Lawrence Livermore National Laboratory

Improved Solvers for Advanced Engine Combustion Simulation

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Project ID # ACS076

2017 DOE Vehicle Technologies Office
Annual Merit Review and Peer Evaluation Meeting
June 5-8, 2017 - Washington, DC

This presentation does not contain any proprietary, confidential or otherwise restricted information

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Acknowledgements

We gratefully acknowledge the support and guidance of the Advanced Combustion Systems' program leaders, Leo Breton, Gurpreet Singh, and Michael Weismiller, and the director, Michael Berube of U.S. Department of Energy's Vehicle Technologies Office.

Overview

Timeline

- Ongoing project with yearly direction from DOE
- FY17-FY20 program plan approved, but will be realigned with Co-Optima*

Barriers

Barrier 1: Efficient, Low-Emissions Engine Knowledge Gap

Barrier 2: Predicting the Impact of Fuel Properties

Computational cost and accuracy limits role of simulation in engine design.

Budget

- FY16 funding: $460K
- FY17 funding: $400K*

* Core funding to LLNL through ACS012 and ACS076 reduced to $570K, while ACS013 moved to Co-Optima program.

Partners

- GM and Convergent Sciences Inc.
- ANL, NREL, ORNL and SNL
- AEC MOU, CRC & FACE working groups, Combustion Inst., SAE, ICCK, and Co-Optima Program
- LLNL Industrial Partnership Office hosts collaboration call for Zero-RK**

** https://ipo.llnl.gov/technologies/zero_rk

Relevance: the Advanced Combustion Numerics project at LLNL addresses two main barriers

from the DOE Vehicle Technologies Office Program Plan*:

1. Efficient, Low-Emissions Engine Knowledge Gap

   "Lack of fundamental knowledge of advanced engine combustion regimes. Engine efficiency improvement, engine-out emissions reduction, and minimization of engine technology development risk are inhibited by an inadequate understanding of the fundamentals of … in-cylinder combustion/ emission formation processes over a range of combustion temperature for regimes of interest, as well as by an inadequate capability to accurately simulate these processes."

2. Predicting the Impact of Fuel Properties

   "Inadequate data and predictive tools for fuel property effects on combustion and engine efficiency optimization. Existing data and models for engine efficiency, emissions, and performance based on fuel properties and fuel-enabled engine designs or operating strategies are inadequate."

* https://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/vt_mypp_2011-2015.pdf

Relevance: better fuel chemistry models elevate all in Advanced Combustion Systems R&D

Objective

Create faster and more accurate combustion solvers.

Barrier 1: Efficient, Low-Emissions Engine Knowledge Gap

Barrier 2: Predicting the Impact of Fuel Properties

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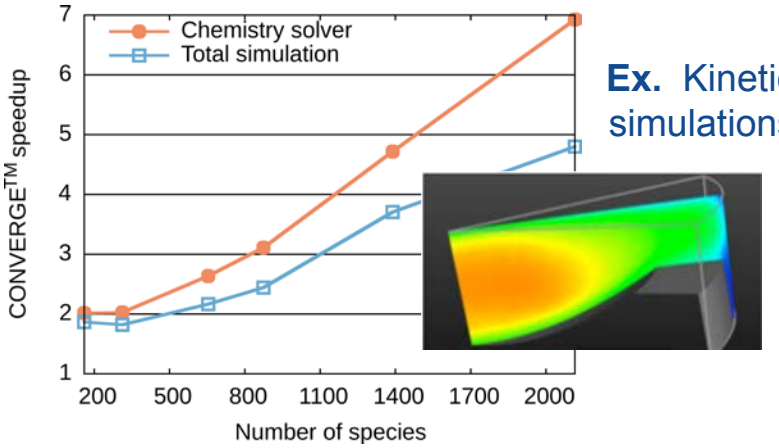

Ex. Kinetically controlled engine simulations with +1K species

- Project increases the predictive power available to the engine design process

Barrier 2: Predicting the Impact of Fuel Properties

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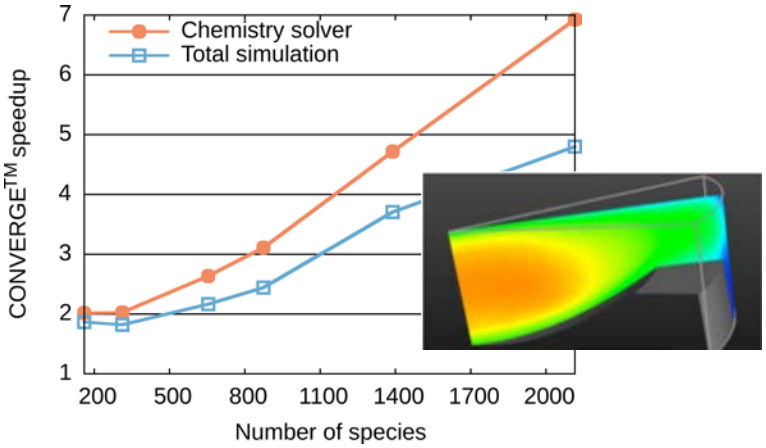
Barrier 1: Efficient, Low-Emissions Engine Knowledge Gap



- Project increases the predictive power available to the engine design process

Barrier 2: Predicting the Impact of Fuel Properties

Ex. Is Fuel A better than B?

- Detailed chemical kinetics captures complex, highly non-linear blending behavior
- Project reduces development and validation time for new mechanisms

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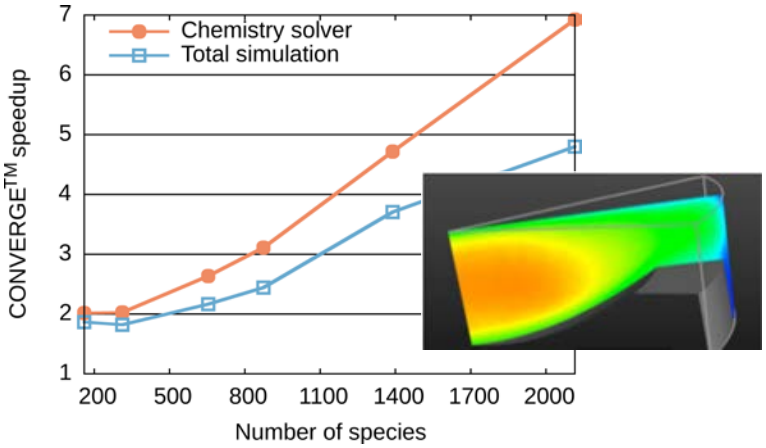
Objective

Create faster and more accurate combustion solvers.

