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

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Overall project objectives and relevance

- **Enable accelerated development of advanced engines meeting fuel economy and emissions goals**
  - Develop and apply ***innovative simulation strategies and tools*** to maximize benefits of predictive information from high performance computing (HPC)
  - Increase computational efficiency through parallelization, automation, and optimization
  - Reduce clock time from ***Months*** to ***Weeks***
  - Translate from ***HPC*** to ***desktop*** to ***on-board diagnostics and controls***
- **Links experimental and modeling capabilities of ORNL and industry partners with DOE's leadership HPC facilities and computational science expertise**
- **Leverages VTO funding with HPC resources at Oak Ridge Leadership Computing Facility (OLCF) funded by DOE Office of Science**
  - TITAN – currently #2 on Top500 Supercomputer list, 27.1 PF peak, ~300k compute cores
- **Addresses specific technology barriers identified by DOE and industry stakeholders**
  - Three ongoing efforts with direct industry involvement
  - Open and proprietary aspects under OLCF User Facility Agreement

Overview

Timeline

- **Project start – May 2012**
- **Ongoing**

Budget

- **FY2012 – $250k**
- **FY2013 – $400k**
- **FY2014 – $400k**

Barriers

- **Directly targets barriers identified in the VTO Multi-year Program Plan**
  - **"Lack of fundamental knowledge of advanced engine combustion regimes"**
  - **"Lack of modeling capability for combustion and emission control"**

Partners

- **Leveraging DOE Office of Science funding for Oak Ridge Leadership Computing Facility**
  - 10M+ CPU-hrs @ $0.03/hr = $300k
- **Three ongoing efforts with direct industry involvement**
  - **Combustion stability**
    - Ford Motor Company
    - General Electric
  - **Injector design optimization**
    - General Motors
  - Convergent Science, Inc. partnering on all three efforts

Ongoing collaborative efforts

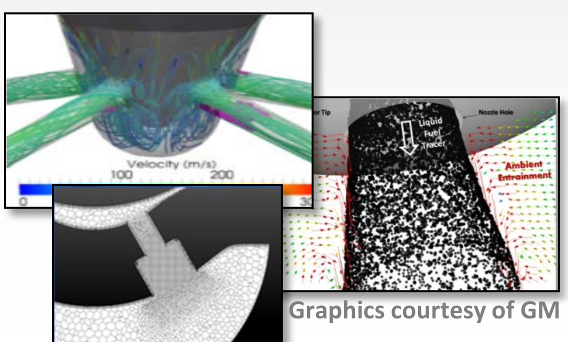
Gasoline DI fuel injector design optimization

Understand and optimize the design of GDI fuel injectors for improved efficiency and reduced emissions.

Computational framework to automate labor-intensive tasks through the iterative design process.

Coupling models of internal injector flow and cavitation with in-cylinder spray and combustion.

Enables massively parallel simulations for thorough and ***rapid*** investigation and optimization across ***operational and geometric*** design spaces.



Graphics courtesy of GM

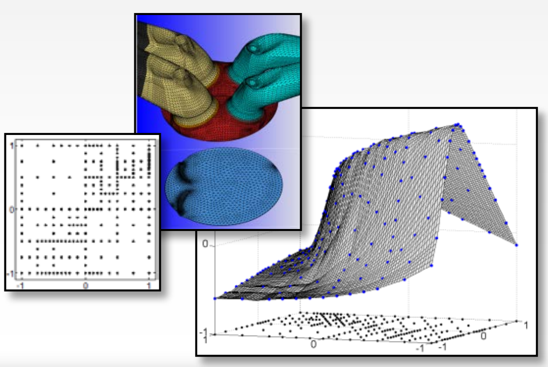
Cycle-to-cycle variation in highly dilute ICEs

Understand the stochastic and deterministic processes driving cyclic variability in highly dilute SI engines.

Novel approach to ***parallel*** simulation of a ***serial*** phenomena.

Detailed CONVERGE simulations at intelligently selected sample points in parameter space.

Enables creation of low-order metamodels that retain key dynamics of CFD model but greatly reduce computational time for thorough exploration of parameter space.



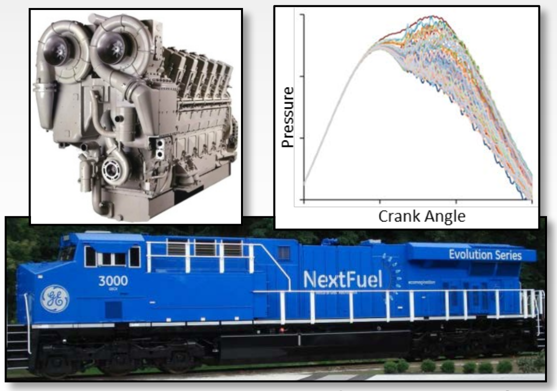
Cycle-to-cycle variation in dual-fuel locomotive engine

Investigate key factors promoting cyclic variability in a dual-fuel (NG/diesel) locomotive application.

Industry-driven with ORNL providing methodology, HPC resources, and limited support.

Similar approach to high-dilution effort with CONVERGE simulations feeding metamodel development.

Stable dual-fuel operation will enable significant displacement of petroleum-based diesel fuel with NG.



