Advanced Combustion Numerics and Modeling

2018 DOE Vehicle Technologies Office Annual Merit Review

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June 19, 2018

Project ID # ACS012

Lawrence Livermore National Laboratory

Overview

Timeline

- Project provides fundamental research to support DOE/ industry Advanced Engine Combustion projects

- Funded by 3-year Lab Call starting FY17

Budget

- FY16 funding: $508K
- FY17 funding: $441K
- FY18 funding: $600K*

*Funding increase is the result of reorganization; ACS076 combined with ACS012 and tasks re-aligned along with Co-Optima Simulation Toolkit Team

Barriers

- Inadequate understanding of the fundamentals of HECC

- Inadequate understanding of the fundamentals of mixed mode operation

- Computational expense of HECC simulations

Partners

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

Relevance – Enhanced understanding of HECC requires accurate, affordable models

Objectives:

- Advance state-of-the art in combustion simulation

  - Enable detailed, predictive models
  - Reduce time to solution

- Use tools to impact industry relevant problems

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.

FY18 Approach – Multi-front development effort

- Continue to accelerate engine CFD with detailed kinetics and apply to ECN diesel spray conditions

- Develop state-of-the-art laminar flame speed solver

- Extend work with GM/ORNL on virtual diesel engine calibration

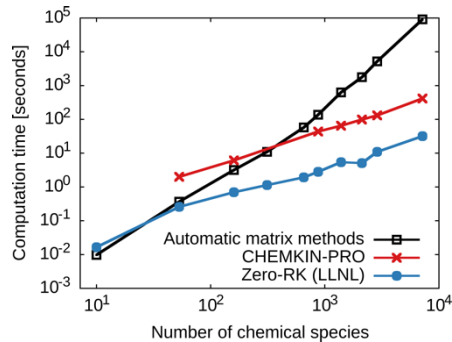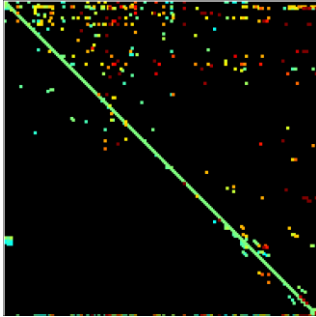- Maintain multiple collaborative projects

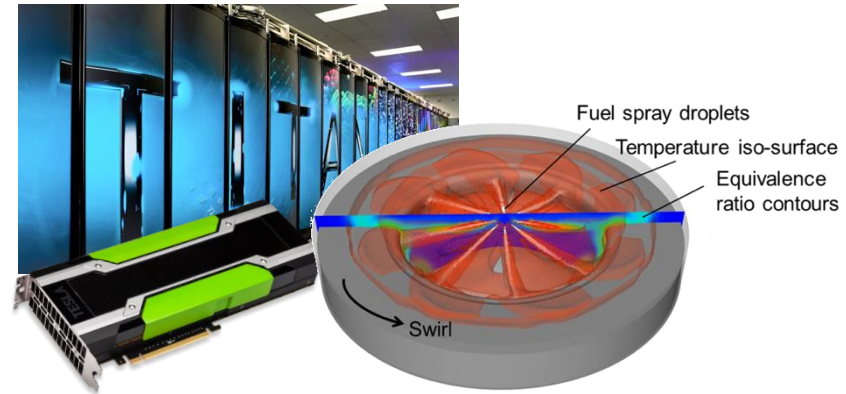**Milestones:**

Quarterly status reports (completed/on-schedule)
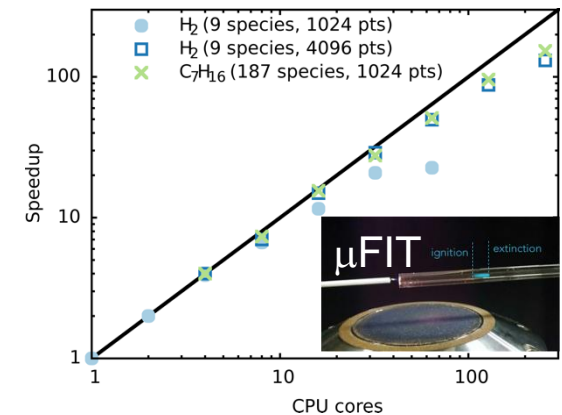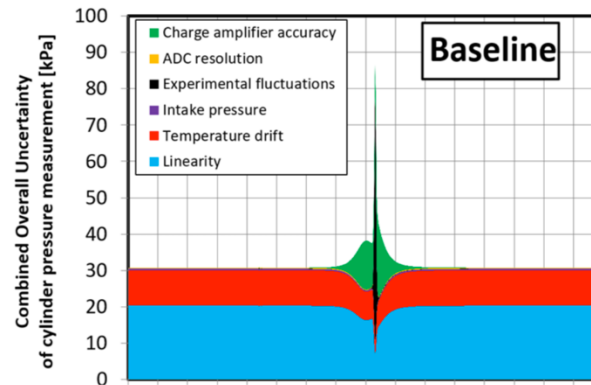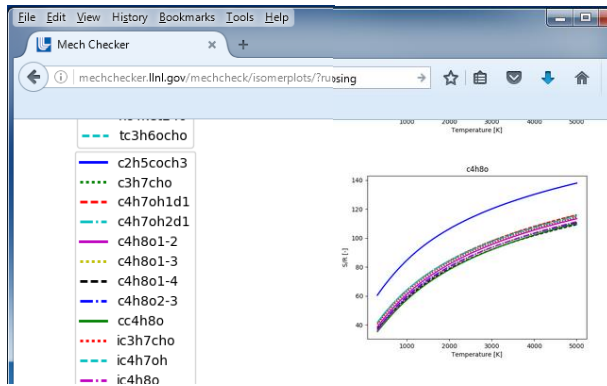
FY18 work builds on previous accomplishments

Algorithms + Numerics

Computation time [seconds] vs Number of chemical species

- Automatic matrix methods
- CHEMKIN-PRO
- Zero-RK (LLNL)

2015 R&D 100 WINNER

Engine CFD with Detailed Chem.

- Fuel spray droplets
- Temperature iso-surface
- Equivalence ratio contours
- Swirl

Applications

Mech Checker — mechchecker.llnl.gov/mechcheck/isomerplots/?running

- tc3h6cho
- c2h5coch3
- c3h7cho
- c4h7oh1d1
- c4h7oh2d1
- c4h8o1-2
- c4h8o1-3
- c4h8o1-4
- c4h8o2-3
- cc4h8o
- ic3h7cho
- ic4h7oh
- ic4h8o

Combined Overall Uncertainty of cylinder pressure measurement [kPa] — Baseline

- Charge amplifier accuracy
- ADC resolution
- Experimental fluctuations
- Intake pressure
- Temperature drift
- Linearity

Speedup vs CPU cores

- H_2 (9 species, 1024 pts)
- H_2 (9 species, 4096 pts)
- C_7H_{16} (187 species, 1024 pts)

µFIT — ignition, extinction

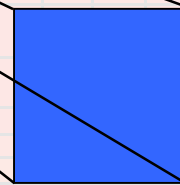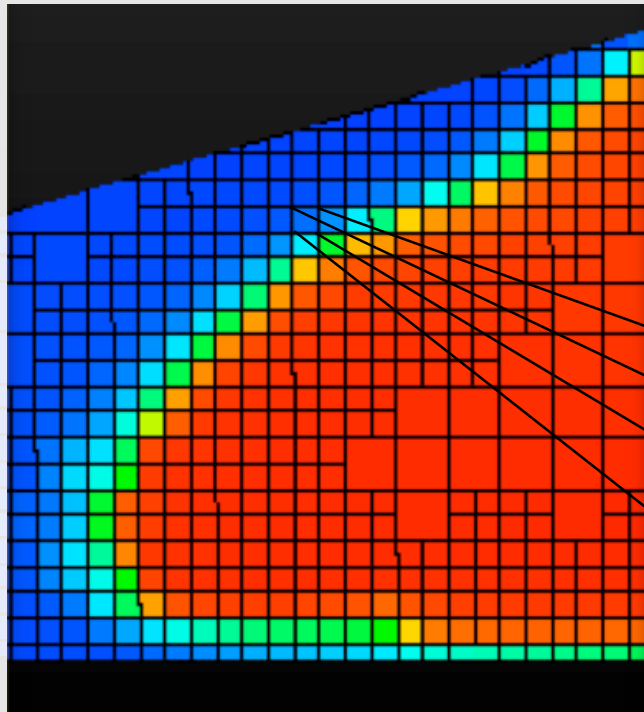### Technical Accomplishments

