

Accelerating predictive simulation of IC engines with high performance computing (ACE017)

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Overall project *objectives and relevance*

Address technical barriers facing the transportation industry through innovative use of predictive simulation and leveraging of DOE's ASCR leadership HPC facilities and fundamental research tools

- **Reduce time-to-market**
 - Enable accelerated development of advanced engines meeting fuel economy and emissions goals
 - Parallelization, automation, and optimization of the design process
 - **Solve the unsolvable**
 - Apply massively parallel, peta-scale HPC to address problems historically limited by computational resources
 - **Develop and evolve new capabilities**
 - Develop and apply *innovative simulation tools and strategies* that maximize benefits of predictive information from HPC
 - Translate capabilities from *HPC* to *desktop* to *on-board diagnostics and controls*
-
- **Project supports multiple, multi-year efforts with industry and university partners**
 - Addresses specific technology barriers identified by DOE and industry stakeholders
 - DOE funds support open, pre-competitive efforts
 - Tools and approaches developed are available to industry for proprietary efforts
 - **Specific efforts evolve in response to direction from DOE and industry stakeholders**
 - Accommodates new efforts in addition to existing efforts and/or as existing efforts come to completion



Overview

Timeline

- Project start – May 2012
- Ongoing

Budget

- FY2012 – \$250k
- FY2013 – \$400k
- FY2014 – \$400k
- FY2015 – \$400k
\$100k CRADA

Barriers

- Directly targets barriers identified in the VTO MYPP
 - “Lack of modeling capability for combustion and emission control”
 - “Lack of fundamental knowledge of advanced engine combustion regimes”

Partners

- Leveraging DOE Office of Science funding for ASCR resources
 - 2 ALCC and 1 DDR allocations on OLCF HPC resources
 - 32.5+ Mhrs @ \$0.03/hr = \$975k
- Multiple ongoing efforts with industry and academic involvement



- CRADA effort for GPU acceleration of numeric solvers



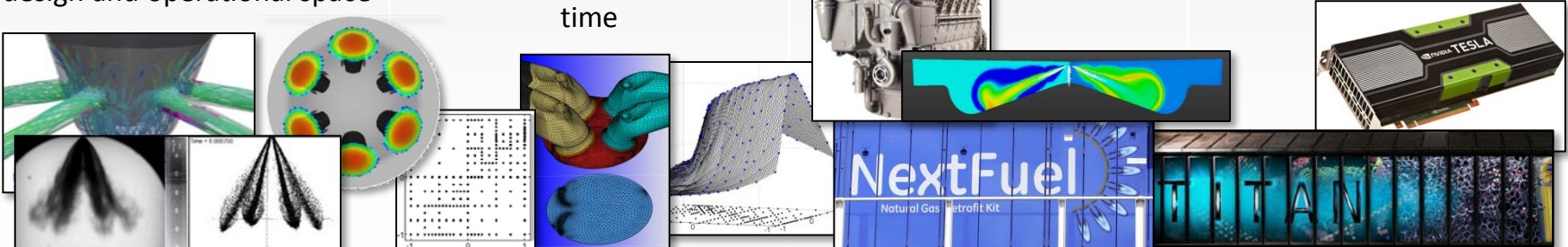
- Supports OPTIMA simulation team



- Developing relationship with Ohio State University on knock modeling

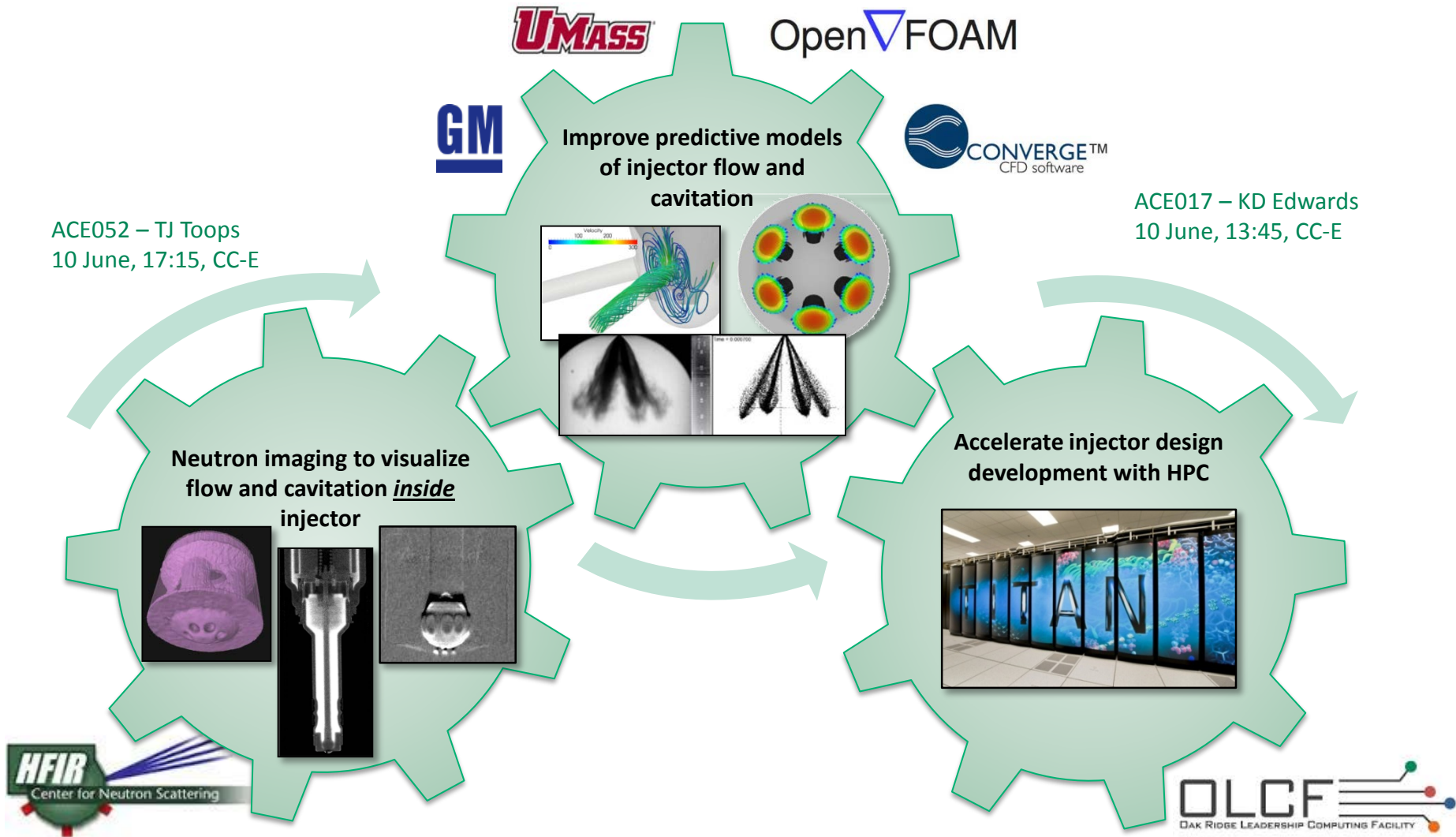


Ongoing collaborative efforts

Reduce time-to-market	Solve the unsolvable		Evolve capabilities
GDI fuel injector design optimization 	Understanding cycle-to-cycle variation Highly dilute ICEs 	Dual-fuel locomotive 	GPU acceleration of numeric solvers 
Understand and optimize GDI injector design for improved efficiency and reduced emissions 2014 ALCC award - 15Mhrs 2015 ALCC submission Parallelization & automation of labor-intensive tasks Coupling models of internal injector flow and cavitation with in-cylinder spray and combustion Enables rapid investigation and optimization across full design and operational space	Understand stochastic and deterministic processes driving cyclic variability in highly dilute SI engines 2014 ALCC award - 17.5Mhrs Novel approach to <u>parallel</u> simulation of a <u>serial</u> phenomena Uncertainty quantification with intelligent sampling Enables creation of low-order metamodels that retain key dynamics of CFD model but greatly reduce computational time	Investigate key factors promoting cyclic variability in a dual-fuel (NG/diesel) locomotive application 2015 ALCC submission Adapting metamodel approach to examine dual-fuel stability Stable dual-fuel operation will enable significant displacement of petroleum-based diesel fuel with NG	CRADA effort seeking to implement GPU acceleration for numeric solvers LLNL – Chemistry solvers ORNL – Flow & combustion solvers Titan & Big Red II – Code evaluation Cummins – Validation data Enables faster runtimes and/or higher-resolution simulations with more-detailed chemistry
			

