Model Development and Analysis of Clean and Efficient Engine Combustion

2019 DOE Vehicle Technologies Office Annual Merit Review

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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
- Transitioning to participate in 5-year Combustion Consortium

Budget

- FY17 funding: $441K
- FY18 funding: $600K
- FY19 funding: $700K

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.

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.

FY19 Approach – Detailed Kinetics in Flows

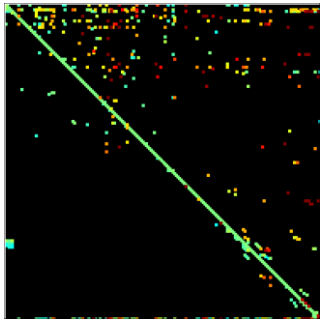
- One-Dimensional Flames
  - Improvements to premixed flame solution
  - New diffusion flame solver
  - Application to fuel sooting propensity (YSI)
- Mechanism Reduction with Zero-RK
- Diesel Spray Simulations with Detailed Chemistry
  - Study on Impact of Mechanism Size
  - Application of hybrid chemistry mechanism
- Maintain multiple collaborative projects

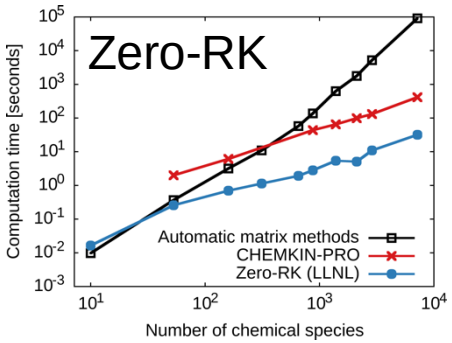
Milestones:

Quarterly status reports (completed/on-schedule)

Building on our previous accomplishments

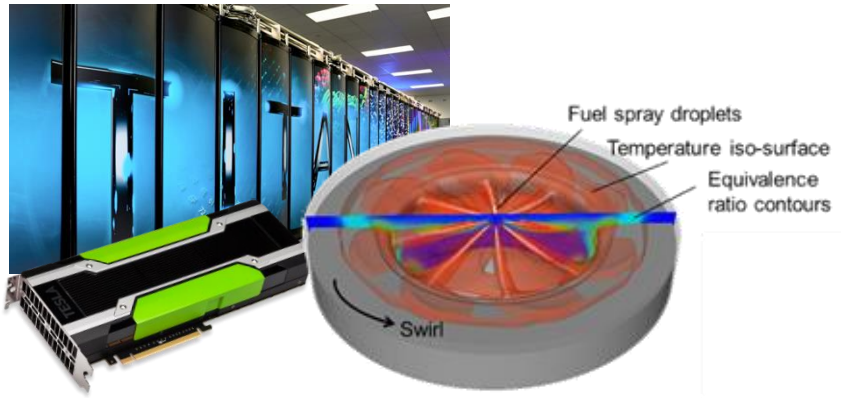
Algorithms + Numerics





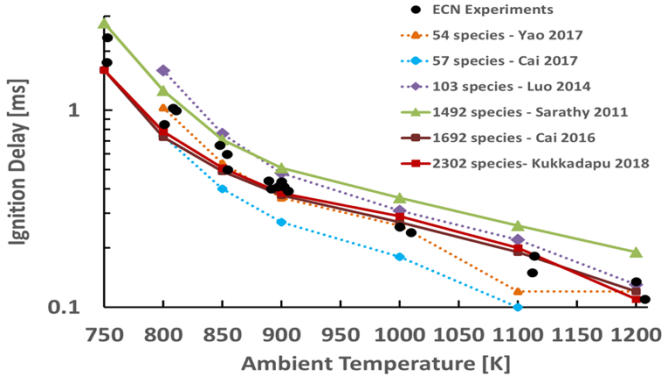
2015 R&D 100 WINNER

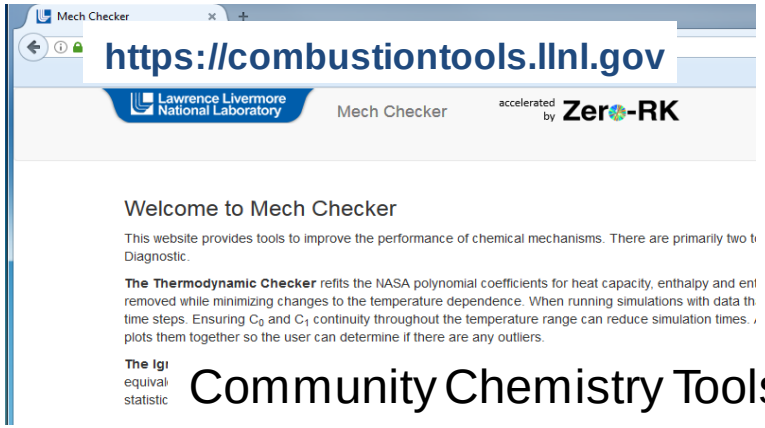
Engine CFD with Detailed Chem.



Applications

ECN Spray Predictions



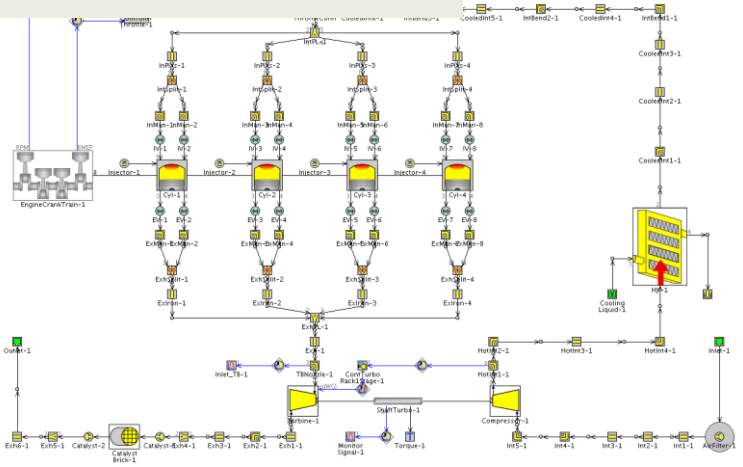


Community Chemistry Tools

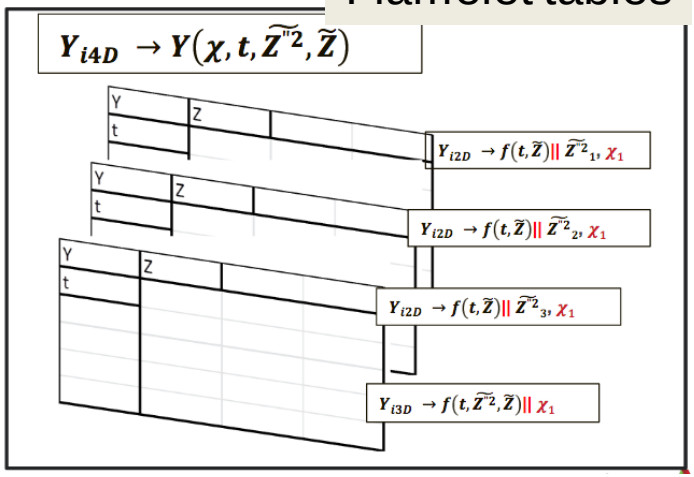
Technical Accomplishments

In FY19, we have dramatically reduced cost of one dimensional flame simulations with wide-ranging applications in Engine R&D

