Model Development and Analysis of Clean & Efficient Engine Combustion

2017 DOE Hydrogen and Fuel Cells Program and Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting

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Lawrence Livermore National Laboratory

Overview

Timeline

- Ongoing project with yearly direction from DOE

Barriers

- Inadequate understanding of the fundamentals of HECC
- Inadequate understanding of the fundamentals of mixed mode operation
- Computational expense of HECC simulations

Budget

- FY15 funding: $508K
- FY16 funding: $508K
- FY17 funding: $441K

Partners

- AEC Working Group:
  - Sandia NL, GM, Oak Ridge NL
- Industrial:
  - Convergent Science Inc.
  - Nvidia

Relevance – Enhanced understanding of HECC requires models that couple detailed kinetics with CFD

Objectives:

- Advance state-of-the art in engine simulation
  - Enable detailed, predictive models
  - Reduce time to solution
- Get tools into the hands of industry

VT multi-year program plan barriers addressed:

A. Lack of fundamental knowledge of advanced engine combustion regimes
C. Lack of modeling capability for combustion and emission control
D. Lack of effective engine controls

Accurate simulations yield improved engine designs.

Approach – Work with partners to achieve objectives.

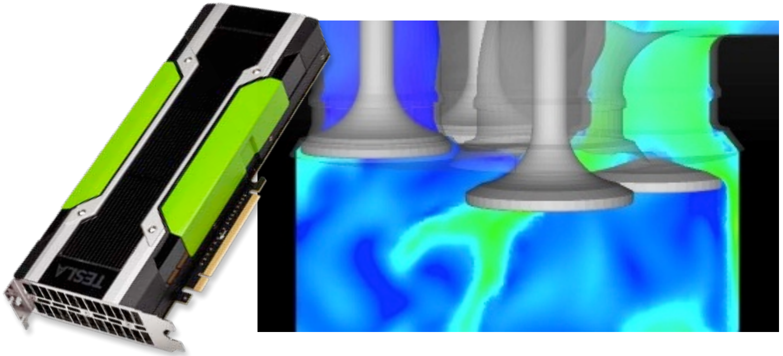
- Development and deployment of fast-chemistry solvers in engine CFD
- Assemble uncertainty quantification framework for robust error bounds on experimental measurements for comparison to models

Milestones:

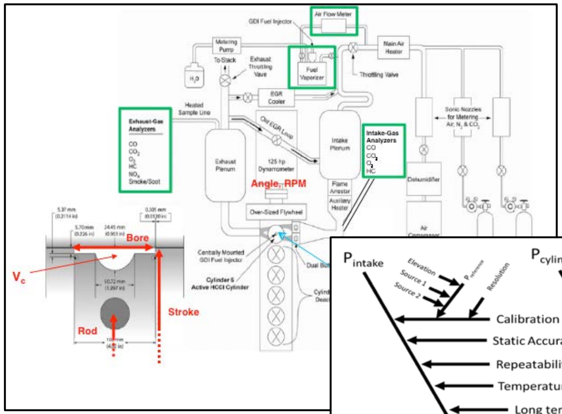
1. *Demonstrate use of fast-chemistry solver by industrial engine partner.*
2. *Publish uncertainty-quantification study and software.*

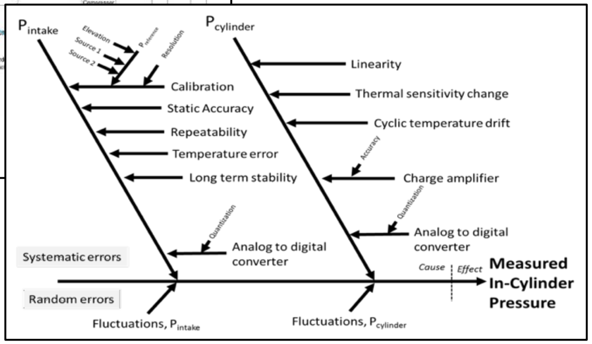
Accomplishments presented at 2016 AMR

- Practical GPU use in engine simulation
  - Heterogeneous & distributed processing
  - New algorithms make best use of available computing resources



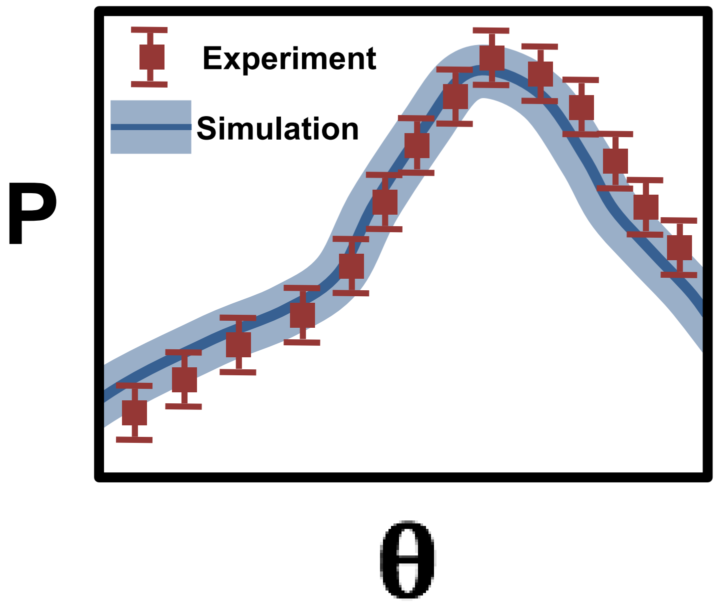
- Uncertainty Quantification of HCCI engine test cell
  - First effort for detailed UQ in engines
  - Uncertainty values vital to comparison of experiments with models