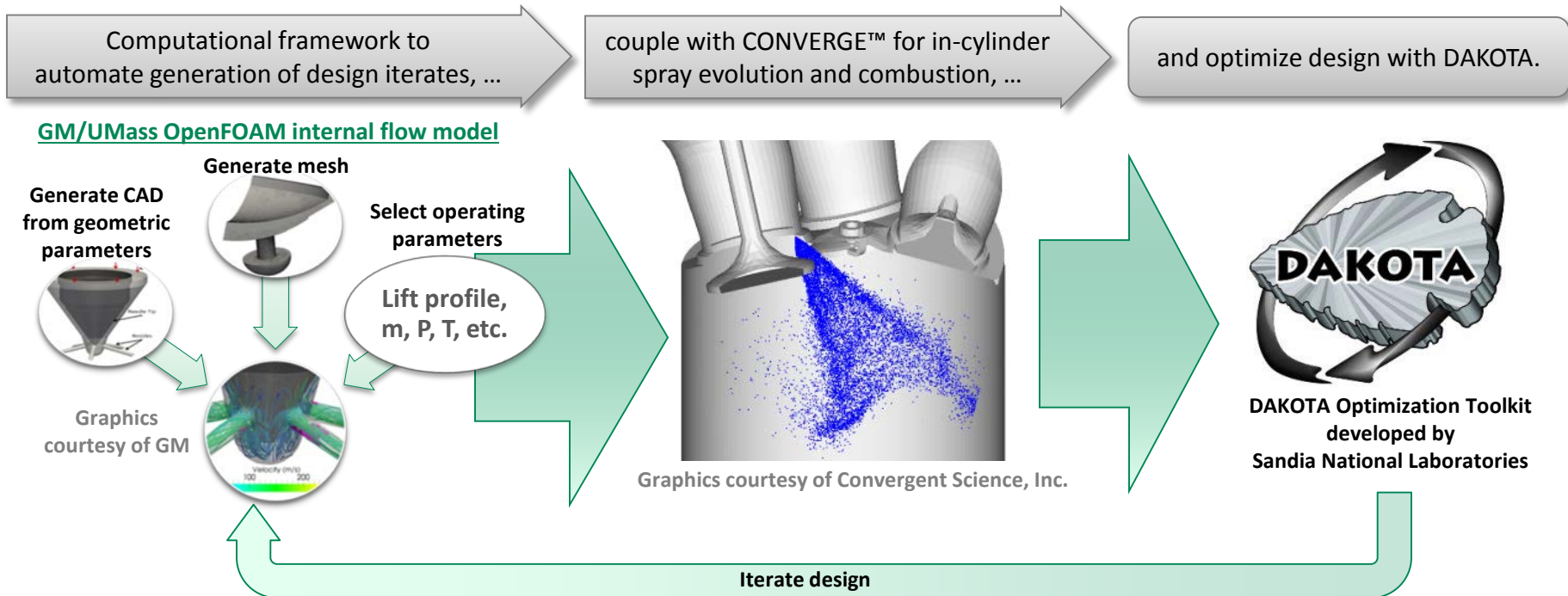
Accelerating GDI fuel injector design optimization

ORNL and GM partnering on multiple projects to validate, improve, and employ predictive injector flow models



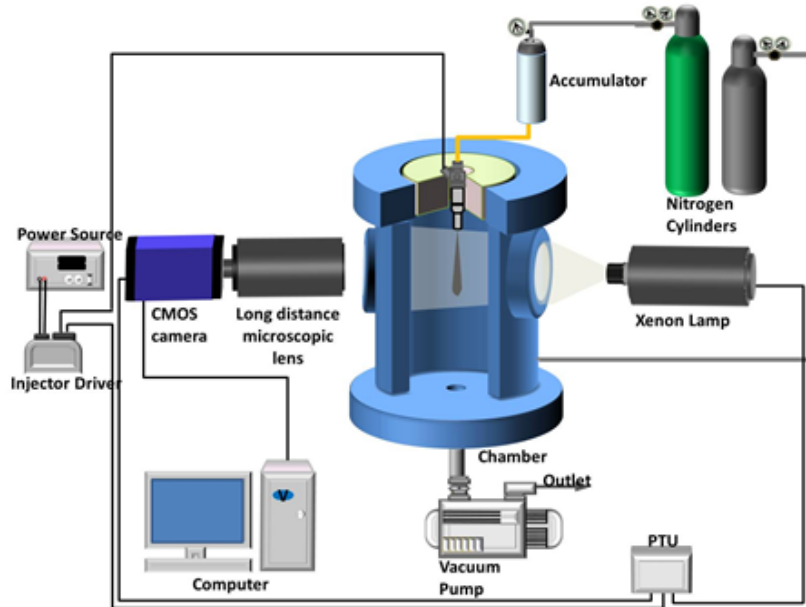
GDI fuel injector design optimization – *Relevance and Approach*

- Collaborative effort with General Motors and University of Massachusetts
- Injector design optimization is currently a lengthy, labor-intensive process
 - Iterative effort requiring several hardware iterations
- HPC enables thorough & rapid investigation of operational & geometric design spaces
 - Reduce design cycle from months to weeks AND more enable thorough coverage of design space
- **Current focus is to validate a methodology towards more accurate spray modeling**
 - Coupling of the internal flow field to initialize an external spray solver
 - Validate the methodology against experimental measurements