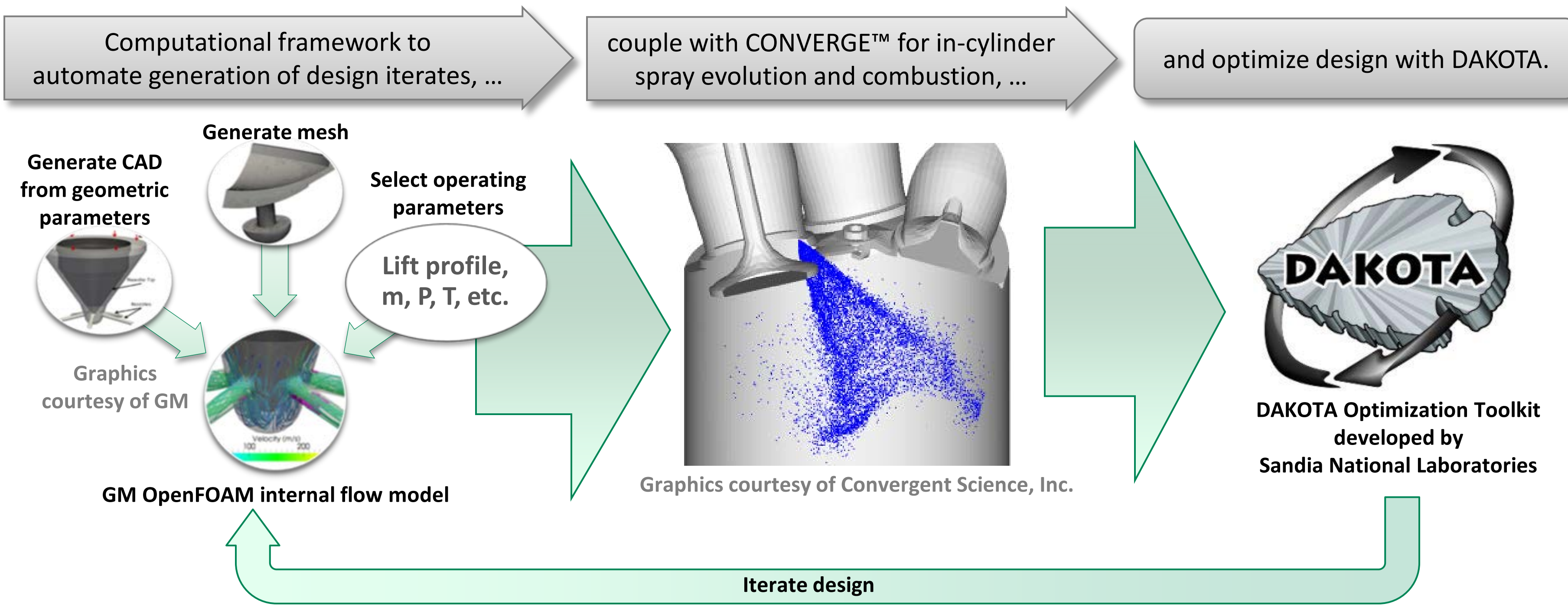
Graphics courtesy of GE

Use of logos and graphics approved by respective industry partners

- **Injector design optimization**
- Highly dilute combustion stability

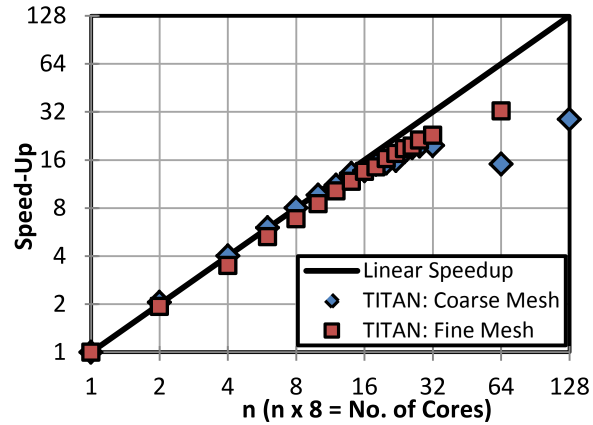
Injector design optimization – Relevance and Approach

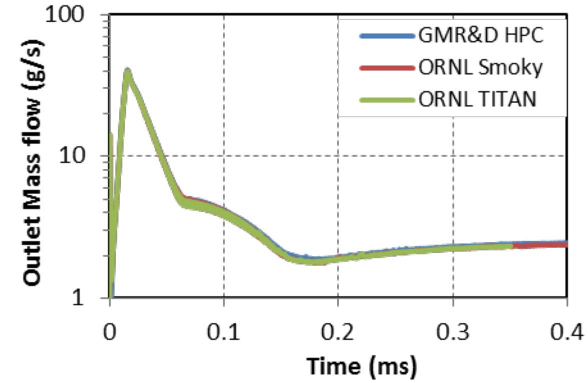
- **Collaborative effort with <u>General Motors</u>**
- **Injector design optimization is currently a lengthy, labor-intensive process**
  - Months of effort to minimally cover design space
- **HPC enables <u>*thorough*</u> & <u>*rapid*</u> investigation of <u>*operational*</u> & <u>*geometric*</u> design spaces**
  - From months to weeks <u>*AND*</u> more thorough coverage of design space
- **ORNL developing computational framework to automate model generation & design optimization**
  - Leveraging experience with automotive batteries (CAEBAT) and fusion (IPS for ITER)

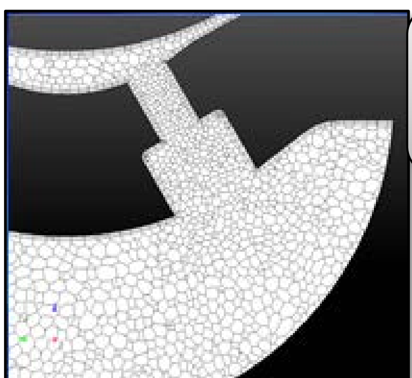


Model validation and grid optimization – Technical Accomplishments

- **Performed initial code validation and operating parameter sweeps**
  - 42 parallel cases using 5000+ cores on TITAN
  - Compared against GM simulations and *experimental data*
- **Repeated sweep with higher-resolution mesh in the nozzle area**
  - 256 cores/simulation => 10,000+ cores on TITAN
  - All cases showed good agreement with coarse grid results
  - Future runs will use the coarse grid
- **Initiated large-scale sweep of geometry and parameter space**
  - 7 nozzle designs at 42 reference operating points
  - 75,000 cores on TITAN
- **Identified file-write issues with OpenFOAM on HPC**
  - Each core writes an output directory, onerous for peta-scale HPC
    - *2.5 million* total files for our large-scale sweep
  - Typical of barriers encountered while adapting code for HPC