Increases R&D bandwidth of ACS and Co-Optima programs

Barrier 1: Efficient, Low-Emissions Engine Knowledge Gap



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Barrier 2: Predicting the Impact of Fuel Properties

Ex. Is Fuel A better than B?

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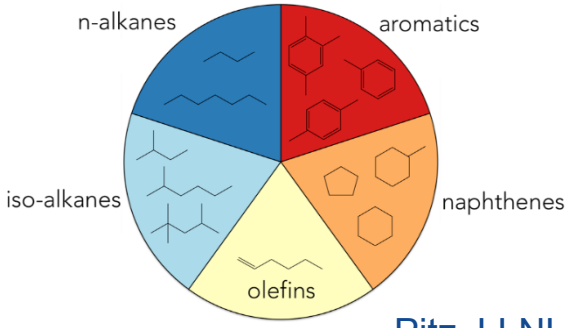
Relevance: the advances made by this project directly impact numerous R&D efforts

Light & Heavy Duty Fuel Model Development (ACS013, FT052)



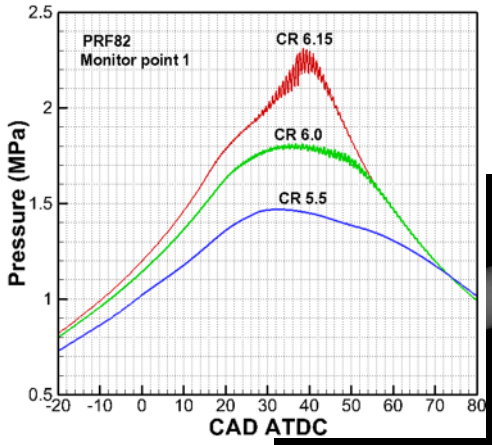
Pitz, LLNL

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

Goldsborough, ANL

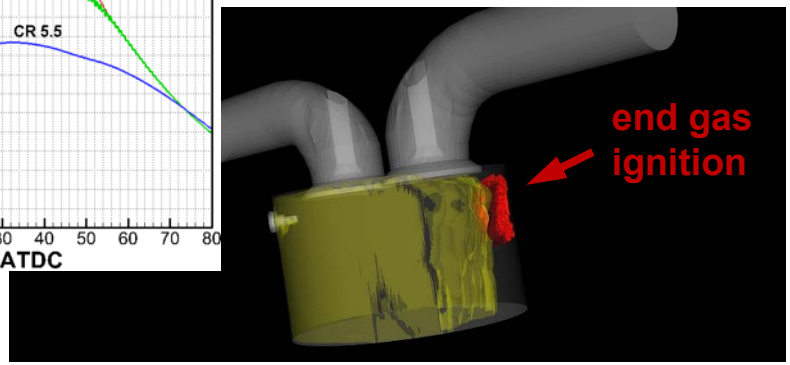
Measuring fuel properties from microliters (LDRD)

McNenly, LLNL

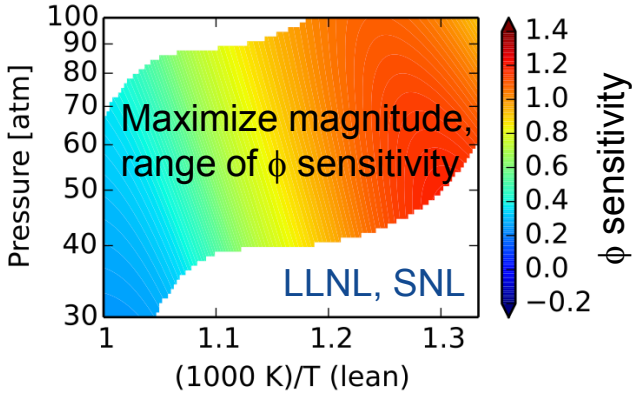


Pal, ANL

Virtual fuel models with matched octane ratings to test the Central Fuel Hypothesis (FT052, FT053)



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



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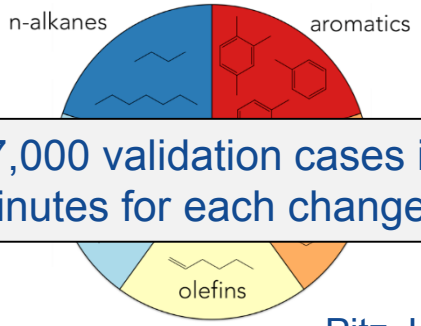


27,000 validation cases in minutes for each change

Pitz, LLNL

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

72,000 reaction sensitivity calculations in hours

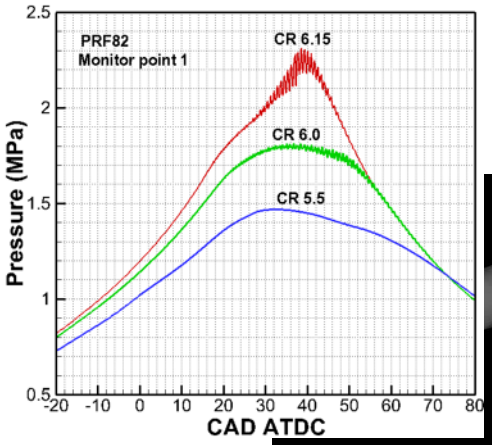
Goldsborough, ANL

Measuring fuel properties from microliters (LDRD)

from I. Schoegl

15,000 unsteady flames to infer reduced model reaction rates

McNenly, LLNL



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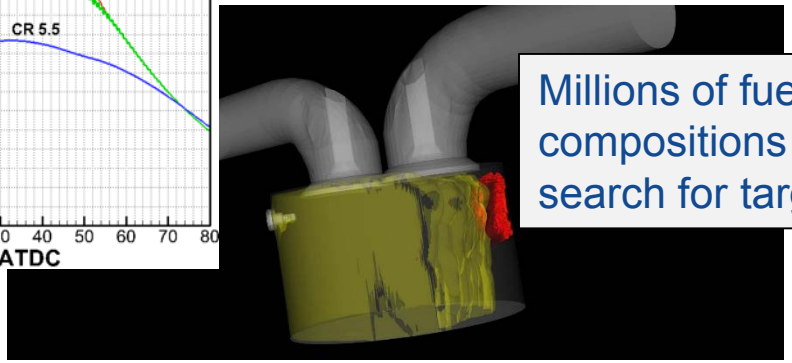
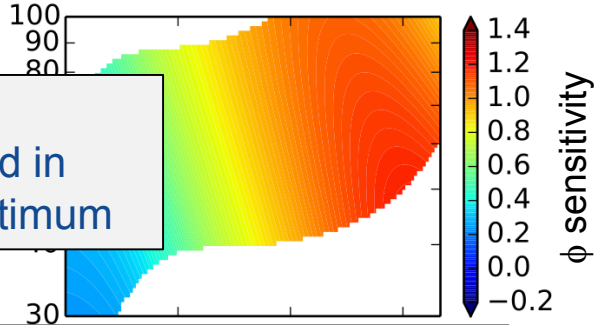


