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

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Overview

Timeline

- **Project start – FY2012**
- **Proposed through FY2019**

Barriers

- **Directly targets barriers identified in the DOE-VTO MYPP**
  - "Lack of modeling capability for combustion and emission control"
  - "Lack of fundamental knowledge of advanced engine combustion regimes"
- **Directly targets the Strategic Focus Areas identified in PreSICE Workshop Report***
  - Improved predictive modeling for **Sprays** and **Cyclic Variability**

Budget

- **FY2015 – $373k**
  - **$100k CRADA**
- **FY2016 – $450k**
  - **$50k CRADA**

Partners

- **Leveraging DOE Office of Science funding for ASCR resources**
  - Multiple ALCC and DD allocations on OLCF HPC resources
  - **45 Mhrs** on Titan @ $0.03/hr = **$1.35M**
- **Multiple ongoing efforts with industry, NL, and academic involvement**

- **Collaboration with LLNL for application of GPU-enabled Zero-RK chemistry solvers on Titan (ACE076)**
- **CRADA effort in development for GPU acceleration of numeric solvers**

- **Strong connectivity to broader simulation portfolios at ORNL and DOE**
  - **Co-Optima simulation team (FT040)**
  - **FOA-supported knock modeling effort with Ohio State University**
  - **Advanced propulsion materials (PM057)**
  - **Simulation support of experimental efforts at ORNL (ACE016, ACE090, etc.)**

* https://www1.eere.energy.gov/vehiclesandfuels/pdfs/presice_rpt.pdf

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Relevance and *Approach*

ORNL is partnering with industry (OEMs and ISVs), universities, and other national labs to accelerate development of advanced engine designs to meet fuel economy and emissions goals

- **Maximizes benefits of predictive simulation with DOE's ASCR leadership HPC resources**

- **Targets key barriers identified in VTO MYPP and PreSICE Workshop**

- **Supports multi-year efforts to address complex technical issues while maintaining flexibility to quickly address emerging issues**

- **Develop and evolve new capabilities**
  - Develop *innovative simulation tools and strategies* to improve predictive capabilities
  - Translate capabilities from *HPC* to *desktop* to *on-board diagnostics and controls*
- **Solve the unsolvable**
  - Apply massively parallel, peta-scale HPC to address problems historically limited by computational resources
- **Enable virtual design**
  - Address barriers to virtual design and calibration of engines and components
  - Parallelization, automation, and optimization of the design process

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Current Task List and *Milestones*

| Projects / Current-year Tasks	Collaborations / Status
Virtual fuel injector design Accelerate virtual design and optimization of GDI fuel injectors	GM
• ALCC project to couple internal injector flow model with in-cylinder spray evolution • Evaluate qualitative accuracy of combined model with spray visualization data	**Completed FY2015-Q4**
Virtual engine design and calibration Address barriers to further enable and accelerate virtual engine design and calibration	GM
• ALCC project to improve speed and accuracy of emissions predictions through use of GPU-enable solvers and detailed kinetics • Evaluate potential reduction in computation time and accuracy improvements over full speed/load range	**On-track for FY2017-Q1**
Cyclic variability in dilute ICEs Understand stochastic & deterministic processes driving CV in highly dilute SI ICEs	Ford
• ALCC project to refine metamodel approach with LES turbulence modeling • Transition simulation efforts to modified GM 2.0-L GDI	**Completed FY2015-Q4** **On-track for FY2016-Q4**
Cyclic variability in dual-fuel ICEs Investigate key factors promoting cyclic variability in dual-fuel engine applications	GE
• DD project for initial study of impact of initial and boundary condition variability on CV	**Completed FY2015-Q4**
CRADA to develop GPU-enabled numeric solvers Implement hardware acceleration for CFD numeric flow solvers	Cummins, IU
• Kick-off CRADA	**Pending**

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# *Technical Accomplishments* – Virtual injector design (1/2)

Virtual design has potential to significantly accelerate and expand exploration of the design space

- **Reduce design cycle from months to weeks while considering more potential design candidates**
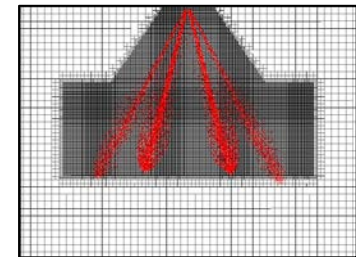- **Downselect candidate designs to reduce physical build and testing efforts**

OpenFOAM HRM model for
internal injector flow
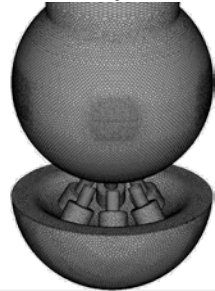
Detailed velocity profiles provide
accurate BCs for each plume
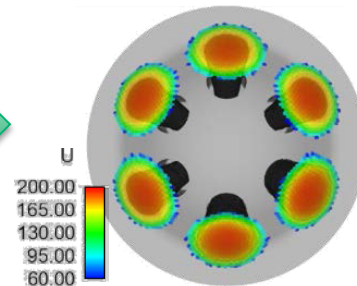
CONVERGE for in-cylinder
spray evolution

U
200.00
165.00
130.00
95.00
60.00

Collaborative effort to enable virtual fuel injector design

- **Coupled internal injector flow model with in-cylinder spray model**
  - Homogeneous Relaxation Model (HRM) developed by University of Massachusetts
  - Improved definition of boundary conditions and reduced "tuning" of spray parameters
  - Qualitative validation with spray visualization data
- **Evaluate potential improvement with 2-fluid HRM**
- **Validate for additional conditions and geometries**

Supported by ALCC allocation

- **15 Mhrs on Titan**

GM · CONVERGE™ CFD software · OLCF Oak Ridge Leadership Computing Facility

TITAN

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Technical Accomplishments – Virtual injector design (2/2)