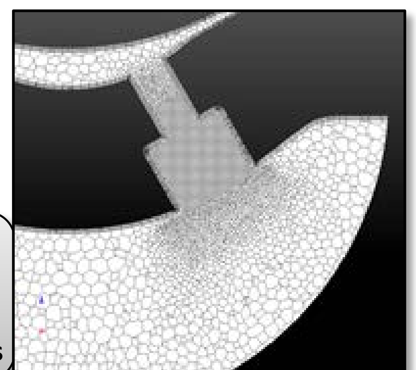


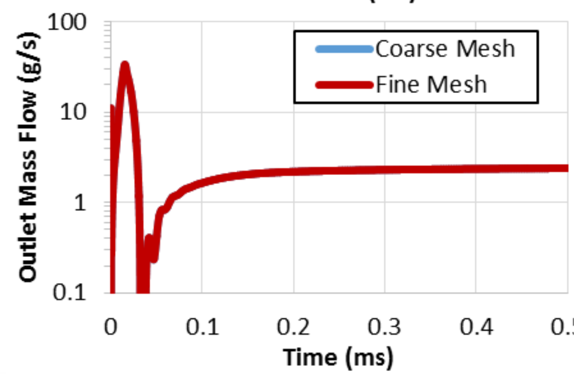




Coarse Grid
- 383k Total Cells
- Δx ≈ 30µm in counter bore
- 2 cells in 20µm prism layers

Fine Grid
- 688k Total Cells
- Δx ≈ 10µm in counter bore
- 4 cells in 20µm prism layers

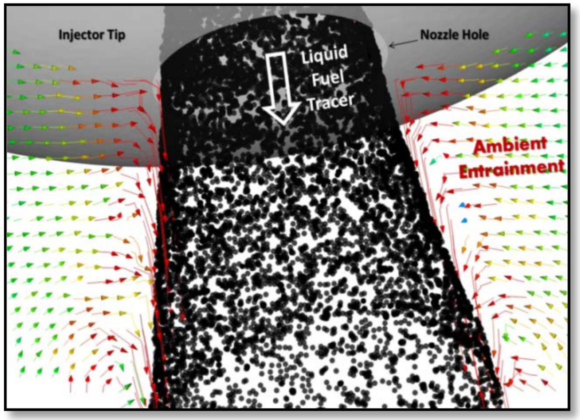




Graphics provided by General Motors

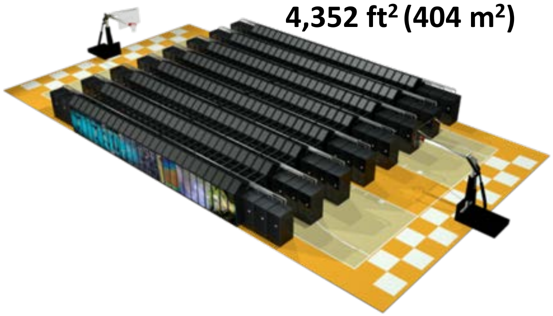
Ongoing and future activities

- **<u>Remaining challenges and barriers:</u>**
  - Address file-write bottleneck with OpenFOAM
  - Couple internal flow model with in-cylinder spray evolution and combustion
  - Adapt codes for GPUs to take full advantage of TITAN's speed
- **Submitted ALCC application for 15M CPU-hrs for future efforts**
- **Couple with CONVERGE™ for downstream spray evolution**
  - Validate with available experimental measurements
  - Fully coupled model for in-cylinder simulations with combustion
- **Improve scalability of OpenFOAM & CONVERGE™ models through use of GPUs**
  - Talking with NVIDIA, FluiDyna, Convergent Science
  - Possible collaboration with LLNL
- **Demonstrate automated optimization of injector geometry for…**
  - Improved fuel economy
  - Lower emissions
  - Lower shot-to-shot variability
- **Transfer of knowledge and methodology to GM for proprietary runs**



Graphics provided by General Motors

4,352 ft^2 (404 m^2)



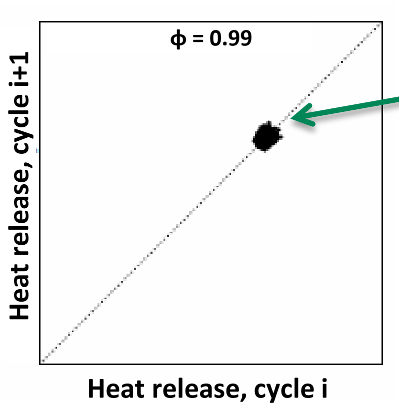
<u>TITAN SPECIFICATIONS:</u>

- **Peak performance of 27.1 PF**
  - 24.5 GPU + 2.6 CPU
- **18,688 compute nodes each with:**
  - 16-core AMD Opteron CPU (299,008 total compute cores)
  - NVIDIA Tesla "K20x" GPU