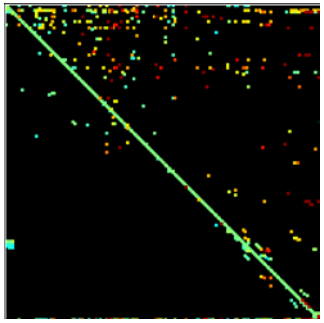
Millions of fuel blend compositions evaluated in search for target or optimum

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



Plus more shown by Whitesides in ACS012

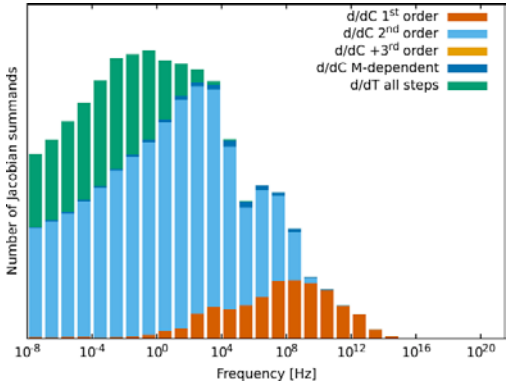
Approach: create faster and more predictive engine models along three research fronts



1. Better algorithms and applied mathematics
   – same solution only faster

2. New computing architecture
   – more flops per second, per dollar, per watt

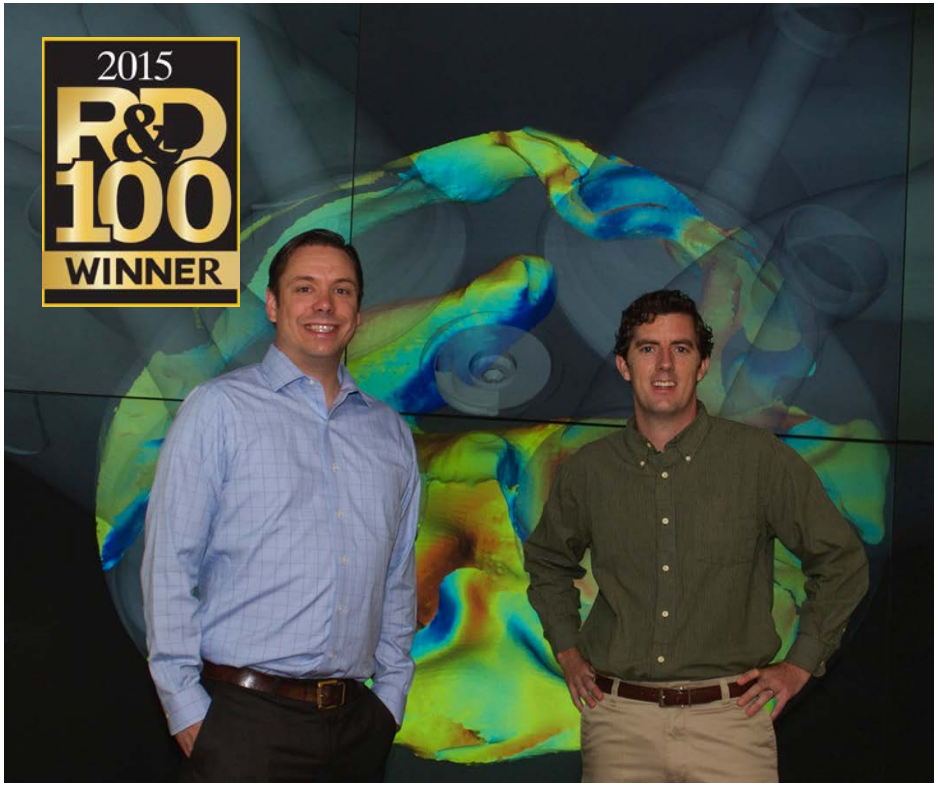
Accomplishments discussed in more detail in Whitesides' presentation (ACS012)

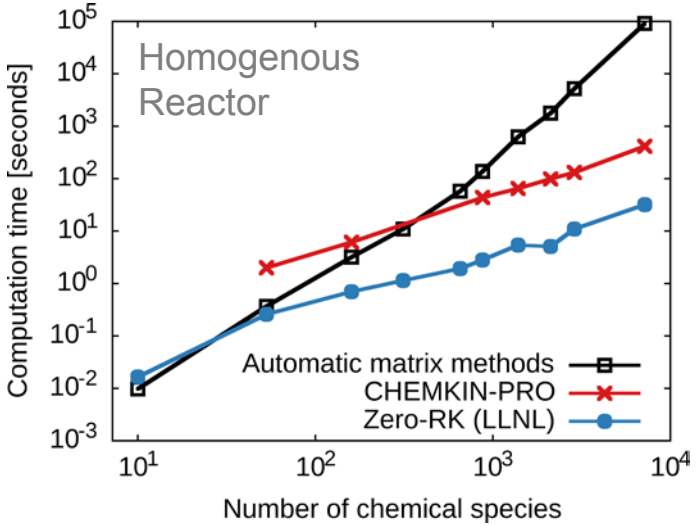


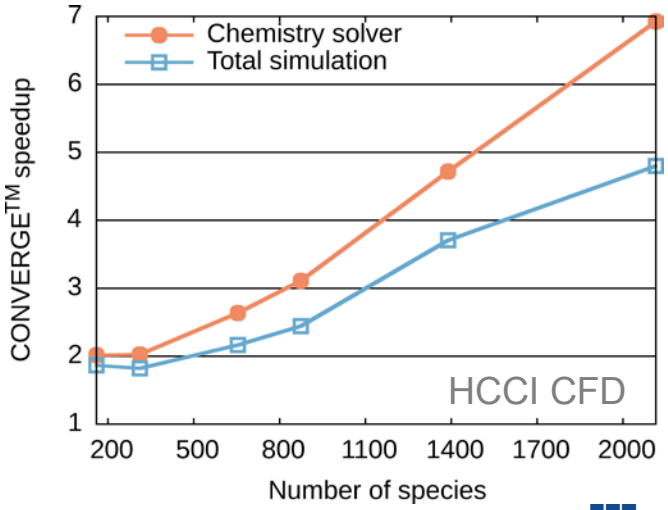
3. Improved physical models
   – more accuracy, better error control