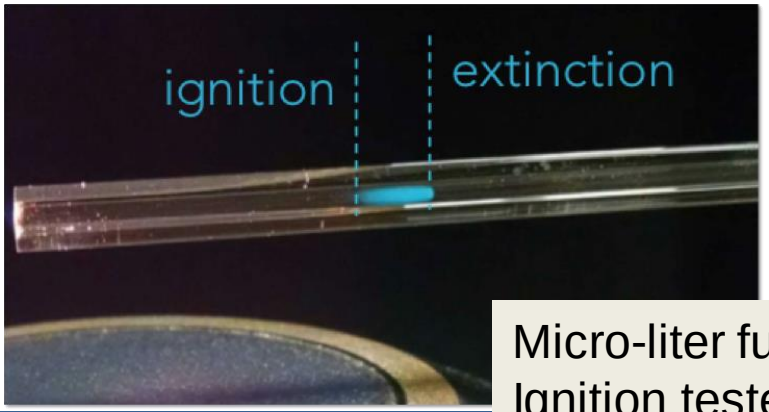
System level simulations



Flamelet tables



Sooting experiments (YSI)

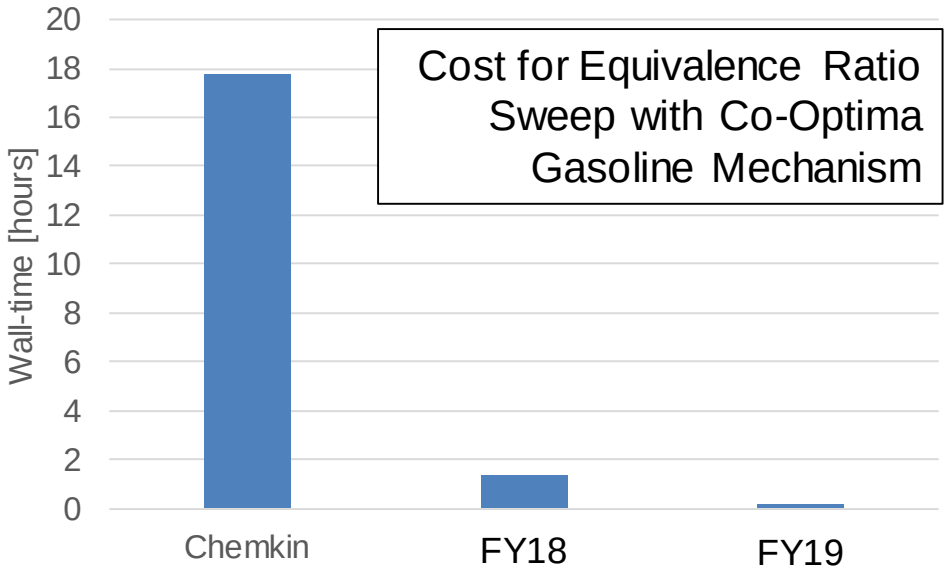


Micro-liter fuel Ignition tester

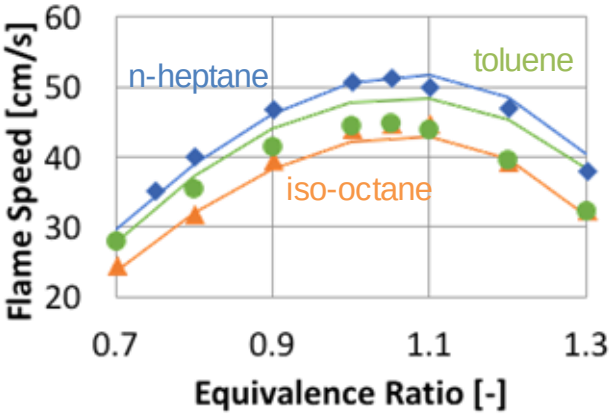
Technical Accomplishments

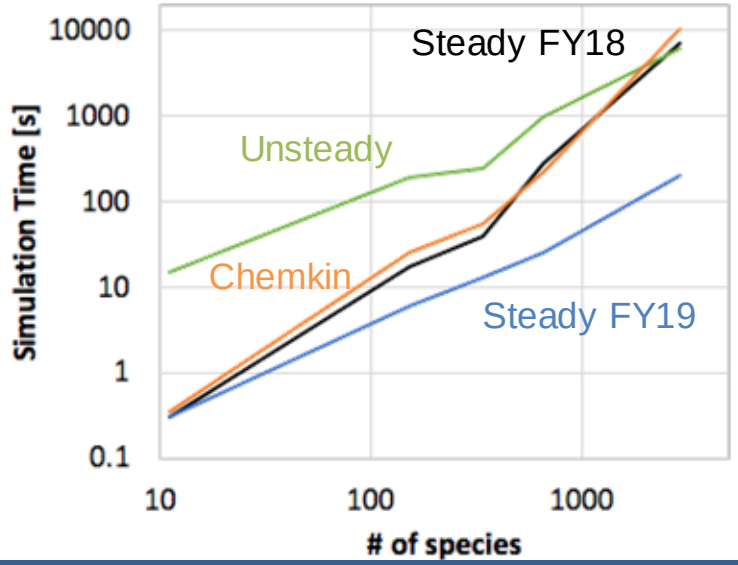
Our development of algorithms to achieve linear scaling for steady solvers provides new dramatic improvements in simulation time

10 minutes for ϕ sweep (previously 18 hours with Chemkin or > 1 hour with FY18 results)!



Result depends on sophisticated manipulation of linear system solution in implicit solvers

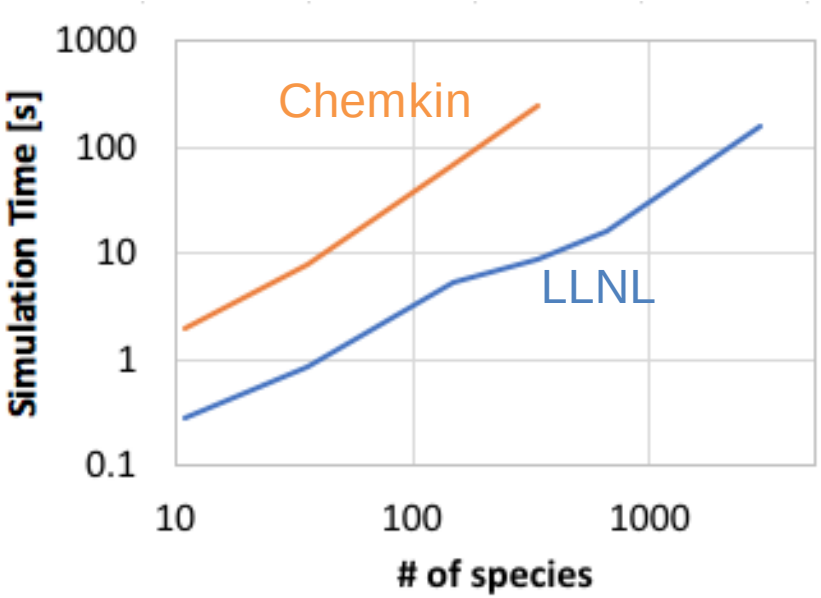




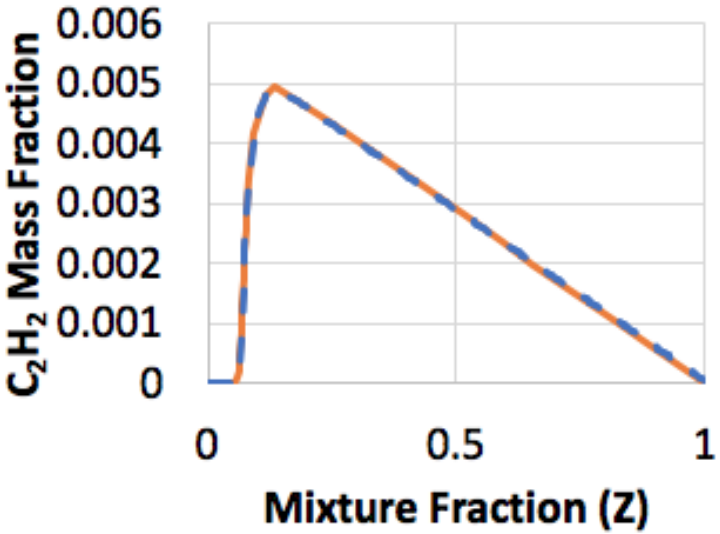
Technical Accomplishments

Our new diffusion flame solver extends methodology to new applications with performance similar to premixed solvers