Importance of Uncertainty Analysis in Engine Research

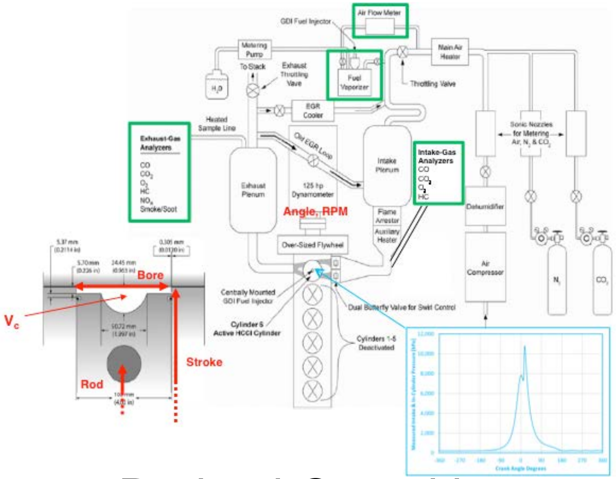
- Comparisons among experiment and between experiments and simulations still suffer due to lack of confidence intervals
- Proper confidence interval estimation requires detailed accounting of uncertainty sources
- HCCI experiments at Sandia National Laboratory provide a good platform for this type of analysis in engine context
  - Long history of experiments
  - Rigorous experimental practice
  - Homogeneous operation



Uncertainty analysis of HCCI experiments at SNL (1/3)

- Began analysis in FY16 working to identify as many sources of uncertainty as we could
- Worked with J. Dec and J. Dernotte at SNL to understand the experiments and their data processing/analysis approach
- Developed framework for Uncertainty Quantification/Uncertainty Propagation in HCCI/LTGC engine experiments
- Framework analysis based on conservative assumptions and manufacturers specifications for sensors/transducers

<u>Measured Quantities</u>



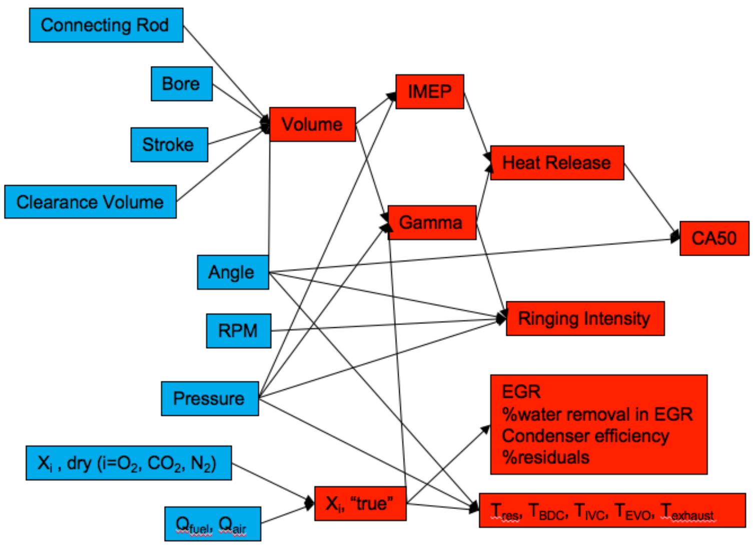
<u>Derived Quantities</u>

Compression Ratio
Air/fuel mixture (phi)
T_{IVC}, T_{EVO}, $T_{exhaust}$, $T_{residuals}$, T_{BDC}
X_i (actual)
%residual, %EGR
%water removal in EGR loop
%water removal upstream gas analyzers
IMEP, heat release, Ringing Intensity

Technical Accomplishments

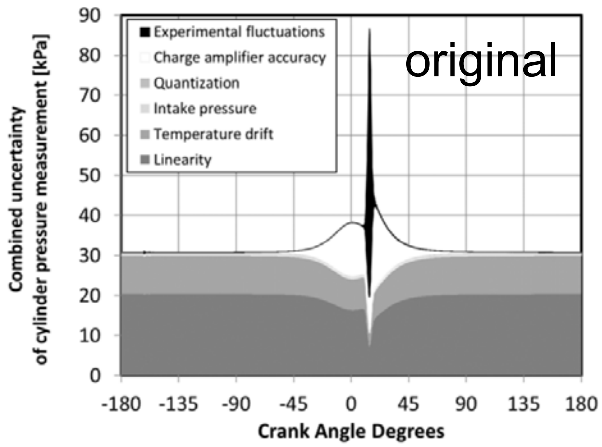
Uncertainty analysis of HCCI experiments at SNL (2/3)