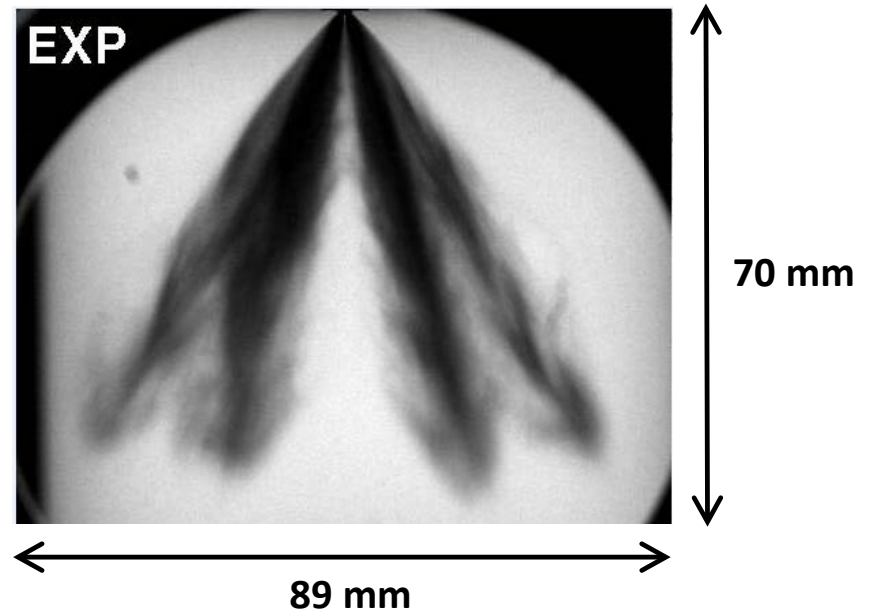


Model validation using experimental spray imaging from GM – Approach

Schematic of GM visual interference imaging setup



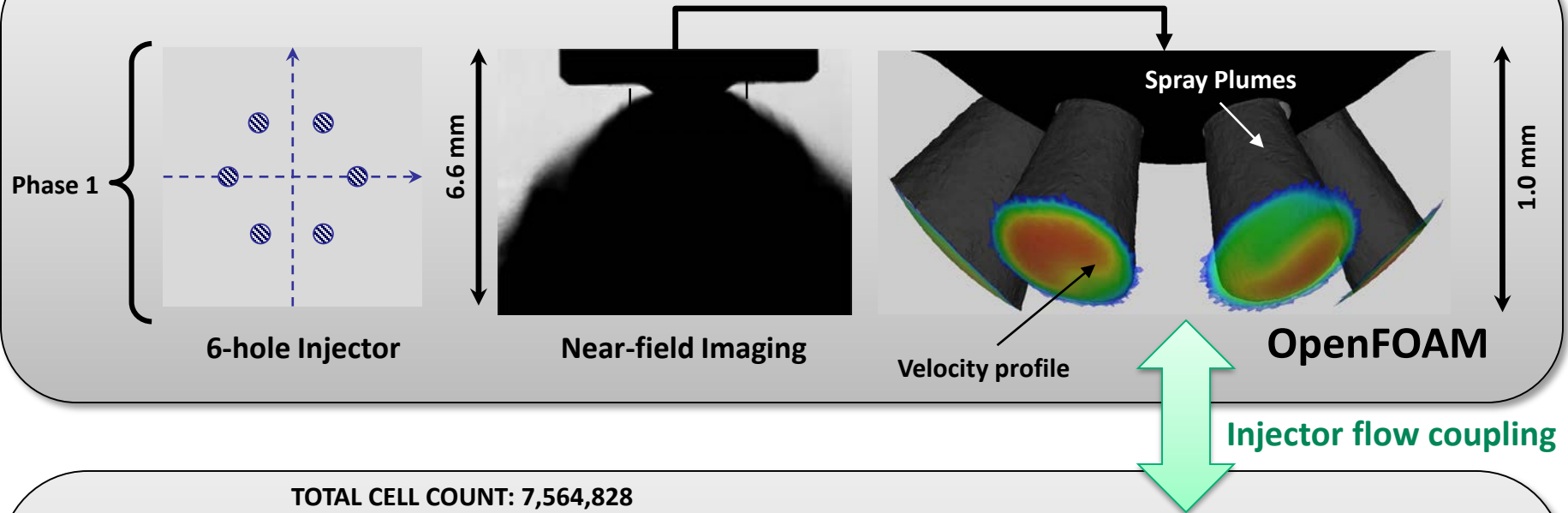
Sample image



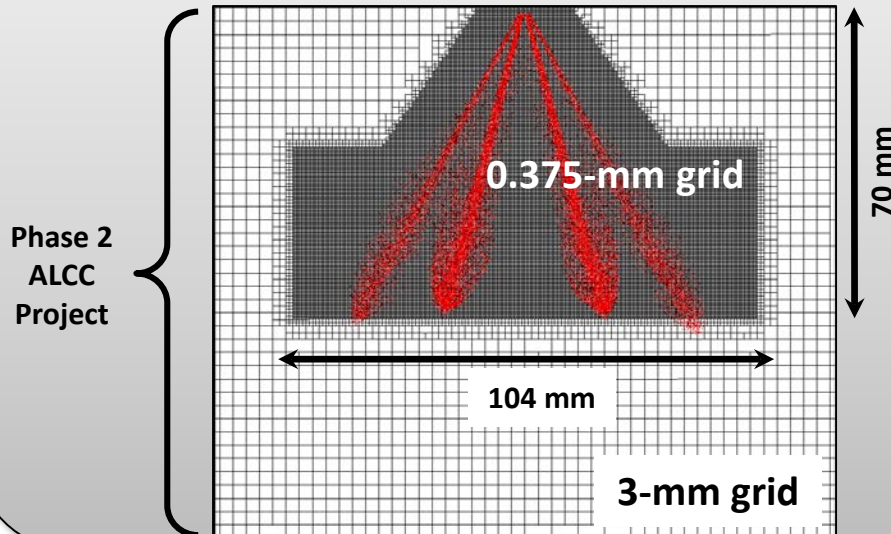
Parameter	Metric
Working fluid	n-hexane
Injection Pressure (MPa)	15
Ambient Pressure (kPa)	40
Fuel Temperatures (°C)	25 – 85
Ambient Temperature (°C)	20

Coupling of internal and in-cylinder spray – *Technical Accomplishments*

Internal Flow simulations



TOTAL CELL COUNT: 7,564,828



External Spray Simulations

CONVERGE™ External Spray Simulations

- Customized UDF to read in nozzle internal flow velocity profile from OpenFOAM simulations
- Fixed mesh embedding to resolve the propagation of the spray
- Semi-empirical injection routine
 - Droplets injected post primary atomization
 - Collision & Coalescence model turned OFF

Internal nozzle flow simulations capture flash boiling impacts on plume angle – *Technical Accomplishments*

Inlet

Fluid property table based on REFPROP

$$P_{inj} = 15 \text{ MPa}$$

$$T_{fuel} = 25 - 85 \text{ }^{\circ}\text{C}$$

Flow Through

Tracks two species

1. Liquid Fuel
2. Fuel vapor (HRM)

$$\frac{Dx}{Dt} = \frac{\bar{x} - x}{\theta}$$

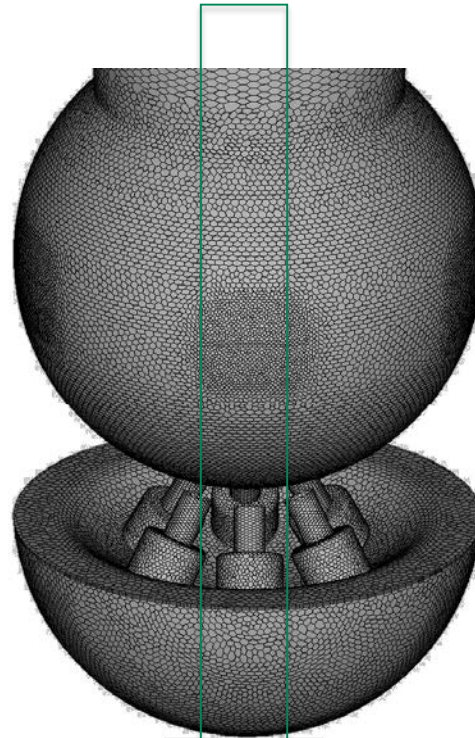
$$\theta = \theta_0 \alpha^{-0.54} \psi^{-1.76}$$