Recognition of approach: Zero-RK chemistry software earns an R&D 100 award in FY16

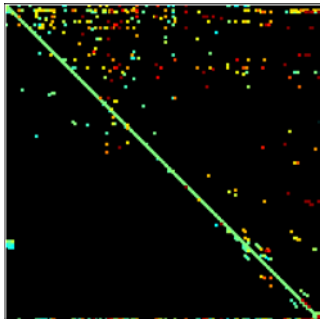
Zero-RK







Outline for accomplishments



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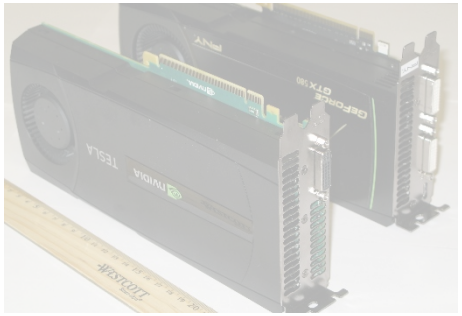

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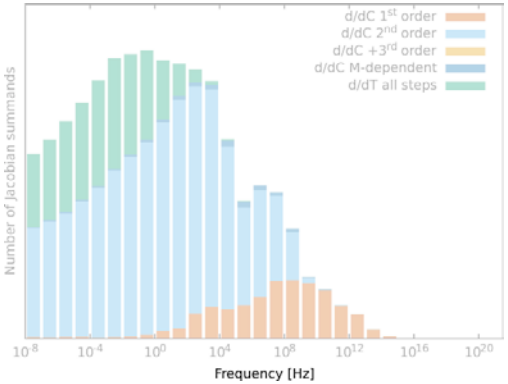

3. Improved physical models
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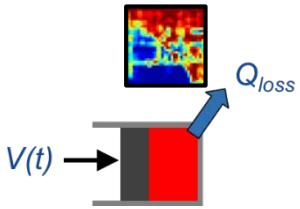
Extend Zero-RK chemistry solver to more applications impacting VTO research

The Jacobian matrix is the key to fast solvers for real fuel chemistry:

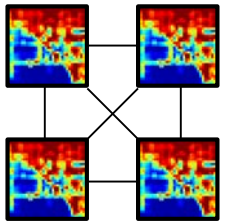
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

Slow/No reaction coupling

Fast reaction coupling

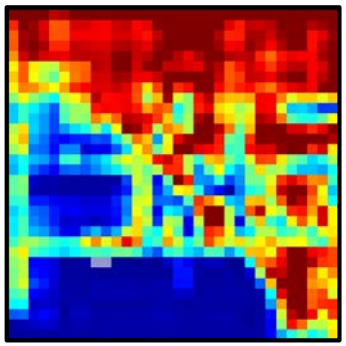


Variable Volume

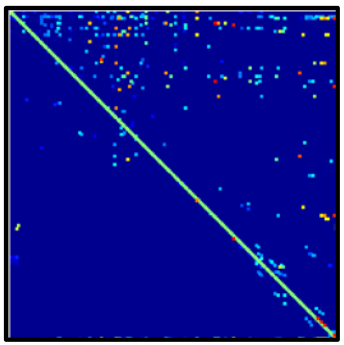


Engine Multizone

$J =$



Reduced *i*-C_8H_{18}
63 species



Detailed *i*-C_8H_{18}
874 species

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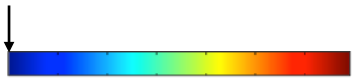
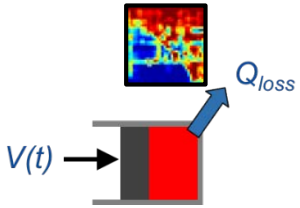
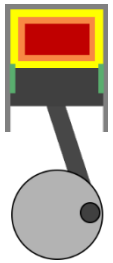
Slow/No reaction coupling

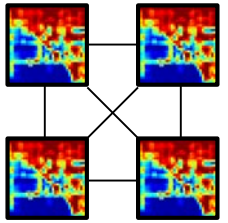
Fast reaction coupling





Variable Volume

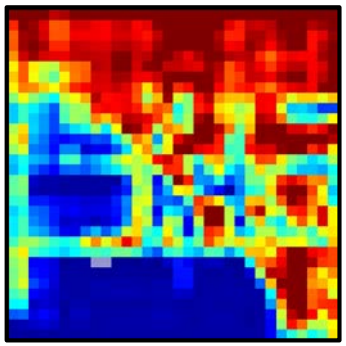




Engine Multizone

Zero-RK speedup shown in previous AMRs is now accelerating VTO research at other labs:

$J =$



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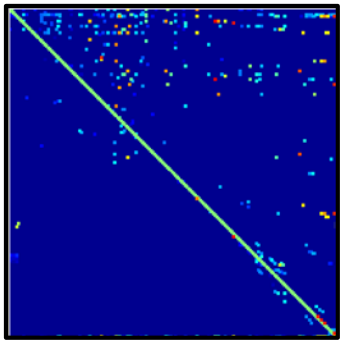

Detailed *i*-C_8H_{18}
874 species

2 journal papers, and 2 conference papers with ANL RCM group led by Goldsborough.

Extend Zero-RK chemistry solver to more applications impacting VTO research

The Jacobian matrix is the key to fast solvers for real fuel chemistry:

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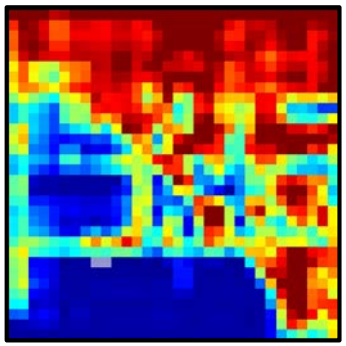
$J =$ 

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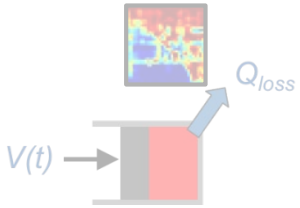
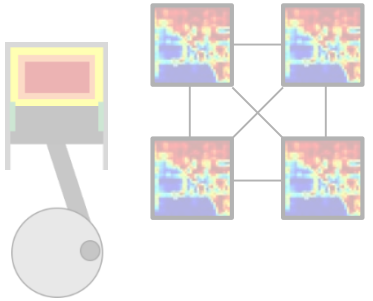
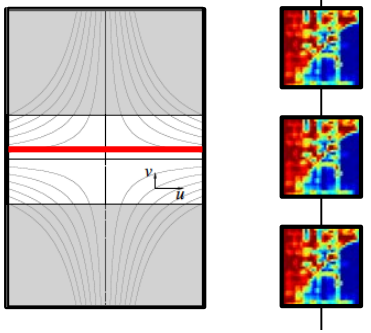