NNSA National Nuclear Security Administration

Detailed chemical kinetics in reacting flow simulations

Operator Splitting Technique
Solve independent Initial Value Problem in each cell (or zone) to calculate chemical source terms for species and energy advection/diffusion equations.
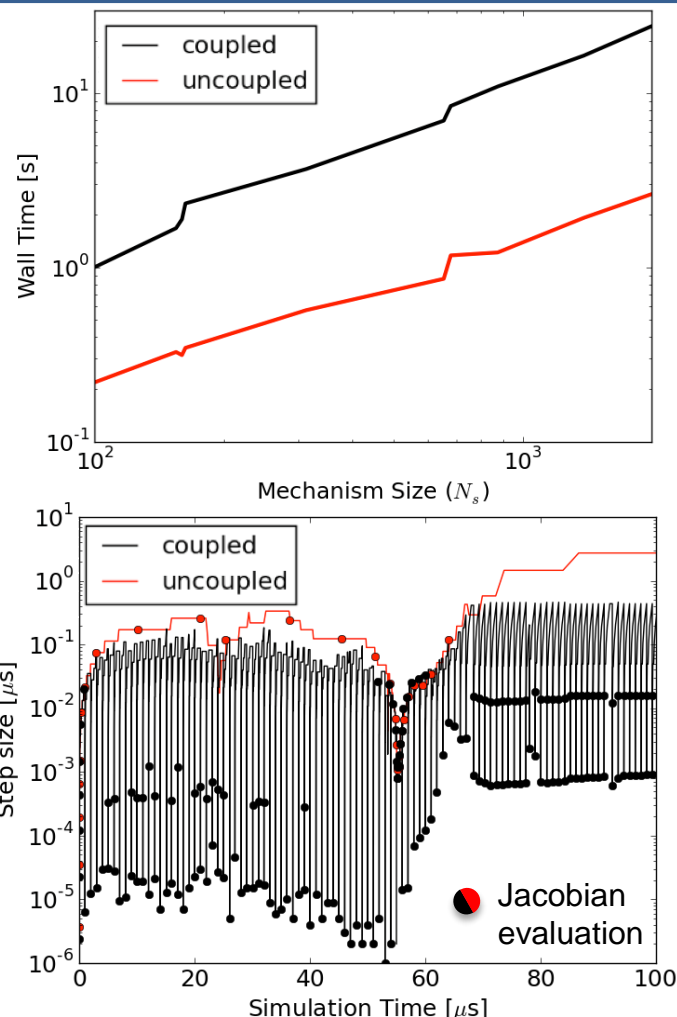
t

t+Δt

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Accelerating Detailed Kinetics in Engine CFD

- CFD coupling via operator splitting introduces discontinuity, requiring restart of chemical integration
- Our preferred solver for un-coupled systems (CVODE) builds up accuracy by using history of system which is thrown out on restart
- New published research (Imren & Haworth*) shows other solvers may be better for this problem
- We have implemented SEULEX solver in Zero-RK which doesn't require history information but maintains high accuracy
- Our implementation maintains features we have built previously (Jacobian, linear algebra, GPU) and can switch between CVODE and SEULEX
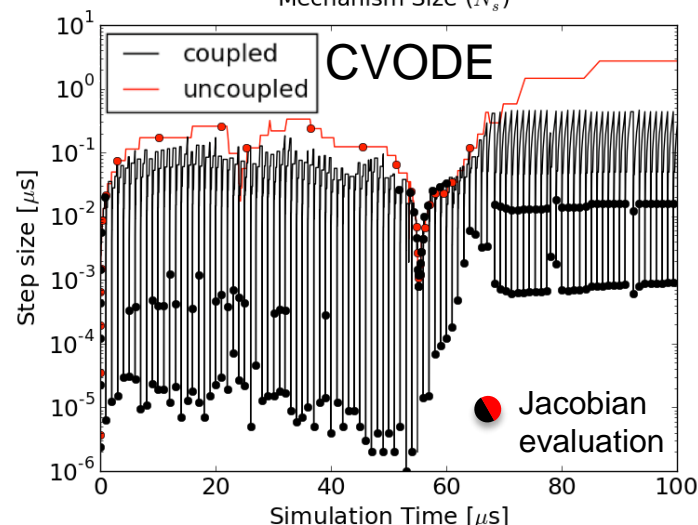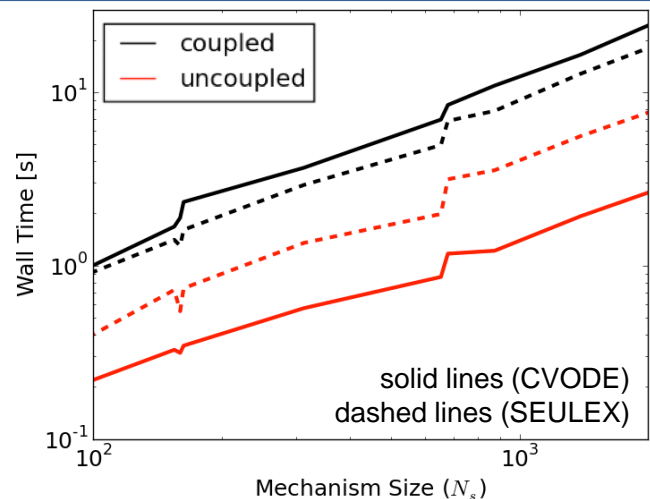
*https://doi.org/10.1016/j.combustflame.2016.09.018

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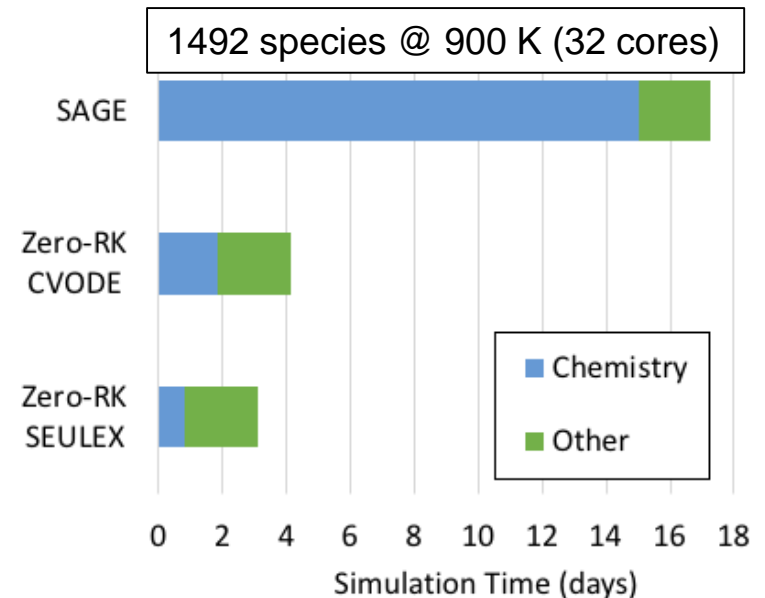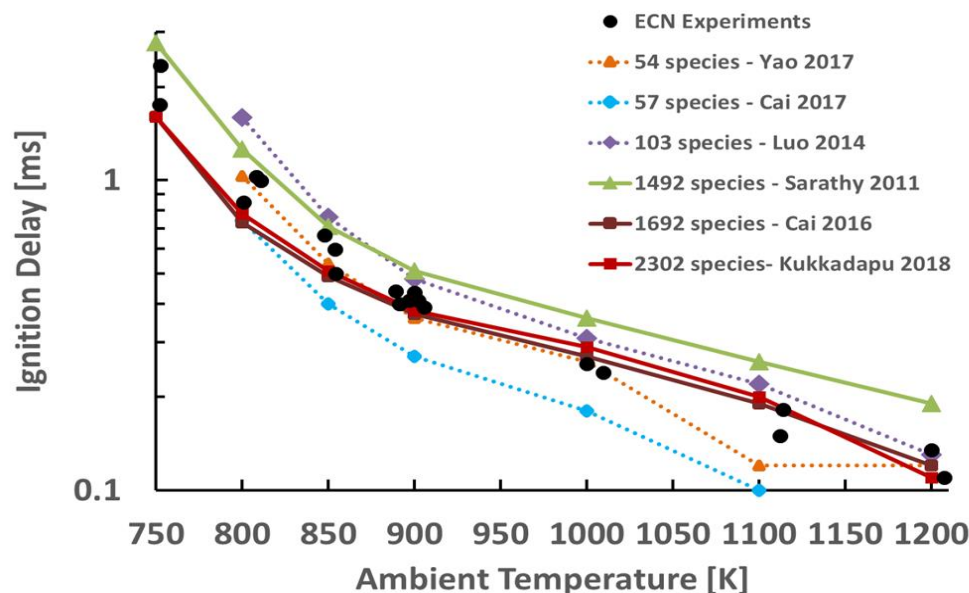
*https://doi.org/10.1016/j.combustflame.2016.09.018

solid lines (CVODE)
dashed lines (SEULEX)

