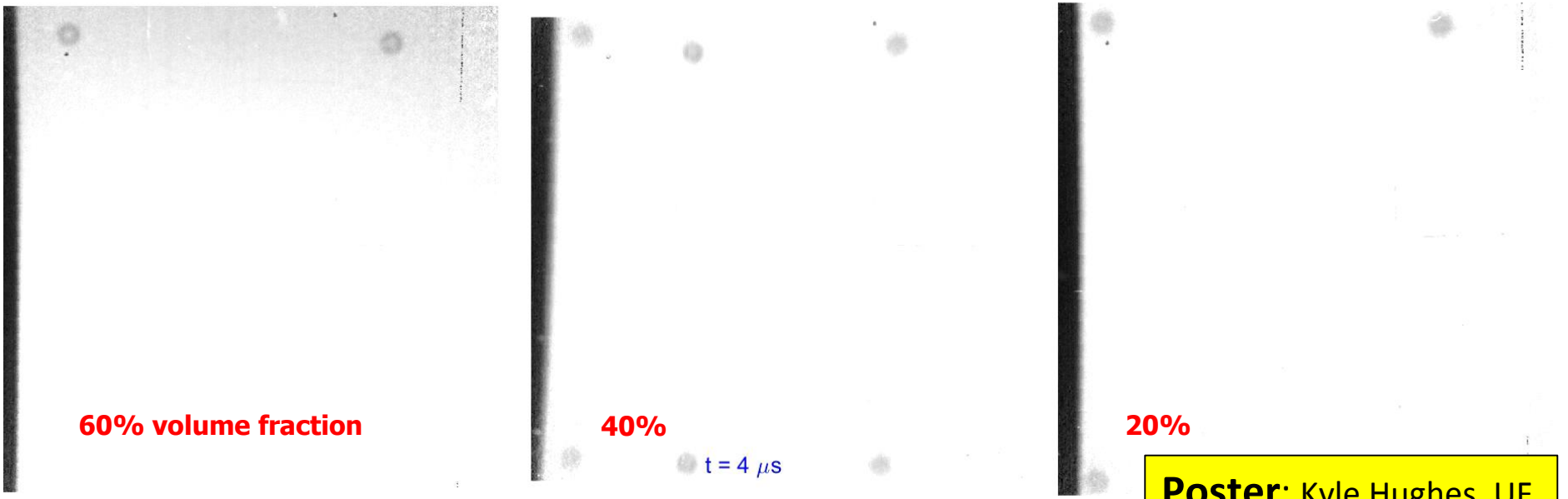
Camera 3 at 1.067 ms after detonation showing the differing results for shock position

CCMT

Other Microscale & Mesoscale Experiments







Poster: Kyle Hughes, UF

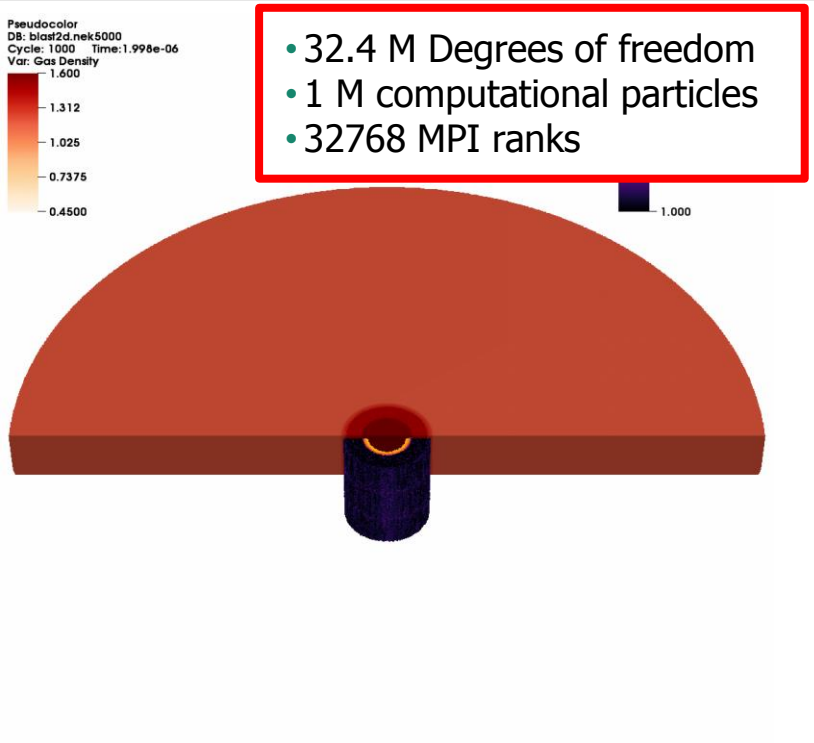
Mesoscale P-rad experiments performed at LANL