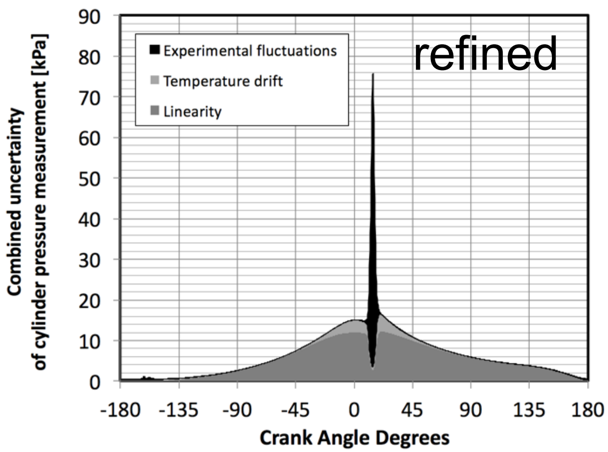
- Using the developed framework allows us to study uncertainty relationships and sensitivities of key quantities (e.g. IMEP, CA50, PRR).
- Framework published in this years SAE Congress (SAE 2017-01-0736) and code open sourced and available at https://github.com/LLNL/UQ_combustion
- We want feedback from engine community and hope that UQ becomes more common among engine researchers.



Uncertainty analysis of HCCI experiments at SNL (3/3)

- Currently refining our estimates of sensor uncertainty
  - Close collaboration with J. Dec on sensor calibration
  - Accounting for actual sensors being used as opposed to manufacturers specifications
- Refined estimates for sources of uncertainty significantly reduce confidence interval for pressure measurement
- Multiple studies in the works making use of the engine UQ framework



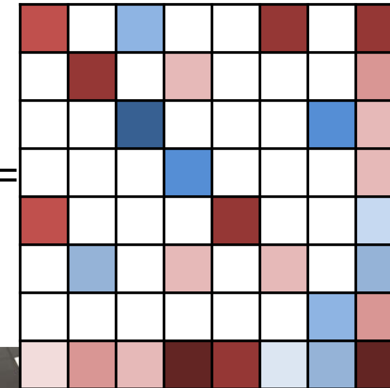


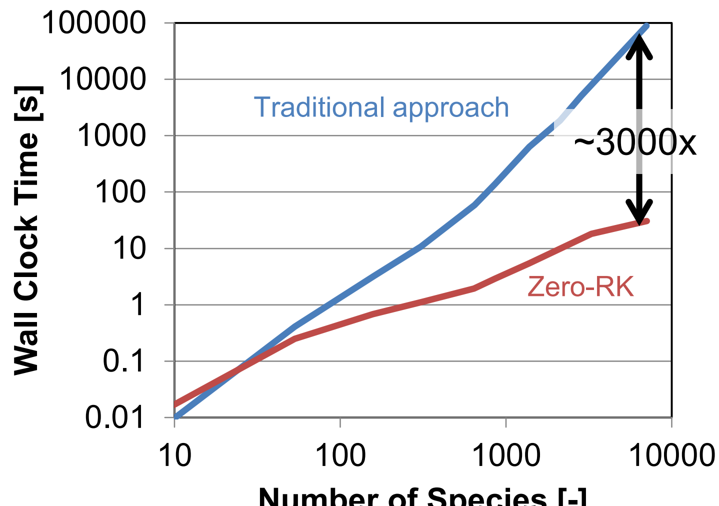
Technical Accomplishments

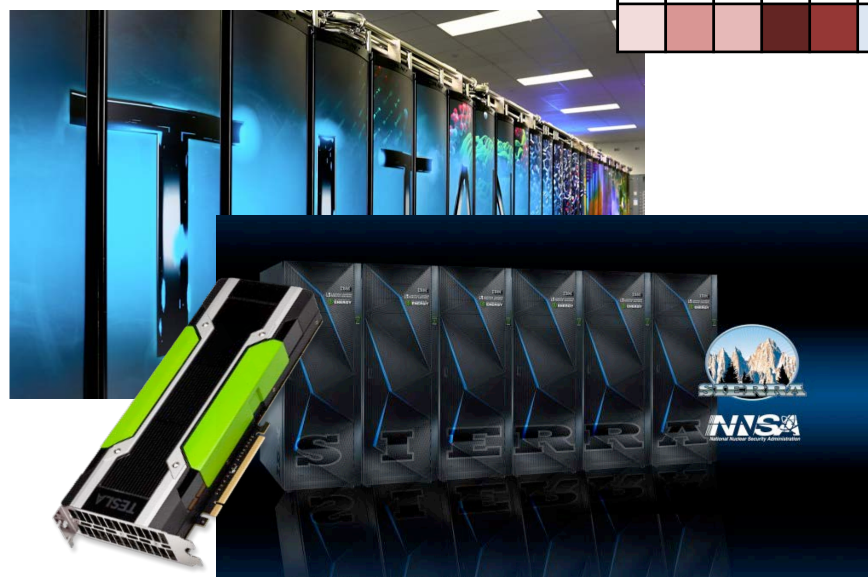
Fast-solver CFD Development Overview

- Integrating work in ACS076 into engine CFD codes (collectively: Zero-RK)
- Dramatic speed-up with new algorithms
- Targeting current and future architectures