HRM 2-fluid model vs. single-fluid model

- **Tracks liquid & vapor fuel and nitrogen**

- **Includes liquid compressibility**

- **Improved prediction of penetration length at intermediate temperatures**

- **Captures general trend of transition to flash boiling**

- **Additional refinement needed for plume thickness accuracy**
  - Too thin at non-flashing conditions
  - Overpredicts plume interaction at flashing conditions
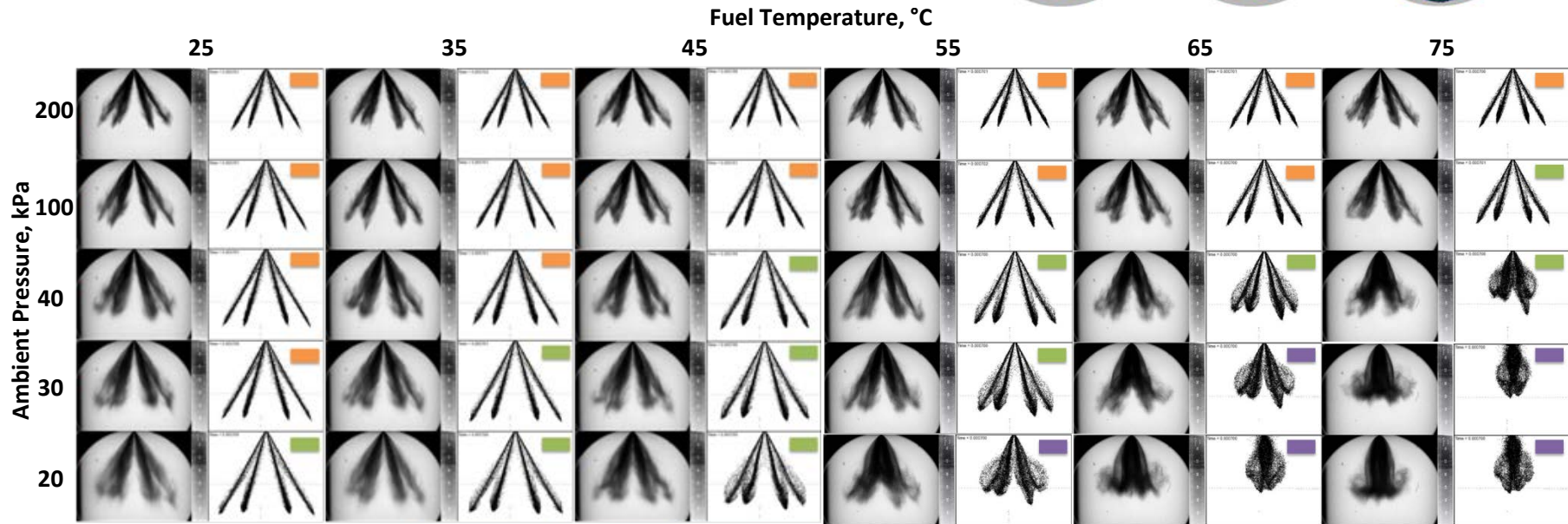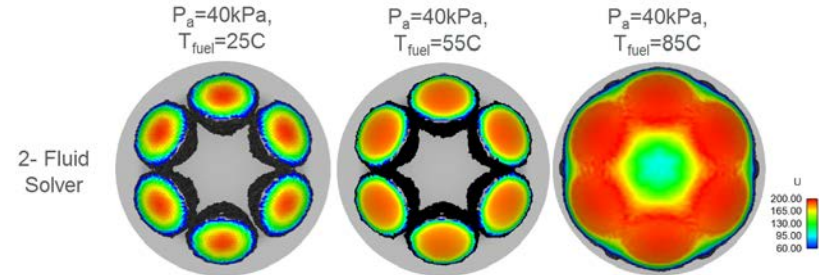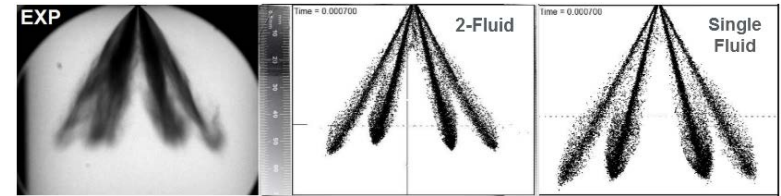
Results to be presented at 2016 ILASS

Technical Accomplishments – Virtual engine design and calibration (1/4)

Virtual engine design and calibration is the "holy grail" for accelerating engine development
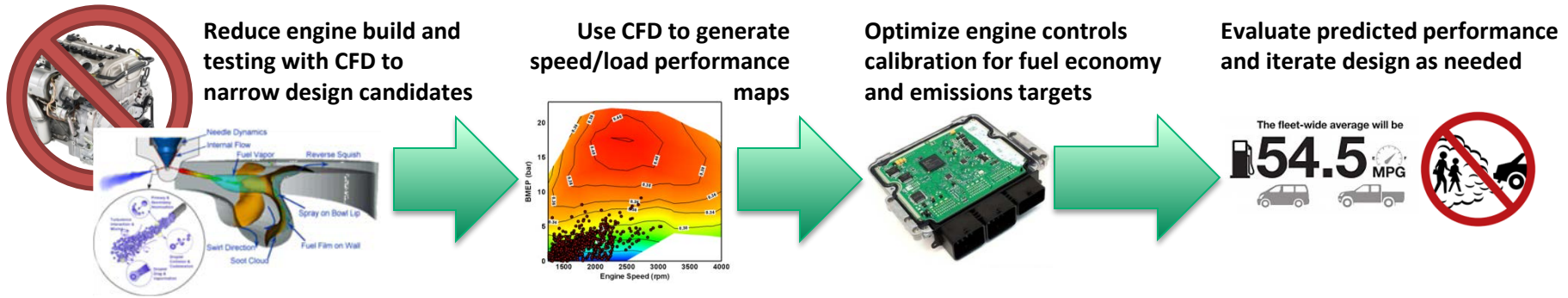

Reduce engine build and testing with CFD to narrow design candidates → **Use CFD to generate speed/load performance maps** → **Optimize engine controls calibration for fuel economy and emissions targets** → **Evaluate predicted performance and iterate design as needed**

- **Fast and accurate emissions predictions are among the many barriers**

Collaborative effort to optimize balance between emissions accuracy and computational speed

- **Parallel ensemble simulations to cover full speed/load range**
- **Detailed chemical mechanisms for improved accuracy**
- **LLNL's GPU-enabled Zero-RK chemistry solvers for computational speed-up**
- **ORNL's TASMANIAN with Adaptive Sparse-Grid sampling to enable transition from HPC to industrial clusters and GPU-enabled workstations**

Supported by ALCC allocation

- **8 Mhrs on Titan**

Technical Accomplishments – Virtual engine design and calibration (2/4)

Scalability study performed on Titan with Zero-RK solvers with and without GPUs

- **CPU Scalability**
  - 1.5x speed-up going from 1 to 2 nodes
  - Benefits plateau around 96 CPU cores

- **GPU scalability**
  - Significant benefit over CPU-only for low #nodes
  - Benefits at higher #nodes limited by #cells
    - Benefits of GPU increase with #cells in model

- **Titan has option to run on <16 CPUs per node**
  - Provides some memory and floating-point processor benefits
  - For fixed #cores, speed-up < 2x for 2x allocation usage
  - Benefits for current case equivalent to that of simply doubling #nodes

Full, single-node runs (16 CPU + 1 GPU) provide best balance between speed-up and allocation usage for current case