>10x in time-to-solution



Same result as Chemkin



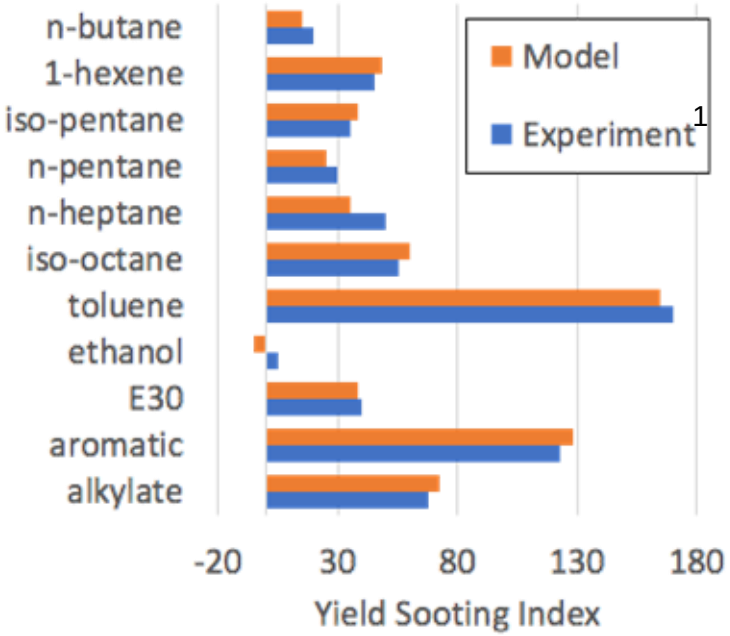
Built on same technology as 0-D and premixed flame solvers

Our model is able to reproduce experimental results for sooting behavior of gasoline components and blends

YSI predictions calculated with Co-Optima Gasoline mechanism (~3000 sp.)

Accelerated solvers allow for sensitivity analysis to determine which reactions drive soot production

Work being extended to investigate diesel surrogate blends and potential before-oxygenate blendstocks (BOBs) in CoOptima program (PSU, Xuan)



Yield Sooting Index Experiment (Yale[2])

Cost for Reaction Sensitivity Calculations

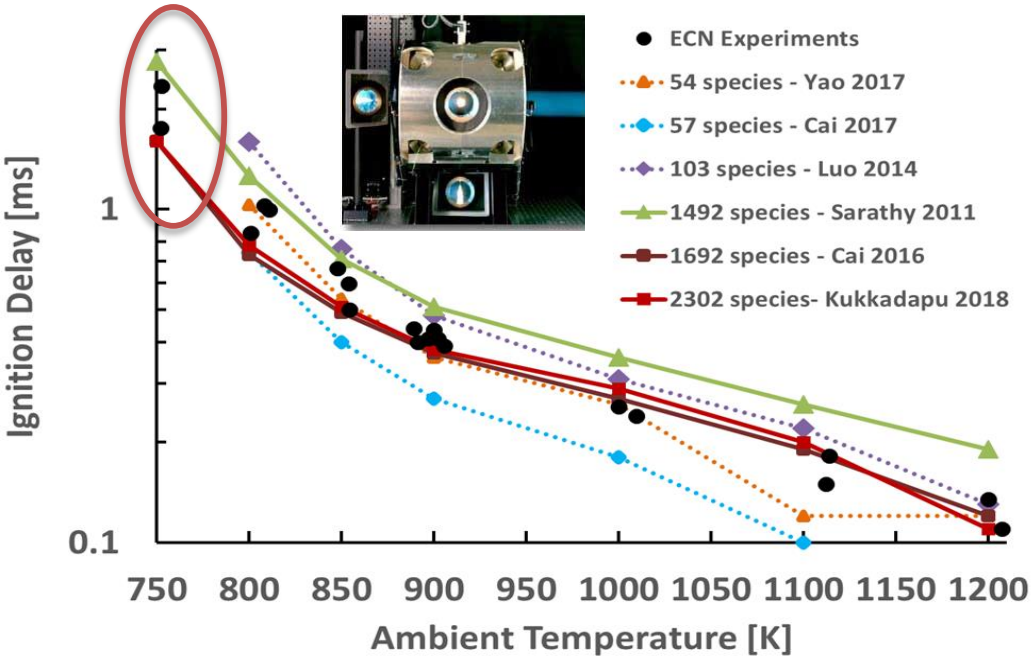
Solver	CPU Time [h]
FlameMaster	> 20,000
LLNL (full Jacobian*)	3570
LLNL (approx. Jacobian*)	33

*see Tech. Backup Slides

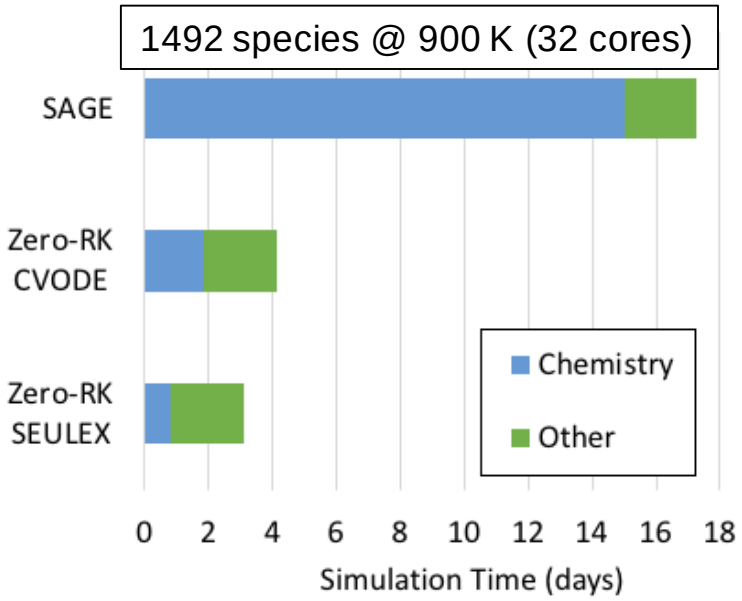
[1]McEnally et al., Proc. Combust. Inst. (2018)
[2]McEnally and Pfefferle, Combust. Flame (2007)

We are continuing to investigate the influence of chemical detail on predictions of combustion of Spray A (ECN)

Previous Results Showed Detailed Kinetics Predict Ignition Where Smaller Mechanisms Failed



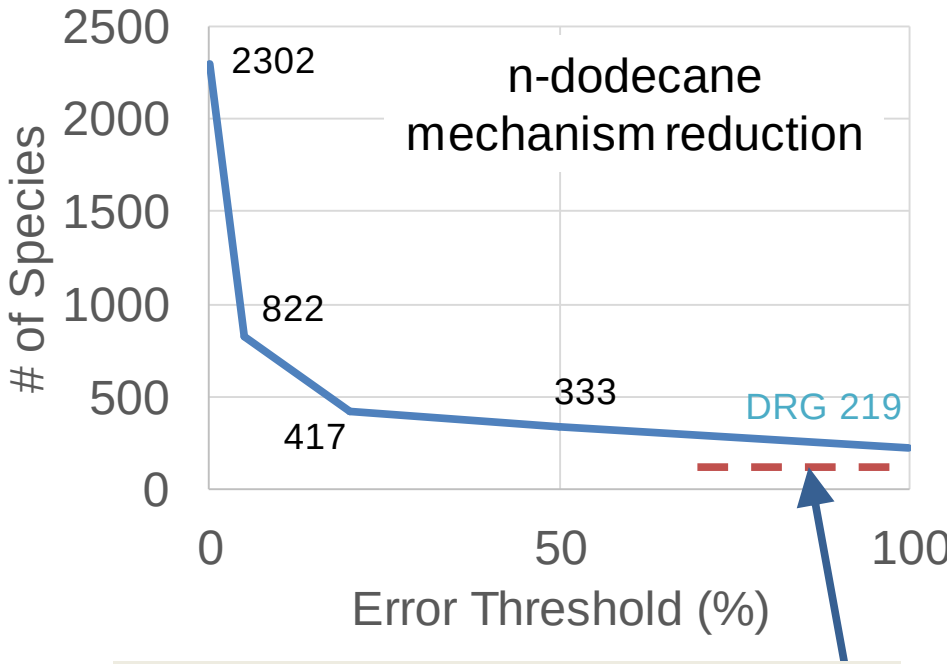
Simulations made possible by fast solvers (Zero-RK) developed in this program