CMT-nek Development

Goals

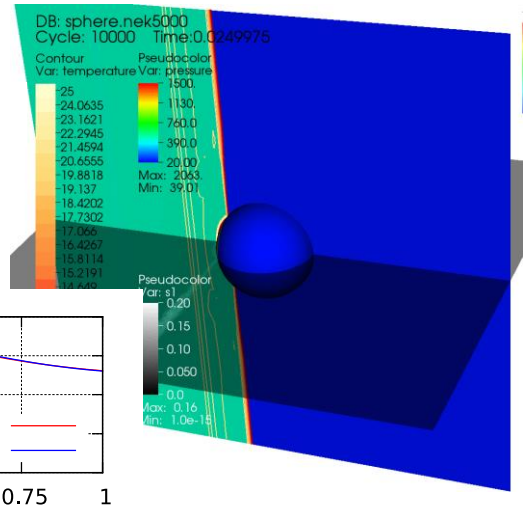
- Co-design an exascale code (CMT-nek) for compressible multiphase turbulence
- Perform micro, meso and demonstration-scale simulations
- Develop & incorporate energy and thermal efficient exascale algorithms

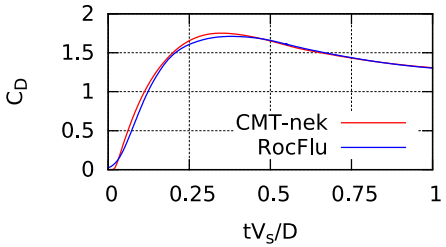
Poster: David Zwick, UF

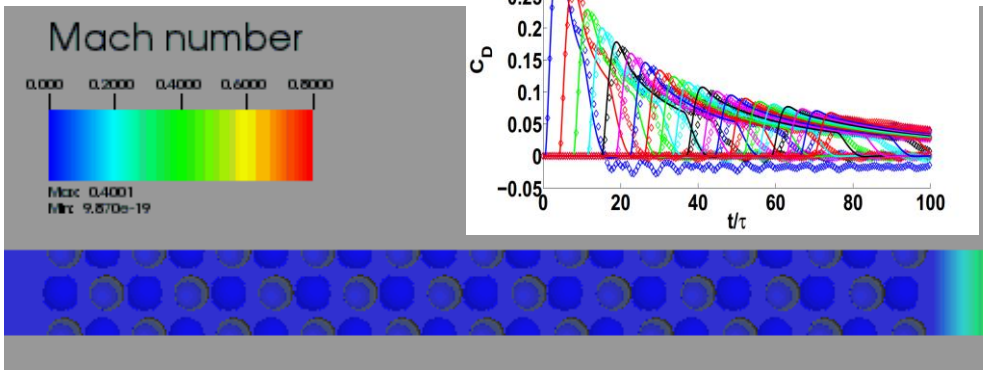


- 32.4 M Degrees of freedom
- 1 M computational particles
- 32768 MPI ranks

Mach 3

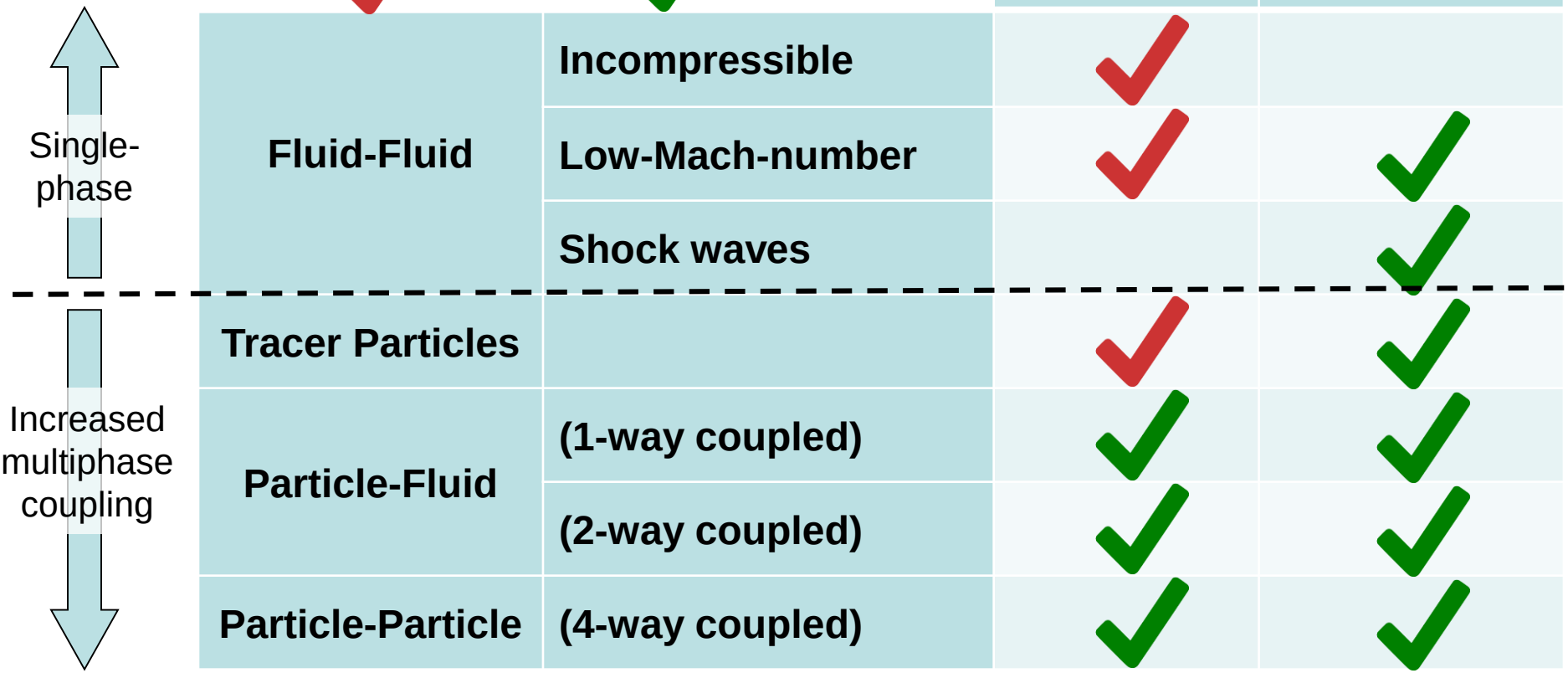