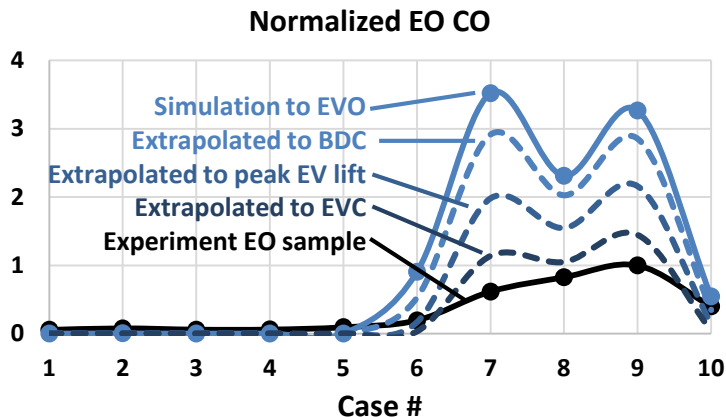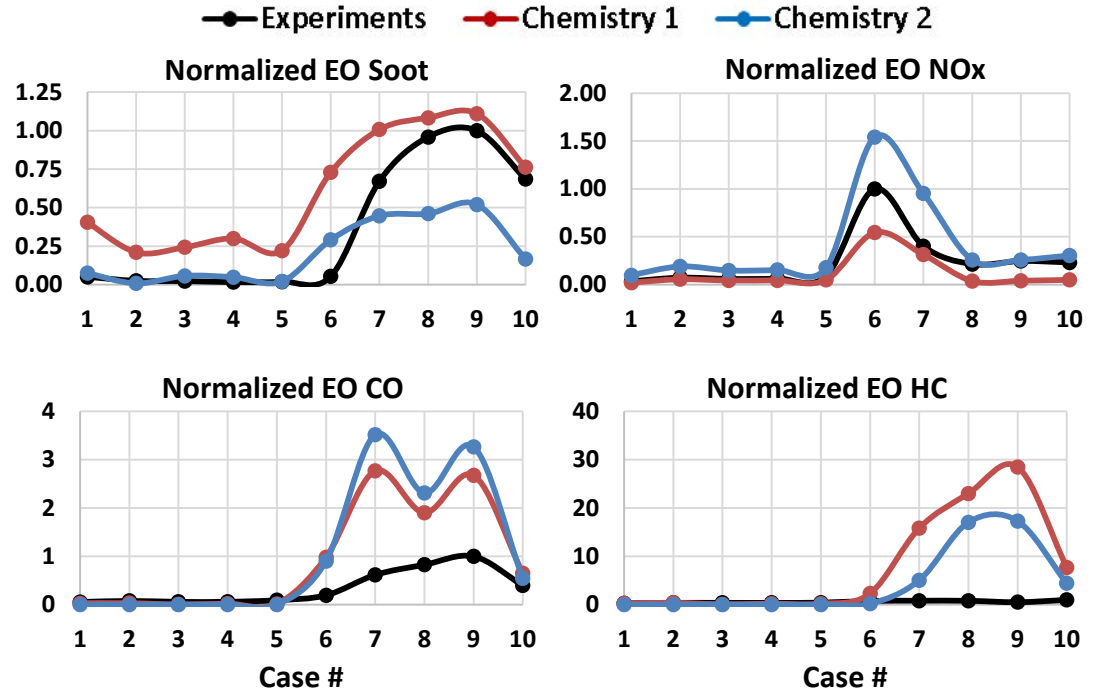- Using 2 nodes doubles allocation usage for < 2x speed-up

- Closed-cycle, diesel sector model
- CONVERGE on Titan with LLNL's Zero-RK chemistry solvers
- ~50k cells with AMR and multi-zone chemistry
- 144 species, 900 reactions

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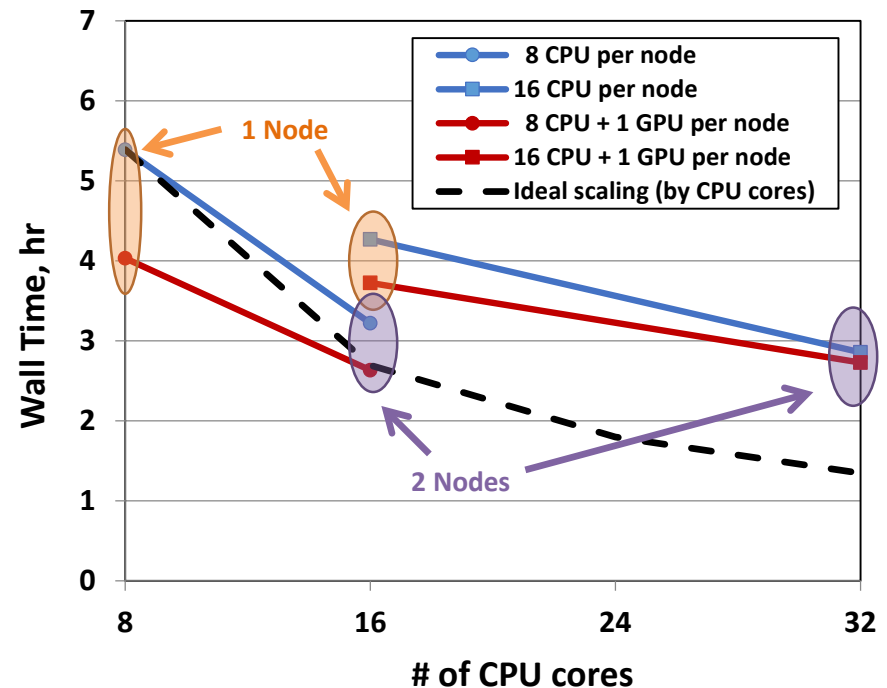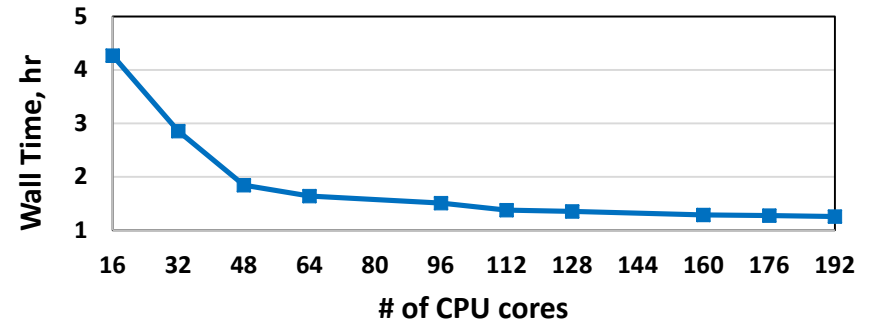
Technical Accomplishments – Virtual engine design and calibration (3/4)

Initial refinements to chemistry details provides notable improvement in HC accuracy