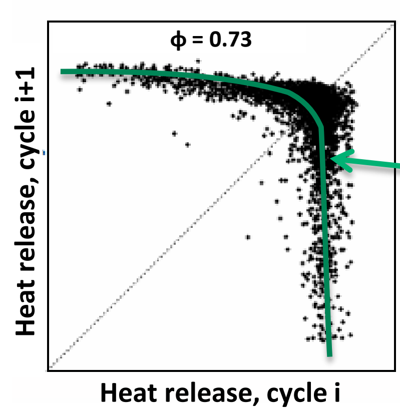
- Injector design optimization
- **Highly dilute combustion stability**

Highly dilute combustion stability – Relevance and Approach

- **Collaborative effort with <u>Ford Motor Company</u> and <u>Convergent Science, Inc.</u>**
- **Potential efficiency and emissions benefits of highly dilute (lean or high-EGR) operation are limited by combustion instability**
  - Instability driven by combined effects of stochastic and deterministic processes
  - Understanding the causes of instability enables potential for redesign and/or control
- **HPC and CFD models enable detailed study of key factors promoting instability**
  - Thousands of simulated cycles required to study problem with statistical accuracy
  - Previous analytical studies used low-order models to avoid excessive computation time
- **ORNL is using detailed HPC CFD simulations to feed development of low-order metamodels to improve understanding of stochastic and deterministic factors promoting combustion instability**



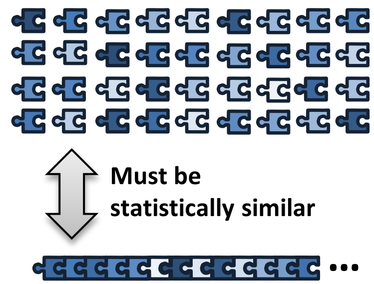
<u>Low dilution</u>
- Stochastic effects dominate
- Relatively low variability
- Minimize by design

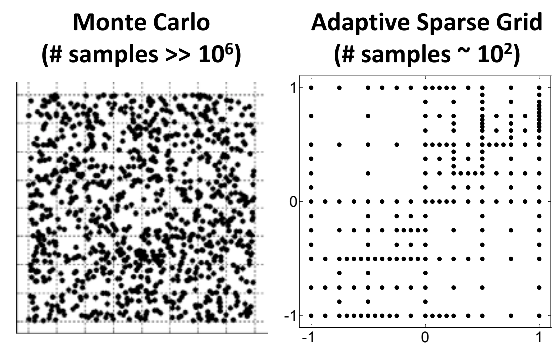


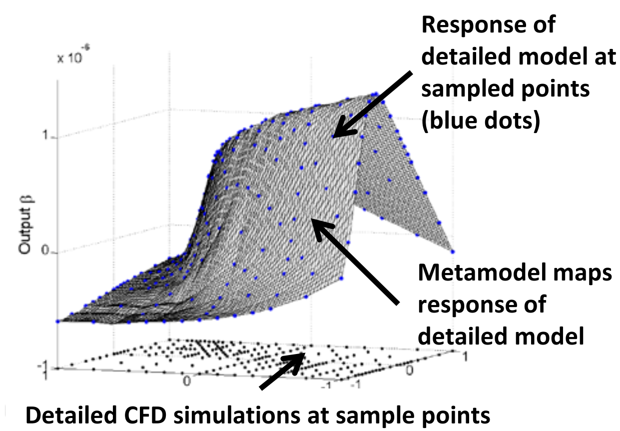
<u>High dilution</u>
- Lean or high-EGR
- Deterministic effects dominate
- Stochastic effects produce additional "noise"
- High variability
- Minimize by active control

Approach

- **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
    - ~10^2 samples vs. >>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
    - Continuous and differentiable set of basis functions
    - Uncertainty Quantification (UQ) and stochastic collocation using ORNL's TASMANIAN algorithm
  - Retains dominant features of detailed model's behavior
  - Allows rapid exploration of parameter space







<u>TASMANIAN</u>

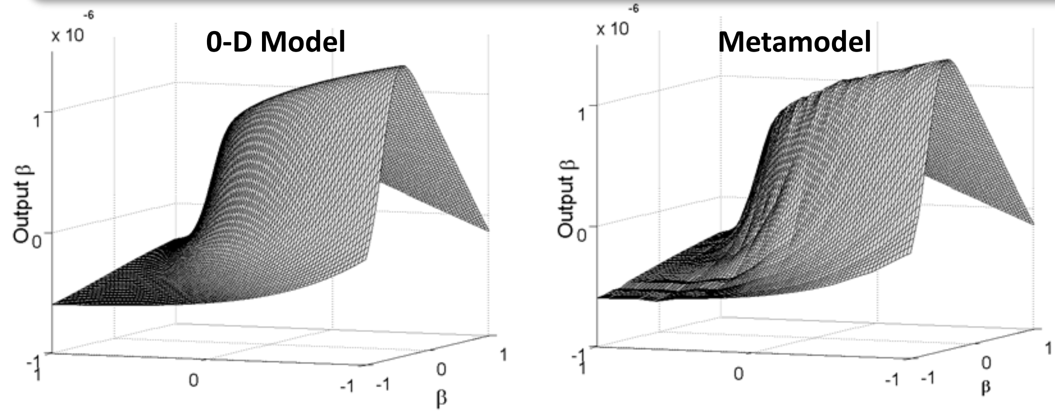
<u>T</u>oolkit for <u>A</u>daptive <u>S</u>tochastic <u>M</u>odeling <u>A</u>nd <u>N</u>on-<u>I</u>ntrusive <u>A</u>pproximatio<u>N</u>