Technical Accomplishments

We have incorporated our fast solvers into mechanism reduction software for in-house reduction and testing

- We coupled MARS* software to Zero-RK
- Directed Relation Graph (DRG) method with error propagation and sensitivity analysis is used
- Our parallel implementation further reduces wall-time
- This capability removes a significant bottleneck in reduction process
- We can now study trade-off between mechanism size and accuracy in CFD



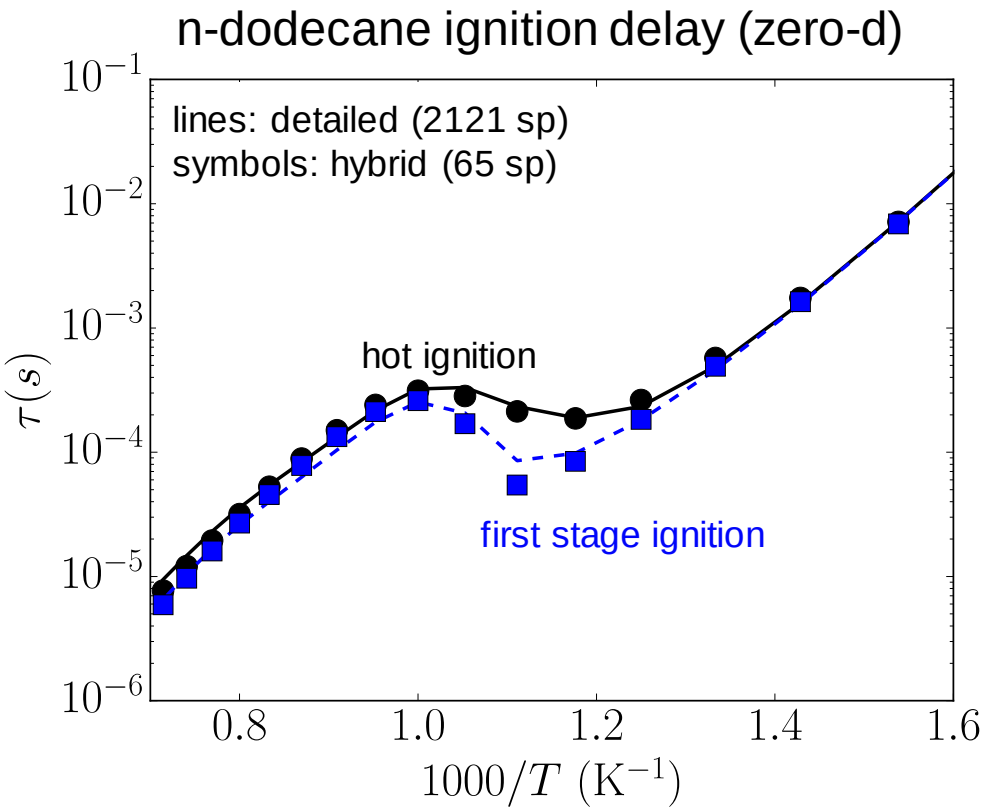
Error grows quickly when reducing to fewer than ~200 species

From 4.5 hours to 26 minutes to reduce Co-Optima gasoline surrogate mechanism to 50% error threshold with 8 targeted ignition points

* References:
doi:10.1016/j.combustflame.2009.12.022
https://niemeyer-research-group.github.io/MARS/

New hybrid mechanism approach is able to match detailed mechanism performance at much smaller size

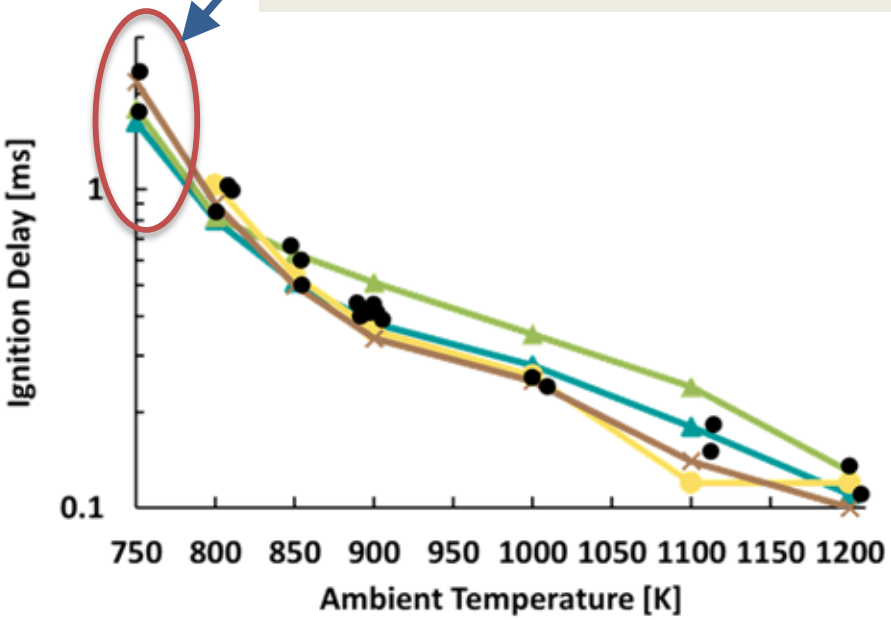
- New approach for reduced chemical models
- Developed as part of internal laboratory funding*, our method can match both high and low-temperature ignition
- Employs a detailed small hydrocarbon core and an empirical fuel specific initiation mechanism trained on detailed model results
- Hybrid n-dodecane mechanism developed in this project has 65 species and can match both first and second stage ignition delays for varying temperature

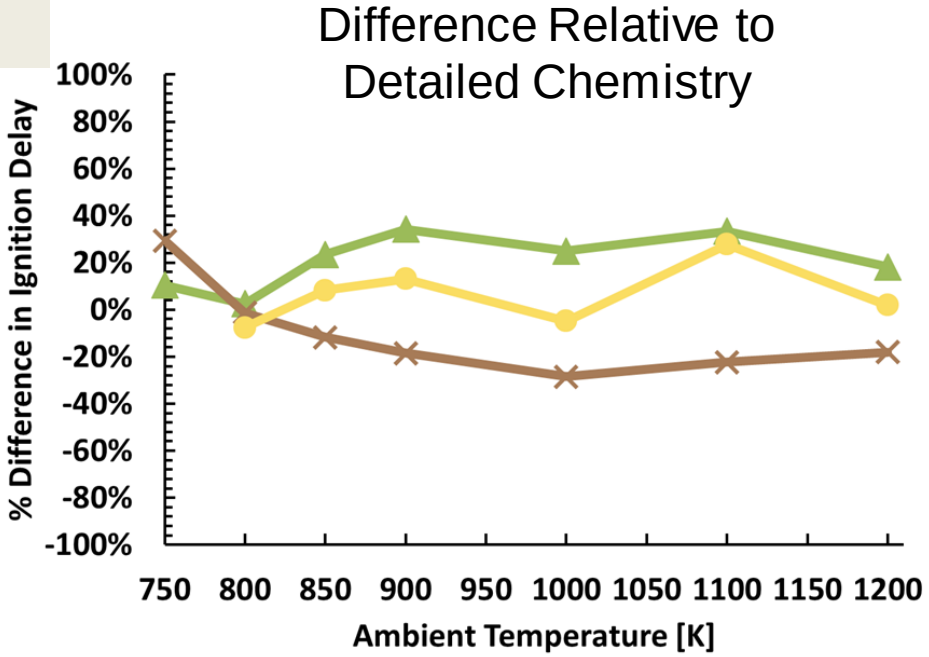


* LDRD: 16-ERD-003

Ignition delay results show both our standard reduced mechanism and hybrid mechanism succeed where the literature reduced mechanisms fail