Ambient

Fuel Properties

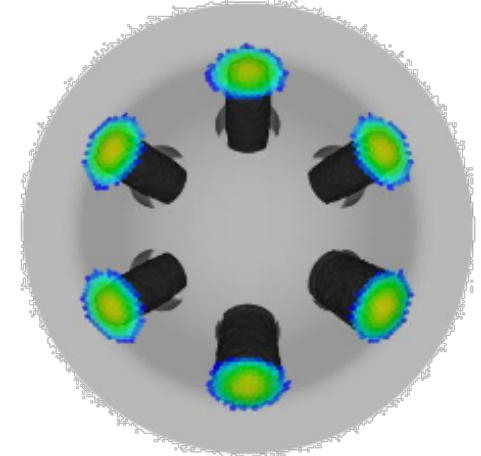
$$P_a = 40 \text{ kPa}$$

$T_a \rightarrow$ based on inlet fuel enthalpy

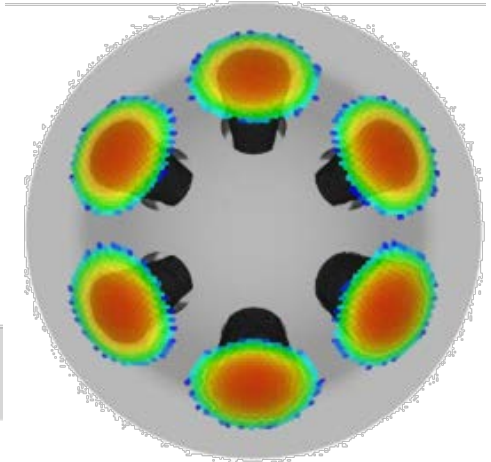
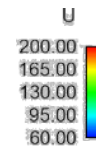


Flow direction

$$P_a = 40 \text{ kPa } T_{fuel} = 25^{\circ}\text{C}$$



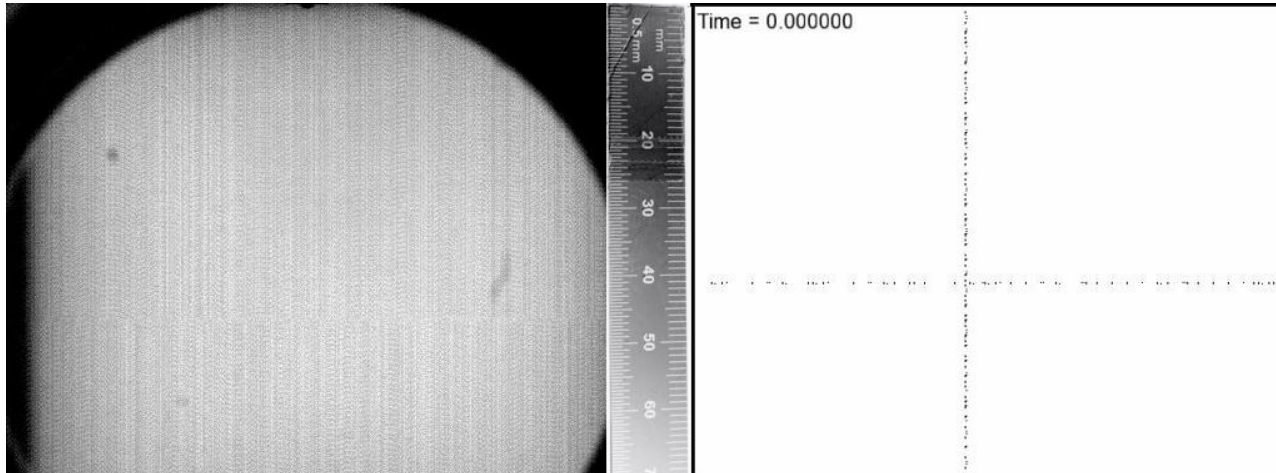
$$P_a = 40 \text{ kPa } T_{fuel} = 85^{\circ}\text{C}$$



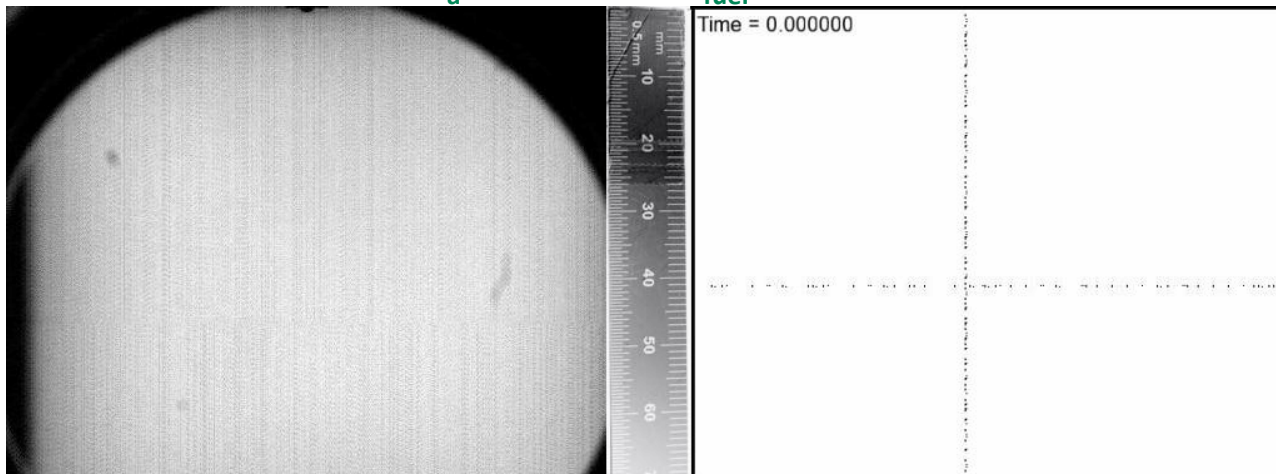
Flash-Boiling leads to increase in nozzle-exit plume angle

External spray simulation results validated with GM spray visualization data – *Technical Accomplishments*

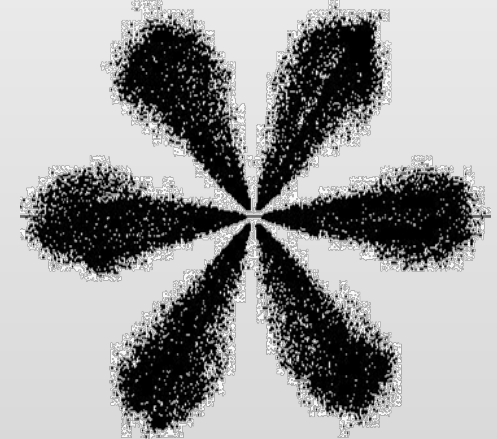
$P_a = 40 \text{ kPa}$ $T_{\text{fuel}} = 25^\circ\text{C}$



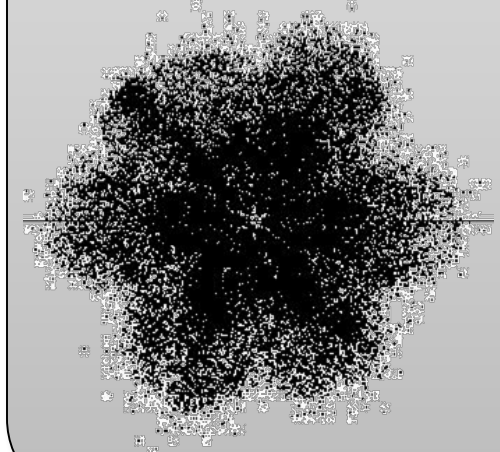
$P_a = 40 \text{ kPa}$ $T_{\text{fuel}} = 85^\circ\text{C}$