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

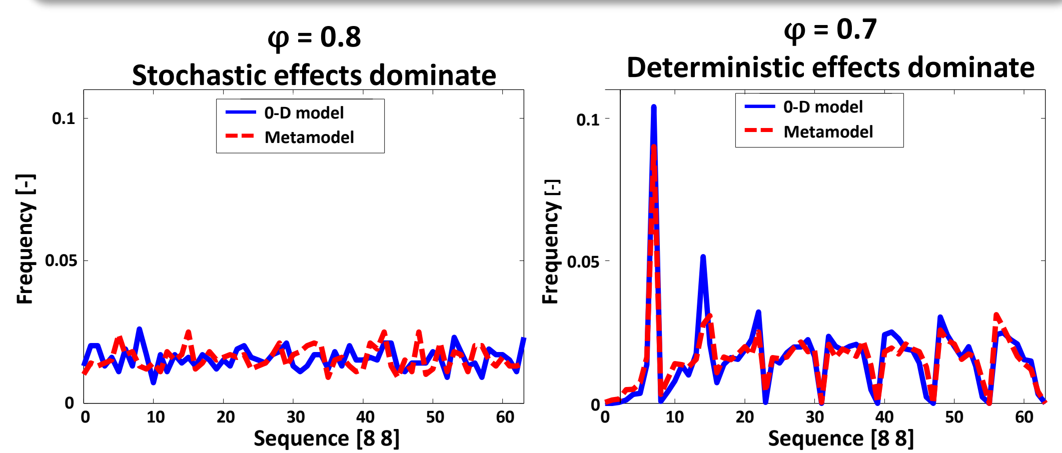
Proof of concept using simple, 0-D engine model – Previous Results

- **Successfully demonstrated our approach using simple SI model with cycle-to-cycle feedback**
  - 0-D, single-zone with prescribed (Wiebe) combustion
  - Combustion efficiency variation with dilution based on experimental observations and percolation theory
- **Metamodel created based on 8 sampled model parameters**
  - No feedback: SOC, φ, Wiebe exponent (m)
  - With cycle feedback: Fueling parameters (α and β), residual fraction and temperature, molar charge at IVC
- **Analysis shows metamodel retains key physics of original model**
  - Predicts transition from stochastic to deterministic behavior with φ

Metamodel captures steepness of response map with limited residual error (seen here as "wrinkles")



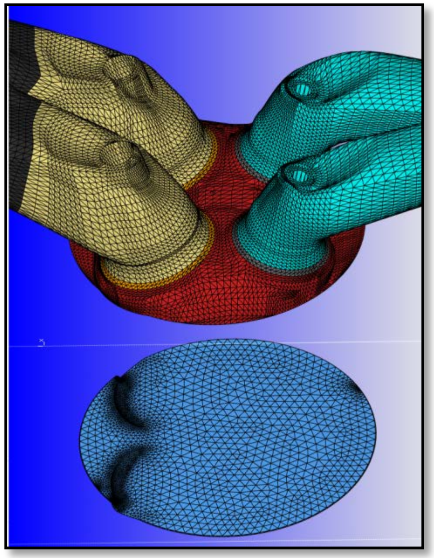
Symbol statistics show metamodel retains key physics of the original model. Residual fuel effects begin to dominate near the lean stability limit.



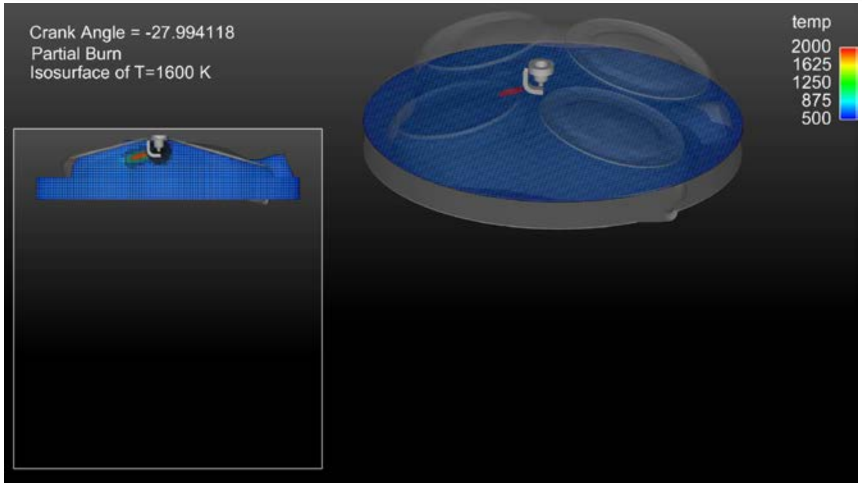
- **Finney, et al. 2012 International Conference on Theory and Applications of Nonlinear Dynamics (ICAND).**
- **Webster, et al. 2013 SIAM Computational Science and Engineering Conference.**

Transition to CFD simulations on TITAN – Technical Accomplishments

- **Ported CONVERGE™ to TITAN**
- **Non-proprietary geometry model provided by Ford**
- **Calibrated open model for high-EGR dilution**
  - Current open-source kinetic mechanisms appear to under-predict combustion performance at high dilution
- **Developed and validated supervisory framework for job management on TITAN**
  - Scripts to generate cases with parametric variations, monitor output quality, and manage restarts (~20-30+ restarts per simulation)
- **Completed initial sparse grid sampling on TITAN**
  - Nominal conditions: 1500 RPM, road load (~3.5-bar IMEP), 17% external EGR
  - Sweep of 4 parameters:
    - Spray mass = 12.8-15.65 mg
    - Spark energy = 0.01-0.03 J
    - P in exhaust manifold = 85-110 kPa
    - T in exhaust manifold = 685-785 K
  - 401 parallel simulations using 6000+ total cores and approximately 1M CPU-hrs