Both of our reduction techniques predict ignition at 750 K





Detailed (2121 species)

Yao (54 species)

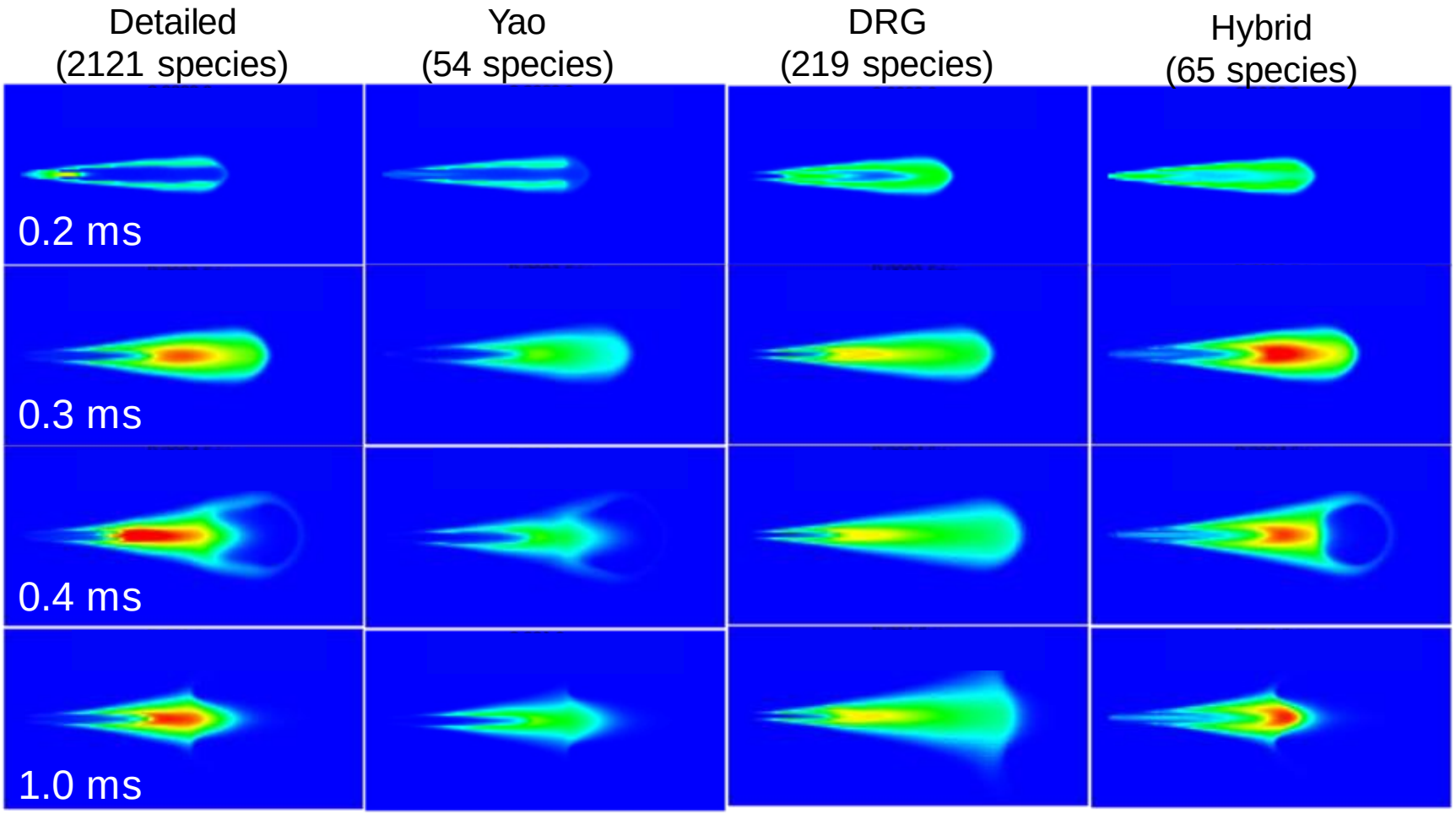
ECN Experiments

DRG (219 species)

Hybrid (65 species)

Technical Accomplishments

Formaldehyde distributions @ 900 K during spray ignition show hybrid mechanism best matches full detailed model

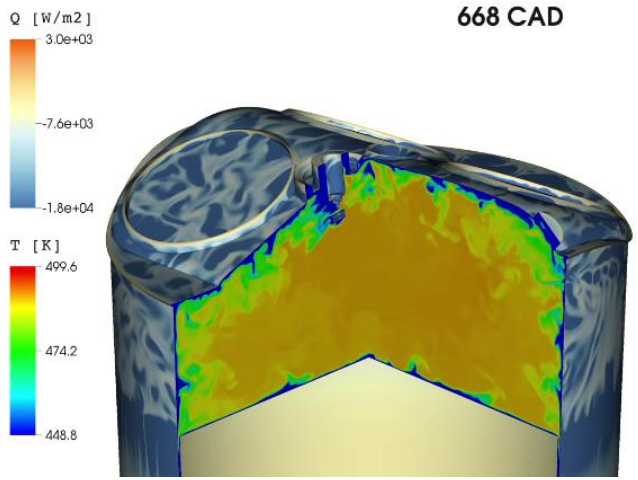


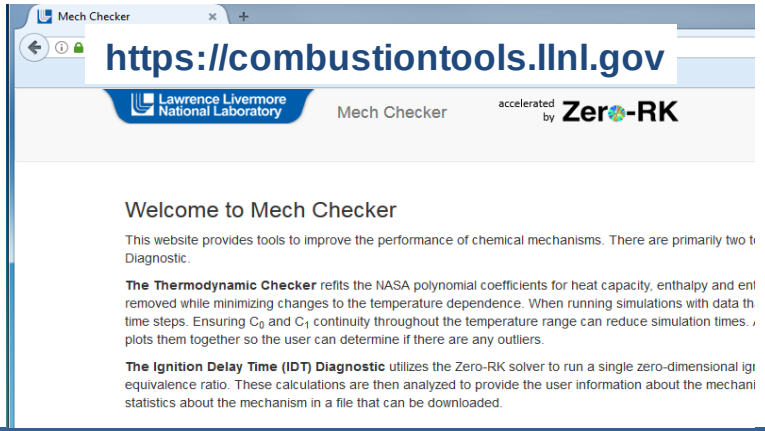
Progress continues in other areas

Coupling Zero-RK to Scalable DOE CFD codes
- NEK5000 (ANL)
- Pele (LBNL/NREL)

Machine learning to further accelerate Zero-RK:
- Building database of engine relevant conditions
- Training a classifier to choose best integrator based on thermodynamic state

CombustionTools Website Community Update:
- 43 users
- 23 institutions

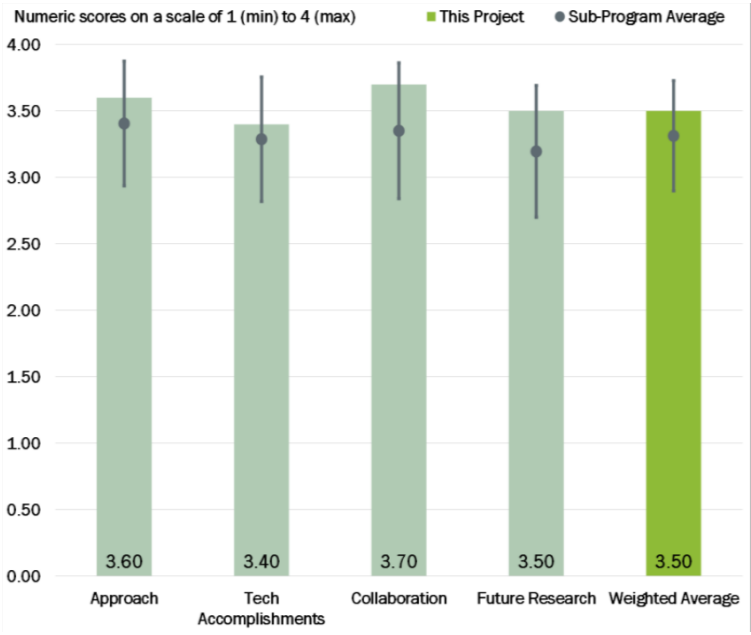




Technical Accomplishments

FY2018 Reviewer's Comments and Our Response

- Mostly positive comments and above average scores
- Zero-RK platform/availability:
  - Software has been designed for flexibility
  - Multiple demonstration licenses signed
  - Ready to work with new partners (both industrial and academic)
- Role of Machine Learning & Data Science:
  - We are taking our first steps in these areas
  - We see potential for significant impact on combustion R&D