$$J_{i,j} = \frac{d}{dy_j}\left(\frac{dy_i}{dt}\right) =$$







Technical Accomplishments

Developing/Deploying Code with GM and ORNL

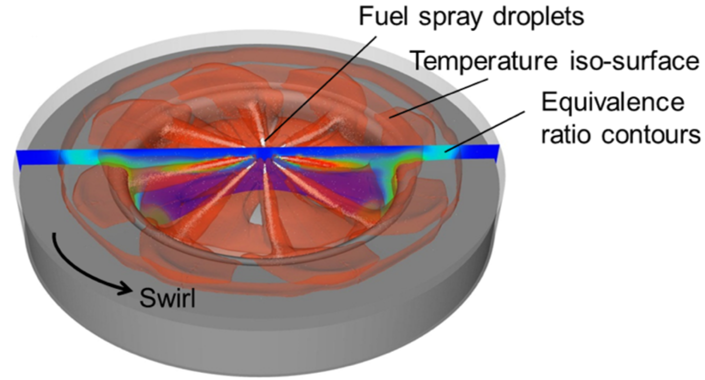
- Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge awards (ALCC)
- FY16 Diesel virtual engine calibration
  - Focused on emissions predictions
  - Range of mechanisms to probe effect of chemical detail
  - OLCF User Meeting Best Poster - PI
- FY17 HCCI/LTGC ignition chemistry
  - Low-temperature chemistry vital
  - Multiple fuel surrogates

GM

Technical Accomplishments

LLNL Fast-solver Integral to ALCC Work

- GPU algorithms a key enabler of ALCC award work
- ALCC award provides world-class computing capability (>25 million CPU-hours)
- Over 1,600 engine simulations with detailed chemistry
- Creating new capability, and developing fundamental knowledge of engine combustion



NOx (Load ↑, Speed →)

			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 (Load ↑, Speed →)

			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 →)

			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

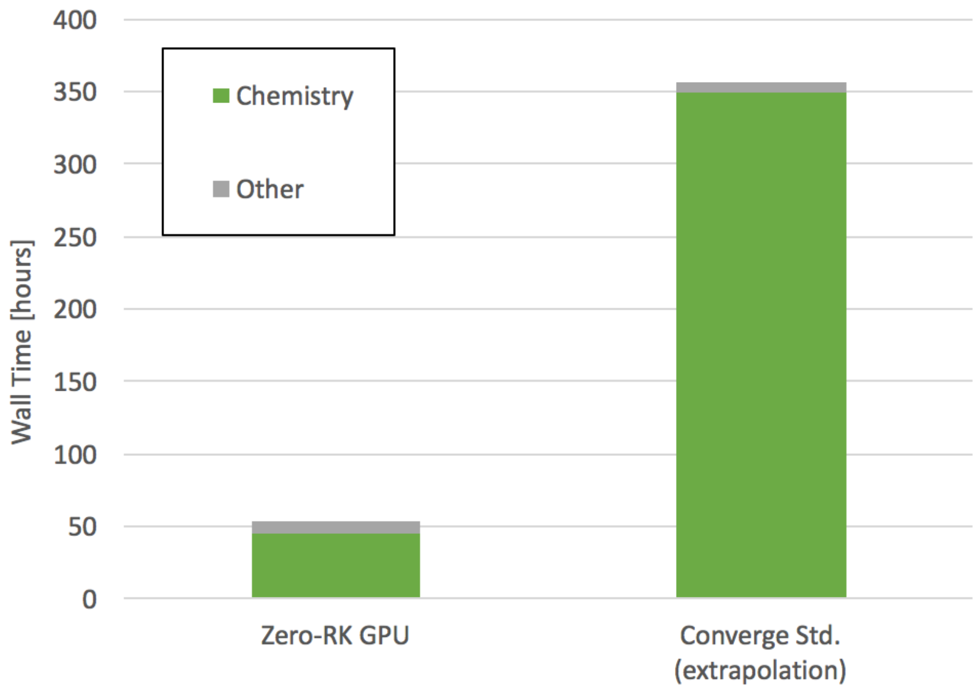
HC (Load ↑, Speed →)

			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

Technical Accomplishments

CFD Benefit/Capability of GPU Fast Chemistry Solver

- Fast-solver + GPU pushes limits of simulation capability
- First reported simulations to include >1,000 species in engine simulation (or any reacting flow simulation)
- Detailed chemistry vital for ignition and emissions predictions
- Further acceleration still possible