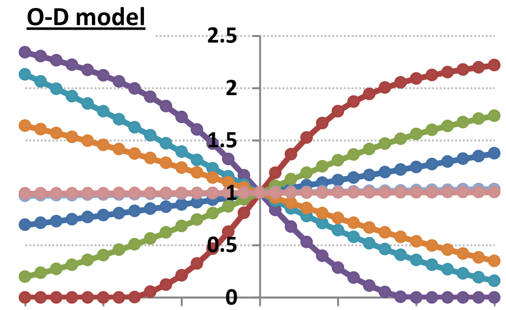
CONVERGE™ simulation at lean conditions showing partial burn

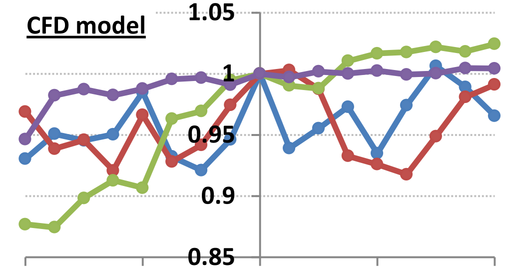


Initial CFD runs reveal variability introduced by spray model – Technical Accomplishments

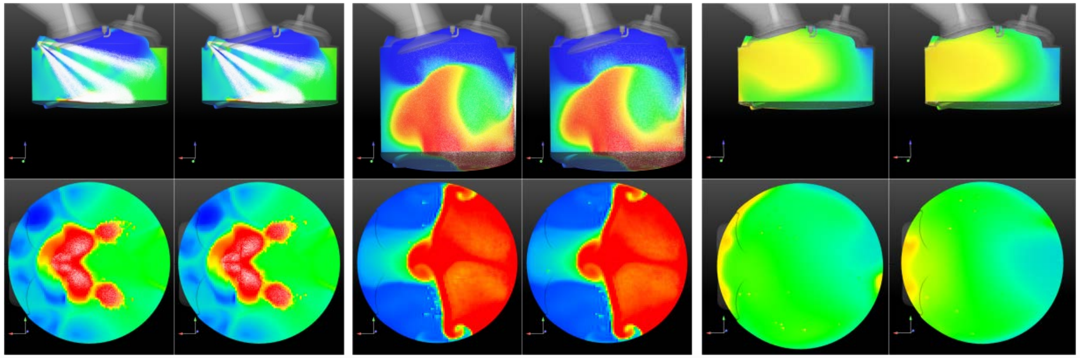
- **Stochastic variability obscuring deterministic behavior**
  - Metamodel approach requires clear, deterministic trends
- **To reduce computation time, state-of-the-art spray models use random number generator and pre-defined probability distributions in Monte-Carlo-like approach to…**
  - Populate initial size and velocity of individual droplets
  - Determine outcome of collisions and spray/wall interactions
- **Introduces *uncontrolled* stochastic variation to initial conditions**
  - Random components impact global performance
  - Harkens back to perturbation theory (e.g., Daw, et al. 2012)
- **Resulting variability not limited to highly dilute cases**
  - Less (but still substantial) variability observed at low dilution levels
  - Real physics or numerical artifact?
  - Perform additional simulations and compare to experimental variability

Sensitivity of HR to varied parameters

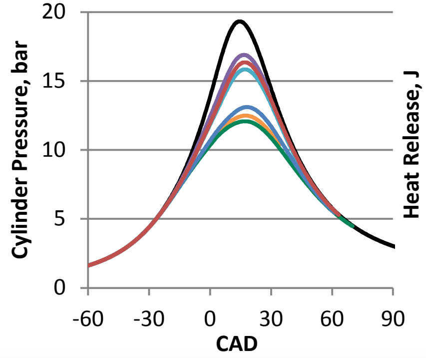


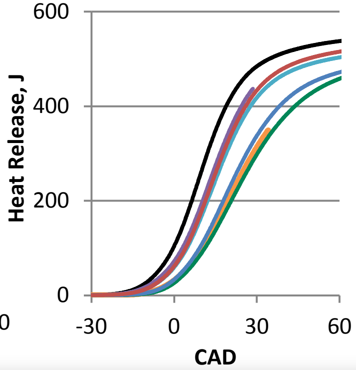


Changing the random seed produces small differences in the spray which evolve during mixing into larger differences in charge distribution at spark…



and significant variation in predicted performance.