On-axis View



Spray collapse driven by
increase in plume-to-plume
interaction



@ 0.5 ms

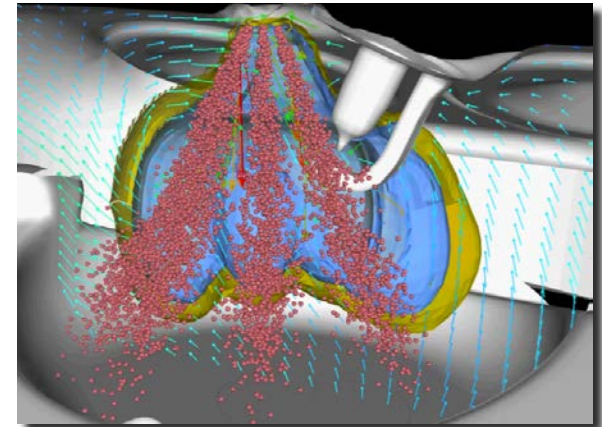
Remaining challenges and Future work

Remaining challenges and barriers

- Validate fully coupled model with combustion
- GPU acceleration to take full advantage of Titan's resources
- Demonstrate accelerated and fully optimized “start-to-finish” injector design

Ongoing and future work

- **Submitted 2015 ALCC application** (20 Mhrs on Titan, 2 Mhrs on EOS)
- **Remainder of FY2015**
 - Validate methodology over a larger test matrix
 - Additional fuel temperatures and pressures
 - Additional injector hole geometries
 - Evaluate improvements to internal flow model by UMass
 - Accounts for fuel (liquid & vapor) and gas (N₂)
- **FY2016**
 - Utilize CONVERGE™ for full engine simulations with combustion
 - Validate with experimental data
 - Optimize nozzle geometry for best mixing
- **FY2017-2018**
 - GPU acceleration of OpenFOAM & CONVERGE™ models
 - Leverage current CRADA
 - Ongoing discussions with NVIDIA, Fluidyna for OpenFOAM
 - Demonstrate accelerated, fully optimized injector design

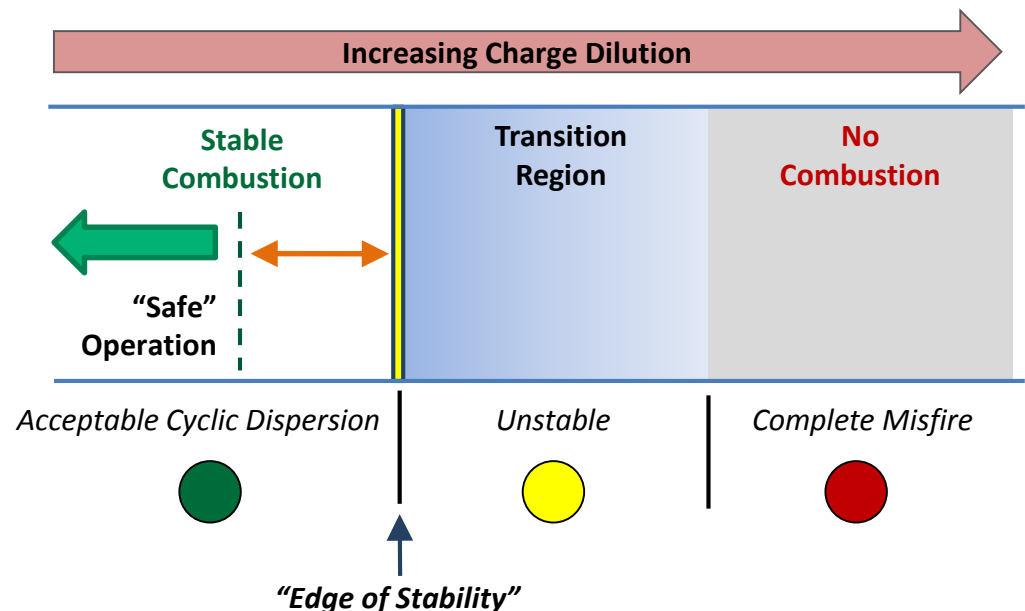


Graphics provided by General Motors

Understanding cycle-to-cycle variation in ICEs

Understanding cyclic combustion variability – *Relevance*

- **Combustion stability is a potential barrier to realizing the full benefits of many advanced combustion strategies**
 - Current approach is to operate a “safe” distance from “edge of stability”
- **ORNL has long history and considerable expertise in studying and controlling combustion variability**
 - Includes ongoing experimental efforts (ACE090 – BC Kaul; next talk)
- **Combustion instabilities typically driven by stochastic (in-cylinder variations) and deterministic (cycle-to-cycle and cylinder-to-cylinder coupling) processes**
 - Short-term predictable
 - Understanding the nature and causes of instability enables potential for redesign and control
- **HPC and CFD models enable detailed study of key factors promoting cyclic variability**
 - Thousands of simulated cycles required to study problem with statistical accuracy
 - Previous studies limited by available computing resources



As an example, the potential efficiency and emissions benefits of high charge dilution (with either high EGR or lean operation) are limited by the need to operate at “safe” conditions for improved driveability and to avoid potential engine damage

Uncertainty Quantification Metamodel Approach

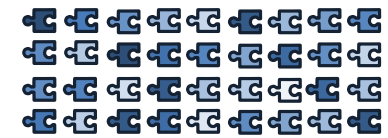
- Apply DOE ASCR tools and resources
 - TASMANIAN
 - OLCF HPC resources
- Parallel cycle simulations which cover the statistical behavior exhibited by serial combustion events
 - Sampling of initial parameter space must match statistics of key feedback parameters to capture cycle-to-cycle interactions
- Intelligent sampling of multi-dimensional parameter space
 - Adaptive sparse grid sampling of multiple parameters
 - Iterative method concentrates samples in high-gradient regions
 - $\sim 10^2$ samples vs. $\gg 10^6$ samples for Monte Carlo
- Detailed CFD combustion and kinetics simulations at sample points using CONVERGE™ on TITAN
 - Must have control over all initial inputs (no randomness)
- Create low-order metamodels of deterministic response
 - Multi-dimensional mapping of CFD model's response at sample points
 - Uncertainty Quantification (UQ) and stochastic collocation
 - Continuous and differentiable set of basis functions
 - Retains dominant features of detailed model's behavior
 - Allows rapid exploration of parameter space

TASMANIAN

Toolkit for Addaptive Stochastic Modeling And Non-Intrusive Approximation

Developed at ORNL with funding from the DOE Office of Science ASCR Program

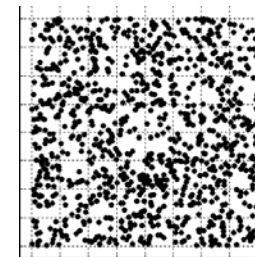
tasmanian.ornl.gov



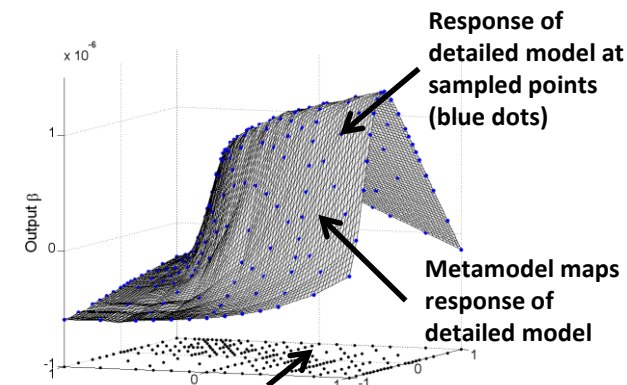
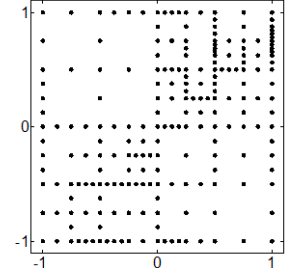
Must be statistically similar



Monte Carlo
(# samples $\gg 10^6$)



Adaptive Sparse Grid
(# samples $\sim 10^2$)



Detailed CFD simulations at sample points

Cyclic variability in highly dilute ICEs

- Relevance

- Enable operation at “edge of stability” to fully realize efficiency and emissions benefits of high dilution
- Collaborative effort with Ford and Convergent Science

