Accelerating predictive simulation of IC engines with high performance computing (ACS017)

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Overview

Timeline

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

Budget

- **FY2016 – $450k**
  $50k CRADA
- **FY2017 – $340k**

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**

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

Partners

- **Leveraging DOE Office of Science funding for ASCR resources**
  - Multiple ALCC allocation awards on OLCF and ALCF HPC resources
  - **49 Mhrs** on Titan and Mira @ $0.03/hr = **$1.47M**
- **Multiple ongoing efforts with industry, NL, and academic involvement**
- **Collaboration with LLNL for application of GPU-enabled Zero-RK chemistry solvers on Titan (ACS076)**
- **Strong connectivity to broader simulation portfolios at ORNL and DOE**
  - **Co-Optima simulation team (FT052, FT053)**
  - **Engine knock prediction with The Ohio State University (ACS110)**
  - **Daimler SuperTruck II team (ACS100)**
  - **Advanced propulsion materials (PM057)**
  - **Simulation support of experimental efforts at ORNL (ACS016, etc.)**

Overall *Relevance* and *Approach*

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

- **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 ***workstations/clusters*** to ***on-board diagnostics and controls***
- **Solve the unsolvable**
  - Apply peta/exa-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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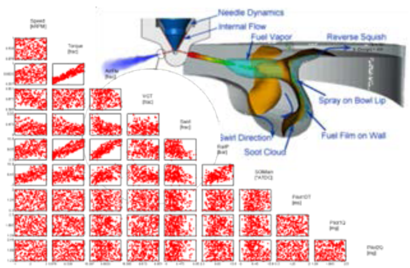
Current Task List and *Milestones*

Projects / Current-year Tasks	Collaborations / Status
Enabling virtual engine design and calibration Address barriers to further enable and accelerate virtual engine design and calibration	
• ALCC project to enable practical use of highly detailed chemistry in ICE CFD simulations	**Completed FY2017-Q1**
• Evaluate impact of increased chemistry details on accuracy and simulation time	**Completed FY2017-Q1**
• Proposed ALCC project to further improve predictive accuracy with open-cycle simulations and conjugate heat transfer	**Target FY2018-Q4**
Simulation of Partial Fuel Stratification HCCI Gain new insight to PFS approach using CFD with highly detailed chemistry	
• ALCC project to enable full-cycle CFD simulations of PFS with highly detailed chemistry • Evaluate impact of various fuel surrogates and increased chemistry detail on accurate simulation of PFS HCCI	**On-track for FY2017-Q4**
Cyclic variability in dual-fuel ICEs Investigate key factors promoting cyclic variability in dual-fuel engine applications	
• ALCC project to study impact of initial and boundary condition variability on CV	**On-track for FY2017-Q4**

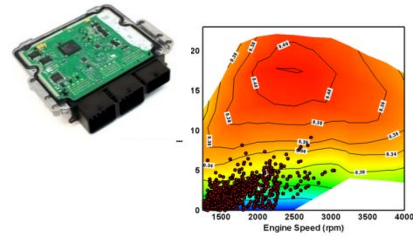
Virtual engine design and calibration (1/9) – *Relevance* and *Approach*

Virtual design and calibration has potential to significantly accelerate engine development

CFD simulations over multi-parameter DoE



Optimize engine controls calibration for fuel economy and emissions targets



Evaluate predicted performance and iterate as needed

- **Compromises for speed and computing resources impact accuracy of CFD simulations**
- **Often need to "tune" model for differing conditions across full operating space**
- **HPC offers potential to reduce need for compromises and achieve better balance of accuracy and speed**

Objective: **Develop and evaluate approaches that use HPC and state-of-the-art predictive simulation tools to better balance speed/accuracy trade-offs**

- Multi-year collaborative effort between OEM, ISV, and national labs

Current focus: **Enable practical use of highly detailed chemical mechanisms in diesel engine CFD simulations**

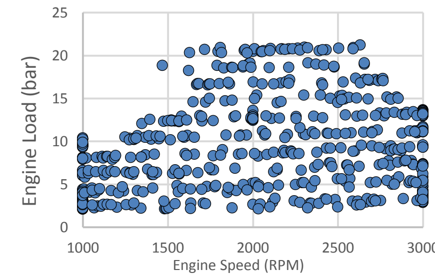
- Parallel ensemble simulations on Titan to cover full DoE
- LLNL's Zero-RK GPU chemistry solvers for computational speed-up
- Evaluate impact on accuracy, speed, and need for "tuning"

Supported by ALCC allocation

- 8 Mhrs on Titan

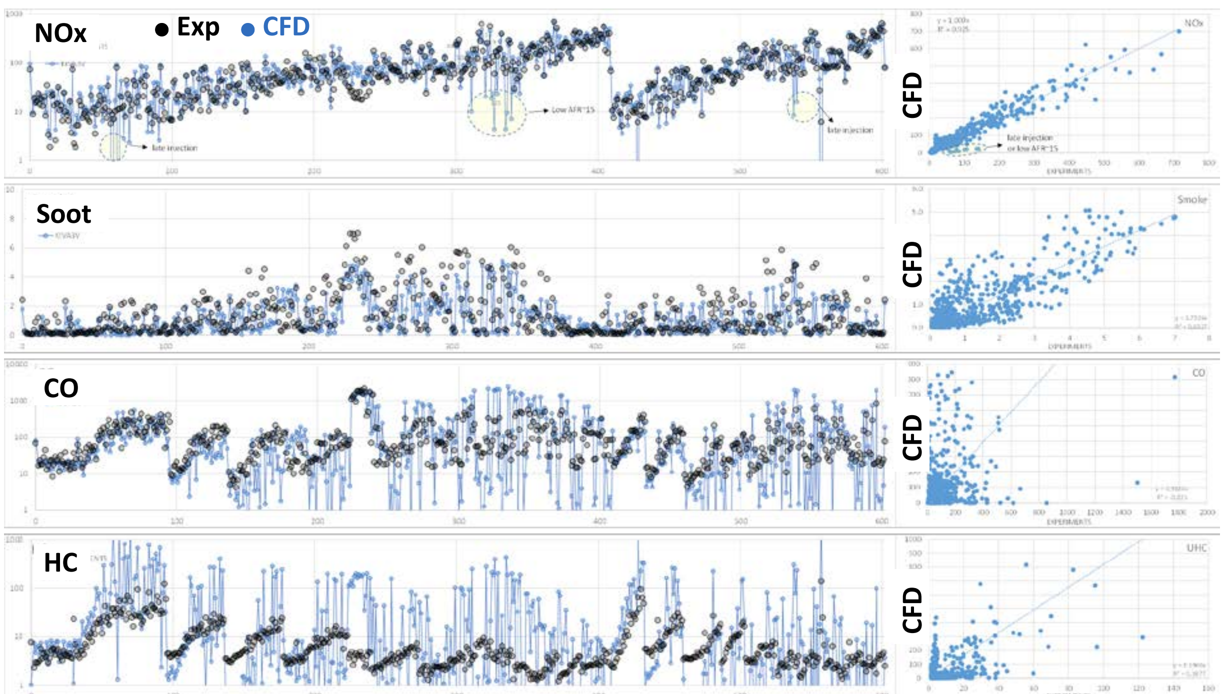
Virtual engine design and calibration (2/9) – *Relevance* and *Approach*