- **CONVERGE with chemistry 1**
  - UW-ERC n-heptane
  - 47 species, 74 reactions
  - Soot: Hiroyasu-NSC
  - NOx: Zel'dovich

- **CONVERGE with chemistry 2**
  - **Merged Chalmers n-heptane & Stanford PAH**
  - **144 species, 900 reactions**
  - **Soot: PSM detailed model**
  - **NOx: Reduced GRI NO**

- **Results shown here are for selected speed/load cases**
  - Simulations for full speed/load range in progress

Legend: ●— Experiments ●— Chemistry 1 ●— Chemistry 2

Normalized EO Soot
Normalized EO NOx
Normalized EO CO
Normalized EO HC
Case #

Normalized EO CO

- Simulation to EVO
- Extrapolated to BDC
- Extrapolated to peak EV lift
- Extrapolated to EVC
- Experiment EO sample

Case #

Investigating several potential reasons for lack of improvement in CO accuracy

- **Added species/reactions mainly target HC & soot precursors**
  - Repeating simulations with more detailed mechanisms

- **CO oxidation continues beyond EVO**
  - Simple extrapolation beyond EVO highlights potential contribution
 - Full-cycle simulations may be needed to fully capture CO

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Ongoing and Future Work

- **Evaluate impact of refined boundary conditions**

- **Evaluate impact of additional chemistry mechanisms**
  - GM multi-surrogate mechanisms
  - LLNL PRF mechanism (1034 species, 4236 reactions)

- **Implement sparse grid sampling to reduce required number of simulations**

- **Assess impact of approach on accuracy and computational time for engine calibration**

Emissions accuracy over the speed/load range
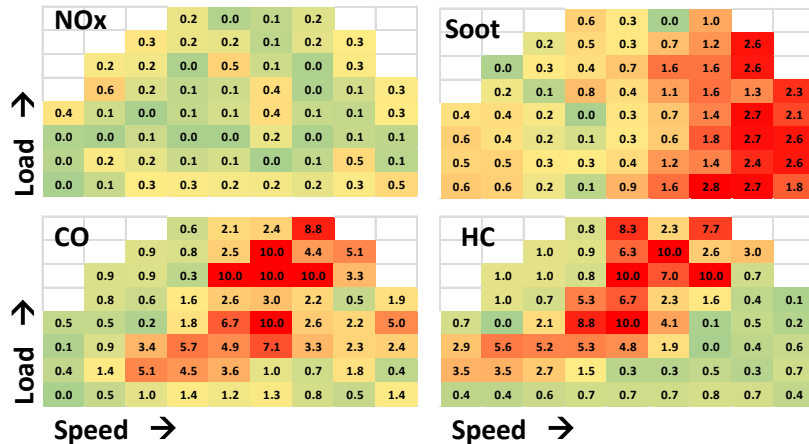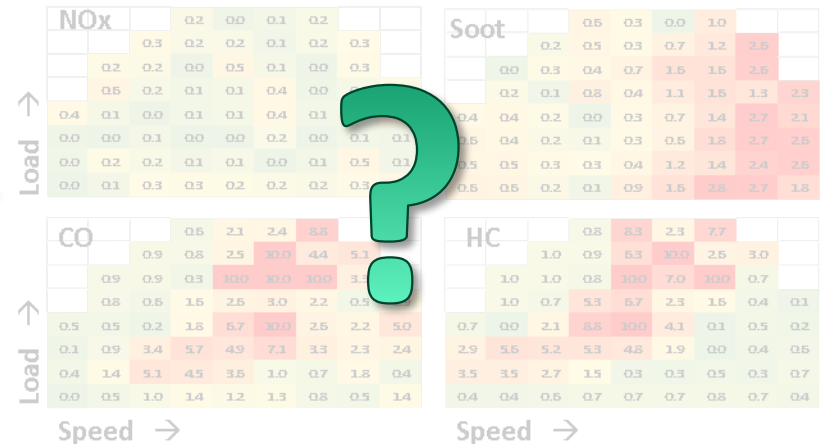
* Note:
NOx and soot contours on same scale.
CO and HC contours on same scale.

Technical Accomplishments – Cyclic variability in dilute ICEs (1/4)

Cyclic variability (CV) is a significant barrier to full realization of efficiency and emission benefits of highly dilute operation

- **PreSICE Workshop identified improved understanding and prediction of CV as a key need**

- **Combustion instabilities typically driven by stochastic (boundary condition variations) and deterministic (cycle-to-cycle and cylinder-to-cylinder coupling) processes**
  - Short-term predictable
  - Understanding the nature and causes of CV enables potential for mitigation and control

- **Study of CV with detailed simulations is complicated by sensitivity to numerically induced variability at highly dilute conditions**

Collaborative effort to gain new understanding into causes of CV at highly dilute conditions

- **Parallel LES cycle simulations with intelligent boundary condition sampling**

- **Uncertainty Quantification (UQ) to investigate impact of key engine and simulation parameters**
  - Ensemble averaging of multiple LES realizations per UQ sample point

Supported by ALCC allocation

- **17.5 Mhrs on Titan**

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Technical Accomplishments – Cyclic variability in dilute ICEs (2/4)

LES realizations effected by perturbations to pseudo-random number generator (PRNG) seed