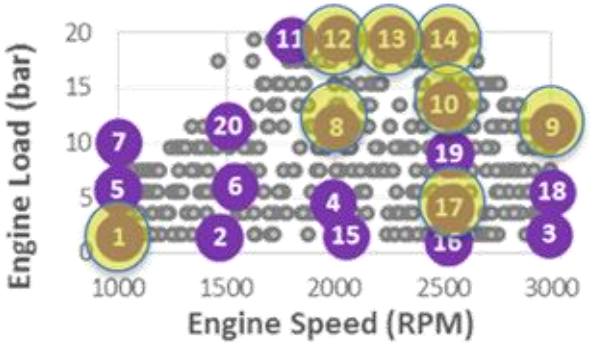


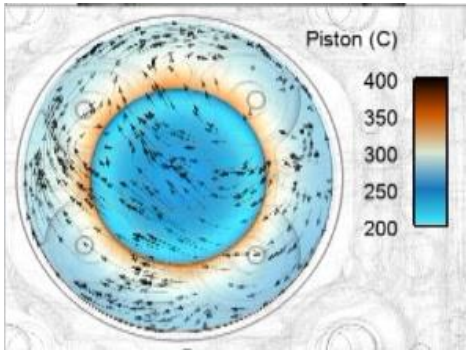
Collaboration – Ongoing interactions with industry, national laboratories, and universities

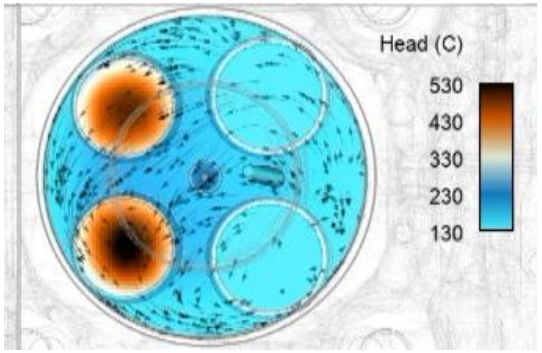
- SNL (Pickett) – ECN Spray A Simulations
- PSU (Xuan) –YSI Evaluation of Diesel Fuel Surrogates/BOBs
- GM/ORNL (Grover/Edwards) – Virtual Diesel Engine Calibration
- LBNL/NREL/ANL – Exa-scale ready CFD Codes (NEK5000/Pele)
- LLNL (Pitz) – Mechanism/Surrogate Development/Tools
- Convergent Science Inc. (CSI) – Current development platform for engine chemical kinetics coupling
- Advanced Engine Combustion (AEC) working group – twice annual research update meetings and informal collaboration

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
- Pushing fidelity to identify requirements for accurate prediction of combustion and emissions for diesel operation
- Past simulations had pointed to need for improved wall temperatures
- Current campaign includes multi-cycle LES simulations of diesel engine including 3D heat transfer through piston and head including water jacket
- *Zero-RK GPU capability integral to project*





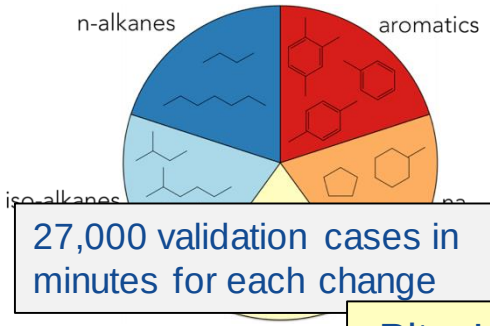


see ACE017 (Edwards) for more details

Collaboration

Collaboration Highlights: Connecting across ACS and Co-Optima Programs

Light & Heavy Duty Fuel Model Development (ACE013, FT052)



27,000 validation cases in minutes for each change

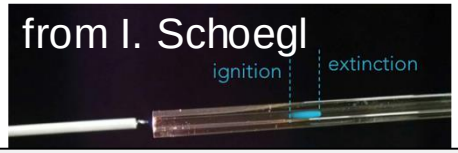
Pitz, LLNL

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

72,000 reaction sensitivity calculations in hours

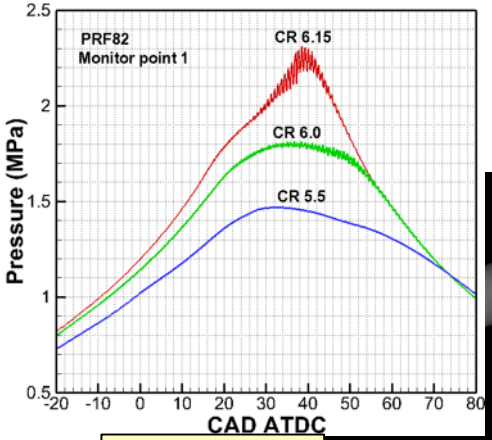
Goldsborough, ANL

Measuring fuel properties from microliters (FT063)



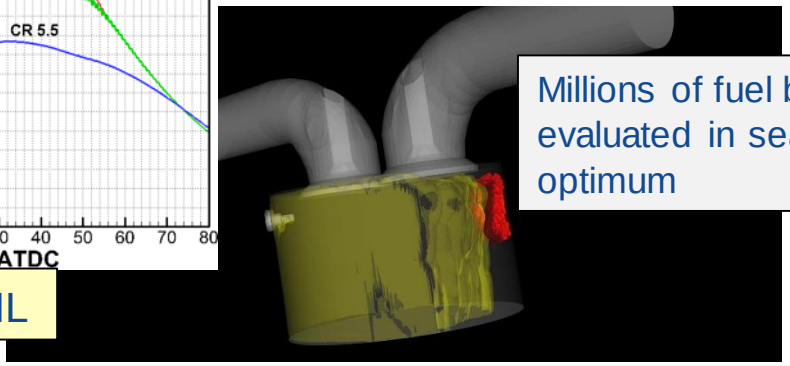
15,000 unsteady flames to infer reduced model reaction rates

McNenly, LLNL



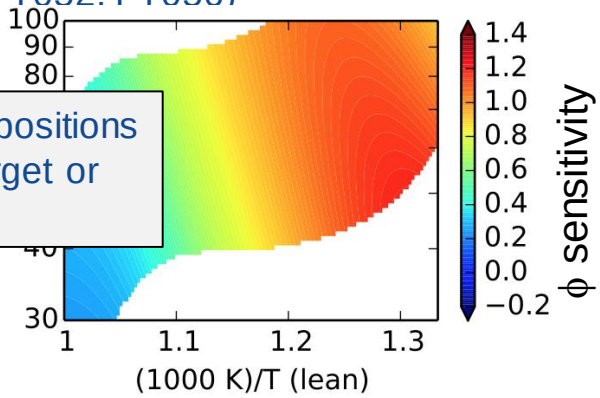
Pal, ANL

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

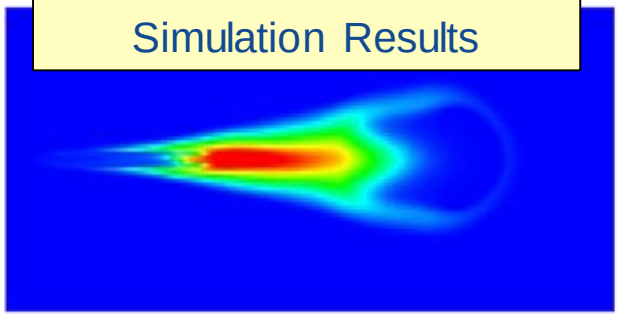
- FY19
  - Evaluate exa-scale ready CFD codes (Pele (LBNL), NEK5000 (ANL))
  - Machine learning to optimize simulation cost and accuracy
  - Continue ALCC work with GM & ORNL
- FY20
  - Coupling of Zero-RK to exa-scale ready CFD codes
  - Accelerate species transport for reacting flow with detailed chemistry
- FY21+
  - Reduction in time-to-solution for engine CFD in both super-computer and workstation hardware
  - Methods and practices for developing predictive models and simulations