- Approach

- ALCC award for 17.5 Mhrs on OLCF resources (Titan)

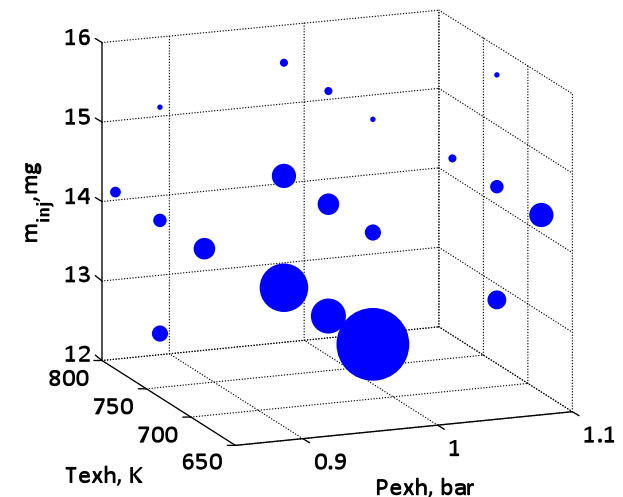
- Technical Accomplishments

- Adapted UQ metamodel approach to account for numeric variability introduced by stochastic inputs
 - High dilution cases are extremely sensitive to these stochastic inputs
 - e.g., Lagrangian spray models with Monte Carlo seeding of PDFs, LES turbulence model
 - Using Monte Carlo sampling of stochastic inputs to create multiple cycle simulations at each sample point
 - Increases computational effort
 - Pending publication
- Development and calibration of engine model with LES turbulence model underway

- Remaining Challenges and Future Work

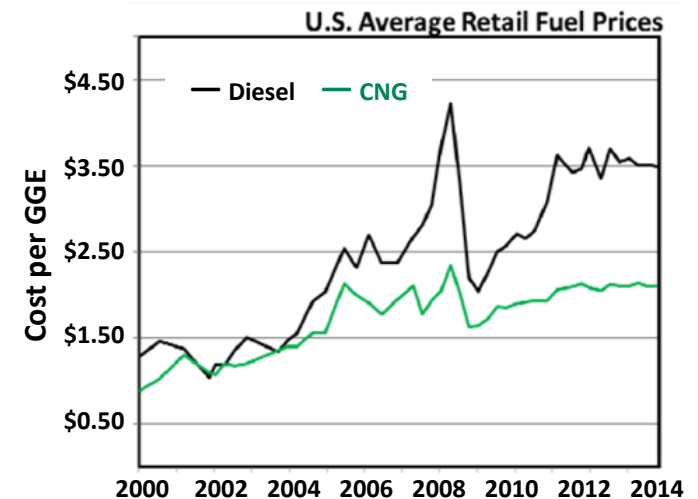
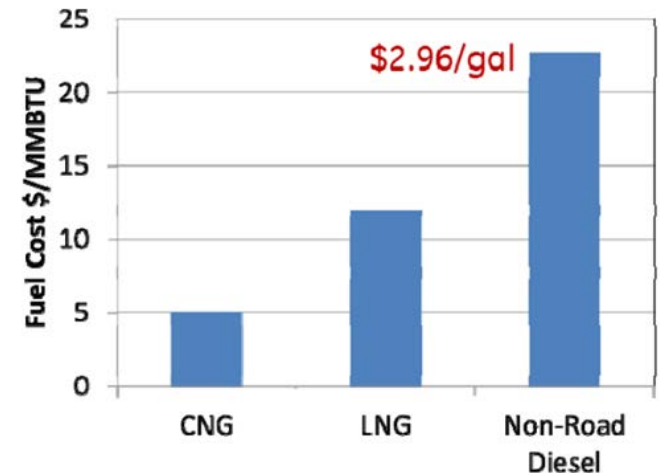
- Remainder of FY2015
 - Evaluate impact of LES turbulence model on combustion stability simulation and metamodel development
- FY2016-2018
 - Apply approach developed here to real-world engines including experimental high-dilution control efforts at ORNL (ACE090 – BC Kaul; next talk)

Standard deviation of predicted heat release over the sampled parameter space (20 iterates at each point varying only random seed for Lagrangian spray model).



Cyclic variability in dual-fuel locomotive applications – *Relevance*

- Collaborative effort with General Electric and Convergent Science
- Natural-gas (NG) substitution reduces costs and pollutant emissions compared with diesel-only operation
- Locomotive applications have great opportunity:
 - 70% NG, 30% diesel operation could save **\$250-300k** in annual fuel costs *per locomotive*
 - For $\approx 12,000$ Class 1 locomotives, this represents up to **\$3.6B** *annual savings* at current fuel costs
- Diesel-only operation is very regular with well-established controls
- Dual-fuel operation involves flame propagation in a premixed NG-air mixture ignited by a pilot diesel flame
 - Complete combustion (or aftertreatment) of NG can be problematic
 - Cyclic variability can be much more pronounced than with diesel-only
 - Higher cyclic variability reduces entitlement on operating range, efficiency, and emissions reduction
- A combined experimental and computational program is being undertaken to identify significant contributors to cyclic variability
- Approach and learnings are applicable to on-road HD



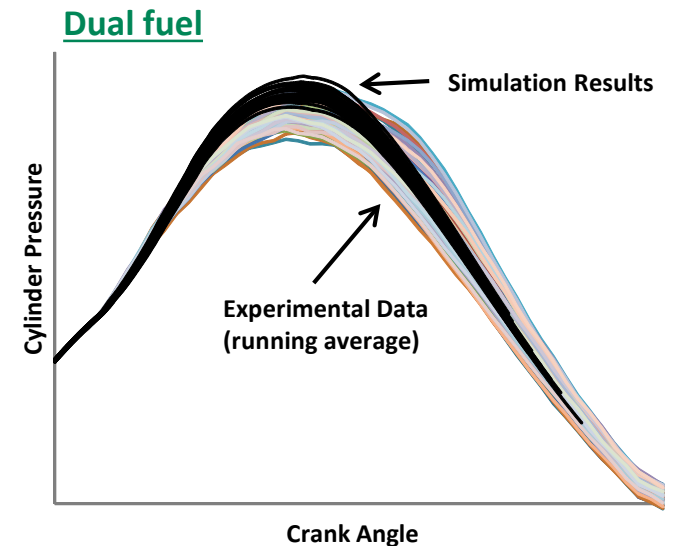
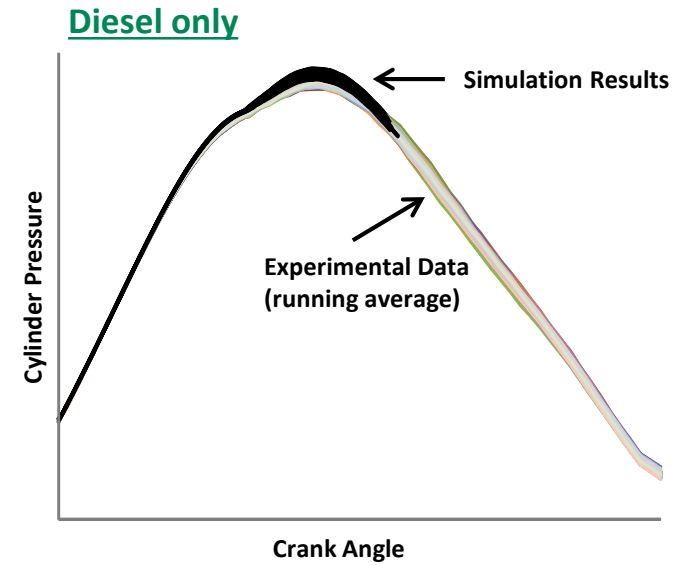
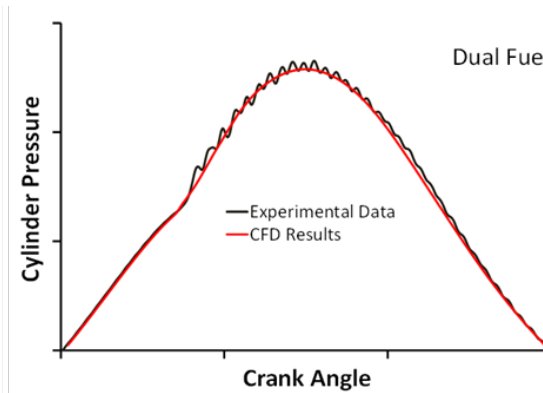
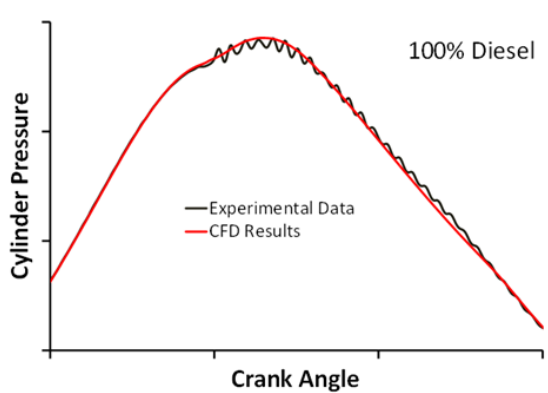
www.afdc.energy.gov/data