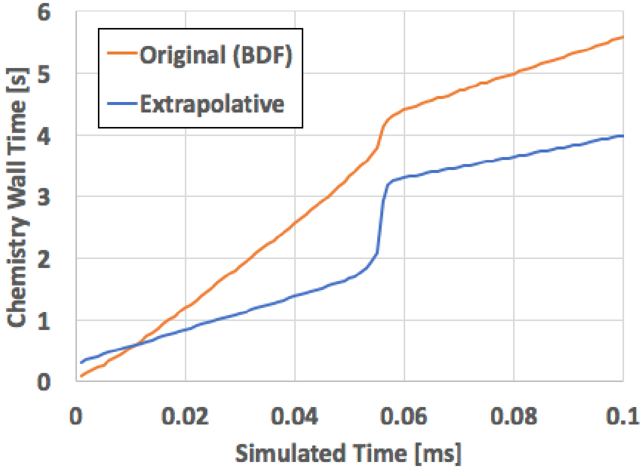


Diesel sector simulation
1034 species chemical mechanism
Every-cell chemistry

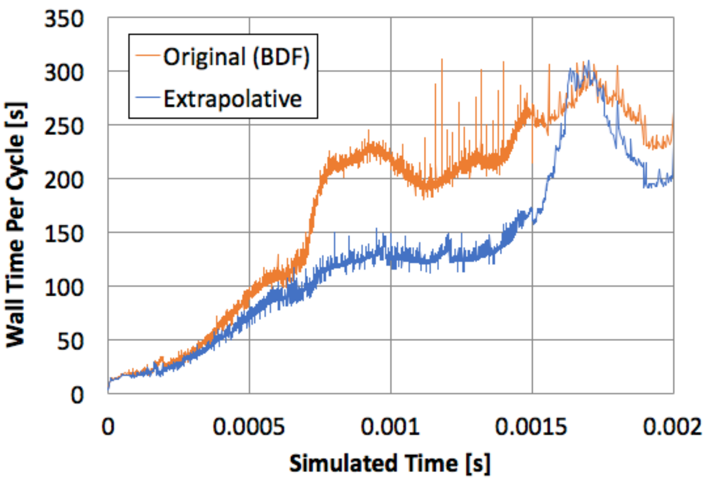
Technical Accomplishments

Continuing Effort to Accelerate Engine CFD

- Working on alternative integration techniques with specific advantages for CFD
- Motivated by interaction with D. Haworth (PSU)
- Implemented extrapolative technique that has less "startup" cost
- GPU implementation included



Constant Volume



Spray Bomb

Technical Accomplishments

FY2016 Reviewer's Comments and Our Response

- Code platform/availability:
  - Software has been designed for flexibility
  - Working on licensing/distribution
- Broader collaboration:
  - Working more closely with collaborators this year on both research fronts
- Multi-component fuels:
  - Part of ALCC HCCI/LTGC work
  - Enabled by fast-solver development

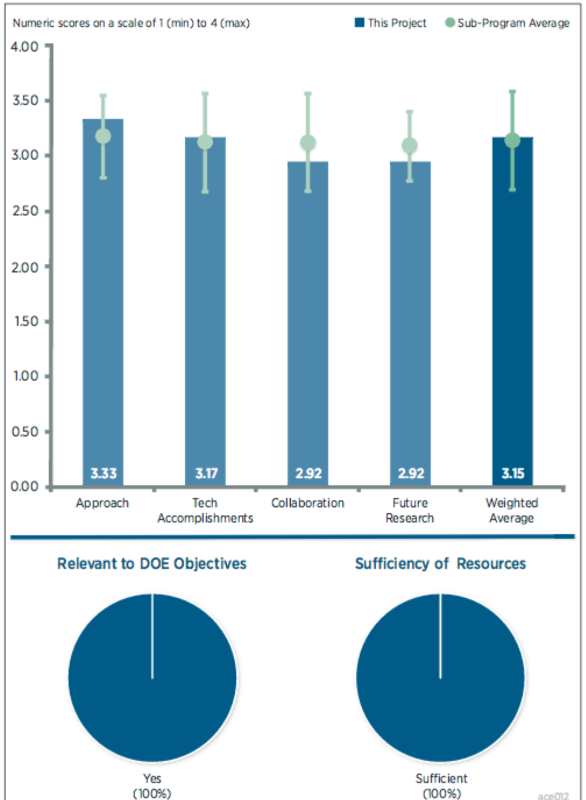


Figure 4-9 - Model Development and Analysis of Clean and Efficient Engine Combustion: Russell Whitesides (Lawrence Livermore National Laboratory) - Advanced Combustion Engines

Mostly positive comments and above average score.

Collaboration – Ongoing interactions with industry, national laboratories, and universities

- Sandia National Laboratory – J. Dec Uncertainty Quantification
- General Motors/Oak Ridge National Lab – Ron Grover/K. Dean Edwards ALCC
- Convergent Science Inc. (CSI) – Current development platform for
- NVIDIA – Hardware, software and technical support for GPU chemistry development
- Advanced Engine Combustion (AEC) working group – twice annual research update meetings and informal collaboration

Remaining Challenges and Barriers

- Fast-solver distribution/availability
  - Currently only available to small list of partners
  - Research code; still requires tech. guidance/support
- Further simulation acceleration needed
  - 1000 species feasible, but challenging
  - Want to include more physics (better turbulence, spray models, etc.)
- Large model uncertainties
  - Tradeoffs in fidelity required for feasibility
  - Error incurred by approximations not quantified

Proposed Future Research

- FY17
  - Work with LLNL Industrial Partnerships Office on licensing/distribution
  - Analyze performance of two/three alternative time integrators in CFD
  - Continue refinement of UQ analysis including cost-benefit analysis of sensor improvements

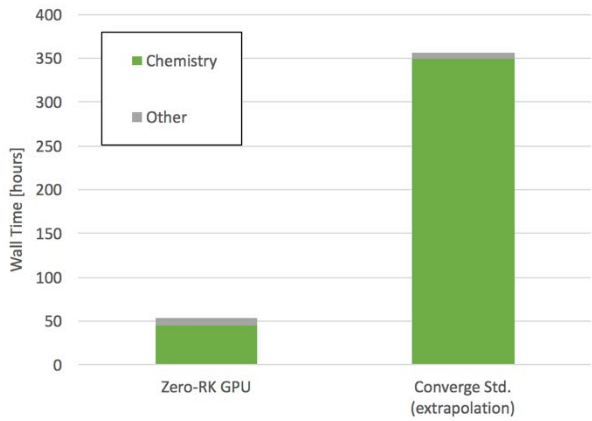
- FY18
  - Implement smart solver (best integrator chosen for each reacting zone)
  - UQ in reacting flow CFD