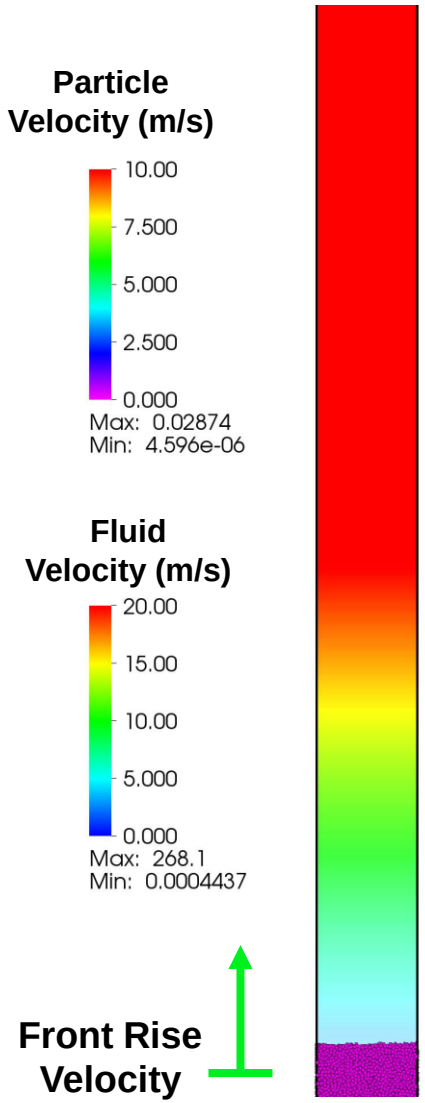
CCMT

Nek5000 + CMT-nek = Powerful Tool



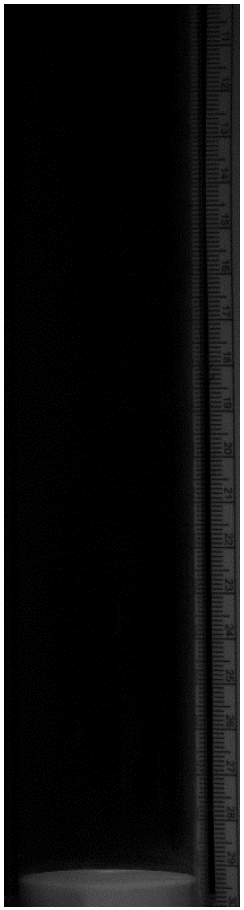
- Goal is to expand from current ~250 users to O(1000) worldwide users
- Last month UF hosted the nek5000/CMT-nek developer/user meeting
- Key features: higher-order accuracy and scalability to O(10^6) MPI ranks

Expansion Fan – Particle Bed Interaction



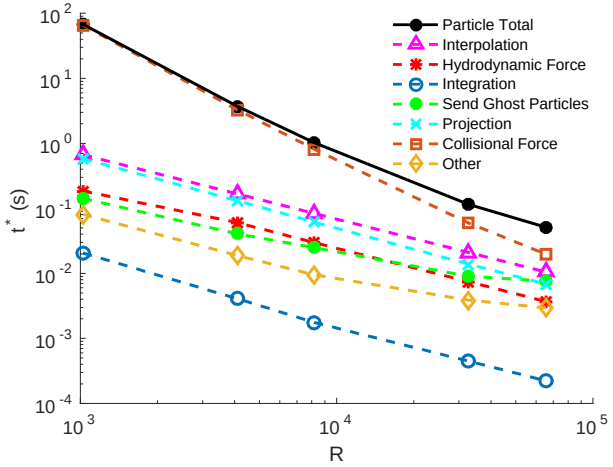
Case 2

ASU Experiment



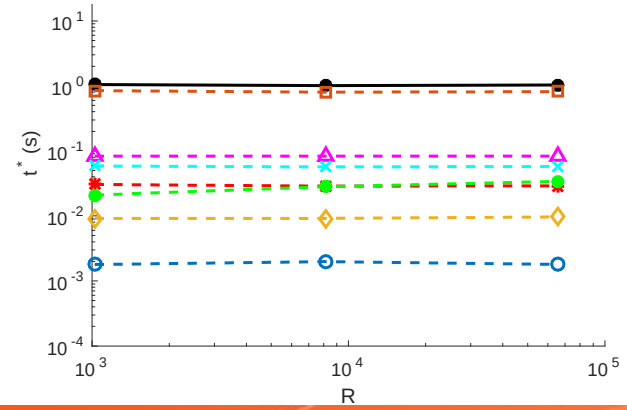
Strong Scaling:

- 15 million grid points
- 8.4 million particles

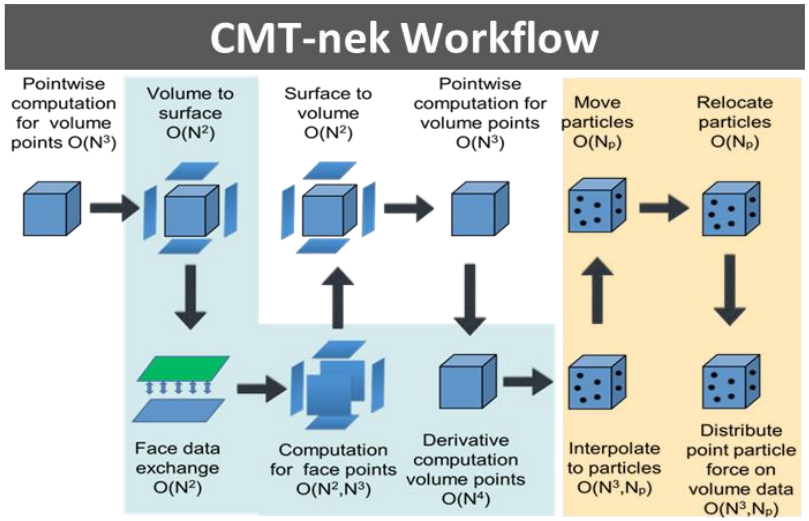


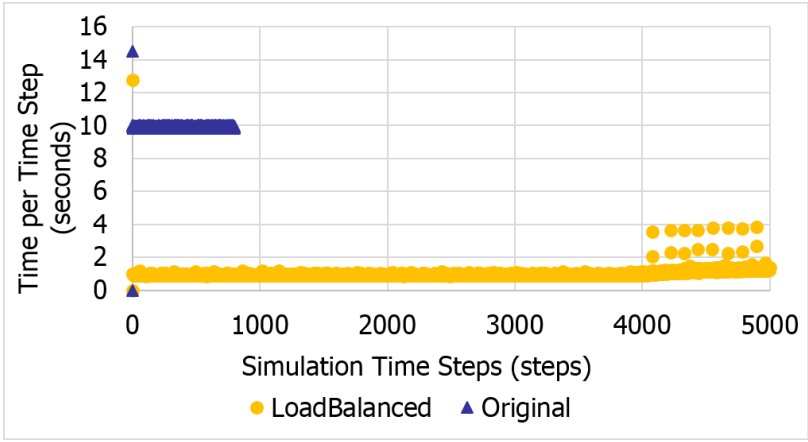
Weak Scaling:

- 864 grid points/rank
- 1024 particles/rank



Co-Design & Dynamic Load Balancing





- Ghost particle algorithm
- Crystal-tuple inter-node data transfer for particles
- Dynamic load balancing: Centralized, distributed and hybrid algorithms
- Adaptive automated triggering of load balance
- Novel trace-based performance predictor

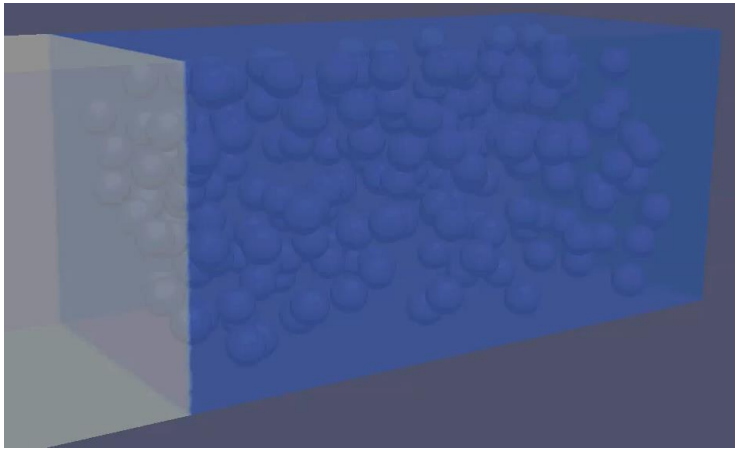
67,206 MPI ranks
1,867 nodes,
36 cores/node
112 Million grid points
1,125,000,000 particles
Rarefaction test
9.97x improvement in performance

Poster: David Zwick, UF

Fully-Resolved Microscale Simulations

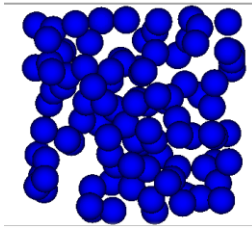
Purpose

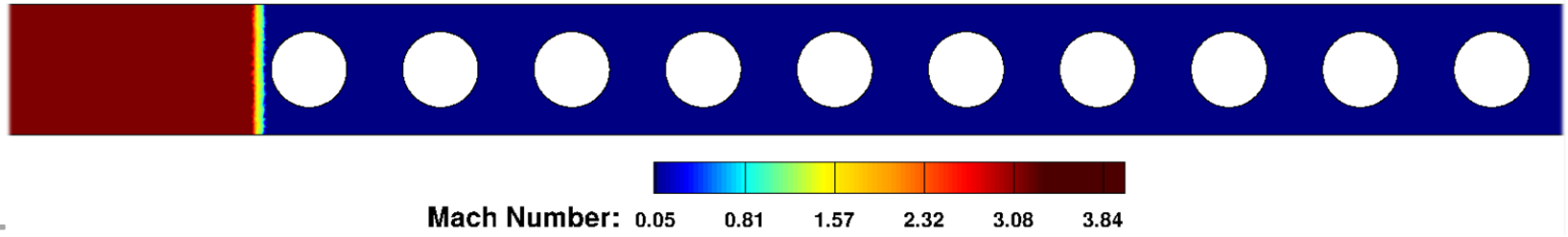
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation



- Shock propagation over a structured array
- Shock propagation over a random array
- Shock + Contact + particles
- Shock over deformable particles