- **Model overview**
  - Diesel, sector-mesh, closed-cycle, RANS model in CONVERGE (v2.3)
  - GT-Power simulations provide initial boundary conditions
  - 600+ cases in DoE of engine control parameters over full engine calibration
    - 10 parameters: Speed, SOI and PW for pilot and main, rail P, EGR, wastegate, etc.
  - Includes extreme operating points that stretch capabilities of model



- **Simulations with simple chemistry and coarse mesh fail to accurately capture combustion for many cases**
  - Burn rate under-predicted resulting in incomplete combustion due to quenching at EVO
  - Worst performance at extreme conditions (late injection, high EGR, high load, rich-mode, etc.)

Will more-detailed chemistry and refined meshing improve predictive accuracy?



Simulation results shown are for coarse mesh and very simple chemistry (47 species) with Zel'dovitch NOx

Difference in emissions over speed-load map using engine calibrations developed using experimental data and simulation data to left

NOx (Load ↑, Speed →)

NOx			0.2	0.0	0.1	0.2		
		0.3	0.2	0.2	0.1	0.2	0.3	
	0.2	0.2	0.0	0.5	0.1	0.0	0.3	
	0.6	0.2	0.1	0.1	0.4	0.0	0.1	0.3
0.4	0.1	0.0	0.1	0.1	0.4	0.1	0.1	0.3
0.0	0.0	0.1	0.0	0.0	0.2	0.0	0.1	0.1
0.0	0.2	0.2	0.1	0.1	0.0	0.1	0.5	0.1
0.0	0.1	0.3	0.3	0.2	0.2	0.2	0.3	0.5

Soot

Soot			0.6	0.3	0.0	1.0		
		0.2	0.5	0.3	0.7	1.2	2.6	
	0.0	0.3	0.4	0.7	1.6	1.6	2.6	
	0.2	0.1	0.8	0.4	1.1	1.6	1.3	2.3
0.4	0.4	0.2	0.0	0.3	0.7	1.4	2.7	2.1
0.6	0.4	0.2	0.1	0.3	0.6	1.8	2.7	2.6
0.5	0.5	0.3	0.3	0.4	1.2	1.4	2.4	2.6
0.6	0.6	0.2	0.1	0.9	1.6	2.8	2.7	1.8

CO (Load ↑, Speed →)

CO			0.6	2.1	2.4	8.8		
		0.9	0.8	2.5	10.0	4.4	5.1	
	0.9	0.9	0.3	10.0	10.0	10.0	3.3	
	0.8	0.6	1.6	2.6	3.0	2.2	0.5	1.9
0.5	0.5	0.2	1.8	6.7	10.0	2.6	2.2	5.0
0.1	0.9	3.4	5.7	4.9	7.1	3.3	2.3	2.4
0.4	1.4	5.1	4.5	3.6	1.0	0.7	1.8	0.4
0.0	0.5	1.0	1.4	1.2	1.3	0.8	0.5	1.4

HC (Speed →)

HC			0.8	8.3	2.3	7.7		
		1.0	0.9	6.3	10.0	2.6	3.0	
	1.0	1.0	0.8	10.0	7.0	10.0	0.7	
	1.0	0.7	5.3	6.7	2.3	1.6	0.4	0.1
0.7	0.0	2.1	8.8	10.0	4.1	0.1	0.5	0.2
2.9	5.6	5.2	5.3	4.8	1.9	0.0	0.4	0.6
3.5	3.5	2.7	1.5	0.3	0.3	0.5	0.3	0.7
0.4	0.4	0.6	0.7	0.7	0.7	0.8	0.7	0.4

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Virtual engine design and calibration (3/9) – *Approach*

Overview of mechanisms evaluated

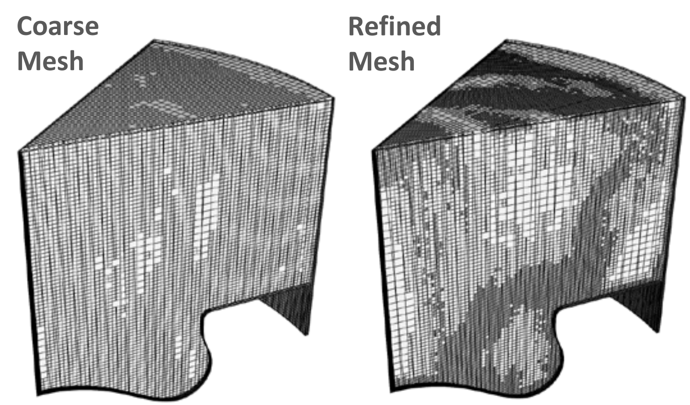
Mechanism	Fuel Surrogate	Species	Reactions	Soot	Chemistry Solver	Zones	Mesh
Very simple ERC n-heptane + Zel'dovitch NOx	nC7H16	47	74	Hiroyasu + PSM model	SAGE	MultiZone	Coarse
						Every cell	Refined
Reduced Chalmers n-heptane + Stanford PAH + GRI NOx	nC7H16	144	900	Hiroyasu + PSM model	SAGE	MultiZone	Coarse
				Hiroyasu	ZeroRK+GPU	Every cell	Refined
Detailed GM	4-component surrogate (GM)	766	6787	Hiroyasu	SAGE	Multi-comp MultiZone	Refined
					ZeroRK+GPU	Every cell	
Fully Detailed GM	4-component surrogate (GM)	5155	31,058	Hiroyasu	ZeroRK+GPU	Every cell	Refined

MultiZone model for multi-component fuels (CONVERGE v2.3)

- Allows binning according to concentration of each fuel component

Mesh details

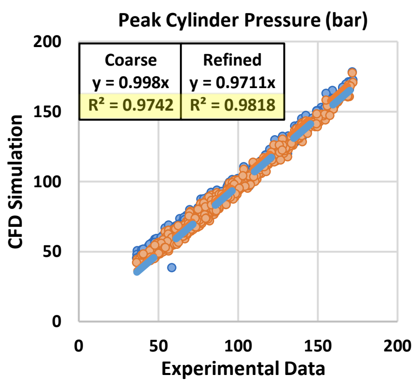
Mesh	Base Grid	Embedding	AMR	Max Cell Count
Coarse	0.002 m	Same	Same	~170k
Refined	0.001 m			~615k