CVODE

Jacobian evaluation

Technical Accomplishments

# Applying Detailed Kinetics to ECN Spray A

- Accelerated kinetics allows us to use highly detailed chemistry at engine relevant configurations
- Detailed kinetics are required to predict ignition at 750 K ambient
- SEULEX is twice as fast as CVODE for this problem, reducing total simulation time by 25% (i.e. multiple days)

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NNSA
National Nuclear Security Administration

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Accelerating Prediction of Laminar Flame Speeds

- Laminar flame speeds are used in the validation of chemical mechanisms and to study knocking behavior in SI engines

- Simple geometric configuration allows for 1-D solution, but approaches have been stagnant for many years

- Standard approach works fine for chemical mechanisms with less than 100 species

- We applied the same ideas we used for 0-D chemical kinetic problems to this problem which adds fully coupled mass and energy transport equations

- Significant improvements in the last year have reduced turn-around time by an order of magnitude in some cases
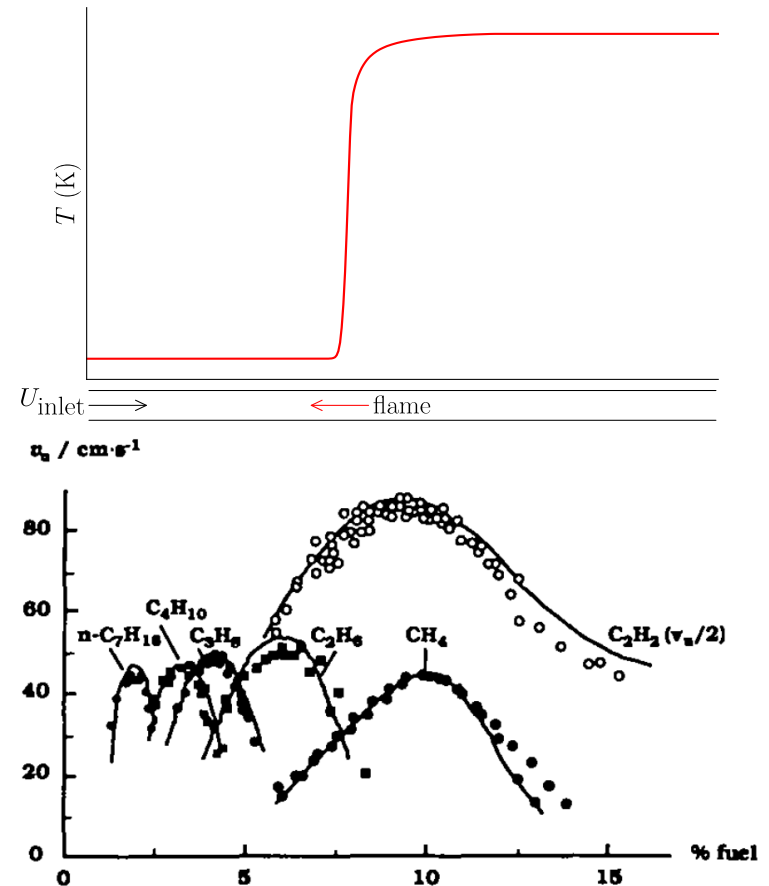

Warnatz, Symposium (International) on Combustion. 24 (1992) 553–579
https://doi.org/10.1016/S0082-0784(06)80070-6

Technical Accomplishments

Design of Flame Speed Solver Provides Attractive Scaling with Problem Size, Grid Resolution, and Processors

- Linear increase in wall-time with number of species (N_S)
- Linear speed-up with number of processors (N_P)
- Quadratic increase in accuracy with number of grid points (N_G)
- For large mechanisms, our approach is >10x faster than Chemkin Pro

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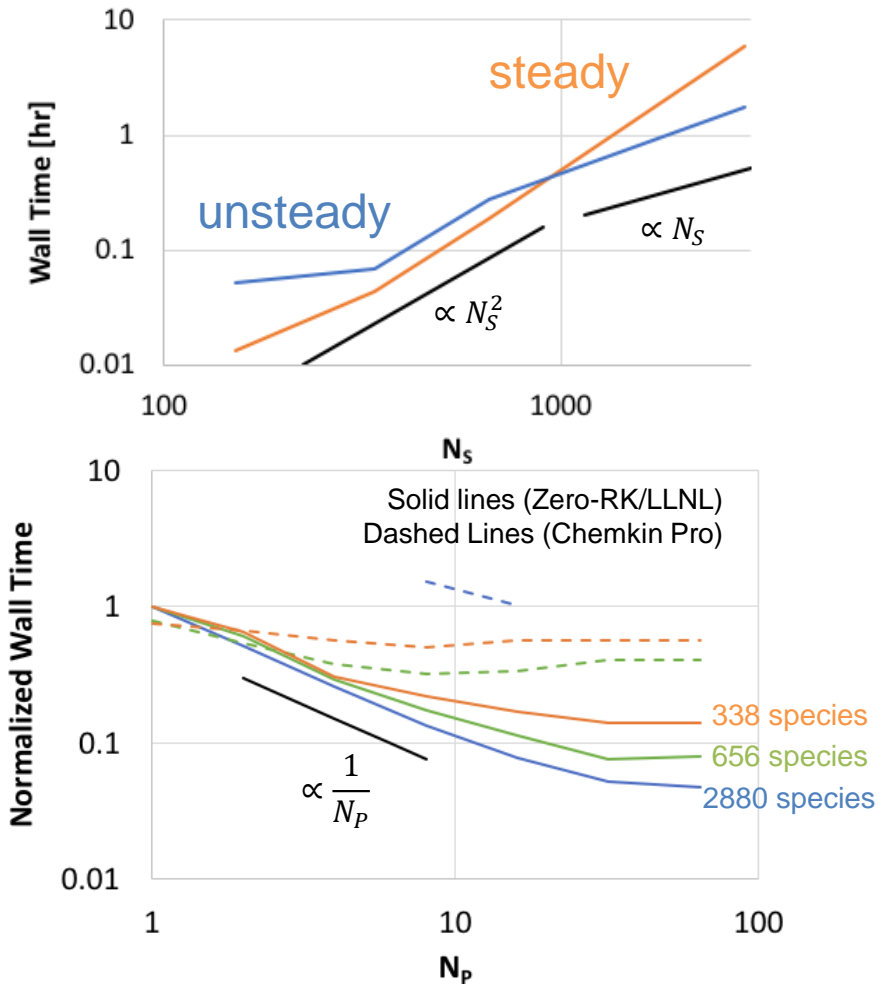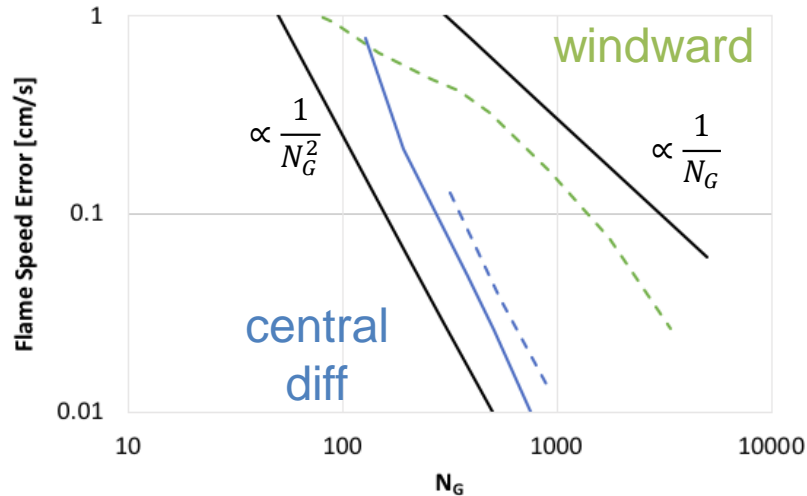
# Accelerated Flame Speed Calculations Enable Entirely New Applications