“High Performance Computing unlocks the fundamental physics of our machines and is critical to the development of next generation technologies in GE.”

— Mark Little, Senior Vice President, GE Global Research

Model development and validation – *Technical Accomplishments*

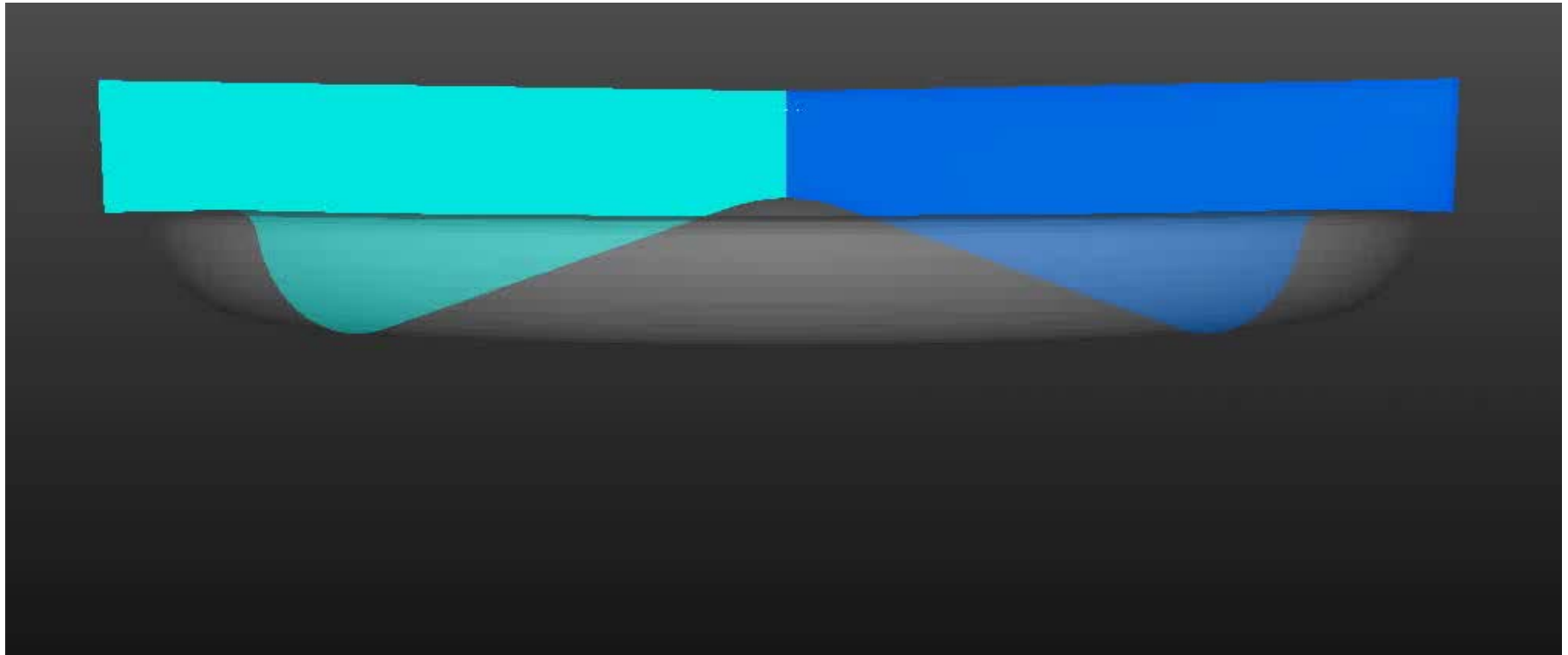
- **Initial model development complete and validated with experimental data**
 - Diesel-only and dual-fuel operation
 - Larger minimum timestep in Titan simulations resulted in increased peak pressure as shown here
 - Higher resolution simulations will be performed with next OLCF allocation
- **Initial, limited UQ sampling of stochastic engine parameters complete**
 - Diesel simulations mostly captured extent of experimental variation
 - Dual-fuel experiments exhibited more variation than seen in this set of simulations
 - Impact of additional stochastic parameters and deterministic feedbacks to be examined in next round of simulations



Visualization shows flame quenches before reaching the cylinder wall – *Technical Accomplishments*

Methane Concentration Contours

Cell Temperature Contours



Remaining challenges and Future work

Remaining challenges and barriers

- **Due to scale and complexity, initial investigations were limited by allocated computing resources (DDR allocation)**
 - Need larger allocations (e.g., ALCC) for full investigation of all parameters and feedbacks

Ongoing and future work

- **Requesting additional allocations on DOE's HPC resources at OLCF**
 - Director's Discretionary Research – Continuation of 2014 DDR project to address follow-up questions
 - ASCR Leadership Computing Challenge (ALCC) – Submitted proposal for 2015 call for 25 M CPU-hours to study advanced issues in dual-fuel and diesel-only combustion
- **Remainder of FY2015 and FY2016**
 - Identify and refine additional stochastic parameters and deterministic feedback effects
 - Explore sensitivity magnitude and functional form for factors not examined to date
 - Develop and exercise a dynamical metamodel to generate simulated time series
 - Publish results in open literature
- **FY2017-2018**
 - Apply learnings to experimental efforts and iterate
 - Leverage numeric solvers developed in CRADA for GPU acceleration

GPU acceleration of numeric solvers

CRADA for GPU acceleration of numeric solvers

- Relevance

- OEMs desire < 24-hr simulation run times
 - Cummins ready to use GPUs “today”
- GPU implementation has significant potential to accelerate detailed CFD engine simulations
 - Reduce runtimes
 - Include more detail – higher resolution, more chemistry
- Bulk of modern HPC systems are GPU-based
 - At least 50 of Top500 SuperComputers utilize GPUs
 - Titan: 27.1 PF peak performance = 2.6 PF (CPU) + 24.5 PF (GPU)
- CONVERGE™ only has partial GPU implementation
 - LLNL has shown significant acceleration of chemistry solvers
 - Flow and combustion solvers need GPU implementation
- Builds foundation for future implementation on new and emerging architectures (e.g., Intel MICs)