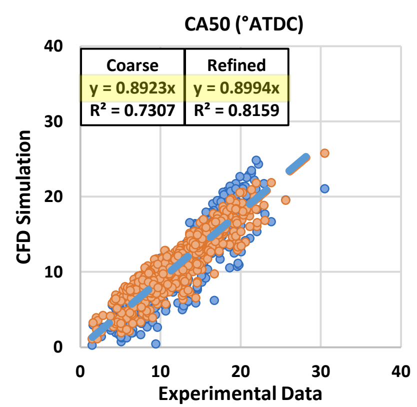


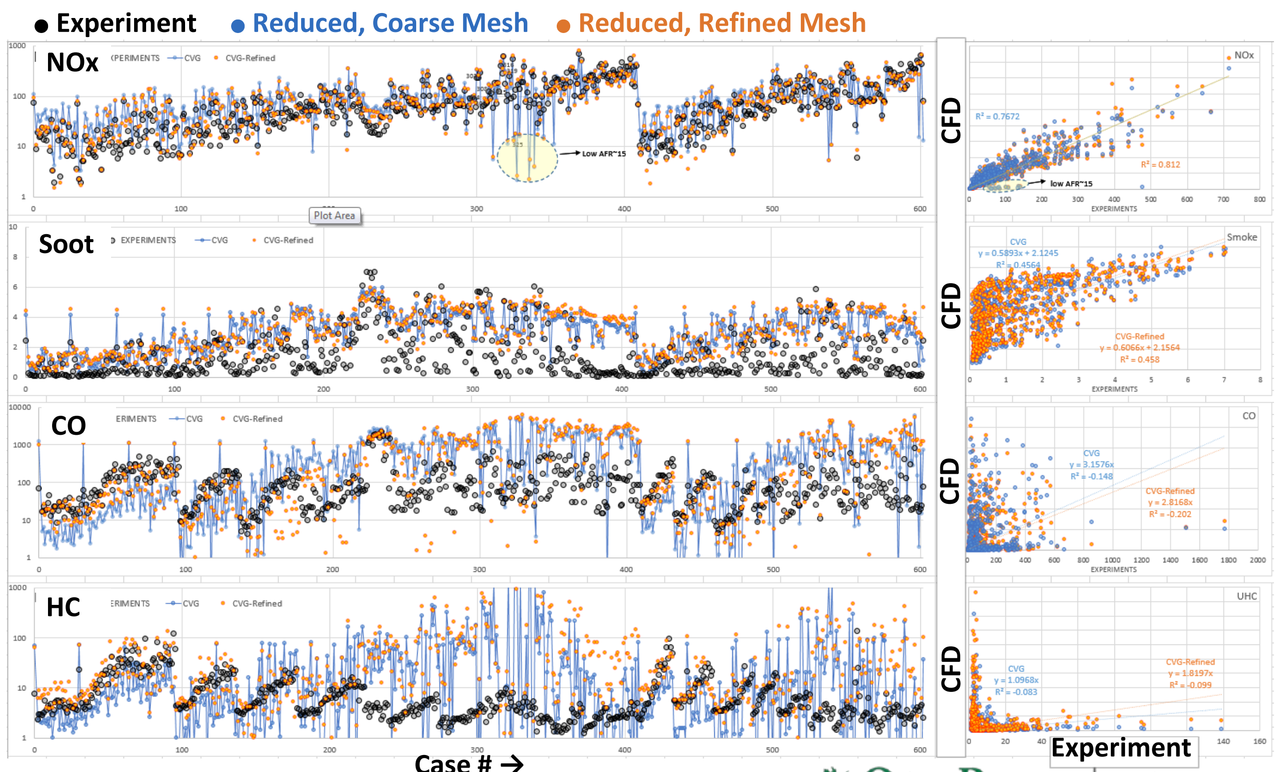
Virtual engine design and calibration (4/9) – *Technical Accomplishments*

Mesh refinement study with reduced mechanism (144 species) and MultiZone model

- **Refined mesh (~615k cells) improves overall correlation with experimental combustion metrics**
  - Good agreement with peak Pcyl, but predicted CA50 ~10% early on average
  - Continues to under-predict burn rate for many cases resulting in quenching at EVO
    - Especially at high speed and load conditions with rich operation and high EGR
- **Emissions results with refined mesh are mixed**
  - NOx – significantly improved correlation
  - Soot – little change
  - CO and HC – significantly improved at low-load points, unchanged (or worse) for quenched cases



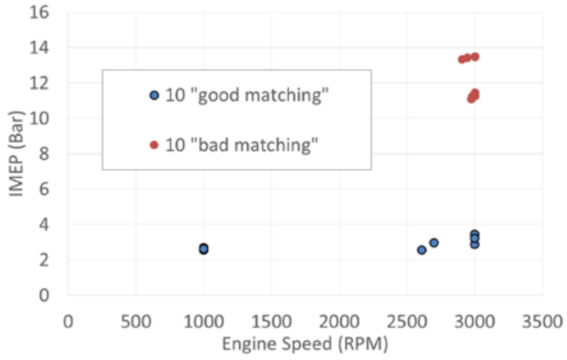




Virtual engine design and calibration (5/9) – *Technical Accomplishments*

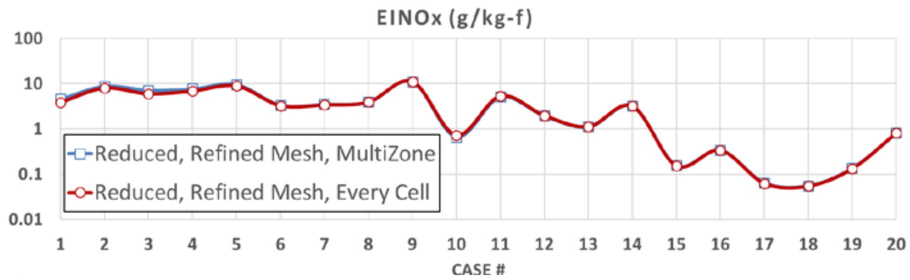
Every-cell vs. MultiZone chemistry study with reduced mechanism (144 species) and refined mesh