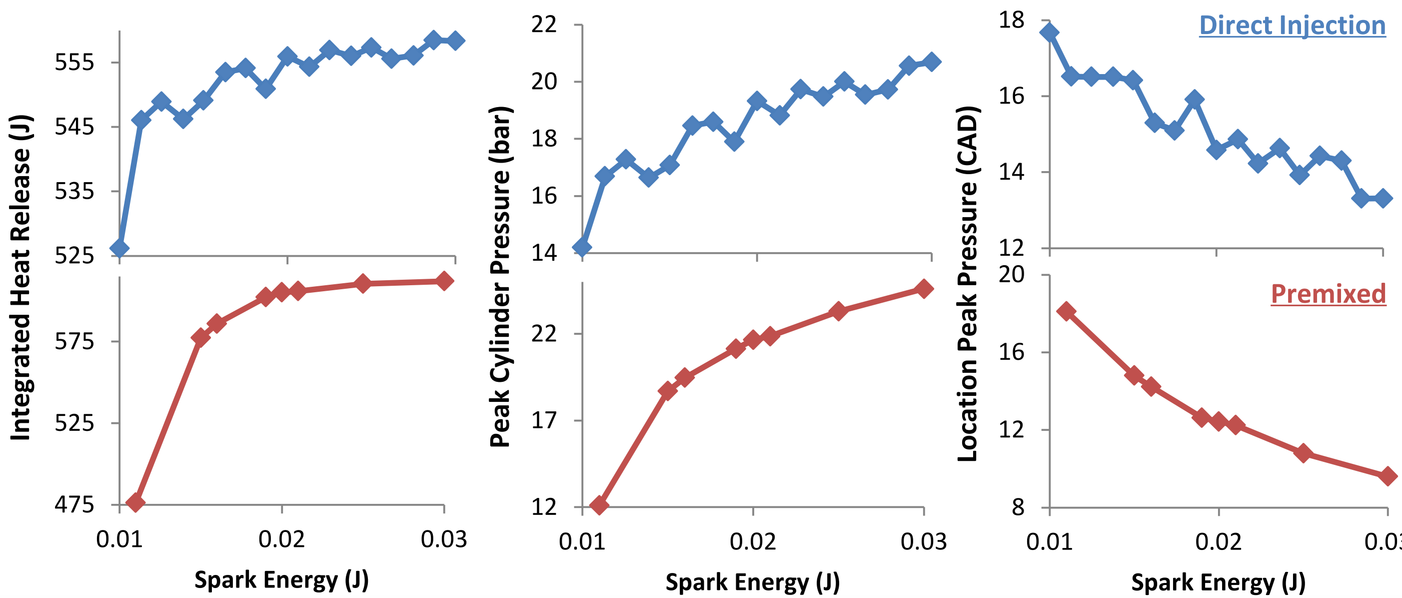




Steps forward to resolve stochastic and deterministic contributions

- **Metamodel approach requires separation of stochastic and deterministic contributions**
- **Option 1: Cycle average at each sampling point**
  - For statistical accuracy would require ~100 runs/point x 401 points = 40,100 simulations
  - Computationally prohibitive
- **Option 2: Pursuing control over spray model's random components with Convergent Science**
  - Enables systematic study of the impact spray model parameters have on stability
- **Option 3: Premixed simulations to remove stochastic effects of spray model**
  - Resolves deterministic contributions of other parameters of interest
  - Removes any fuel stratification, but retains residual mixing
  - Initial runs are currently underway, preliminary results promising

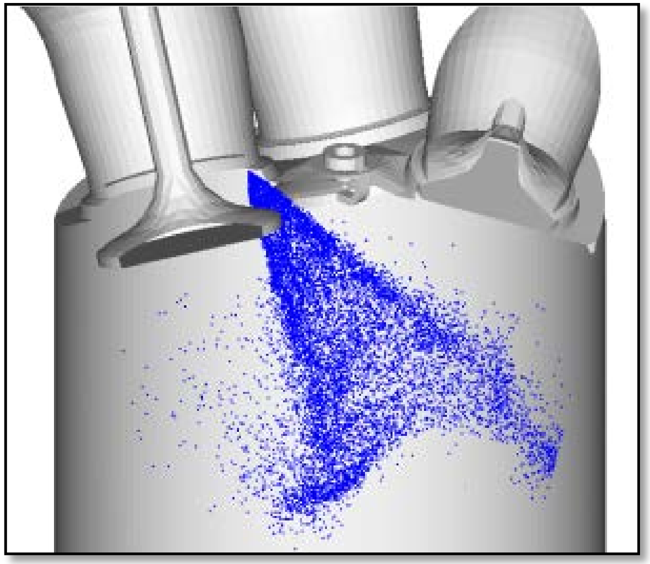
Preliminary results from premixed simulations show smoother trends over parametric sweeps



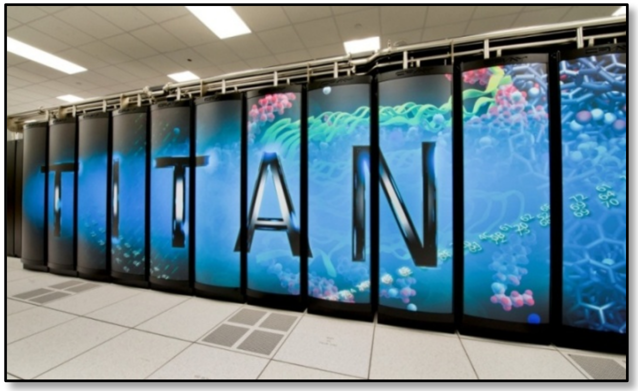
Ongoing and future activities

- **<u>Remaining challenges and barriers:</u>**
  - Continue to resolve stochastic and deterministic contributions to combustion variability
  - Understand and control variability created by spray model
  - Potential for similar stochastic variability with LES
  - Medium-sized cluster (500-1000 cores) needed to accelerate model development

- **Submitted ALCC application for 17.5M CPU-hrs for future work**
- **Use GPUs to improve scalability of CONVERGE™ flow models**
  - Talking with NVIDIA and Convergent Science
  - Potential for collaboration with LLNL
- **Develop and exercise refined metamodel to identify and understand impact of engine parameters which promote combustion instability**
- **Transfer of knowledge and supporting software to Ford for proprietary runs**
  - Coordinating Ford access to OLCF resources for proprietary runs
  - Transferring methodologies and learnings



Graphics courtesy of Convergent Science, Inc.