- **Pseudo-random submodel components introduce numerical stochasticity to in-cylinder conditions**
  - Seeding of initial spray parcel distributions, collision and break-up decisions, etc.
- **At low dilution, the resulting CV is relatively low**
- **However at highly dilute conditions, combustion can be very sensitive to these small changes resulting in large variability**
- **Additional studies needed to investigate potential impact of grid and parcel refinement on reducing numerical variability**
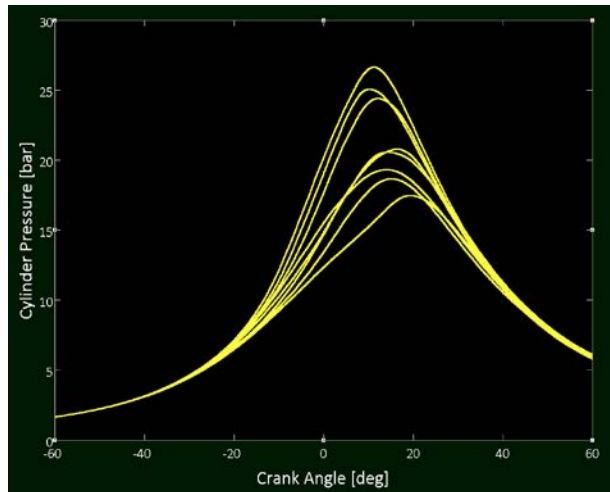
Results from multiple LES realizations with identical inputs except PRNG seed show extreme sensitivity to numeric variability at highly dilute conditions
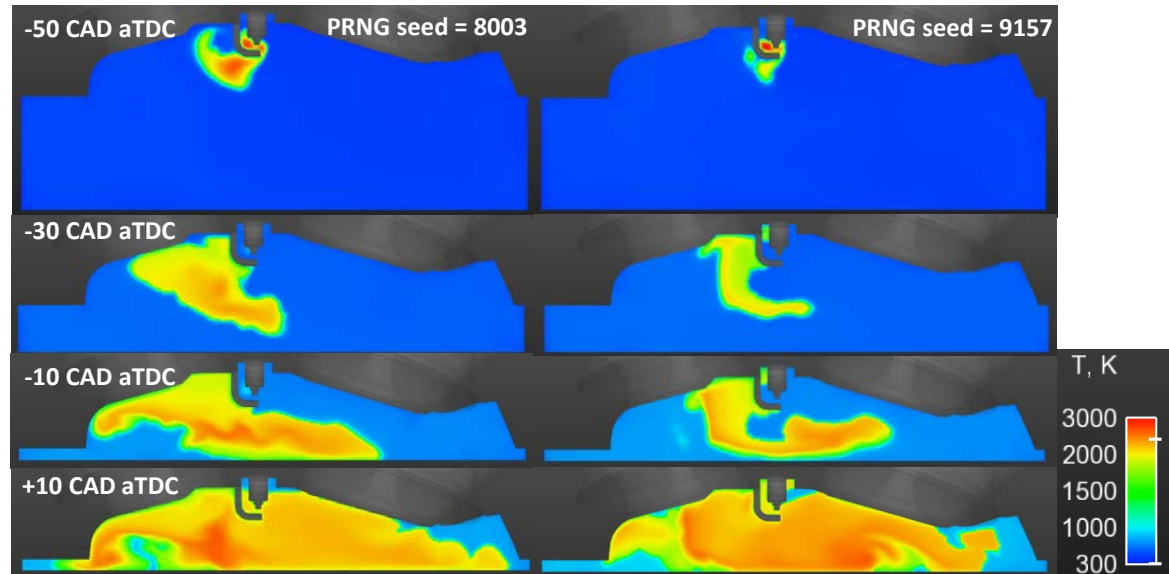
ASME ICEF2015-1172

Technical Accomplishments – Cyclic variability in dilute ICEs (3/4)

Limited sparse-grid UQ study to examine combustion sensitivity to variability in key boundary conditions which impact dilution

- **Exhaust P (residual fraction)**
- **Exhaust T (residual fraction and temperature)**
- **Mass of injected fuel (equivalence ratio)**

Parameter	Minimum	Maximum
P exhaust, kPa	**98.5**	**110**
T exhaust, K	**685**	**785**
Fuel injected, mg	**12.8**	**15.6**

Variability strongest at lower phi

- **20 realizations at each sample point**
- **Ensemble averaging allows study of parameter sensitivities**

At target operating condition, combustion most sensitive to variations in equivalence ratio
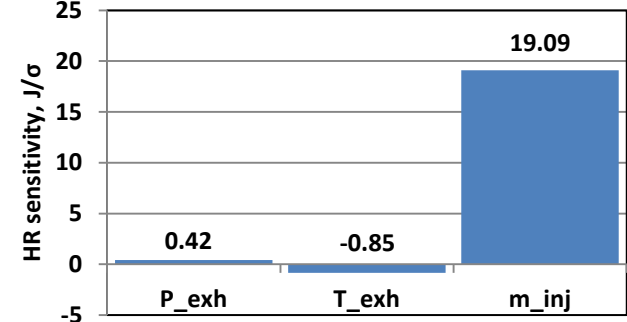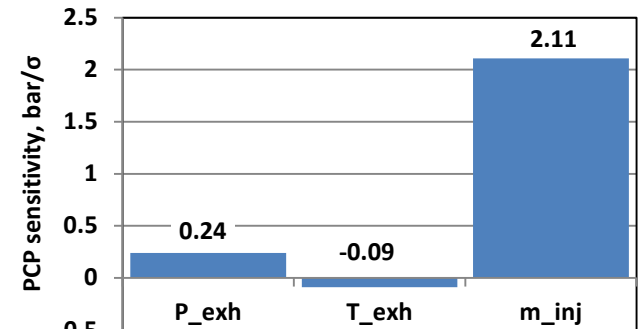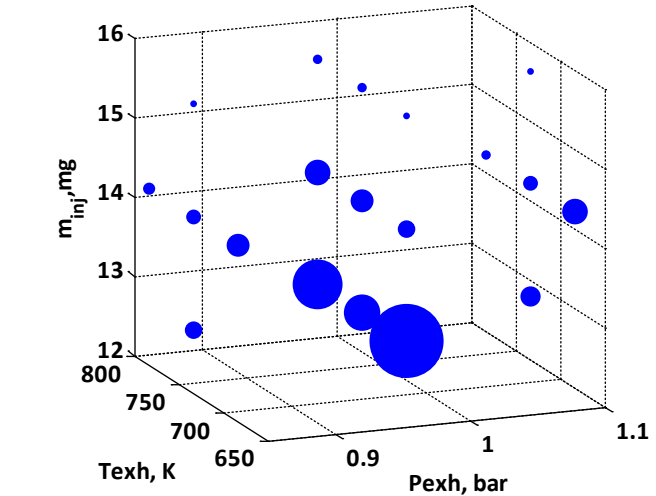
ASME ICEF2015-1172

Technical Accomplishments – Cyclic variability in dilute ICEs (4/4)

Simulation efforts are transitioning to modified GM 2.0-L Ecotec engine

- **Provides better alignment with CV experimental efforts at ORNL (ACE090)**
- **Rapid coordination of simulations and experimental data**
- **Advanced controls hardware for on-engine evaluation of metamodel-based control strategies**
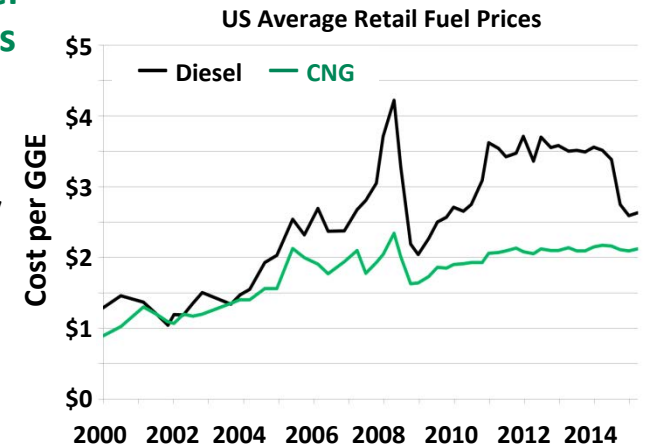
Ongoing and Future Work