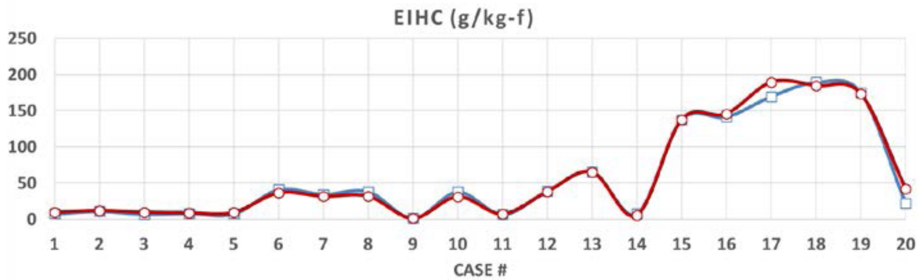
- **MultiZone model gives excellent agreement with every-cell approach**
  - Binning thresholds: T = 5 K, φ = 0.05
- **Significant reduction in wall time with MultiZone model**
  - Every-cell: 10-13 days
  - MultiZone: 90% of cases completed in 48 hrs

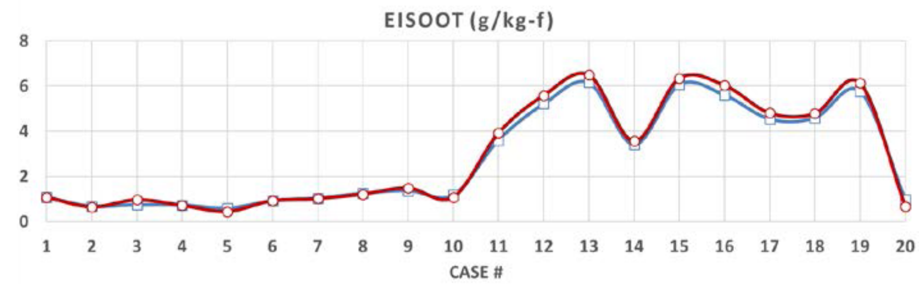


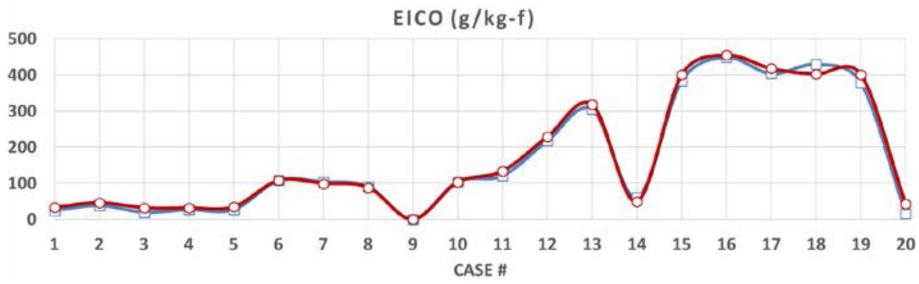
Results below are for 20 down-selected cases

- **1-10: low load "normal" operation, generally good agreement with experiment**
- **11-20: high speed & load "extreme" operation, generally poor agreement**









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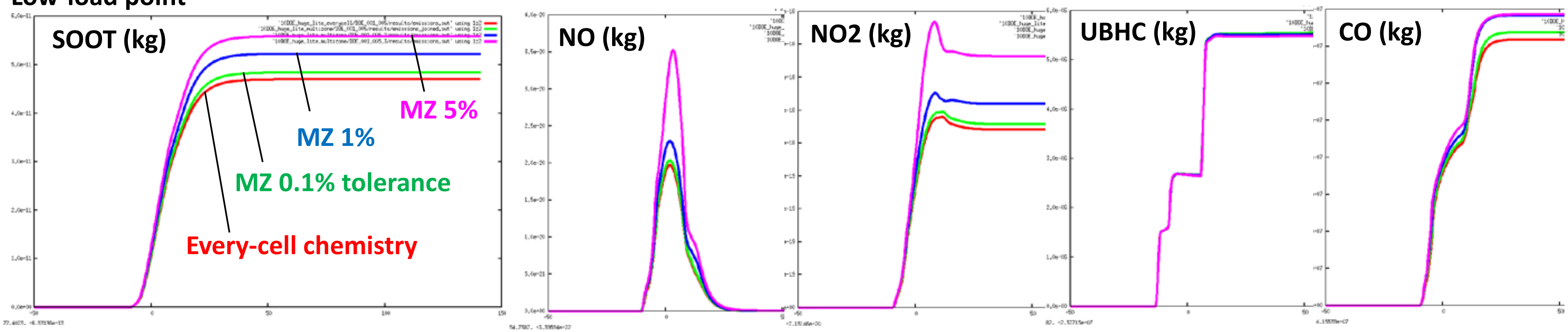
Virtual engine design and calibration (6/9) – *Technical Accomplishments*

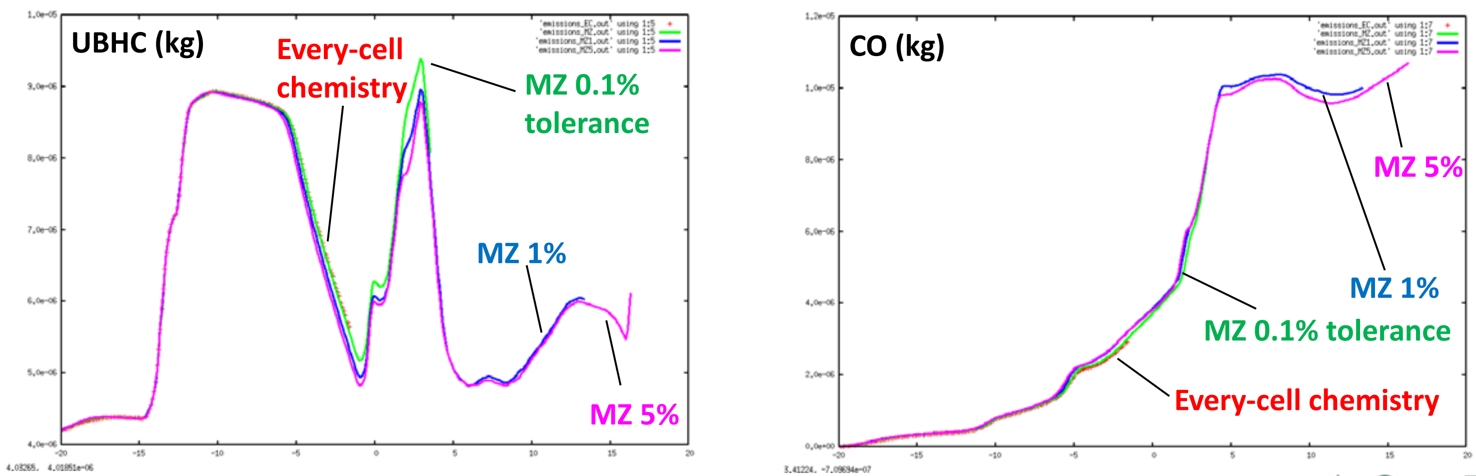
<u>Every-cell vs. MultiZone study with detailed mechanism (766 species), multi-species surrogate, refined mesh</u>