- Chemical kineticists can now include flame speed comparisons *during* model development instead of only at the end

- Engine experimenters can use flame speeds to investigate fuel effects on knocking behavior at a *wider* range of engine operating points (Sjoberg (SNL))

- Other applications:
  - Flame speed tables
 - Octane number correlations
  - Small volume fuel testing

$$RH + H^* = R^* + H_2$$
$$O_2 + H^* = O + OH^*$$

warm
cold
cold/dilute
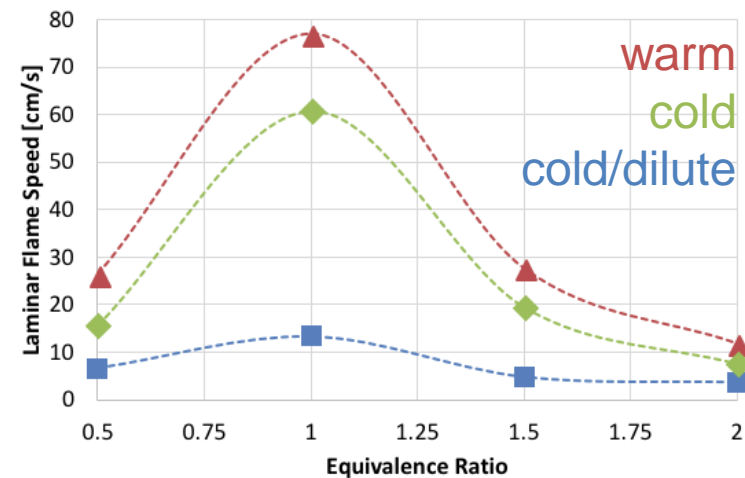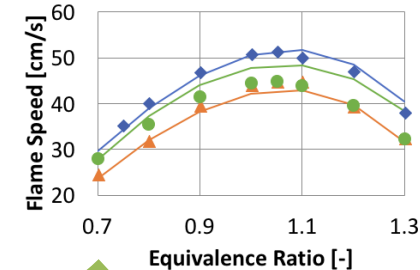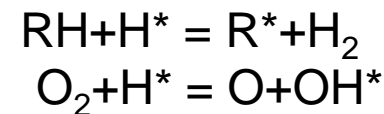
Continuing collaboration with GM and ORNL is pushing the boundaries of simulation fidelity for engines

- Project leverages resources and expertise at all three institutions to advance state-of-the-art in engine simulations

- Diesel virtual engine calibration simulations have been extended to include full-cycle simulations including intake and exhaust flows

- 20 cases have been selected from the full speed-load map to test predictions with full-cycle simulations

- Simulations including heat flux through engine head and coolant flow in the water jacket are in progress
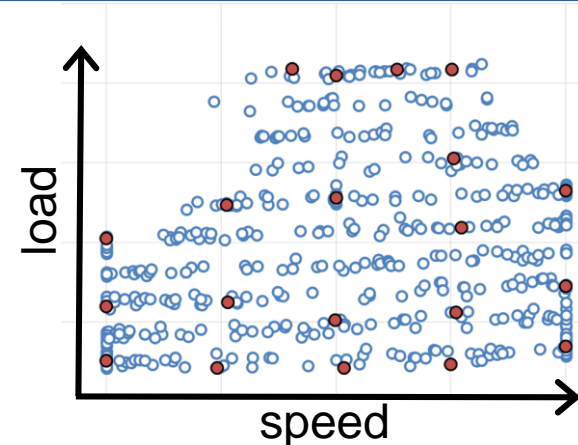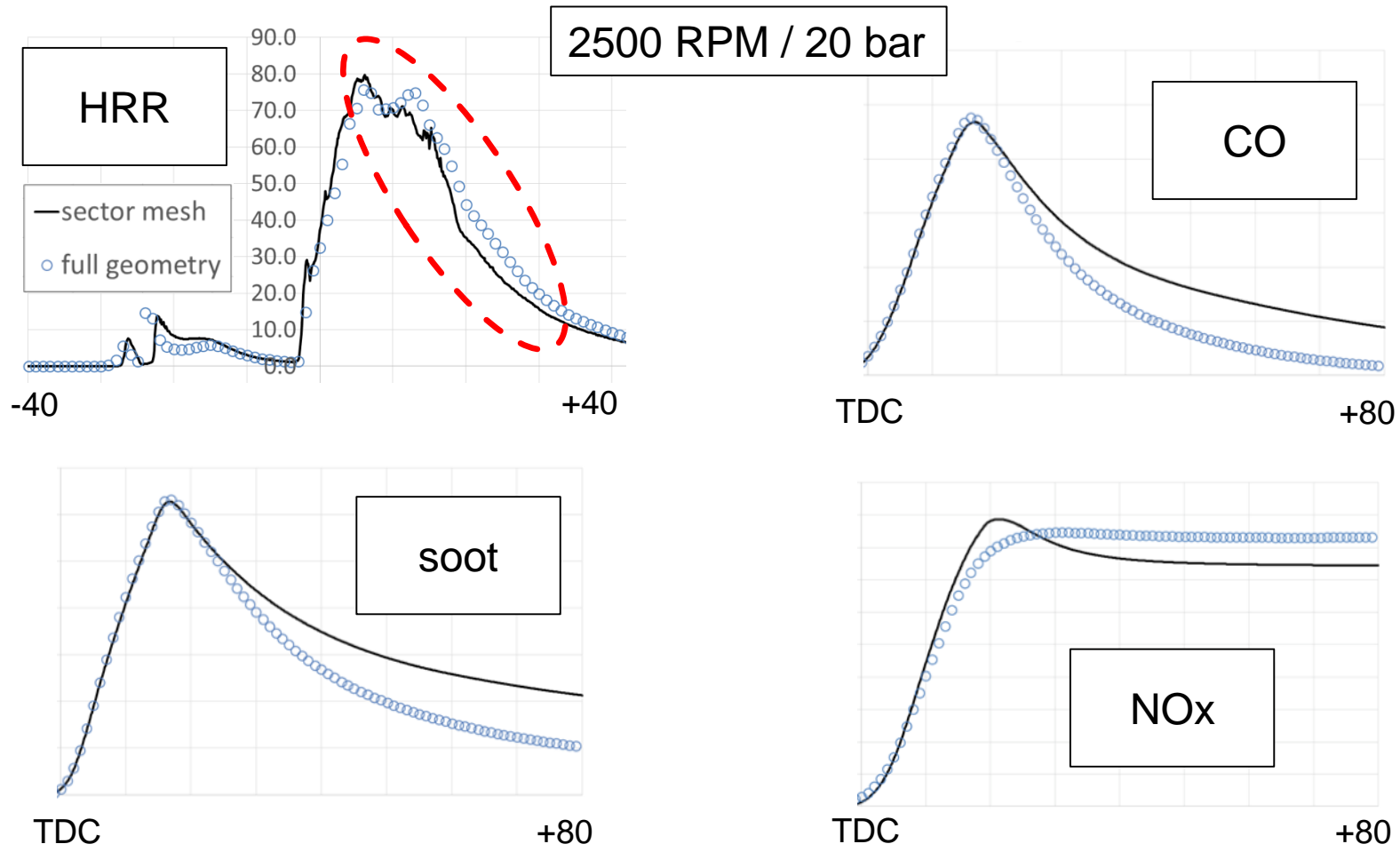