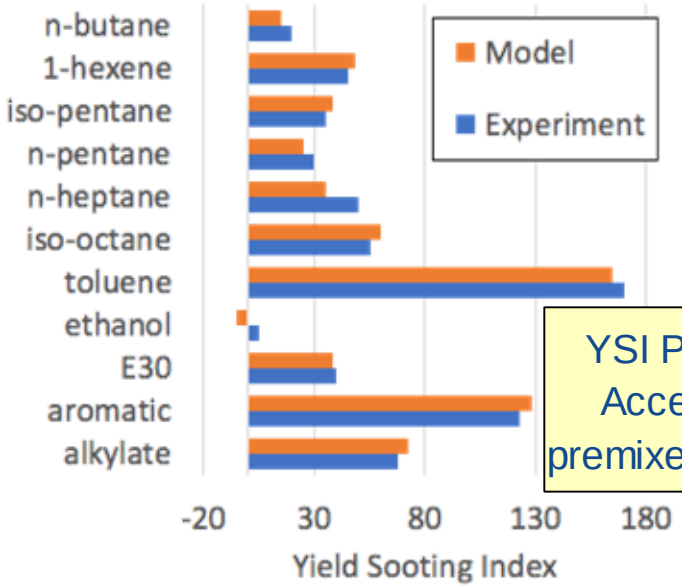
Any proposed future work is subject to change based on funding levels

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

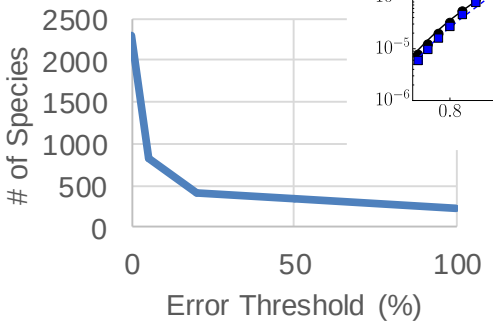
Highlighting the Impact of Mechanism Size on Detailed Simulation Results

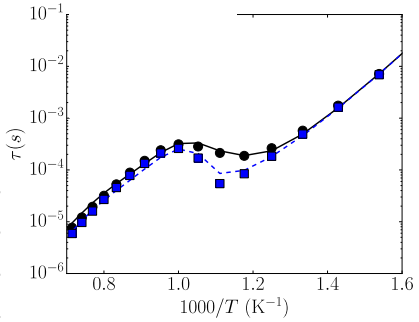




YSI Prediction with Accelerated Non-premixed Flame Solver

New Reduced Mechanism Capabilities



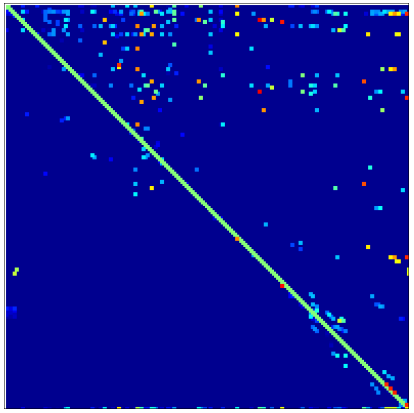


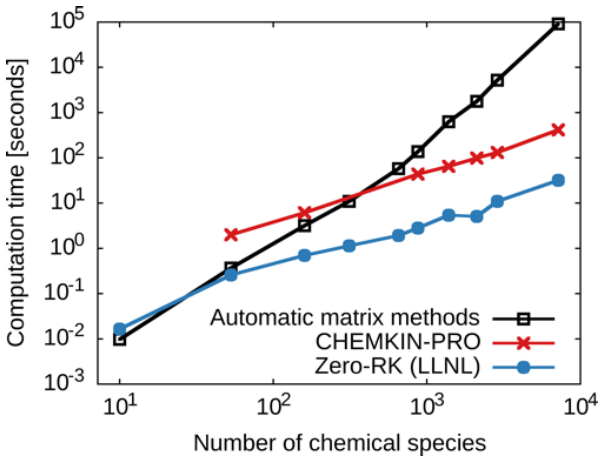
Technical Backup Slides

Zero-RK: Accelerated Solution for Chemically-Reacting Systems

- Combustion chemistry is stiff, $\frac{\tau_{max}}{\tau_{min}} \ggg 1$
- Implicit solvers /Jacobians are needed
- We pioneered methods to accelerate solutions of these systems:
  - Fast computation of chemical derivatives
  - Semi-analytic Jacobian formulation
  - Iterative solutions with adaptive preconditioning
- For isolated systems, solutions scale linearly with system size (n_s)

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \frac{\partial f_N}{\partial x_2} & \cdots & \frac{\partial f_N}{\partial x_N} \end{pmatrix}$$

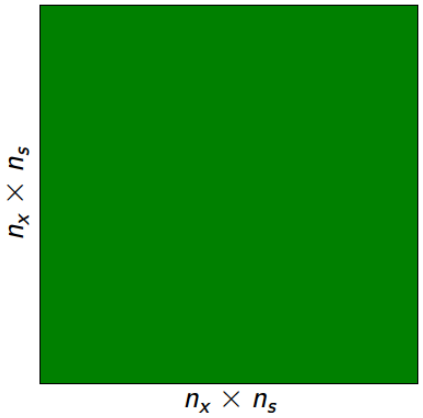




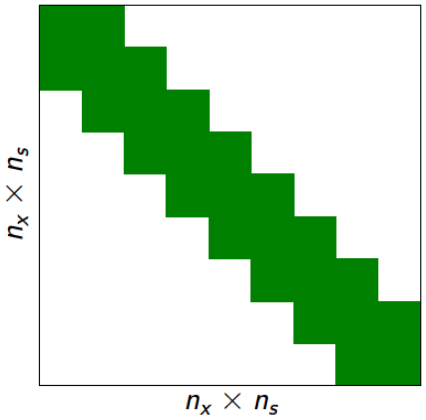
Improvements in steady state solvers dependent on novel method for implicit solution

No knowledge/use of the Jacobian structure

$\text{cost} \sim n_x^3 * n_s^3$



$\text{cost} \sim n_x * n_s^3$

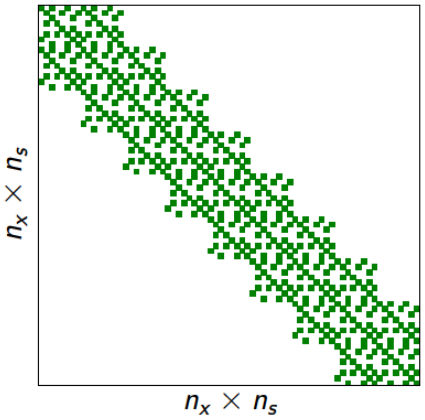


Block-tridiagonal structure with dense blocks*

*Assuming second order centered differences to compute derivatives

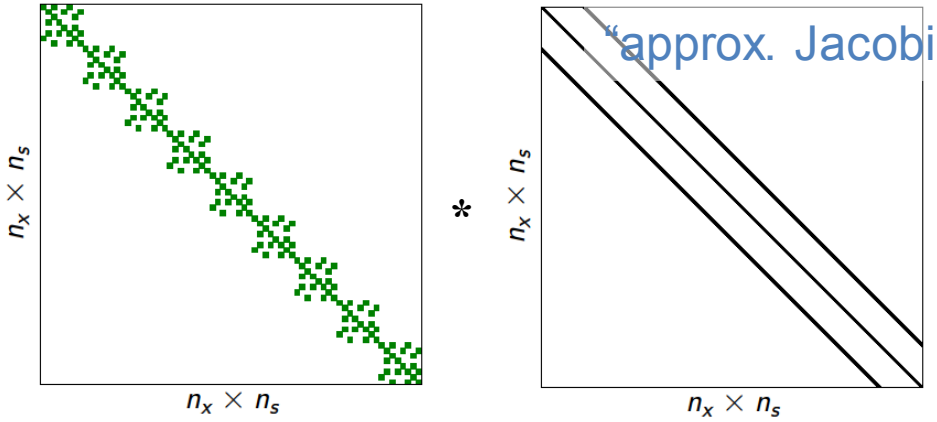
"full Jacobian"