- **Scan engine hardware and import to CONVERGE CFD model – COMPLETE**
- **Calibrate model for high-EGR operation – On Track**
- **Further refine metamodel approach and evaluate potential for model-based control (FY2017-18)**
- **Develop and evaluate metamodel-based control strategy on-engine (FY2019)**
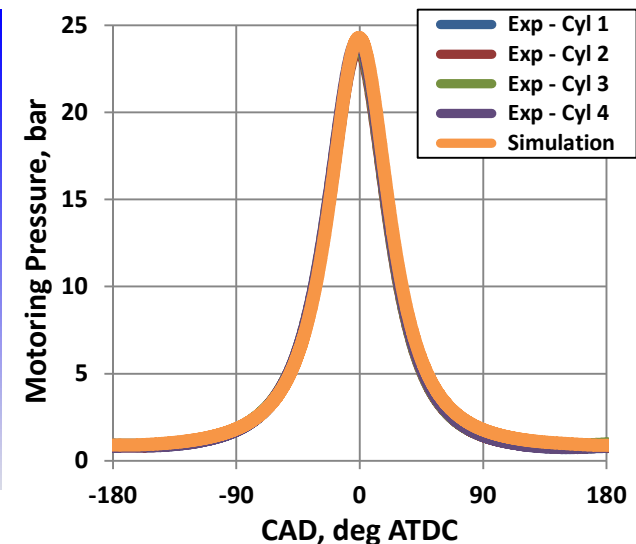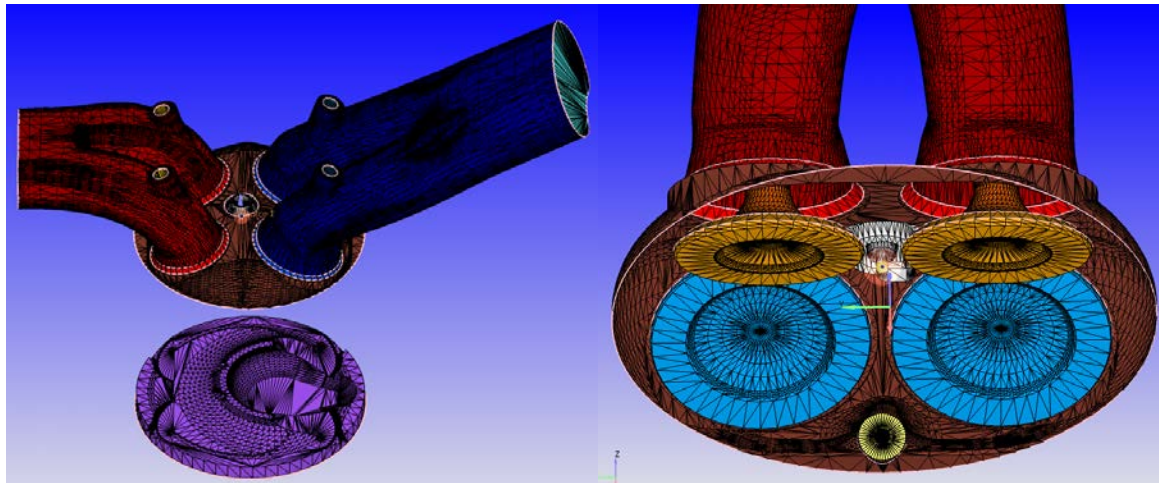
Technical Accomplishments – Cyclic variability in dual-fuel ICEs (1/3)

Cyclic variability (CV) in dual-fuel (diesel/NG) operation is a barrier to significant cost savings and petroleum reduction in locomotives and HD regional fleets

- **Diesel pilot ignites propagating flame in premixed NG**

- **CV for dual-fuel is much more pronounced than for diesel-only at certain engine conditions**
    - Decreased performance
    - Increased methane emissions

US Average Retail Fuel Prices

— Diesel — CNG

Cost per GGE

$5
$4
$3
$2
$1
$0

2000 2002 2004 2006 2008 2010 2012 2014

US-DOE Alternative Fuels Data Center
www.afdc.energy.gov/data
Updated 10/2015

Collaborative experimental and computational effort to investigate the contributing factors to CV in dual-fuel operation

- **Experiments to quantify on-engine variability in operating and boundary conditions**

- **CFD simulations and uncertainty quantification to study contribution of individual variabilities on CV**

Supported by Director Discretion (DD) allocation

- **5 Mhrs on Titan**

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Technical Accomplishments – Cyclic variability in dual-fuel ICEs (2/3)

Initial study using RANS simulations to examine contribution of limited set of boundary conditions

- **Focused on single operating point (1050 RPM, 20-bar BMEP) for 100% diesel and dual-fuel**
  - Full cylinder, closed cycle simulations (2-3M cells with AMR)
  - ~80 species, ~450 reactions
  - 256-512 CPU cores on Titan per simulation

Good agreement with experimental data at baseline cases
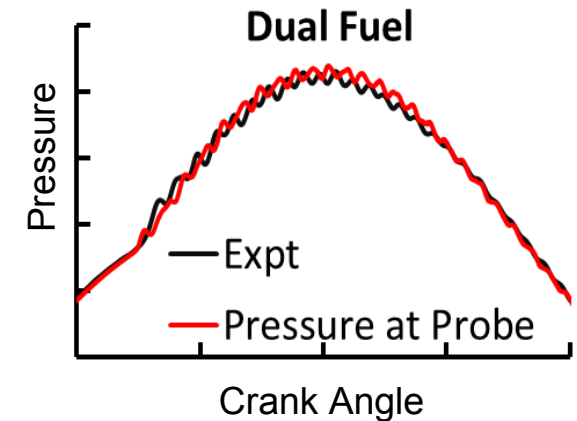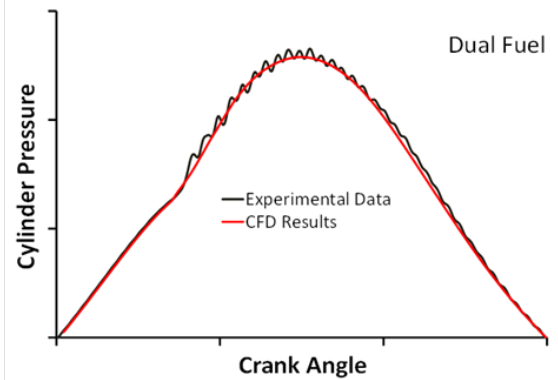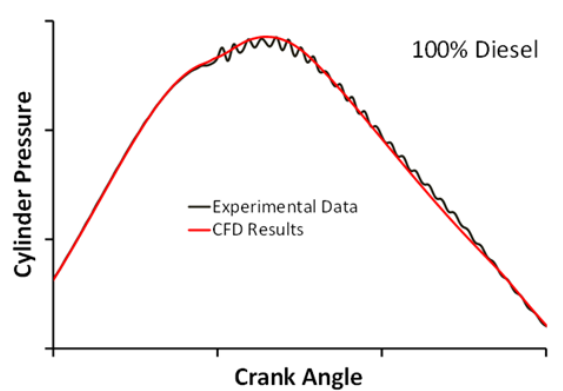
Averaged bulk cylinder pressure does not reflect oscillations in experimental measurements