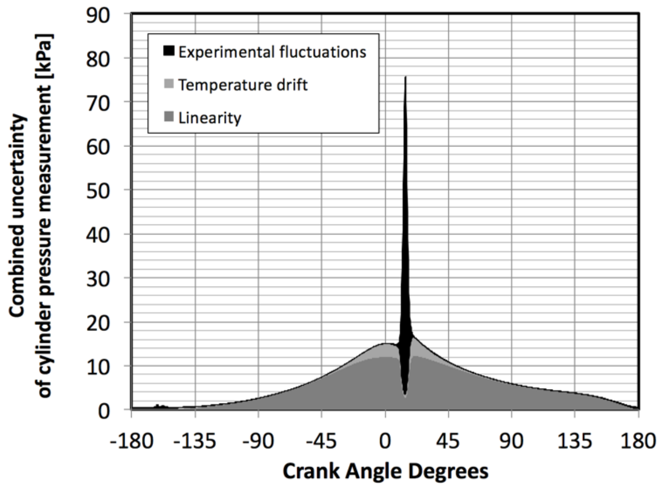
- FY19+
  - Reduction in time-to-solution for engine CFD in both super-computer and workstation hardware
  - Methods and practices for developing predictive models and simulations

Any proposed future work is subject to change based on funding levels

Summary: Our modeling work is impacting present and future engine research

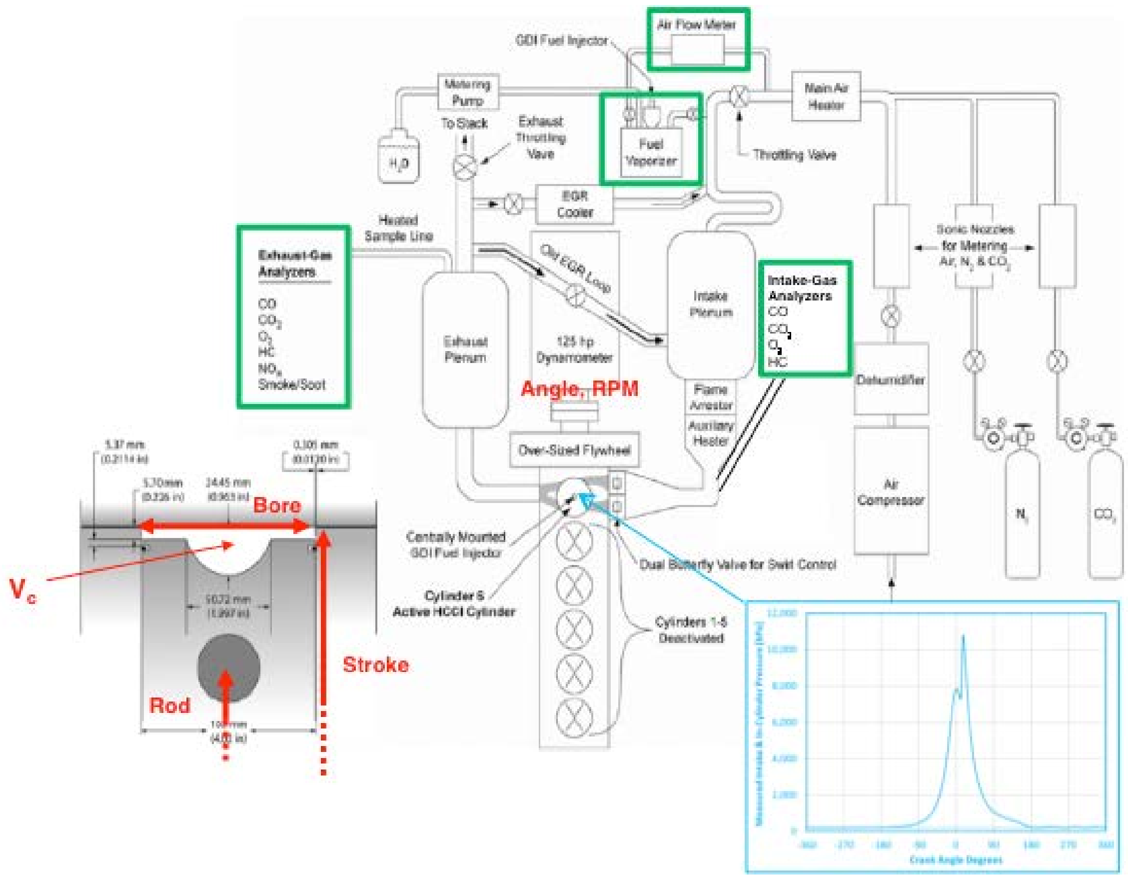
- Chemistry acceleration in CFD:
  - Brings new capability to engine CFD
  - Integral to start-of-art engine simulation campaign
  - Working toward wider availability
- Uncertainty analysis:
  - Published uncertainty framework study
  - Open sourced software for other researchers to use and improve: https://github.com/LLNL/UQ_combustion
  - Refined pressure uncertainty measurements with J. Dec (SNL) with plans for further studies as collaboration.