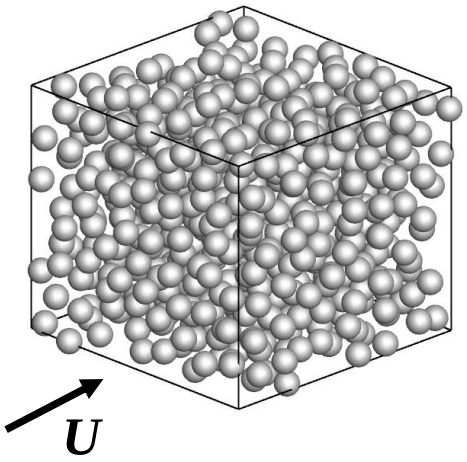
With Kambiz Salari (LLNL)



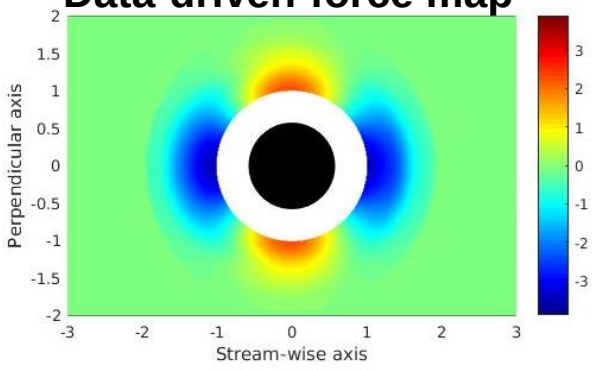


PIEP Modeling Through Machine learning

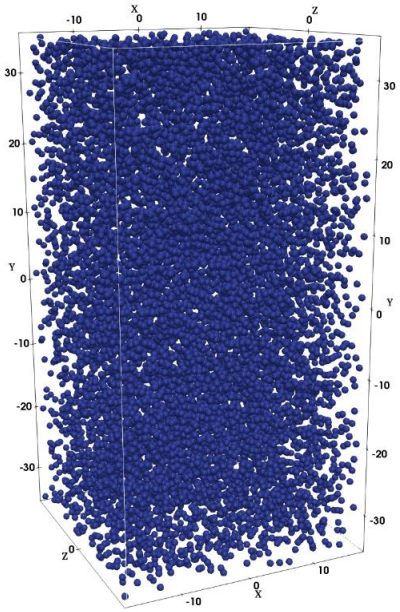
$\phi = 44\%, Re = 20, \mathrm{N} = 459$