- **Virtual probe placed at measurement location does reveal local pressure oscillation**
  - Potential future publication

SAE 2016-01-0798

Initial study examined contribution to CV of variation in limited set of key boundary conditions

- **Initial simulations did not fully capture experimental CV**
  - Particularly the highest levels of CV during flame propagation
- **Variability in diesel injection and T at IVC are largest contributors**
  - Need to evaluate additional parameters

	Diesel-only		Dual Fuel	
	Min	**Max**	**Min**	**Max**
P @ IVC	ā - 1.3 σ	ā + 0.67 σ	ā - 0.36 σ	ā + 1.52 σ
T @ IVC	ā * 0.99	ā * 1.01	ā * 0.99	ā * 1.01
Air flow	ā - 3 σ	ā + 3 σ	ā - 1.35 σ	ā + 1.35 σ
Residual %	ā * 0.62	ā * 1.63	ā * 0.7	ā * 1.7
DI SOI	ā - 1 σ	ā + 1 σ	ā - 1 σ	ā + 1 σ
Diesel flow	ā - 3 σ	ā + 3 σ	ā - 2.7 σ	ā +2.7 σ
NG flow	—	—	ā - 1.35 σ	ā + 1.35 σ
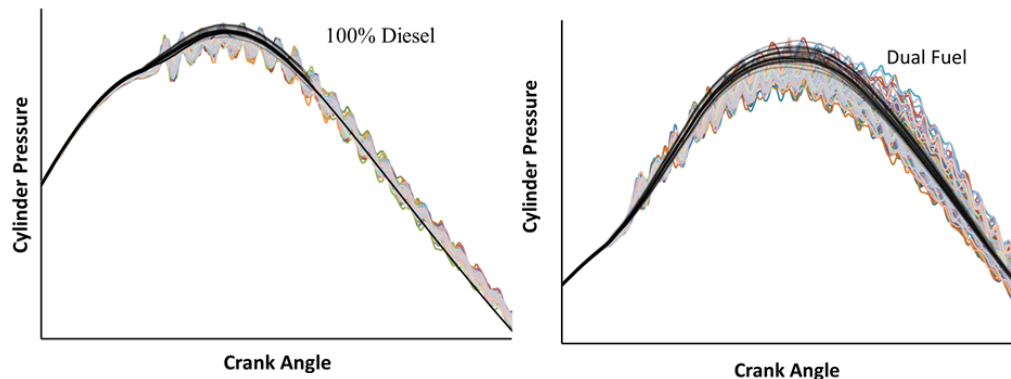
Parameter	**Diesel %COV (Rank)**	**Dual-Fuel %COV (Rank)**
P @ IVC	0.16 (3)	0.04 (5)
Air flow	0.04 (4)	0.04 (5)
T @ IVC	0.16 (3)	0.95 (2)
DI SOI	0.72 (1)	1.61 (1)
Diesel flow	0.29 (2)	0.64 (3)
NG flow	—	0.39 (4)

100% Diesel — Cylinder Pressure vs Crank Angle

Dual Fuel — Cylinder Pressure vs Crank Angle

SAE 2016-01-0798

Ongoing and Future Work

- **Pending DD proposal on Titan**
  - LES simulations with fuel stratification and additional parameter variability
- **Proposed 2016 ALCC effort on Mira – GE, ORNL, ANL, Convergent Science**
 - LES simulations of injector needle wobble

Stratification　**Needle Wobble**

Courtesy: Som, ANL

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Summary of *Future Work*

Virtual engine design and calibration	
• Evaluate with larger chemistry mechanisms • Implement sparse grid sampling to reduce required number of simulations • Assess impact of approach on accuracy and computational time for engine calibration	**FY2016-17**
Cyclic variability in dilute ICEs	
• Calibrate 2-L GDI model for high EGR operation with data from ACE090 • Develop metamodel and evaluate potential for model-based control • Develop and evaluate metamodel-based control strategy on-engine	**FY2016** **FY2017-18** **FY2019**
Cyclic variability in dual-fuel ICEs	
• LES simulations on Titan with fuel stratification and additional parameter variations • LES simulations on Mira with nozzle wobble	**FY2016-17** **FY2016-17**

Submitted 2016 ALCC proposal aimed at gaining new insight into Partial Fuel Stratification strategy

• **CFD simulations on Titan**

• **Detailed chemistry with GPU-enabled Zero-RK chemistry solvers**

• **Experimental optical engine data from SNL (ACE004)**

Courtesy: Dec, SNL

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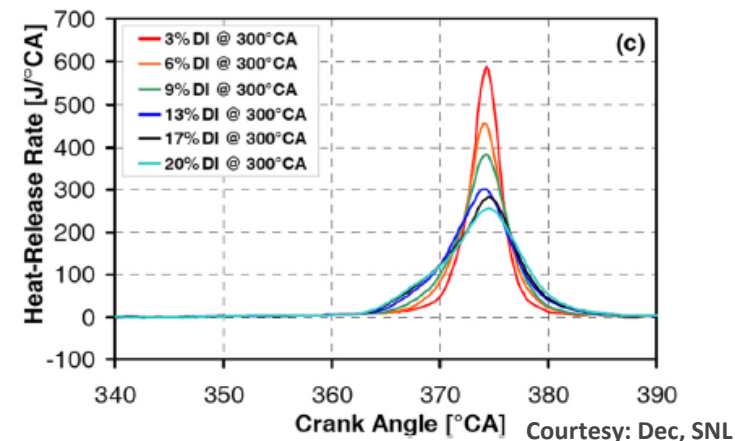
Response to reviewer comments

Overall reviewer responses were positive citing strong collaboration and relevance to DOE-VTO objectives.

Many questions raised sought a deeper dive into technical details.
- **Response:** The nature and intent of this presentation limits the level of detail we are able to provide. Additional technical details for each project are available upon request and in the cited publications.

Our lowest scores (Approach and Technical Accomplishments) seem to have been partially impacted by the presenter's choice to focus the presentation on a couple of subtasks. For example, reviewers expressed the desire for more status information on the remaining subtasks which only received single-slide summaries.
- **Response:** This year we hope to provide a better overview of the overall project approach and goals and provide a more even balance to presentation of results from the many subtasks (while recognizing that will likely come at the expense of providing a deeper technical dive).