- Bin tolerance of 0.1% on surrogate species concentration required for good agreement with every-cell results
- Speed vs. accuracy trade-off:
  - 5% tolerance = ~50x speed-up vs every-cell, ~10x for 1%, ~2x for 0.1%

Low-load point



High-load point



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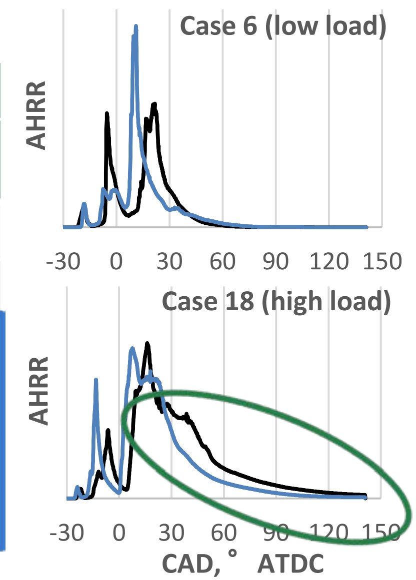
Virtual engine design and calibration (7/9) – *Technical Accomplishments*

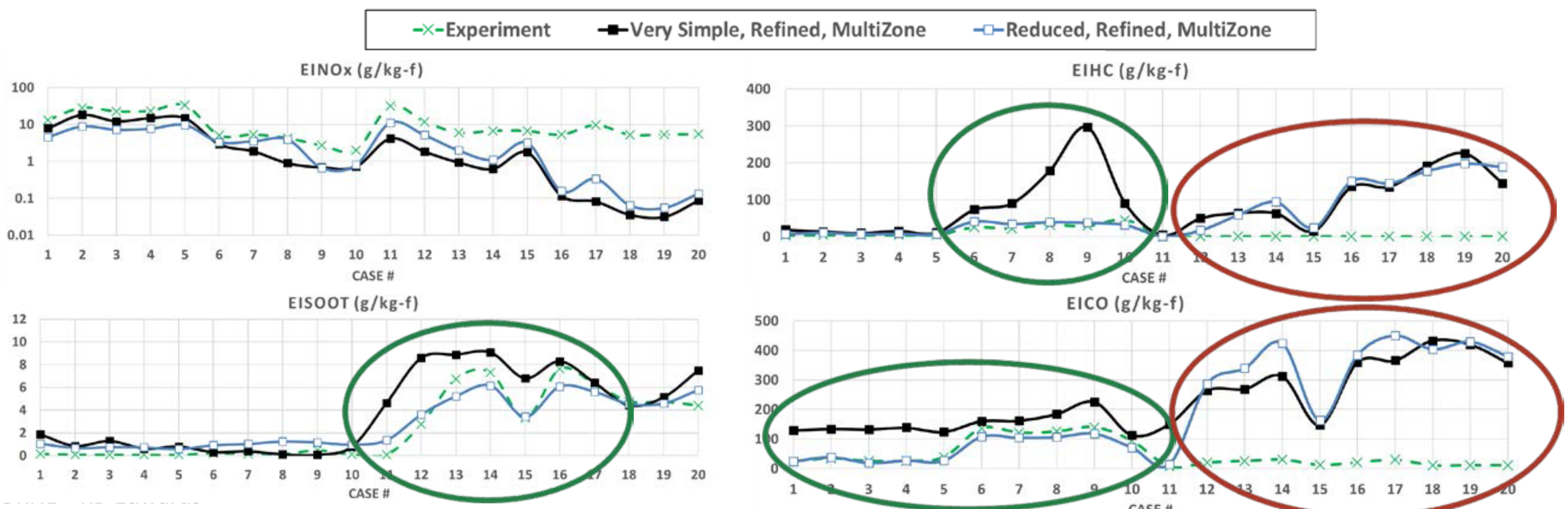
Mechanism comparison: very simple (47 species) vs. reduced (144 species)

- **Low-load points (cases 1-10):**
  - Significant improvement in UHC, CO
- **High-load points (cases 11-20):**
  - Some improvement in NOx
  - Significant improvement in soot
  - But little difference in UHC and CO
- **High speed/load points (rich, high EGR) have long burn duration quenched by EVO**
  - Significant increase in partial burn species and soot precursors vs. low load
  - Reduced mechanism provides some reduction of tail burn

Comparison of key species mass fractions at EVO

	Case 6		Case 18	
	Very Simple	Reduced	Very Simple	Reduced
O2	0.143	0.143	0.017	0.028
nC7H18	4.69e-4	1.23e-4	7.13e-6	4.58e-6
CH4	1.10e-4	4.40e-5	3.04e-3	3.93e-3
C2H2	4.68e-7	1.57e-7	1.49e-3	1.03e-3
Benzene		1.36e-8		3.80e-4
Napthalene		4.26e-8		3.56e-4





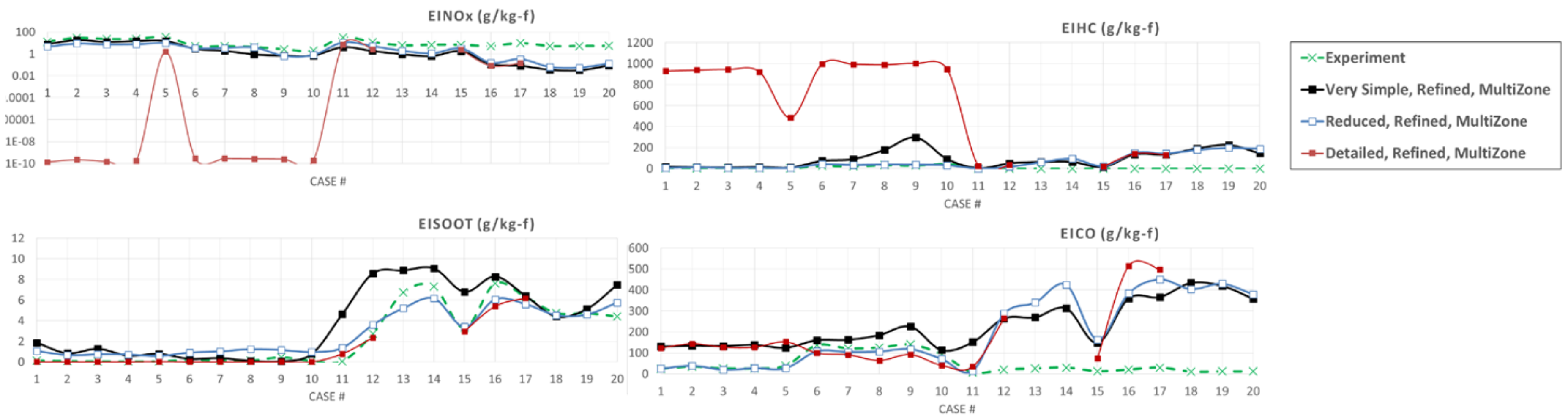
Virtual engine design and calibration (8/9) – *Technical Accomplishments*