load
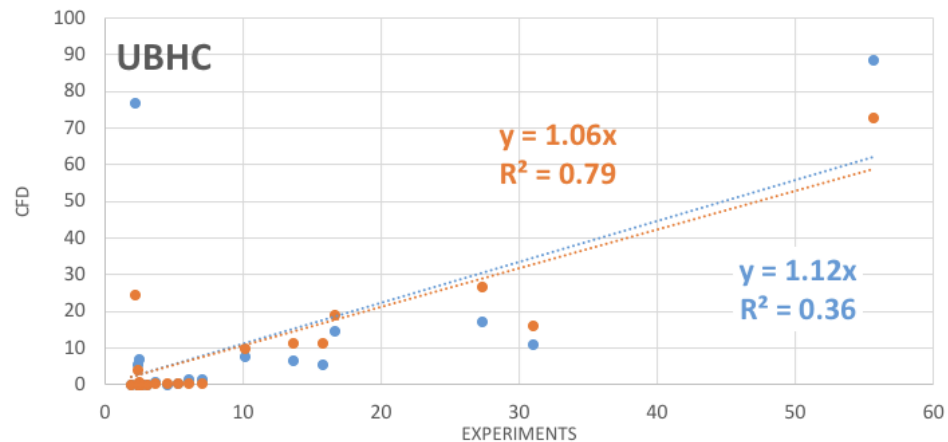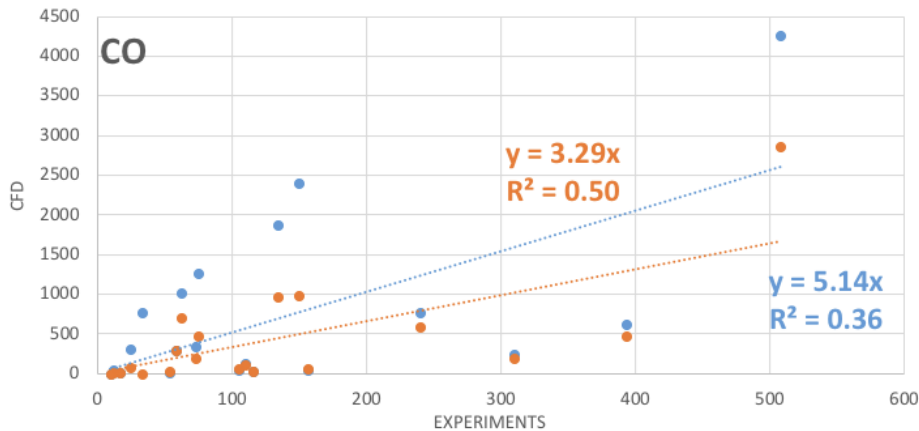speed

sector/closed cycle
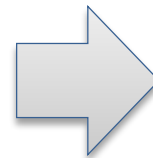
intake+exhaust/ full cycle
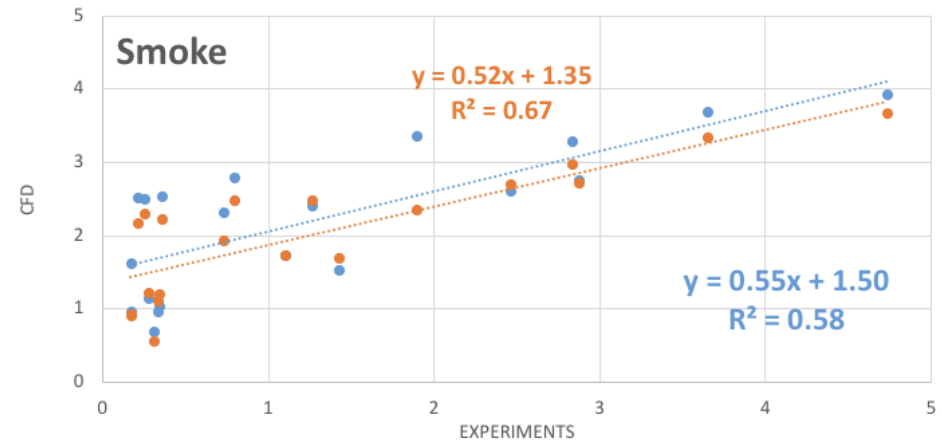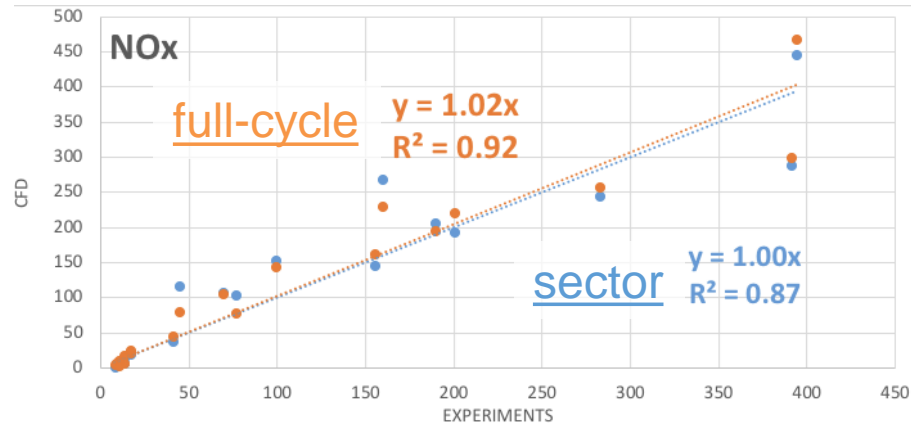

Technical Accomplishments

National Nuclear Security Administration

Gas exchange and better geometry representation increase late heat release, reduce soot and CO for high speed/load case

2500 RPM / 20 bar

HRR

— sector mesh
○ full geometry

-40   +40

CO

TDC   +80

soot

TDC   +80

NOx

TDC   +80

More detailed model improves emissions predictions across speed-load map
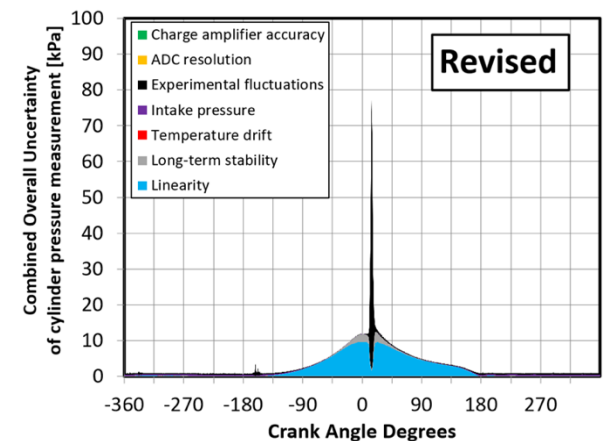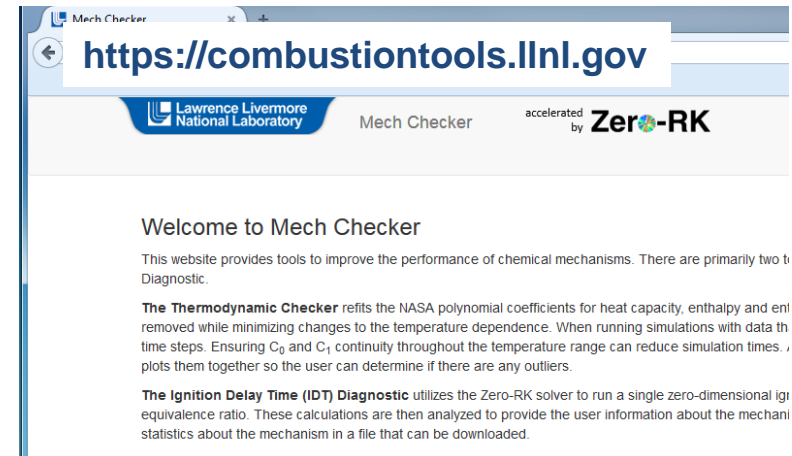
# Progress continues in other numerics/modeling areas

- LLNL Combustion Tools Website:
  - Now open to the public
  - 27 users from 14 institutions (April 2018)
  - Manuscript being prepared for Combustion and Flame
- Paper on Uncertainty Quantification for LTGC Engines presented at SAE World Congress and in revision for Int. J. Engines
- Zero-RK availability: Working with multiple companies on demonstration/evaluation licenses (1 signed, 2 in process)

https://combustiontools.llnl.gov

Lawrence Livermore National Laboratory   Mech Checker   accelerated by Zer⊕-RK

Welcome to Mech Checker

This website provides tools to improve the performance of chemical mechanisms. There are primarily two t
Diagnostic.