1D Flames



New since 2016 AMR

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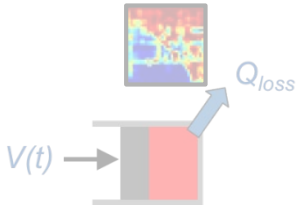

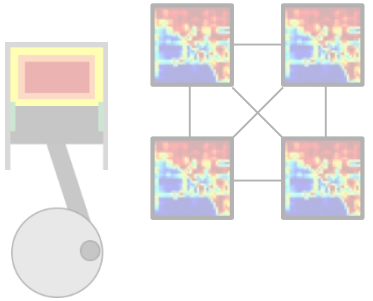

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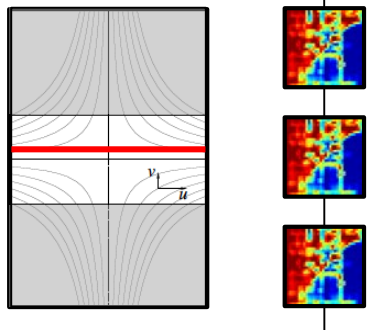
- Key simulations for the design and validation of detailed fuel chemistry
- Demonstrates adaptive preconditioners for multi-dimensional applications

1D Flames



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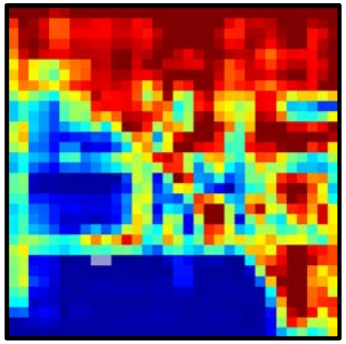

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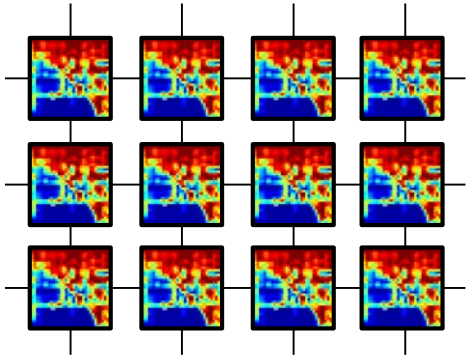
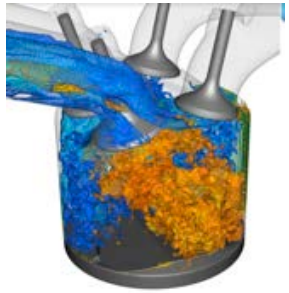
63 species

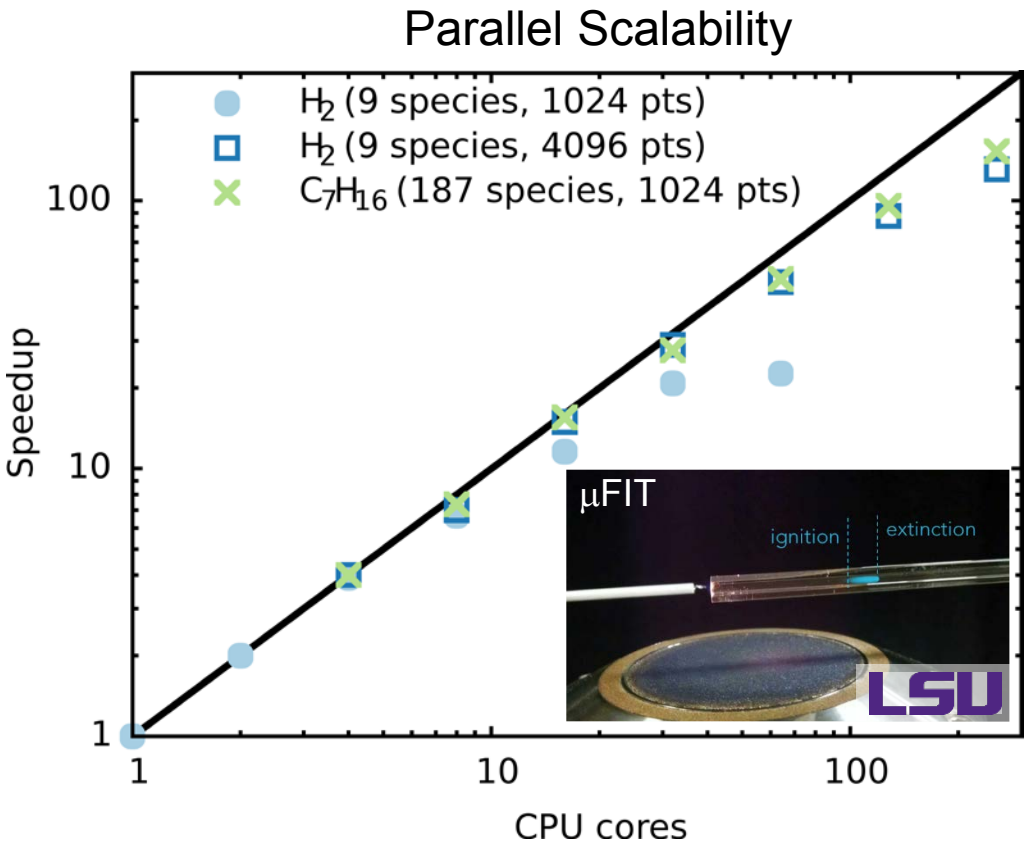
Detailed Fully-Coupled CFD





Flame solver demonstrates adaptive preconditioner approach accelerates coupled reaction-diffusion models

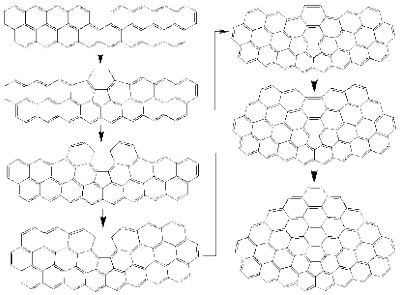
- 100x speedup possible on modest 128 CPU (8-node cluster)
- Time-resolved flame speed has similar wall clock time as steady solution from Chemkin-Pro
- Only turn-key option when steady solver fails, plus it avoids false equilibria
- Zero-RK's adaptive preconditioner produces a faster simulation without losing accuracy