Some comments on the injector design study indicated a lack of clarity in conveying the objectives of that year's efforts and contribution to the overall goal of the study.
- **Response:** The specific goal of that ALCC project is to use an HRM-based internal injector flow model to provide more accurate boundary conditions for each plume to a CONVERGE cylinder model for spray evolution and to *qualitatively* validate results with spray visualization data for multiple injector geometries and spray conditions. A more *quantitative* assessment of the model is pending as resources become available.

Recurring comments addressed both sides of the balance between DOE-funded open, pre-competitive efforts and desire of industry for more proprietary efforts.
- **Response:** This DOE-funded project supports pre-competitive efforts which utilize computing resources at OLCF (a DOE-funded user facility). As such, open publication of some results is expected. Other avenues exist for proprietary efforts.

Recurring comments addressed the use of CONVERGE for the various efforts over other CFD options.
- **Response:** The OEM partner for each task selects the CFD platform and often provides additional licenses for use on Titan. The ISV is typically given the opportunity to join as a partner to provide additional support as needed. OLCF gives preference to proposed efforts which scale well in parallel and make use of Titan's CPU-GPU architecture (which CONVERGE does). ORNL makes use of other CFD options (including KIVA, Forté, and OpenFOAM) as appropriate.

Numeric scores on a scale of 1 (min) to 4 (max) — This Project, Sub-Program Average. Approach 3.07, Tech Accomplishments 3.14, Collaboration 3.43, Future Research 3.14, Weighted Average 3.16.

Relevant to DOE Objectives: Yes (100%). Sufficiency of Resources: Sufficient (100%).
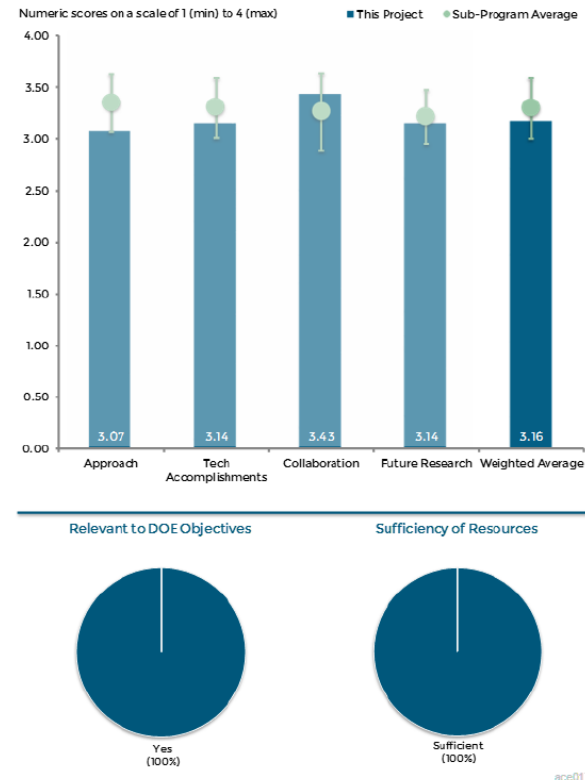
Collaborations

Project supports collaborative efforts with industry (OEMs and ISVs), other NLs, and universities to accelerate development of advanced engines capable of meeting fuel economy and emissions goals

Virtual fuel injector design	GM	⬤	🌱
Virtual engine design and calibration	GM	⬤	🌱 ⬛
Cyclic variability in dilute ICEs	Ford	⬤	🌱
Cyclic variability in dual-fuel ICEs	GE	⬤	🌱 🔺
CRADA to develop GPU-enabled numeric solvers	Cummins	⬤	🌱 ⬛ 🟥
Partial Fuel Stratification simulations	GM	⬤	🌱 ⬛ 🟦

Applies DOE ASCR fundamental tools and HPC resources to address technical barriers identified by VTO MYPP and PreSICE Workshop

- **Oak Ridge Leadership Computing Facility (OLCF) and Titan**
- **TASMANIAN**

Strong coordination with broader simulation portfolios within ORNL and DOE

Co-Optima simulation team (FT040)	⬛ 🔺 🌱 ⬡ 🟦
Predictive knock modeling (FOA)	Ohio State 🌱
Advanced propulsion materials (PM057)	Cummins 🌱 ⬤
Support of ORNL experimental efforts (ACE016, ACE090, etc.)	⬤ ANSYS KIVA GT AUTONOMIE

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Remaining challenges and barriers

Applying simulation tools on HPC resources requires a different mindset

- **Scalability is vital to maximize benefits of parallel architectures**
  - Both single jobs and ensembles
- **Maximizing benefits of HPC (reduced wall time, larger jobs, etc.) must often be balanced with HPC administration rules and hardware limits (fixed allocations, memory & I/O limitations, scheduling rules, etc.)**
- **Software must continually adapt to evolving hardware technologies**
  - Hardware independence (CPU, GPU, MIC, etc.)
  - OLCF gives preference to allocation proposals which make full use of Titan's GPUs
  - DOE-ASCR developing exa-scale HPC platforms (OLCF – Summit in 2018, ALCF – Aurora in 2019)
- **Software must adapt to scale of HPC environments**
  - Memory usage, file I/O, load balancing, restart management, licensing, etc.

Numerically induced variability in highly dilute simulations can mask CV we wish to study

- **Physics of highly dilute combustion is extremely sensitive to variability of in-cylinder conditions**
- **Variability introduced by pseudo-random submodel components can be quite pronounced at highly dilute conditions (less so at lower dilution)**

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Summary

- **Relevance**
  - Addresses barriers identified in VTO MYPP and PreSICE Workshop through innovative use of HPC and predictive simulation to accelerate advanced engine designs to meet fuel economy and emissions goals

- **Approach**
  - Collaborative efforts with OEMs, ISVs, NLs, and universities to…
    - Develop and evolve new predictive capabilities
    - Gain new insight to areas where understanding historically limited by computational resources
    - Further enable virtual engine and component design

- **Technical Accomplishments**
  - Improved spray evolution predictions with 2-fluid HRM injector flow model coupled with CONVERGE
  - Used Zero-RK GPU solvers to enable detailed chemistry and improve emissions prediction for virtual engine calibration
  - Evaluated sensitivity of highly dilute combustion to variability in key BCs which impact dilution level
  - Performed initial characterization of impact of BC variability on CV in dual-fuel ICEs

- **Collaborations**
  - Multiple collaborative efforts with OEMs, ISVs, NLs, and universities
  - Strong coordination with broader simulation portfolios within ORNL and DOE

- **Future Work**
  - Assess potential of our approach to improve accuracy and reduce wall-time for virtual engine calibration
  - Evaluate potential of metamodel-based control to reduce CV in dilute ICEs
  - Further investigate of impact of BC variability (e.g., NG stratification, needle wobble) on CV in dual-fuel ICEs
  - Use detailed simulations to gain new insight to Partial Fuel Stratification approach

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