The Thermodynamic Checker refits the NASA polynomial coefficients for heat capacity, enthalpy and ent
removed while minimizing changes to the temperature dependence. When running simulations with data th
time steps. Ensuring C_0 and C_1 continuity throughout the temperature range can reduce simulation times.
plots them together so the user can determine if there are any outliers.

The Ignition Delay Time (IDT) Diagnostic utilizes the Zero-RK solver to run a single zero-dimensional ig
equivalence ratio. These calculations are then analyzed to provide the user information about the mechani
statistics about the mechanism in a file that can be downloaded.

FY2017 Reviewer's Comments and Our Response

- Mostly positive comments and above average scores (scores shown from **ACS012** and ACS076)

- Code platform/availability:
  - Software has been designed for flexibility
  - Open call to software vendors was made (fbo.gov: FBO329-17)
  - Multiple demonstration licenses being pursued

- Validation vs. Applications/Users:
  - Have to find balance
  - End use/user is always our goal
  - Feedback through review/collab. is vital

- Combining ACS076/ACS012 will inhibit progress
  - Combination happened as part of re-organization
 - Co-Optima program is helping fill the gap
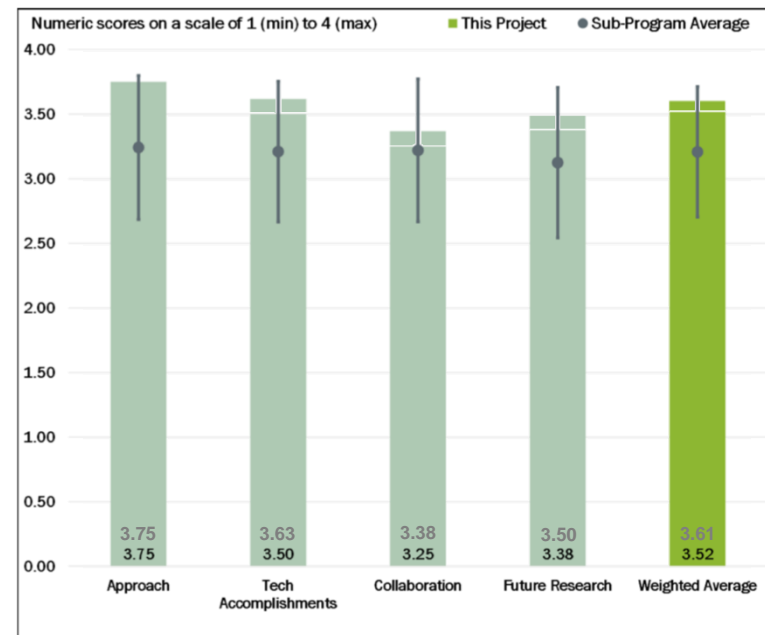
Collaboration – Ongoing interactions with industry, national laboratories, and universities

- Sandia National Laboratory – J. Dec Uncertainty Quantification, M. Sjoberg Flame Speed Dependence on Fuel

- General Motors/Oak Ridge National Lab – Ron Grover/K. Dean Edwards ALCC

- Convergent Science Inc. (CSI) – Current development platform for engine chemical kinetics coupling

- NVIDIA – Hardware, software and technical support for GPU chemistry development

- Advanced Engine Combustion (AEC) working group – twice annual research update meetings and informal collaboration

Collaboration Highlights: Connecting across ACS and Co-Optima Programs

Light & Heavy Duty Fuel Model Development (ACS013, FT052)
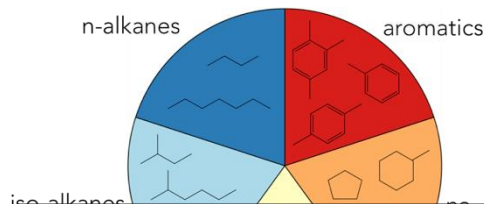
27,000 validation cases in minutes for each change

Pitz, LLNL

Unraveling the kinetic origins of phi-sensitivity and knock onset with ANL RCM (FT045, FT052)

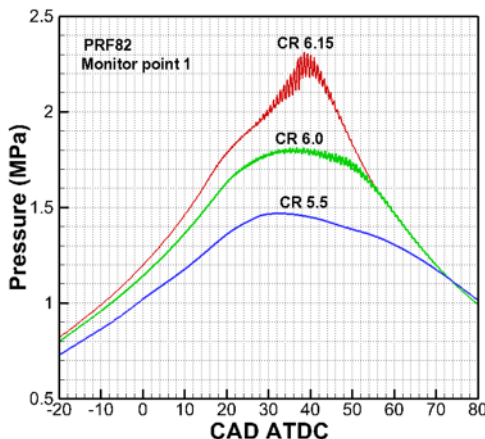72,000 reaction sensitivity calculations in hours

Goldsborough, ANL

Measuring fuel properties from microliters (FT063)
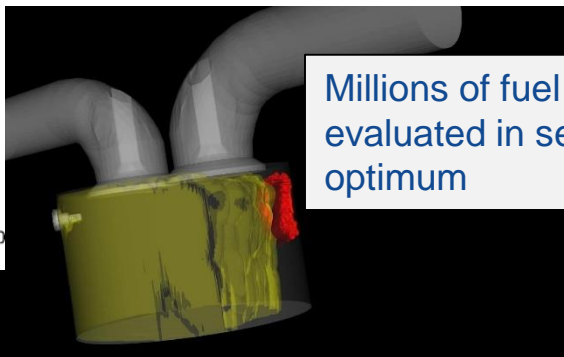

from I. Schoegl

15,000 unsteady flames to infer reduced model reaction rates
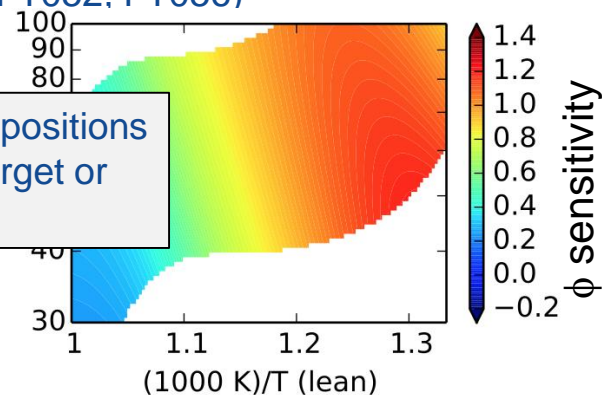
McNenly, LLNL

Pal, ANL

Virtual fuel models with matched octane ratings to test the Central Fuel Hypothesis (FT052, FT054)

Millions of fuel blend compositions evaluated in search for target or optimum

Fuel blend optimization for partially stratified compression ignition (FT052, FT056)

Remaining Challenges and Barriers

- Simulation cost
  - Computational cost for multi-species transport in engine CFD
  - Cost of highly detailed turbulence models

- Simulation accuracy
  - Coupling between chemistry and transport models
  - Detailed (predictive) spray dynamics
  - Soot reaction pathways
  - Nonlinear fuel component interactions