Verified – with NGA DNS code & Chemkin-Pro

Validated – with μFIT data in S. Lapointe *et al.*, *US Natl Combust Mtg.*, 2017. (separate program)

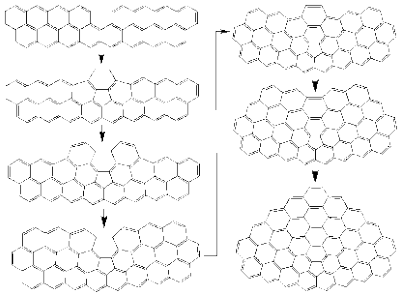
Remaining research* in FY17 accelerates soot models, mechanism validation, and simulation-led optimization



FY17 Q4 Milestone – Performance report on the implementation of the sectional method for soot formation in Zero-RK for realistic fuel surrogates (Mehl, LLNL)

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

Remaining research* in FY17 accelerates soot models, mechanism validation, and simulation-led optimization



FY17 Q4 Milestone – Performance report on the implementation of the sectional method for soot formation in Zero-RK for realistic fuel surrogates (Mehl, LLNL)

Complete parallel, multi-strategy, steady-state solver for jet-stirred reactor and flame speed validation cases using Sundials library

from LLNL

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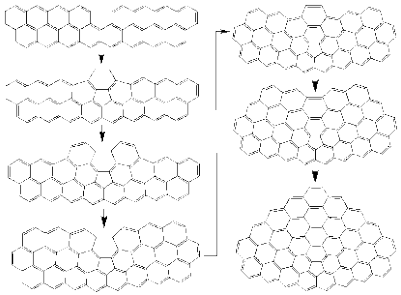
Remaining research* in FY17 accelerates soot models, mechanism validation, and simulation-led optimization



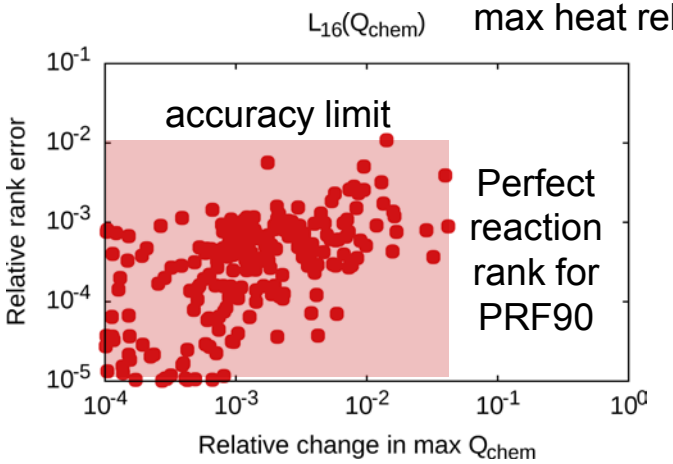
FY17 Q4 Milestone – Performance report on the implementation of the sectional method for soot formation in Zero-RK for realistic fuel surrogates (Mehl, LLNL)

Complete parallel, multi-strategy, steady-state solver for jet-stirred reactor and flame speed validation cases using Sundials library

from LLNL

Ex. Integral approximation to max heat release rate

$$L_n(f) = \left(\frac{1}{b-a} \int_a^b |f(t)|^n \, dt \right)^{1/n}$$

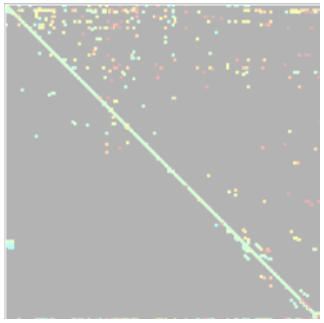


Complete adjoint sensitivity extension to Zero-RK for rapid reaction rate screening

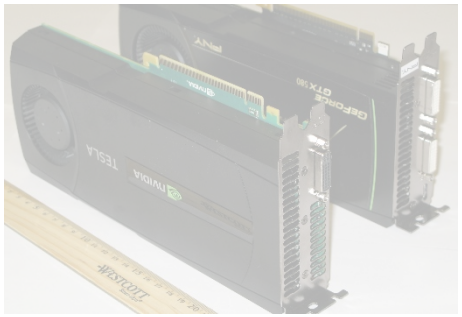
- sensitivity of integrated outputs of the kinetic simulations can be solved order(s) of magnitude faster than brute force perturbation

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

Outline for accomplishments

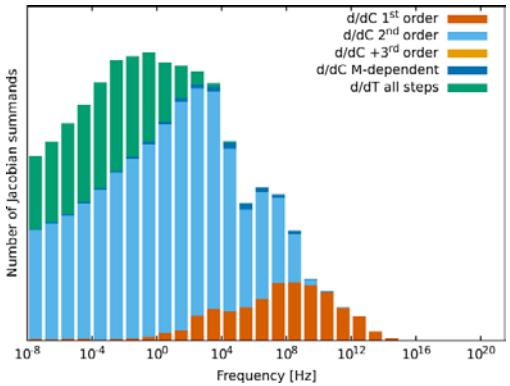


1. Better algorithms and applied mathematics
   – same solution only faster



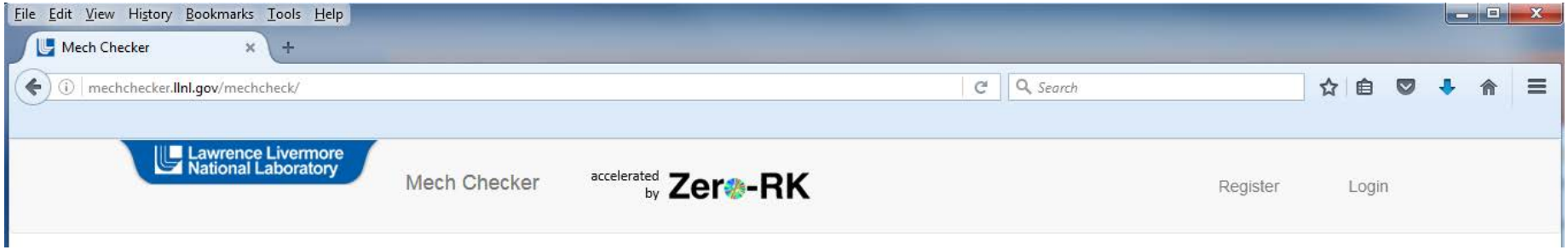
2. New computing architecture
   – more flops per second, per dollar, per watt