Technical Backup Slides

Uncertainty Quantification Background: Test cell diagram and quantities of interest



Measured Quantities

Crank angle

Engine speed

Geometry (Bore, stroke, rod, V_c)

Intake air and fuel flow

X_i (dry), i=CO,CO_2,O_2, Nox, HC

Intake pressure

In-cylinder pressure

Derived Quantities

Compression Ratio

Air/fuel mixture (phi)

T_{IVC}, T_{EVO}, $T_{exhaust}$, $T_{residuals}$, T_{BDC}

X_i (actual)

%residual, %EGR

%water removal in EGR loop

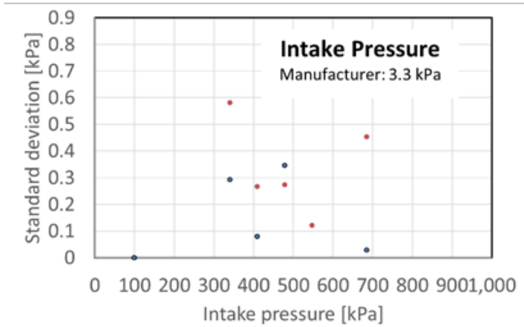
%water removal upstream gas analyzers

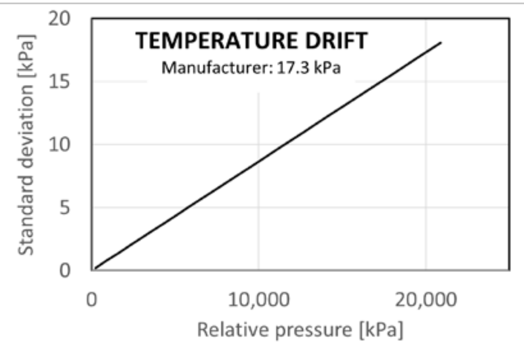
IMEP, heat release, Ringing Intensity

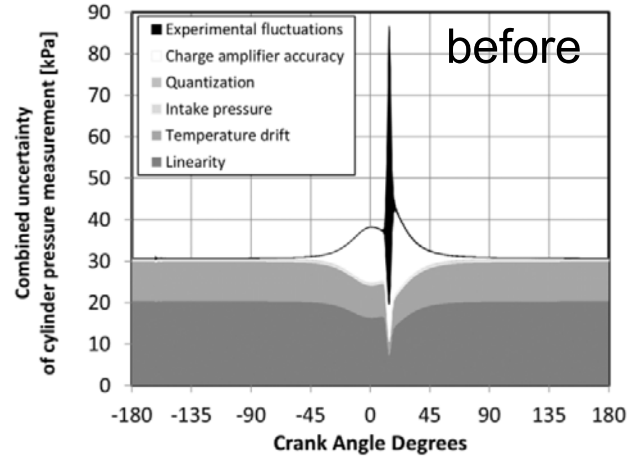
Uncertainty Quantification Background: Measurement uncertainty estimates for HCCI/LTGC operation at SNL

Category	Experimentally measured quantity	Typical Mean Value	Experimental error	Assumed Distribution	Standard uncertainty
Geometry	Bore	0.10223 m	±3e-6 m	Uniform	1.7e-6 m
Geometry	Stroke	0.12 m	±2.5e-5 m	Uniform	1.4e-5 m
Geometry	Connecting rod	0.192 m	±2.5e-5 m	Uniform	1.4e-5 m
Geometry	Clearance volume	75.77 mL	±0.25 mL	Uniform	0.14 mL
Geometry	Crank angle	0 to 360 CAD	±0.05 CAD	Uniform	0.03 CAD
Geometry	Engine speed	1200 RPM	±24 RPM	Normal (95%)	12.2 RPM
Pressure	BDC Pressure	240 kPa	±6.62 kPa	Normal (95%)	3.31 kPa
Pressure	In-cylinder Pressure	240 to 10,900 kPa	±60 to 320 kPa	Normal (95%)	31 to 162 kPa
Composition	Air flow intake	10.98 g/s	±0.02 g/s	Normal (95%)	0.01 g/s
Composition	Fuel flow intake	0.59 g/s	±2% (relative)	Normal (95%)	6 mg/s
Composition	CO_2 intake	5.59%	±0.075 % (absolute)	Normal (95%)	0.04%
Composition	O_2 intake	12.5%	±0.22 % (absolute)	Normal (95%)	0.11%
Composition	CO_2 exhaust	11.4%	±0.16 % (absolute)	Normal (95%)	0.08%
Composition	O_2 exhaust	5.01%	±0.22 % (absolute)	Normal (95%)	0.11%
Composition	Combustion efficiency	98.42 %	1 % (absolute)	Triangular	0.4%