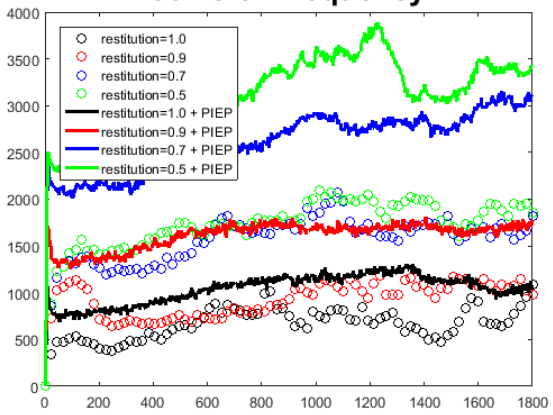
Data-driven force map



Nek5000 simulation with PIEP



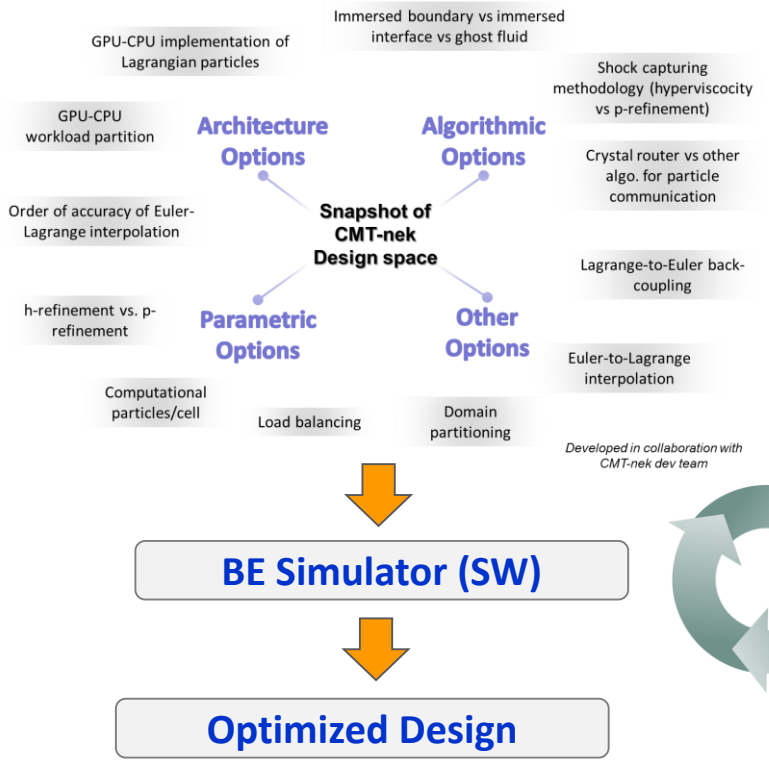
collision frequency



R² Values:		PIEP-Physics			PIEP-Hybrid		
ϕ	*Re*	Drag	Lift	Torque	Drag	Lift	Torque
0.1	**40**	0.70	0.68	0.75	0.72	0.75	0.79
0.1	**70**	0.65	0.68	0.65	0.67	0.72	0.72
0.1	**173**	0.35	0.59	0.45	0.44	0.60	0.58
0.2	**16**	0.38	0.34	0.48	0.66	0.74	0.71
0.2	**89**	0.50	0.48	0.72	0.62	0.63	0.77
0.45	**21**	0.01	0.09	0.47	0.55	0.59	0.76
0.45	**115**	0.21	0.19	0.51	0.63	0.57	0.65

CCMT **PIEP:** Pairwise Interaction Extended Point-particle

FPGA-Accelerated Design Space Exploration (DSE)



CMT-nek design space:

- **20 values for lelt, lx1, lpart**
- **10 different numbers of cores**
- **10 different core types**
- **10 different memory configurations**
- **4 different network topologies**

32 million options to explore

~Minutes per simulation

- **BE Advantage:** significantly faster than existing simulators
- **BE Limitation:** still not fast enough for DSE of exascale systems
- **Approach:** Use FPGA acceleration to improve exploration
  - Sacrifice analysis capabilities to prune design space
  - Use BE-SST to analyze remaining candidates

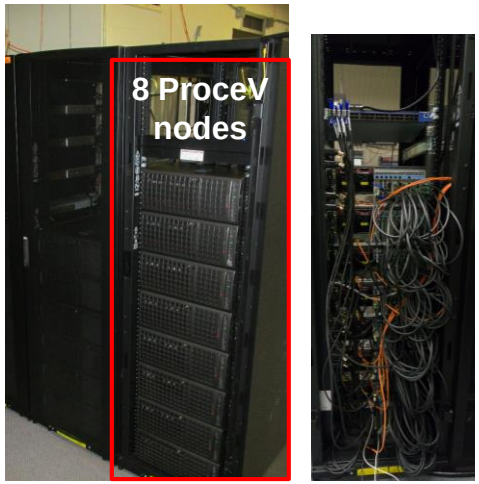
Collapsed Pipeline Multi-FPGA Performance

CMT-Bone-BE is the proxy app