Accomplishments discussed in more detail in Whitesides' presentation (ACS012)



3. Improved physical models
   – more accuracy, better error control

LLNL developed a web-based software platform for the two main mechanism debugging tools



Thermodynamic Repair Utility:

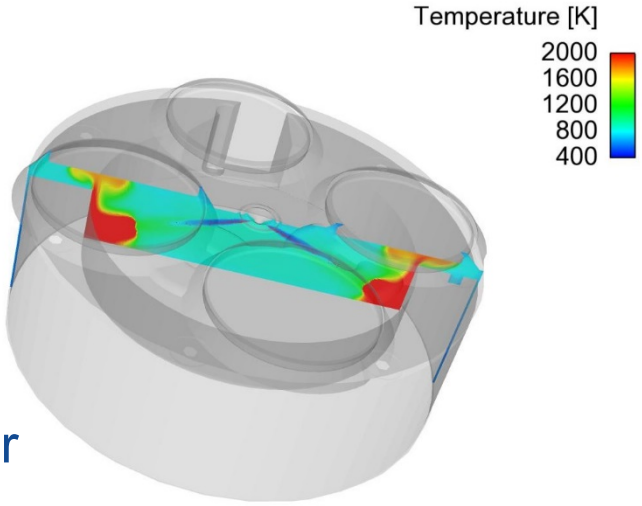
- Refits specific heat, enthalpy and entropy to maintain C_0 & C_1 continuity
- Minimizes changes to original thermodynamics over user-specified temperature range
- Flags non-monotonic species for human review

Ignition Delay Diagnostic:

- Reports integrator performance: time step distribution, negative species, Jacobian timescales & zero-crossings
- Flags mechanism connectivity errors
- Flags and limits (optional) non-physical reaction rates

New web tool quickly uncovers errors affecting the performance of VTO simulations

3299 species bio-diesel mechanism used to simulate methyl decanoate experiments in SNL's SCORE single cylinder diesel engine (C. Mueller)



- Simulation proceeded very slowly compared to previous mechanism and unexpectedly crashed
- IDT web tool allows easy investigation into solver issues:
  - Flagged unimolecular reaction rate at 1.24×10^{20} Hz for the reverse rate $C_2H_5COCH_3 + H = sC_4H_9O$
  - This reverse rate is calculated from the forward rate and equilibrium constant

$$k_{\mathrm{rev}} = k_{\mathrm{fwd}} / K_{\mathrm{eq}}$$

  - Equilibrium constant is calculated using thermodynamic data (entropy and enthalpy)

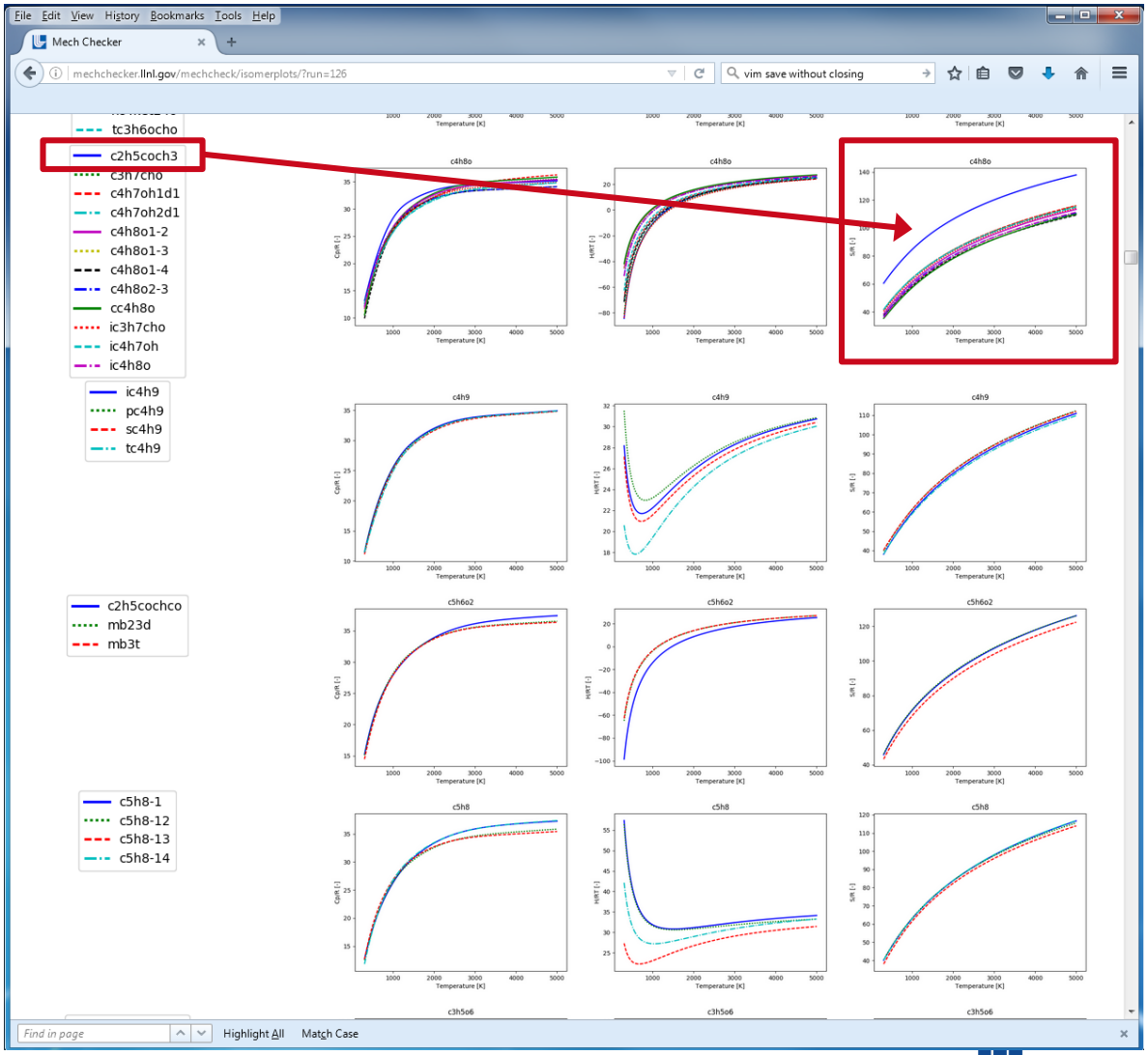
$$K_{\mathrm{eq}} = \left(\frac{p^{\circ}}{R_u T}\right)^{\Delta n} \exp\left(\frac{\Delta S^{\circ}}{R_u} - \frac{\Delta H^{\circ}}{R_u T}\right)$$