Mechanism comparison: multi-component fuel surrogates and detailed mechanisms

- **Every-cell chemistry runs with fully detailed mechanism (5155 species) were halted to preserve allocation**
  - Very slow progress during combustion
  - Future simulations planned using updated MultiZone model for multi-component fuels

- **Initial simulations with detailed mechanism (766 species) produced mixed results**
  - Low-load cases failed to combust
    - Over-predicted spray penetration with large amounts of unburned fuel in wall film
  - High-load cases performed no better than with reduced mechanism (144 species)
- **Revised simulations underway with wall-film model off, revised near-wall treatment, and CONVERGE v2.3.23**
- **Future efforts include recalibration of spray model for multi-component fuels to correct over-penetration**

Paper submitted for 2017 ASME ICEF



Virtual engine design and calibration (9/9) – *Future Work*

Future plans are to complete evaluation of detailed mechanisms and expand efforts to include impact of gas exchange and improved boundary conditions

- **FY2017:**
  - Complete revised simulations with detailed mechanism (766 species)
  - Recalibrate spray model for multi-component fuel surrogate to address over-penetration and wall wetting
- **FY2018:**
  - Perform simulations with fully detailed mechanism (5155 species) using MultiZone model
  - Transition to full-cylinder geometry
  - Full-cycle simulations with gas exchange
    - Include mixing for improved initial cylinder conditions
    - Include combustion during blowdown
  - Include conjugate heat transfer for improved thermal boundary conditions
  - *ALCC proposal submitted for this effort*

Proposed future work is subject to change based on availability of funding and allocation of HPC resources

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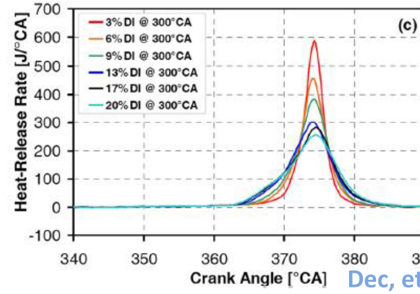
Simulation of PFS HCCI (1/3) – *Relevance* and *Approach*

Dec at SNL has demonstrated that Partial Fuel Stratification (PFS) can reduce knock enabling lean HCCI at high load

Partial Fuel Stratification
- Single-fuel HCCI-like LTC
- Globally lean
- Majority of fuel premixed
- Small DI to control ignition by fuel stratification
- Sensitivity to DI fraction, T intake, fuel's φ sensitivity

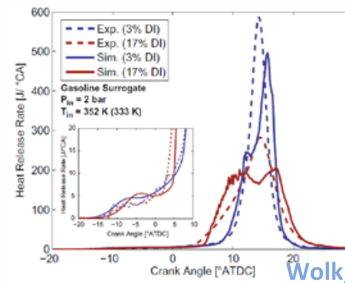


Dec, et al. (2011) SAE 2011-01-0897

Increasing DI fraction produces longer combustion duration and lower peak HRR with less knock.

Provides promise for enabling lean HCCI at high loads.

- **CFD simulations of PFS at UC Berkeley successfully captured…**
  - **Phi sensitivity of gasoline at higher pressures**
  - **Longer combustion duration with increased DI fraction**
- **However, opportunities for improvement were noted…**
  - **Peak HRR under-predicted**
  - **'Double-humped' HRR profile rather different from experiment**
  - **Surrogate calibrated for chemistry and may not fully capture evaporation**



Wolk, et al. (2015) Proc of Comb Inst 35

UCB PFS simulations
- 4-component fuel chemistry surrogate
- 96-species mechanism

Objective: Simulate PFS with detailed chemistry to better capture impact of fuel and thermal stratification

- Collaborative effort between OEM, ISV, and national labs
- Leverage HPC and LLNL's Zero-RK GPU chemistry solvers to enable detailed chemistry
- Evaluate multi-component surrogates for evaporation and chemistry
- Engine validation data from SNL

Supported by ALCC allocation
- 16 Mhrs on Titan

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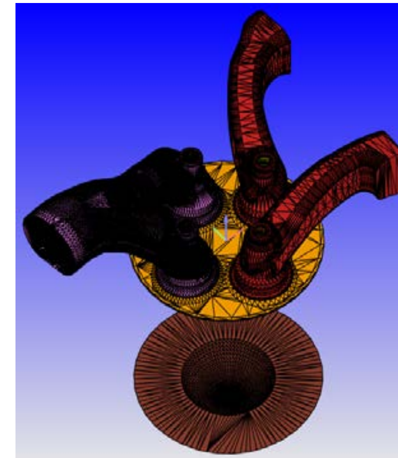
Simulation of PFS HCCI (2/3) – *Approach*

- **Model overview**
  - **Full-cylinder, closed cycle, RANS simulations in CONVERGE**
  - **Revised multi-zone model for multi-component surrogates**
  - **Geometry model of SNL engine**
  - **DoE consists of…**
    - 6 surrogate and mechanism combinations
    - Matrix of initial (IVC) temperature and DI fraction
      - T @ IVC: 350, 360, 370, 380, 390 K
      - DI fraction: 3, 6, 10, 13, 17, 20%



CONVERGE geometry model of engine used in SNL experiments

Liquid Fuel Surrogate	Vaporizes Into	Mechanism
Mehl	Mehl	Mehl 1389 species 5935 reactions **Mehl, et al. (2011) Proc of Comb Inst 33**
	iso-octane	
Styron	iso-octane	
Pitsch	Pitsch	Pitsch 338 species 1610 reactions **Cai, Pitsch (2015) Comb & Flame 162**
	iso-octane	
Styron	iso-octane	

- **Mehl surrogate (liq. %vol)**
  - n-heptane: 16%
  - iso-octane: 57%
  - toluene: 23%
  - trans-2-pentene: 4%
- **Pitsch surrogate (liq. %vol)**
  - n-heptane: 19.4%
  - iso-octane: 42.4%
  - toluene: 38.3%
- **Styron, et al. surrogate (mass fraction)**
  - nC10H22: 0.20
  - iso-octane: 0.45
  - n-hexane: 0.20
  - iso-pentane: 0.15