- Simulation workflow
  - Tradeoffs in fidelity required for feasibility
  - Error incurred by approximations not quantified
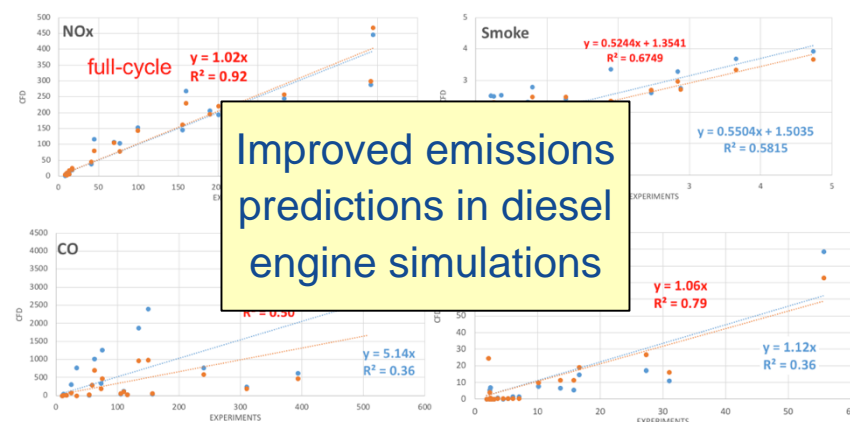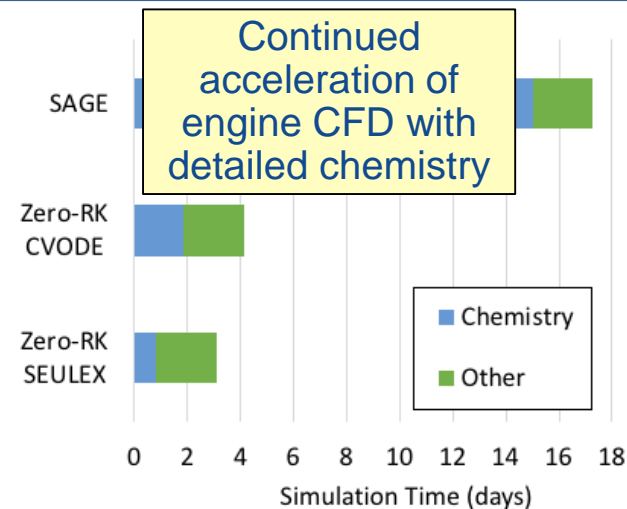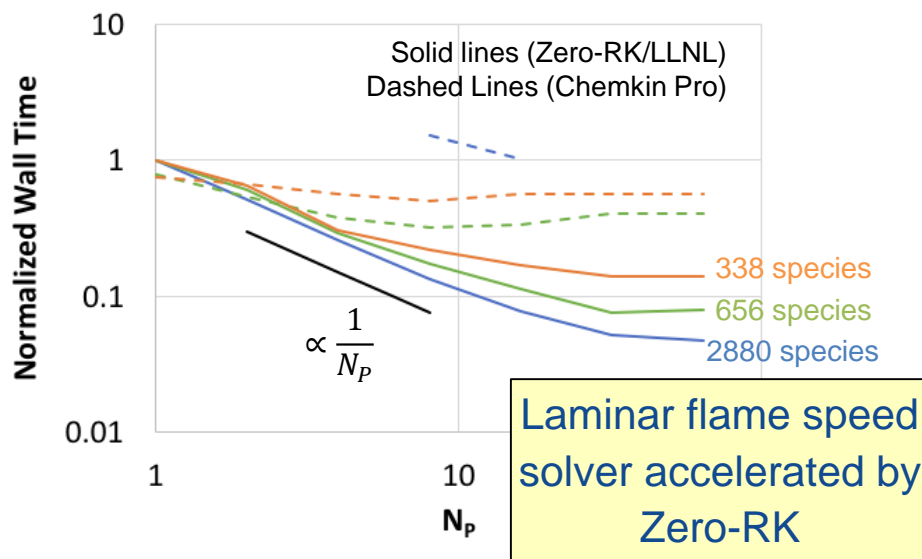 - New, heterogeneous compute architectures

Proposed Future Research

- **FY18**
  - Implement additional alternative time integrators in CFD
  - Work with industrial partners on demonstration/evaluations
  - Continue ALCC work with GM & ORNL

- **FY19**
  - Data science/machine learning to optimize solver performance
  - Multi-fidelity uncertainty quantification and sensitivity analysis

- **FY20+**
  - 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: LLNL modeling work accelerates present and future engine research inside and outside of VTO

Our pursuit of reduction in time-to-solution and increasingly accurate simulations continues to redefine the state-of-the-art in engine modeling and simulation
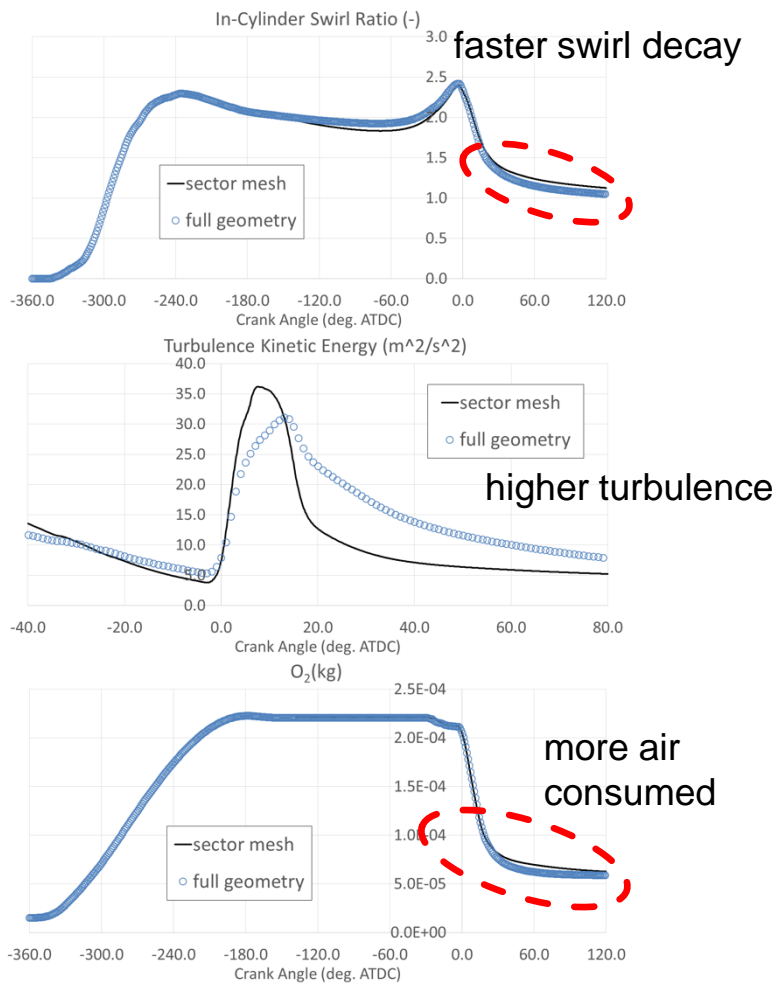

Continued acceleration of engine CFD with detailed chemistry

Laminar flame speed solver accelerated by Zero-RK

Improved emissions predictions in diesel engine simulations
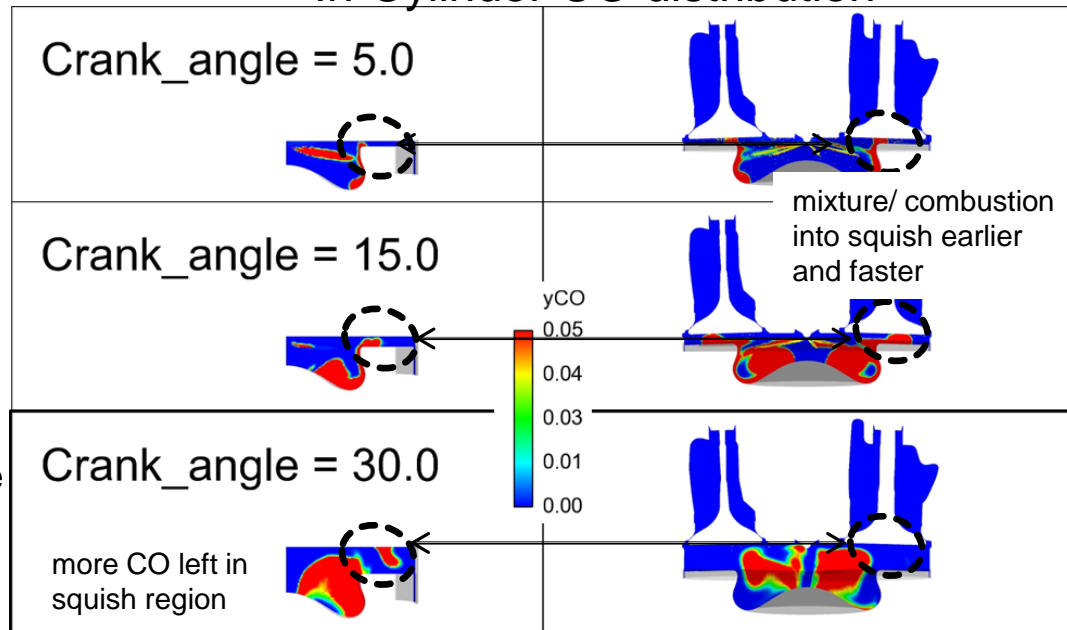
Technical Backup Slides