Block-tridiagonal with sparse blocks



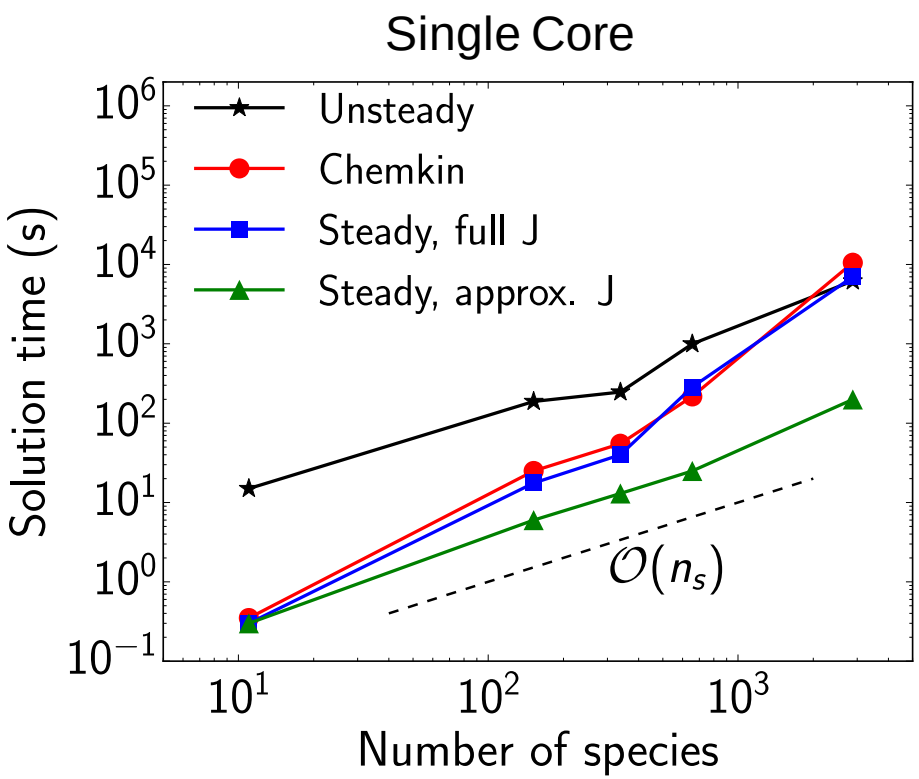
$\text{cost} \sim n_x * n_s^2$

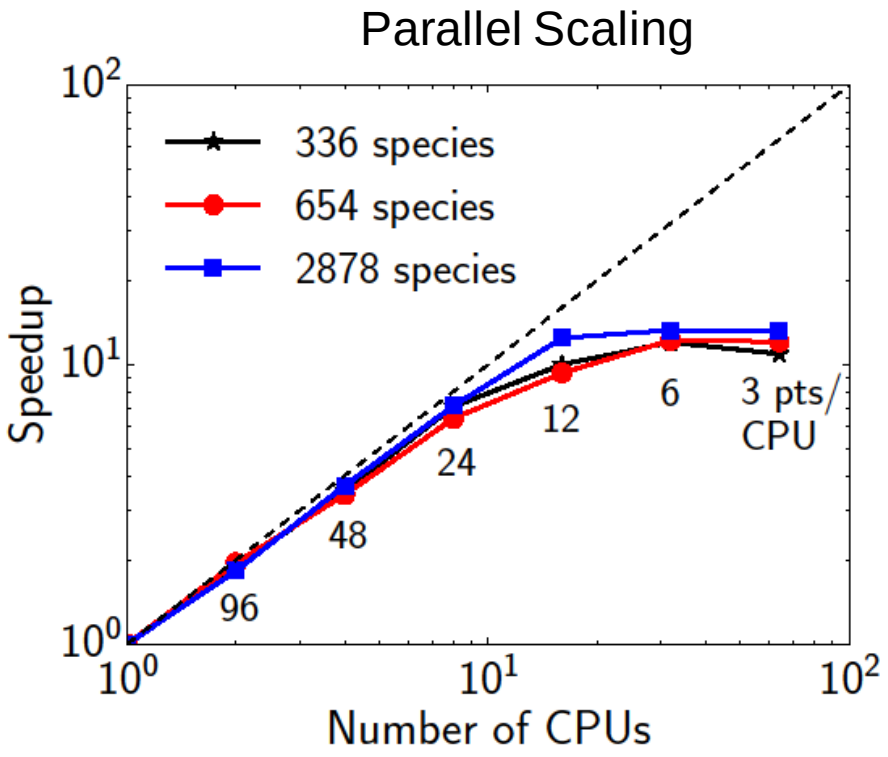
Product of sparse block-diagonal and tri-diagonal



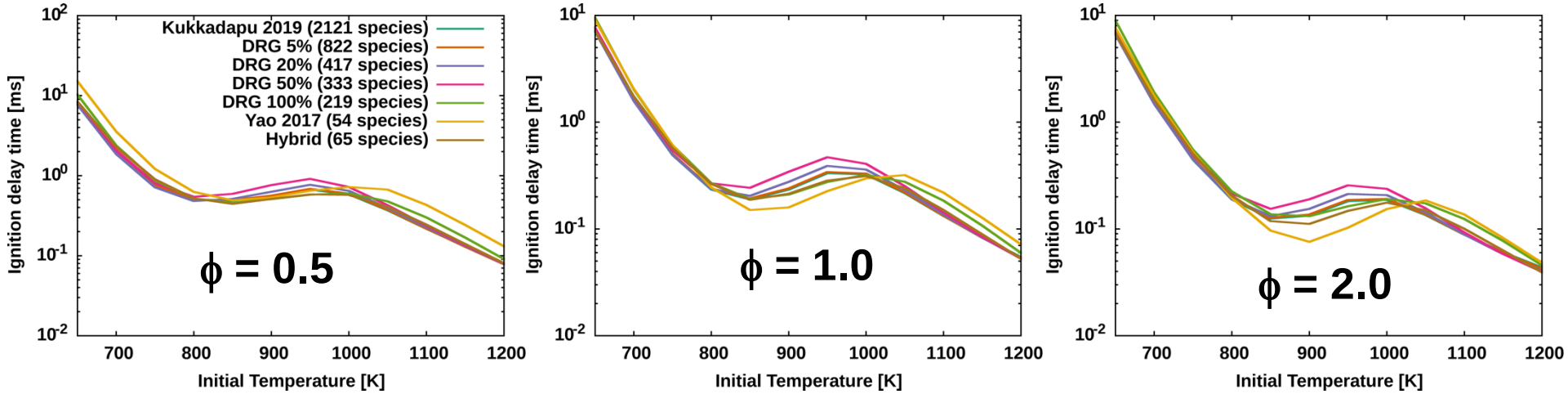
$\text{cost} \sim n_x * n_s$

Acceleration of both Steady and Unsteady Solvers includes Multi-CPU Parallelism





Hybrid mechanism shows ability to model low temperature ignition with very few species



Hybrid mechanism can be adapted to different fuels and fuel surrogates