Styron, et al.
SAE 2000-01-0243

Simulation of PFS HCCI (3/3) – Status and *Future Work*

Initial development runs are complete and production runs are underway

- **These full-cylinder simulations with 1000+ species represent some of the most detailed engine CFD simulations ever performed (in open literature)**
- **Development runs required considerable effort to finalize strategy for running these large simulations on Titan**
  - Significant under-subscription of cores/node required to avoid “out-of-memory” crashes for Mehl cases
    - Mehl cases: 5 nodes using 1 GPU + 2 CPUs per node to achieve 16 GB RAM per CPU core
    - Pitsch cases: 1 node using 1 GPU + all 16 CPUs
    - Simulations with a third mechanism (Abienah, 2957 species, 11,734 reactions) were abandoned due to excessive memory requirements and limited memory/node on Titan

Future work

- **FY2017**
  - Analyze results from production runs
  - Revise and iterate as needed
- **Future efforts (FY2019) may include open-cycle simulations, conjugate heat transfer, and/or LES**
  - Subject to change based on available funding and allocation of HPC resources

Cyclic variability in dual-fuel ICEs (1/2) – *Relevance* and *Approach*

Cyclic variability (CV) in dual-fuel (diesel/NG) operation is a barrier to practical application

- **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

<u>Objective</u>: Experimental and computational effort to investigate the contributing factors to CV in dual-fuel operation

- Multi-year collaborative effort between OEM, ISV, and national labs
- 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 ALCC allocation

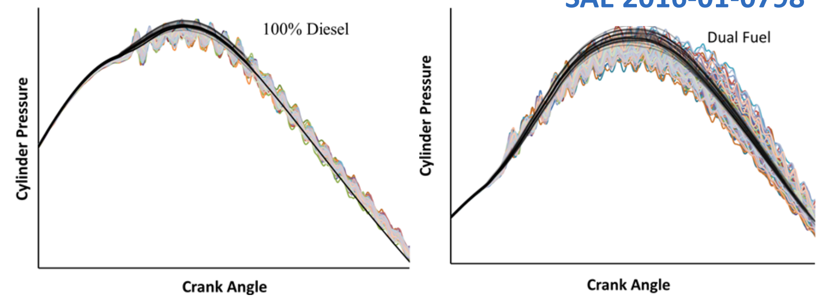
- 25 Mhrs on Mira at ALCF
- Collaboration with KAUST for pilot studies

Cyclic variability in dual-fuel ICEs (2/2) – Past and *Future Work*

Initial study at ORNL simulated the sensitivity of cyclic variability to variation in several key operating parameters

- Full-cylinder, closed-cycle CONVERGE simulations with RANS
- 100% diesel and dual-fuel at 1050 RPM, 20-bar BMEP
- 2-3M cells with AMR
- 7 Parameters considered: P & T at IVC, residual %, DI SOI, and flow rates of air, diesel, and NG
- Predicted variability less than that observed experimentally

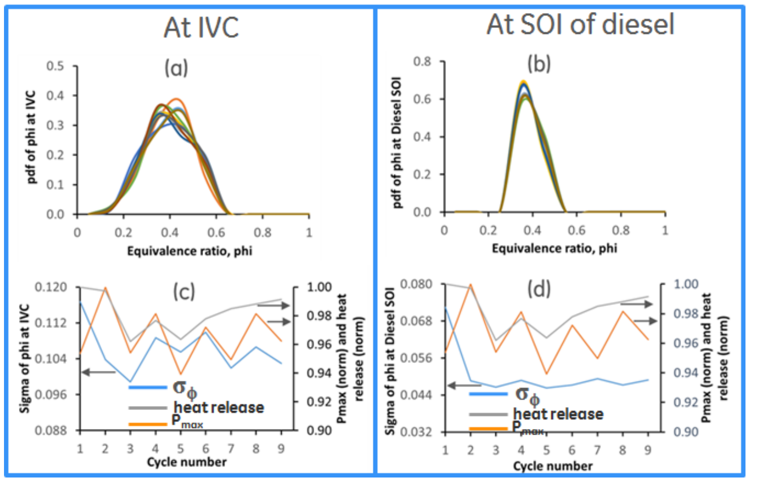
SAE 2016-01-0798



GE conducted a follow-up study at KAUST to evaluate the impact of stratification of premixed fuel

- Full cylinder, **open**-cycle CONVERGE simulations with RANS
- Model included full intake manifold with NG introduction
- Simulated 9 serial cycles
- 100% diesel and dual-fuel at 1050 RPM, 20-bar BMEP
- Model predicted significant cycle-varying fuel stratification
  - Stratification over wide range of φ at IVC
  - More narrow range with less cyclic variability after compression
- Observed correlation between standard deviation of phi in cylinder and cyclic variability in heat release

Predicted equivalence ratio variability



SAE 2017-01-0772

Remainder of FY2017:

Simulation efforts in support of current ALCC project on Mira are in development with CSI and ANL

- Transition to LES simulations
- Evaluate impact of additional sources of variability such as injector needle wobble

Summary of proposed *Future Work*

- **Proposed future work is subject to change based on availability of funding and allocation of HPC resources**

Virtual engine design and calibration	
• Complete simulations for detailed mechanism (5155 species) using MultiZone model • Transition to full-cylinder, open-cycle simulations • Recalibrate spray model for multi-component surrogate • Conjugate heat transfer for improved accuracy on BCs	**FY2017-18**
Simulation of Partial Fuel Stratification HCCI	
• Complete production runs • Iterate as needed based on analysis of results	**FY2017-18**
Cyclic variability in dual-fuel ICEs	
• LES simulations on Mira with additional parameter variations	**FY2017**

Courtesy: Dec, SNL

Response to reviewer comments

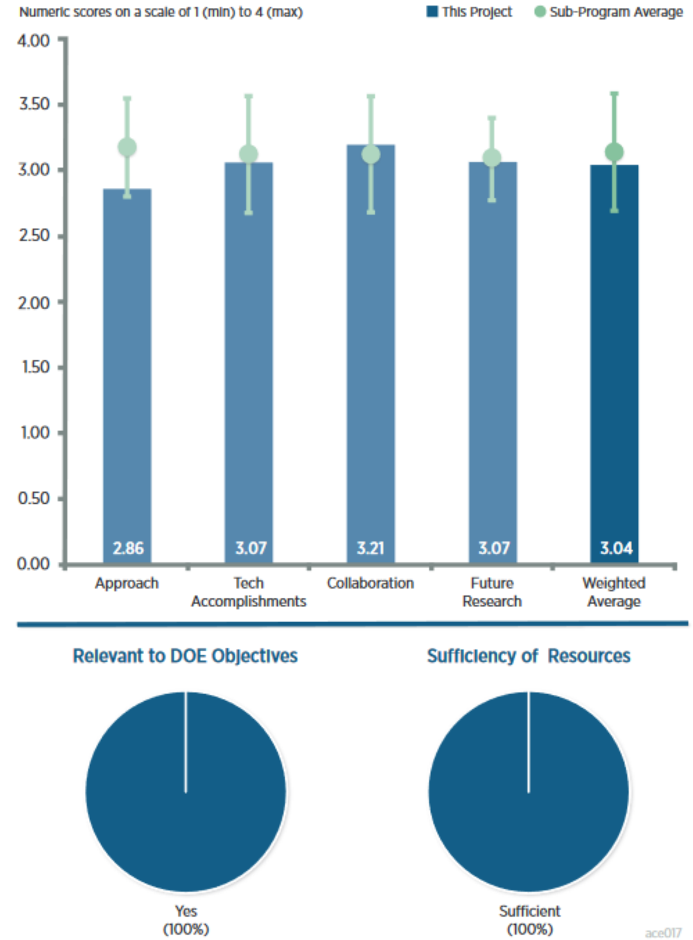
Overall reviewer responses were positive citing strong collaboration and relevance to DOE-VTO objectives.