Performance prediction & DSE on varies MPI ranks

Behavioral emulation: BE-SST (software) vs FPGA (hardware)

Main point: FPGAs achieve similar scalability as BE-SST, but orders of magnitude faster



Ranks	TS	Num. of Events	% LU	Latency (cycles)	Hardware MSPS†	Hardware GEPS‡	BE-SST KEPS‡	Hardware Speedup
32	32	43,008	44	7,532	10.5	450	10.14	$44x10^6$
64	32	92,160	46	10,252	5.23	482	24.91	$19x10^6$
128	32	190,464	47	10,316	2.62	498	24.42	$20x10^6$
256	32	393,216	67	13,516	1.31	515	23.92	$21x10^6$
512	32	811,008	84	20,684	0.65	531	21.47	$25x10^6$
1K	32	1,646,592	84	21,196	0.33	539	18.21	$29x10^6$
32K	32	55,443,456	84	241,868	$1.02x10^{-2}$	567	12.96	$44x10^6$
128K	16	111,673,344	46	333,932	$2.56x10^{-3}$	285	8.91	$32x10^6$
1M	2	112,459,776	5	1,148,056	$3.19x10^{-4}$	36	X	X

Novo-G#

- 64 GiDEL ProceV (Stratix V)
- 4x4x2 3D torus or 5D hypercube
- 6 Rx-Tx links per FPGA
- Measured 32 Gbps per link
- 150 ns latency across links
- Require 64bits/cycle between FPGAs
- 335MHz, 21.4 Gbps, 51 additional lat
- 450MHz, 28.8 Gbps, 68 additional lat
- 500 MHz before link BW saturation

C. Pascoe, S. Chenna, G. Stitt, H. Lam, "A FPGA-Pipelined Approach for Accelerated Discrete-Event Simulation of HPC Systems", Heterogeneous High-performance Reconfigurable Computing (H2RC), Denver, CO, Nov. 13, 2017.