Milestones

- ✓ **Develop and employ computational framework for launching massively parallel ICE simulations on ORNL HPC resources – March 2014, COMPLETE**
- **Identify and understand impact of key engine parameters which promote dilute combustion instability – June 2014, ON TRACK**
- **Development and demonstration of computational framework for accelerated injector design optimization – September 2014, ON TRACK**

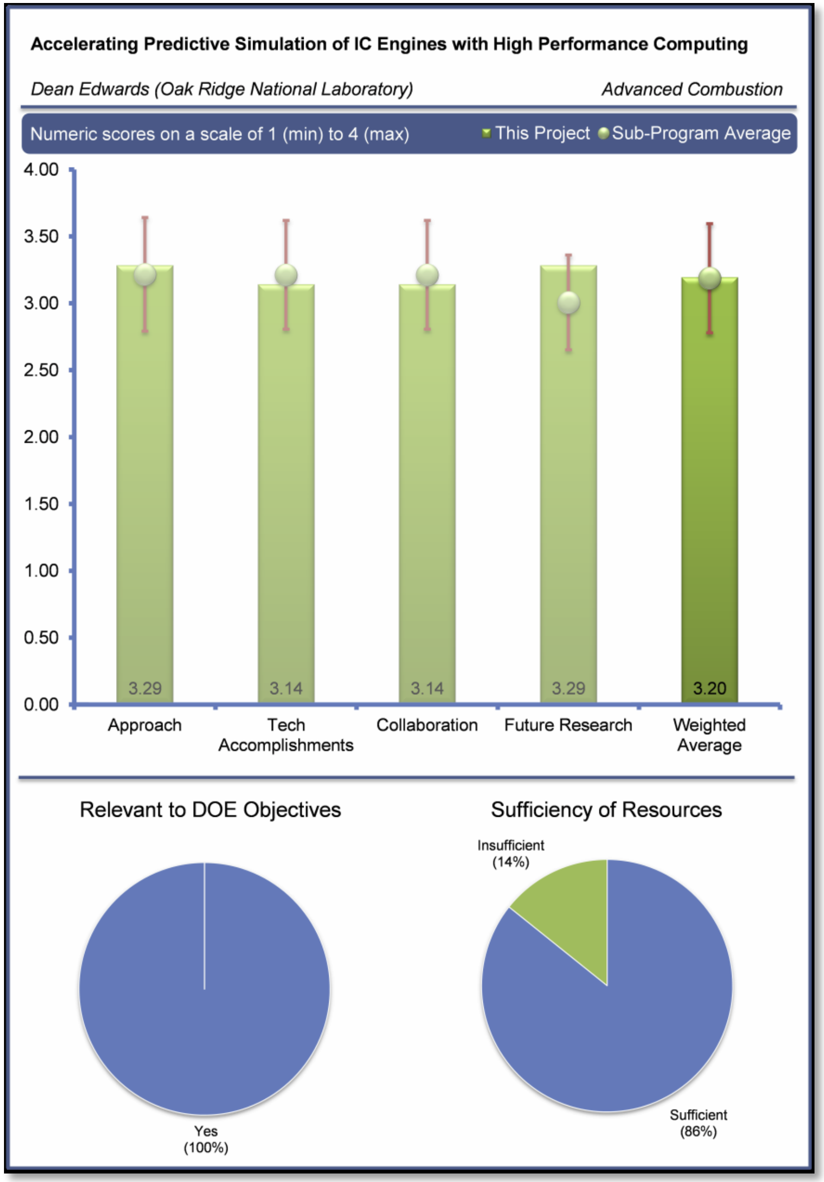
Collaborations

- **Efforts supported through the OLCF user facility agreement**
  - Each effort involves pre-competitive and proprietary aspects
- **Leveraging DOE funds**
  - EERE, Vehicle Technologies Office
    - Support for pre-competitive efforts
  - Office of Science, Advanced Scientific Computing Research (ASCR) Program
    - OLCF user facility and its HPC resources (*e.g.*, Titan)
    - TASMANIAN
  - Multiple internal collaborations within ORNL

- **Ford Motor Company**
  - Brad VanDerWege
  - James Yi
  - Shiyou Yang
- **General Motors**
  - Ron Grover
  - Tang-Wei Kuo
  - Yue Wang
- **General Electric**
  - Roy Primus
  - JS Ravichandra
- **Convergent Science, Inc.**
  - Daniel Lee
  - Keith Richards
  - Eric Pomraning
  - Sameera Wijeyakulasuriya
- **Oak Ridge Leadership Computing Facility (OLCF)**
  - Suzy Tichenor
  - Jack Wells

Responses to reviewer comments

- **Overall the reviewer comments were positive and seemed to agree that the project has a good strategy to address critical issues**
- **Most concerns were regarding two issues…**
- **"Openness" of results**
  - Example comment: "Given the [close partnership] with two OEMS, [will] all of the details of the approach [be] open and publicly available, since it [is] being developed with public funds"
  - Response: For each task, the methods are developed and demonstrated using open models with resulting methodologies openly available. The developed tools are then provided to the partnering OEMs to perform their proprietary studies.
- **Validation with experimental results**
  - Example comment: "Would be beneficial to verify the model prediction at an early stage with some test results from industry partners"
  - Response: Validation with experimental data is vital throughout development stages of each task and perhaps should have received greater emphasis in the presentation. For example, the spray model is being validated with experimental data from GM. However, in later phases of the work, the true benefit of the resulting models will be in exploring portions of the operating space where no experimental data exists.



Summary

- **Relevance**
  - Innovative use of HPC and predictive simulation to accelerate IC engine development to meet future efficiency and emissions goals
- **Approach**
  - 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
- **Technical Accomplishments**
  - Large-scale sweep of injector design and operational parameters currently underway
  - Premixed simulations underway to resolve deterministic contributions to variability
  - Identified critical issues for code evolution to HPC resources and application to our approach
    - File-write issues for large-scale jobs with OpenFOAM
    - State-of-the-art spray models introduce uncontrollable, random variation in initial conditions
- **Collaborations**
  - Three ongoing efforts with direct industry involvement (GM, Ford, GE, Convergent Science)
- **Future Work**
  - Couple injector model with CONVERGE™ for in-cylinder spray evolution and combustion
  - Complete metamodel development and resolve stochastic and deterministic factors promoting instability
  - Transfer learnings and methodologies to industry partners for proprietary runs

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