Verification of SEULEX/CVODE – Heat release profiles for all solvers agree
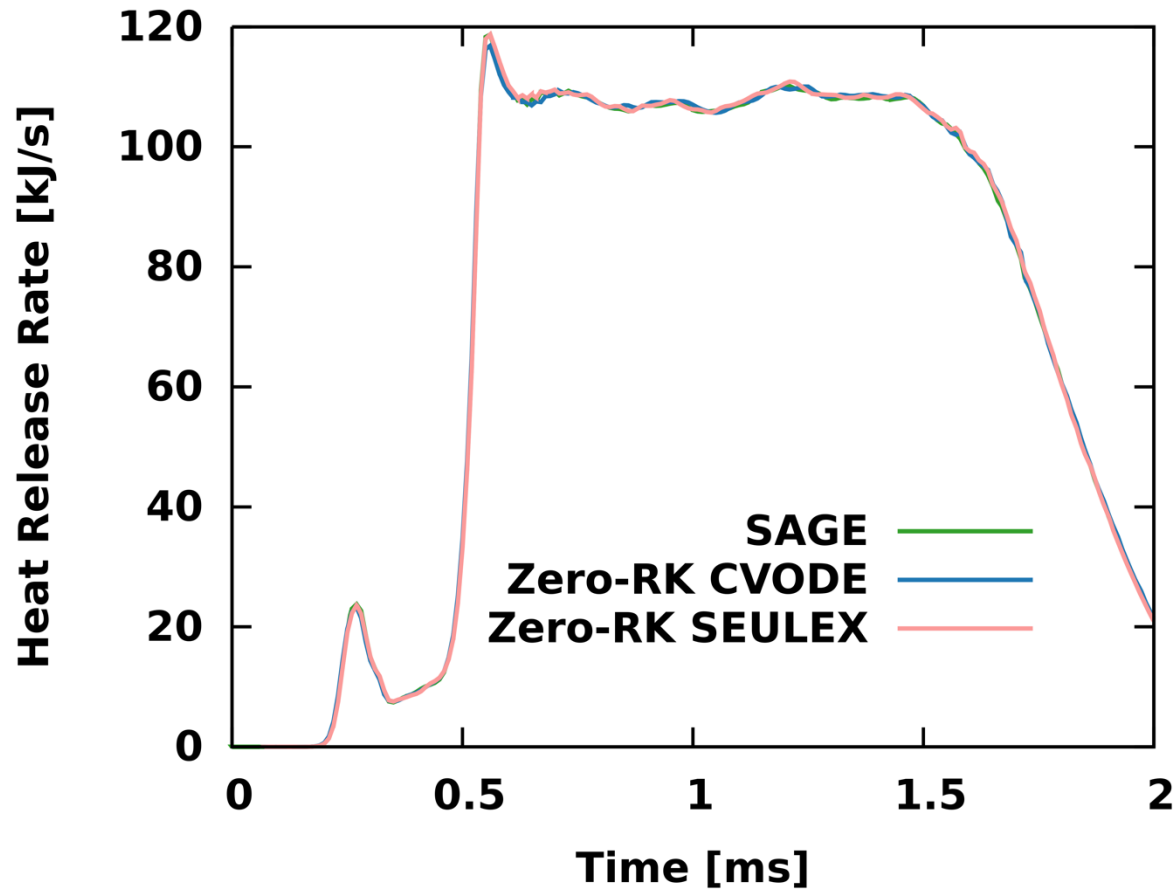
Physics behind more completed combustion with full geometry detailed model

In-Cylinder Swirl Ratio (-)

faster swirl decay

Turbulence Kinetic Energy (m^2/s^2)

higher turbulence

O_2(kg)

more air consumed

In-Cylinder CO distribution

Crank_angle = 5.0

Crank_angle = 15.0

Crank_angle = 30.0

more CO left in squish region

mixture/ combustion into squish earlier and faster

yCO
0.05
0.04
0.03
0.01
0.00

With full geometry detailed model

- Faster swirl decay in the late cycle
- Higher turbulence kinetic energy that helps local mixing
- Lower swirl motion and lower the top edge of the piston allow combustion into squish volume earlier and faster
- Improved air utilization and better soot/CO oxidation

Multi-fidelity uncertainty models provide rich information at dramatically reduced cost
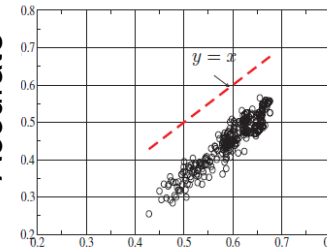
Adapted from Koutsourelakis (2009)*

- Example here from structural mechanics shows 30x reduction in analysis time for well bounded estimates
- Engine combustion problems provide many opportunities to combine approximate models with high fidelity data
- High fidelity data can come from detailed models or experiments
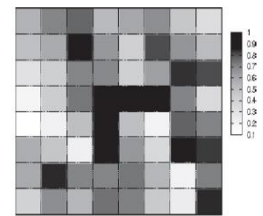
Accurate
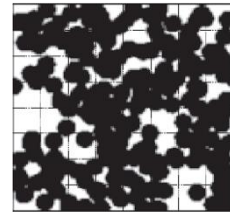
700 (seconds)

Approximate

0.15 (seconds)

Runs necessary to achieve statistical accuracy:
- Accurate: 1,500 = 291 cpu hours
- Approx. (1-model): 100 accurate + 5000 approx. = 20 cpu hours
- Approx. (2-models): 50 accurate + 10,000 approx. = 10 cpu hours
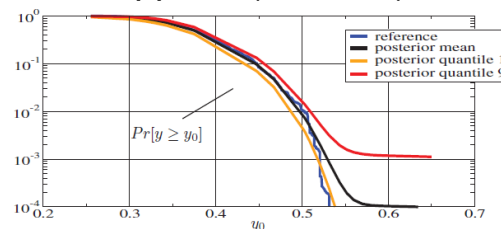
Approx. (1-model)

FIG. 3.11. Posterior for $Pr[y \geq y_0]$ for all y_0 based on 100 training samples.
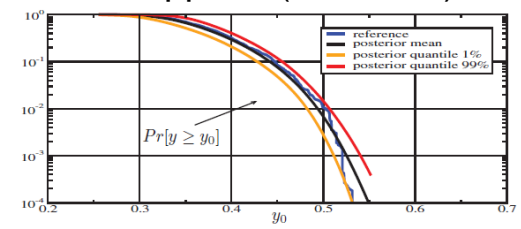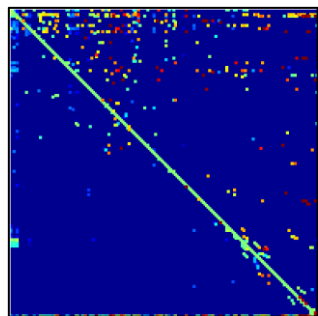
Approx. (2-models)

FIG. 3.14. Posterior mean and quantiles for $Pr[y \geq y_0]$ for all y_0 based on 50 training samples.

*https://doi.org/10.1137/080733565

Adaptive preconditioner using on-the-fly reduction produces the same solution significantly faster

Two approaches to faster chemistry solutions

Ex.   iso-octane
       874 species
       3796 reactions
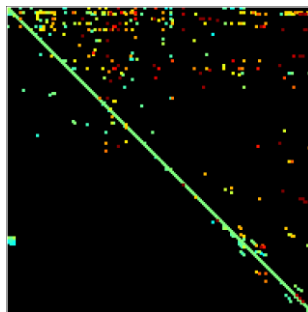

Jacobian Matrix
(species coupling freq.)

slower ⟷ faster

1. Classic mechanism reduction:

Ex.197 species

- Smaller ODE size
- Smaller Jacobian
- Poor low T accuracy

2. LLNL's adaptive preconditioner:

Filter out 50-75% of the least important reactions

- *Identical ODE*
- Reduced mech *only* in preconditioner

Our solver provides reduced mechanism speed without any loss of accuracy

iso-octane (20 bar, phi = 1)

874 species (full mech in solver)
197 species (full mech in solver)
874 species (adaptive preconditioner)