Majority of Titan's speed comes from
NVIDIA K20 GPUs

- Approach

- 3-year CRADA
 - DOE VTO – Funds-in to support NL efforts
 - Convergent Science – Funds-in plus in-kind CONVERGE™ licenses
 - Cummins – Funds-in, experimental validation
 - LLNL – Chemistry solver implementation
 - ORNL – Flow/combustion solver implementation, Titan access for development/demonstration
 - Indiana University – Big Red II access for development/demonstration

- Technical Accomplishments

- New start, just getting underway

Milestones

- Q3 SMART: Evaluate impact of LES on combustion stability simulation and metamodel development
 - ON TRACK
- Q4: Develop and verify parallel infrastructure for coupling spray with engine simulations
 - ON TRACK

Current Collaborations

- **Applies DOE ASCR fundamental tools and HPC resources to address technical barriers of interest to DOE VTO and transportation industry**
 - Oak Ridge Leadership Computing Facility (OLCF) and its HPC resources (*e.g.*, Titan)
 - TASMANIAN
 - DAKOTA
- **Supports pre-competitive efforts with strong industry and university collaborations**
 - Tools and approaches developed are available to industry for proprietary efforts
- **Multiple internal collaborations within ORNL**

OEMs

- **General Motors**
 - Ron Grover
 - Tang-Wei Kuo
- **General Electric**
 - JS Ravichandra
 - Roy Primus
- **Ford Motor Company**
 - Brad VanDerWege
 - Shiyong Yang
 - James Yi
- **Cummins**
 - Siddhartha Banerjee
 - John Deur

ISVs

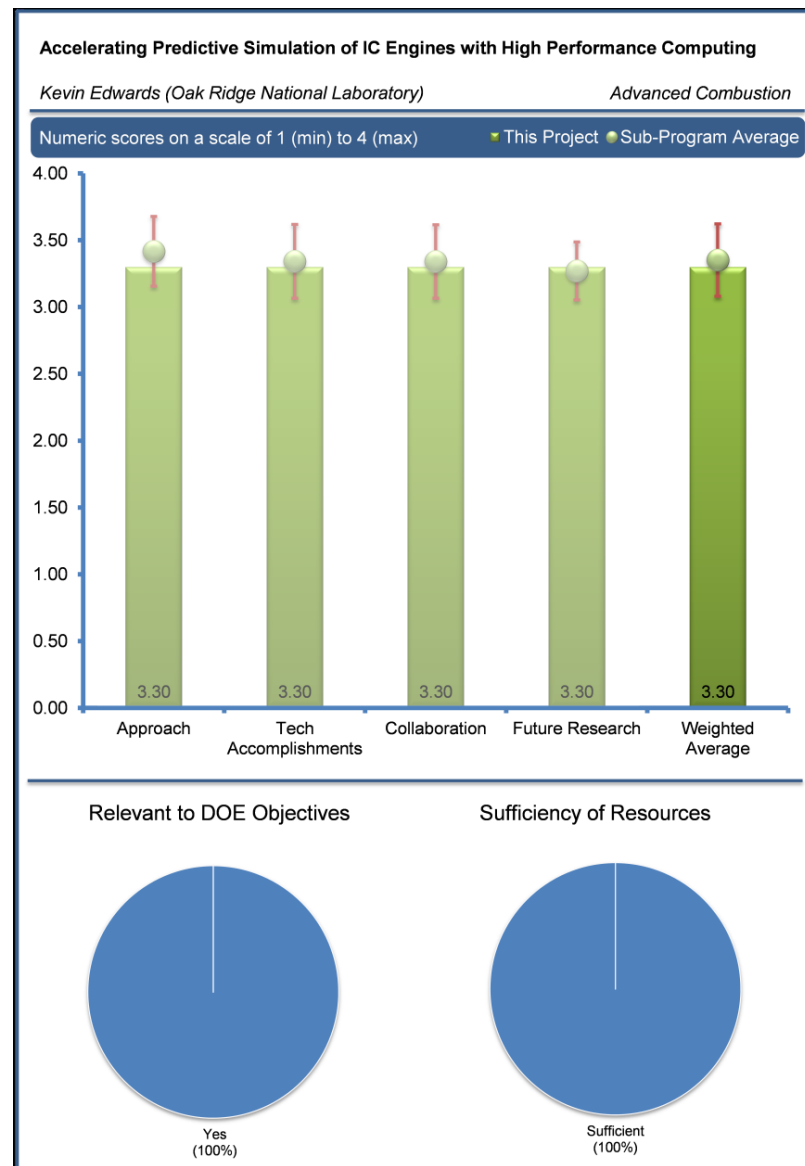
- **Convergent Science, Inc.**
 - Sameera Wijeyakulasuriya
 - Keith Richards
 - Eric Pomraning
 - Daniel Lee
 - Kelly Senecal
- **FluiDyna**

University and National Labs

- **University of Massachusetts**
 - David Schmidt
- **Indiana University**
- **Ohio State University**
 - Seung Hyun Kim
- **Oak Ridge Leadership Computing Facility**
 - Suzy Tichenor
 - Jack Wells
- **Lawrence Livermore National Laboratory**
 - Russell Whitesides
 - Matt McNenly
- **OPTIMA simulation team**

Responses to reviewer comments

- Overall the reviewer comments were *positive* and *supportive* of our approach for applying DOE ASCR fundamental tools and resources to address technical barriers faced by the transportation industry
 - Example comments:
 - “This [is] important work to help industry leverage the capabilities of large-scale computing.”
 - “Accelerating the development of high-efficiency, low-emissions engines by applying innovative uses of HPC and predictive simulation supports DOE goals.”
- Multiple comments expressed the desire for more access to ASCR resources for proprietary efforts
 - Example comments:
 - “A better balance is needed between the project’s “openness” criteria for maximum engagement of these resources [and] the needs of industry to keep at least some aspects of the work proprietary.”
 - “If the latter could be given more flexibility, then this would be an excellent or even outstanding effort.”
 - “Of course, this is just a reflection of higher-level policy.”
 - Response: DOE Office of Science funds the ASCR resources for open, fundamental science and pre-competitive efforts. The OLCF User Agreement *does* allow for hybrid efforts with a *mix of open and proprietary research*. However, ORNL research staff cannot use DOE-funds to directly support the proprietary efforts. Thus, new tools and approaches must be developed for open problems and then transferred to industry partners for proprietary use.



Summary

- Relevance

- Innovative use of HPC and predictive simulation to...
 - Address barriers where understanding has been limited by computational resources
 - Accelerate IC engine development

- Approach

- Applying DOE ASCR HPC resources and fundamental tools to technical barriers for transportation industry
 - Automation and optimization of HPC CFD simulations to greatly accelerate fuel-injector design
 - HPC CFD and metamodel simulations to understand the stochastic and deterministic processes driving cycle-to-cycle variability in highly dilute and dual-fuel engines
 - CRADA to enable GPU acceleration of numeric solvers

- Technical Accomplishments

- Demonstrated coupled predictive model for internal injector flow and in-cylinder spray evolution
- Adapted UQ metamodel approach for impact of stochastic inputs on high-dilution simulations
- Developed and validated dual-fuel model and performed initial UQ sampling for sensitivity analysis

- Collaborations

- Three ongoing efforts and one CRADA with direct OEM, ISV, university, and national lab involvement

- Future Work

- Couple and validate injector model with in-cylinder, predictive combustion model
- Apply metamodel approach to support experimental high-dilution control efforts at ORNL
- Identify and refine additional stochastic parameters and deterministic feedbacks for dual-fuel combustion
- Implement GPU acceleration for flow and combustion solvers

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