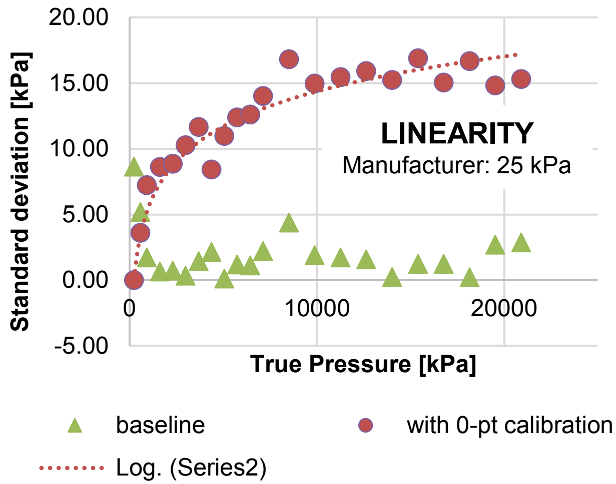
Uncertainty Quantification Background: Data and Methods Used to Refine Estimate for Pressure Uncertainty

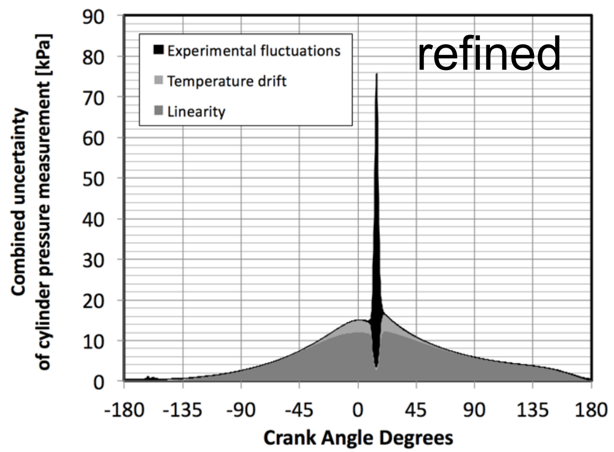




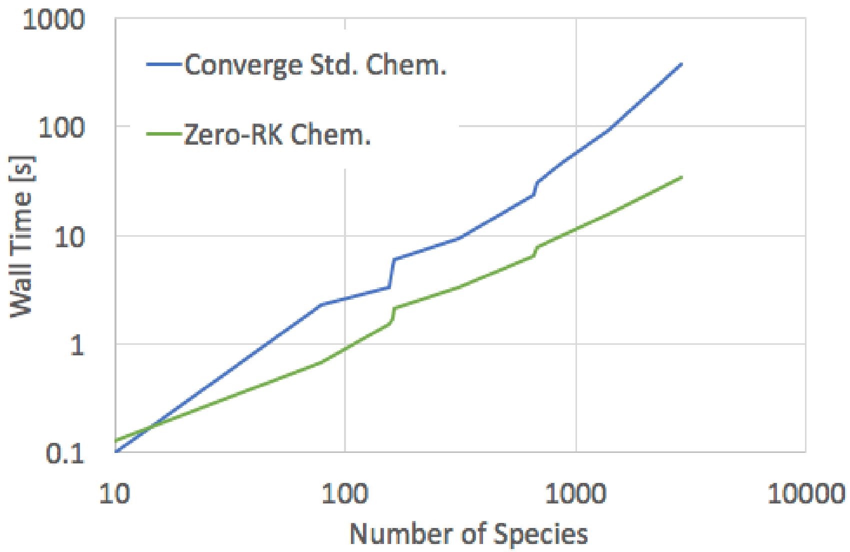


Assumptions:
Charge amplifier error = 0
Pressures identical for both transducers at pegging

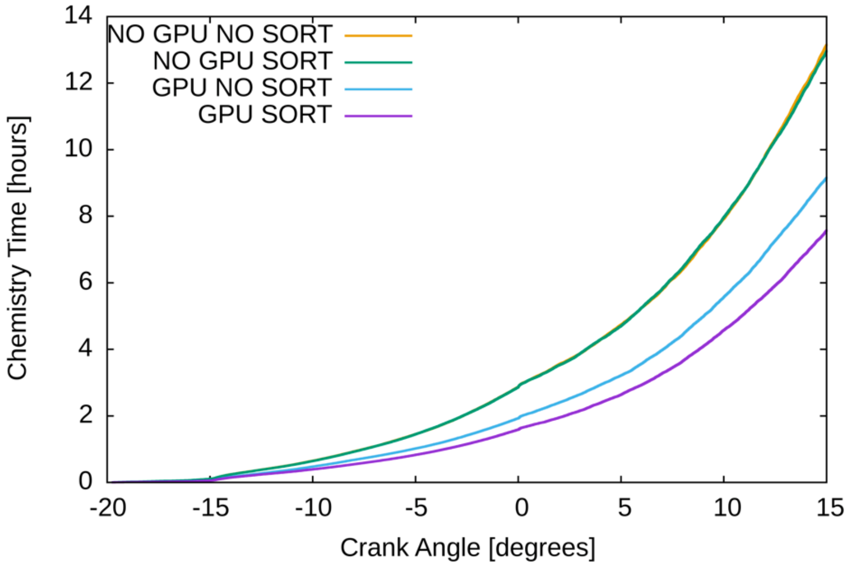




Fast-chemistry Solver Performance in CFD



CPU only scaling with comparison to ConvergeCFD built-in chemistry (5.5x faster at 1000 species)



Performance in test case with and without GPU enabled (1.7x faster with GPU (16 CPU + 2GPU)

Fast-chemistry on GPU Verification

- Outputs for all quantities of interest overlap
- Heat release (HR) rate is noisy based on CFD time step selection, so match is not exact but also true in comparing two CPU runs.