Our lowest score was for Approach. While there were some reviewer comments addressing specific approaches used for each task, the majority of comments seemed to focus on the overall approach with specific attention to virtual engine design and calibration.

- **Response:** **The emphasis on overall approach in last year's presentation was in response to previous requests for more discussion of how specific efforts contributed to overall DOE-VTO objectives. Virtual design has direct potential to accelerate advanced engine design, a key goal of both DOE and GM. Furthermore,** ***HPC resources are particularly well-suited to assist in areas such as virtual design where large DoEs need to be simulated simultaneously in parallel*****. As such, we have selected this as a key focus area and have several ongoing projects related to virtual engine design supported by this project and other DOE- and industry-funded projects. The current multi-year project with GM seeks to take advantage of peta/exa-scale HPC to systematically address barriers to virtual design by targeting various traditional compromises which reduce model complexity (and accuracy) to increase computational speed on smaller computing resources (workstations, clusters, etc.).**

Reviewer comments questioned statements made related to impact on and transitioning to on-board diagnostics and controls.

- **Response:** **This stated goal is specifically related to development of map-based control strategies from the metamodels created in this study that are capable of deployment on advanced engine ECUs for real-time control of cyclic variability. This should not be confused with virtual calibration effort which seeks to improve the accuracy and speed of CFD simulations to allow reduction of physical engine experiments (and replacement with CFD results) in the development of engine calibration maps.**



Recurring comments addressed the use of CONVERGE for the various efforts over other CFD options.

- **Response:** **Our industry partners typically select the desired simulation software. Convergent Science, Inc. are full partners in these tasks. HPC resources at OLCF have a CPU-GPU architecture, and allocations are preferentially given to projects which make full use of the GPUs. With the addition of LLNL's Zero-RK GPU-enabled solvers, CONVERGE has that capability whereas many other CFD software options do not. ORNL does make use of other CFD options (including KIVA, Forté, and OpenFOAM) as appropriate.**

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 engine design and calibration	GM
Partial Fuel Stratification simulations	GM
Cyclic variability in dual-fuel ICEs	

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**

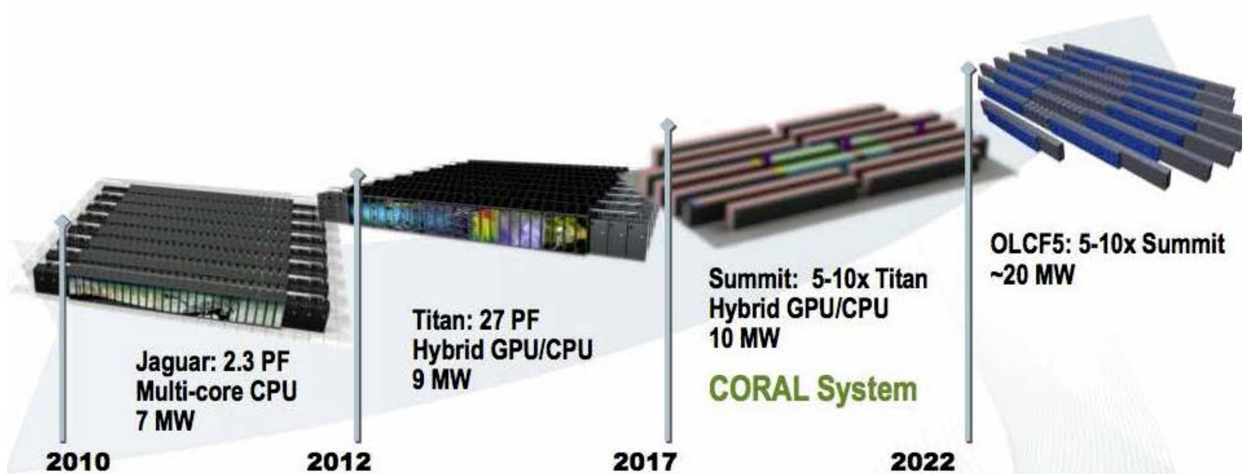
Strong coordination with broader simulation portfolios within ORNL and DOE

Co-Optima simulation team (FT052, FT053)	
Engine knock prediction (ACS110)	
Daimler SuperTruck II team (ACS100)	DAIMLER DETROIT
Advanced propulsion materials (PM057)	
Support of ORNL experimental efforts (ACS016, etc.)	ANSYS KIVA GT AUTONOMIE

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
  - 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.



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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 improve fuel economy and emissions
- **Approach**
  - Collaborative efforts with OEMs, ISVs, NLs, and universities to…
    - Develop and evolve new predictive capabilities
    - Gain new insight to areas where understanding has been historically limited by computational resources
    - Further enable virtual engine and component design
- **Technical Accomplishments**
  - Demonstrated approach using HPC and Zero-RK to enable CONVERGE CFD engine simulations with detailed chemistry containing 1000+ species
  - Demonstrated accuracy improvement with use of detailed chemistry in CFD diesel engine simulations and identified additional areas for improvement
  - Production runs for PSF HCCI simulation underway with 6 surrogate/mechanism combinations
- **Collaborations**
  - Multiple collaborative efforts with OEMs, ISVs, NLs, and universities
  - Strong coordination with broader simulation portfolios within ORNL and DOE
- **Future Work** (subject to change based on availability of funding and allocation of HPC resources)
  - Use multi-zone model to enable diesel simulations with fully detailed mechanism (5155 species)
  - Improve IC and BC accuracy for diesel simulations: full-cylinder open-cycle model, CHT, revised spray BCs
  - Complete evaluation of detailed chemistry impact on PFS HCCI simulations
  - Further investigate of impact of BC variability (e.g., NG stratification, needle wobble) on CV in dual-fuel ICEs

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