NNSA Lab Interaction

Student Internship Completed (19)

- Heather Zunino, Mentor: Dr. Kathy Prestridge (LANL)
- Kevin Cheng, Mentors: Dr. Maya Gokhale, Dr. Scott Lloyd (LLNL)
- Nalini Kumar, Mentor: Dr. James Ang (SNL)
- Chris Hajas, Mentor Dr. Maya Gokhale (LLNL)
- Christopher Neal, Mentor Dr. Kambiz Salari (LLNL)
- Carlo Pascoe, Mentor Dr. Maya Gokhale (LLNL)
- Giselle Fernandez, Mentors: Dr. Greogy Weirs, Dr. Vincent Mousseau (SNL)
- Justin Mathew, Mentor: Dr. Nick Hengartner (LANL)
- Trokon Johnson, Mentors: Drs. Cristina Garcia-Cardona, Brendt Wohlberg, Erik West (LANL)
- David Zwick, Mentors: Dr. John Pott, Dr. Kevin Ruggirello (SNL)
- Mohamed Gadou, Mentor: Dr. Galen Shipman (LANL)
- Goran Marjanovic, Mentors: Dr. Paul Crozier, Dr. Stefan Domino (SNL)
- Georges Akiki, Mentor: Dr. Marianne Francois (LANL)
- Paul Crittenden, Mentor: Dr. Sam Schofield (LLNL)
- Yash Mehta, Mentor: Dr. Kambiz Salari (LLNL)
- Kyle Hughes, Mentor: Dr. Kathy Prestridge (LANL)
- Prashanth Sridharan, Mentor: Dr. Jonathan Regele (LANL)
- Brad Durant & Fred Ouellet, Will finish internship this fall

Graduated PhD Students & Postdocs

- Angela Diggs, PhD (2015), Dr. S. Balachandar, MAE
  - Eglin AFB (continuing)
- Bertrand Rollin, Postdoc in thru August 2014
  - Assistant Professor, Embry Riddle, Daytona Beach FL
- Mrugesh Shringarpure, Postdoc in thru January 2016
  - Research Engineer, ExxonMobil, Houston TX
- Subbu Annamalai, PhD (2015), Dr. S. Balachandar, MAE; Postdoc in thru March 2017
  - Senior Systems Engineer, Optym, Gainesville FL
- Georges Akiki, PhD (2016), Dr. S. Balachandar, MAE; Postdoc thru March 2017
  - Postdoctoral Associate, LANL
- Nalini Kumar, PhD (2017), Dr. H. Lam, ECE
  - Intel, Santa Clara CA
- Yiming Zhang, PhD (2018), Drs. Haftka and Kim, MAE
  - GE Global Research, Niskayuna, NY
- Mohammad Gadou, PhD (2018), Dr. S. Ranka, CISE
  - Bloomberg, New York, NY
- Cameron Stewart, PhD (2018), Dr. Balachandar, MAE
  - Naval Surface Warfare Center, Indian Head, MD

4 More PhDs graduating this summer

Additional Information

- Additional Graduate Program Announcements
  - David Zwick – NSF Fellowship Graduate Program (Aug 2016)
  - Georges Akiki - MAE Best Dissertation Award (TSFD; May 2017)
  - Chandler Moore – NSF Fellowship Graduate Program (Aug 2017)
  - 6 other PhD students – UF Graduate Student Fellowship
- Other metrics (Y1 – Y4)
  - Publications: 134
  - Presentations: 94
- Deep Dive Workshops
  - Exascale & CS Issues, Feb 3-4, 2015, University of Florida
  - Multiphase Physics, Oct 13-14, 2016, Tampa FL
  - CMT-nek/nek5000, April 17-18, 2018, Tampa FL
- Center Webpage
  - http://www.eng.ufl.edu/ccmt/

Do you have any questions?