Plots from web tool indicate a large discrepancy in the entropy for $C_2H_5COCH_3$ compared to isomers

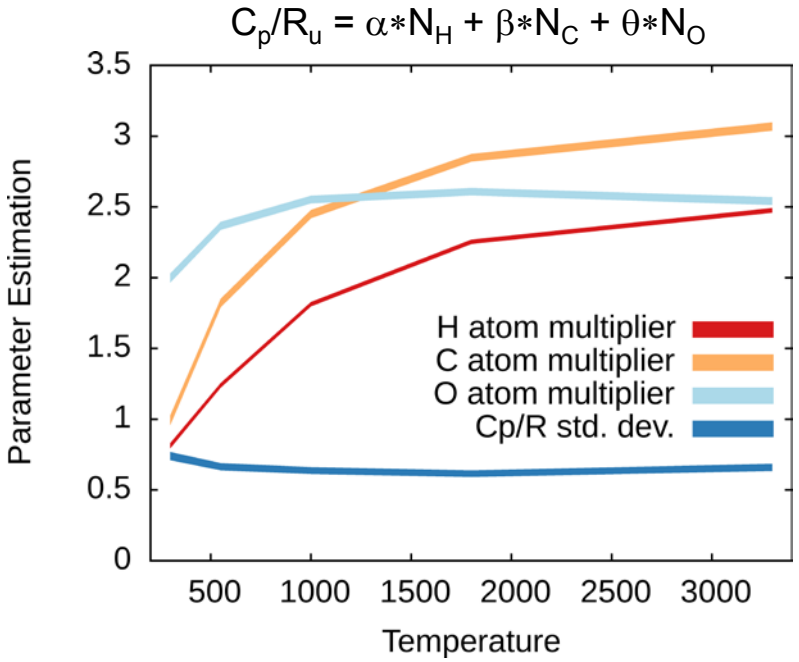
The webtool allows quickly organizes potential errors in large mechanisms difficult for a human to dissect

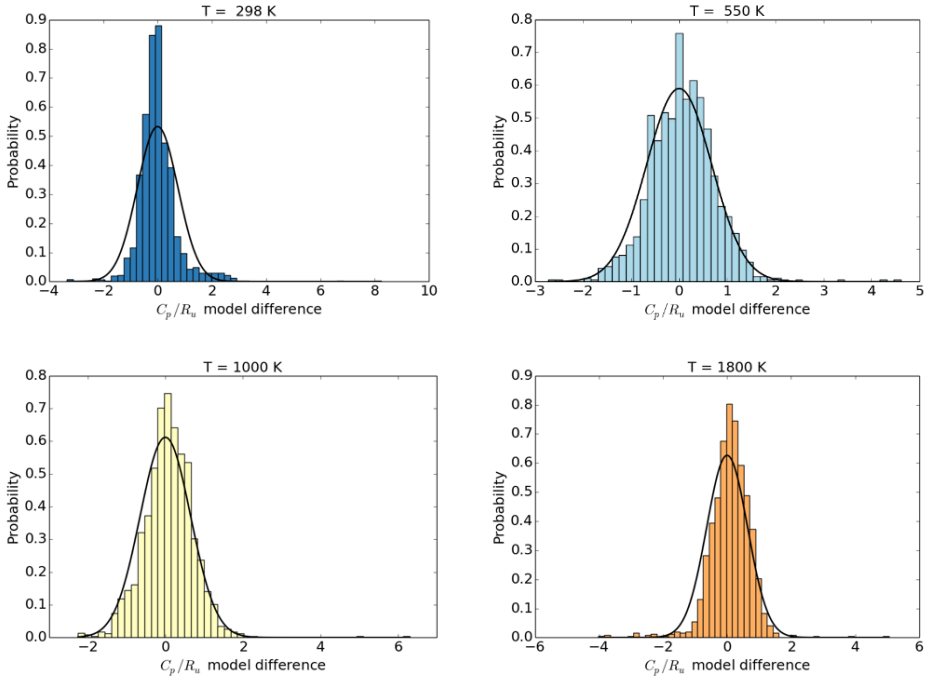
Ongoing work for FY17:

- Develop external version compliant with LLNL cybersecurity
- Increase the number of correction options
- Propose corrections for rapid human review with tracked change log

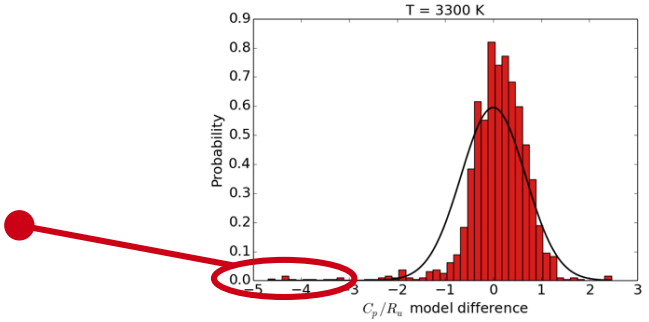


Statistical anomaly detection methods developed to guide mechanism repair



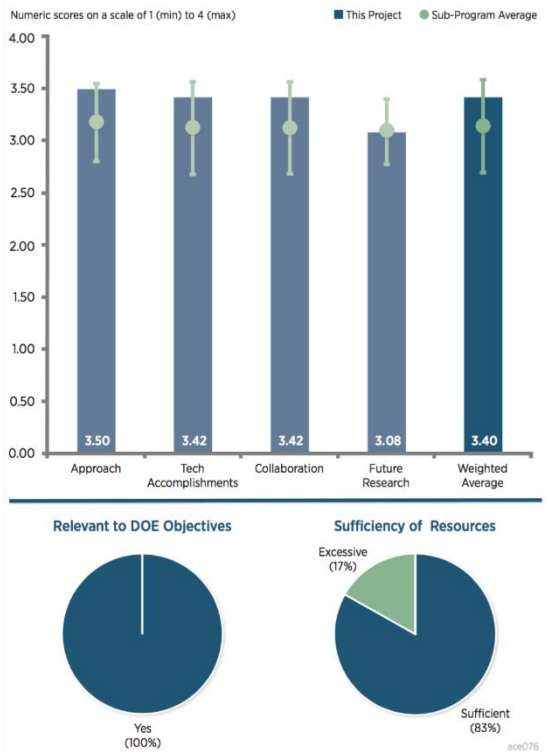


- Estimate the probability an outlier is anomalous in new mechanisms
- Rank and organize high probability anomalies for human review



Response to AMR16 reviewers comments

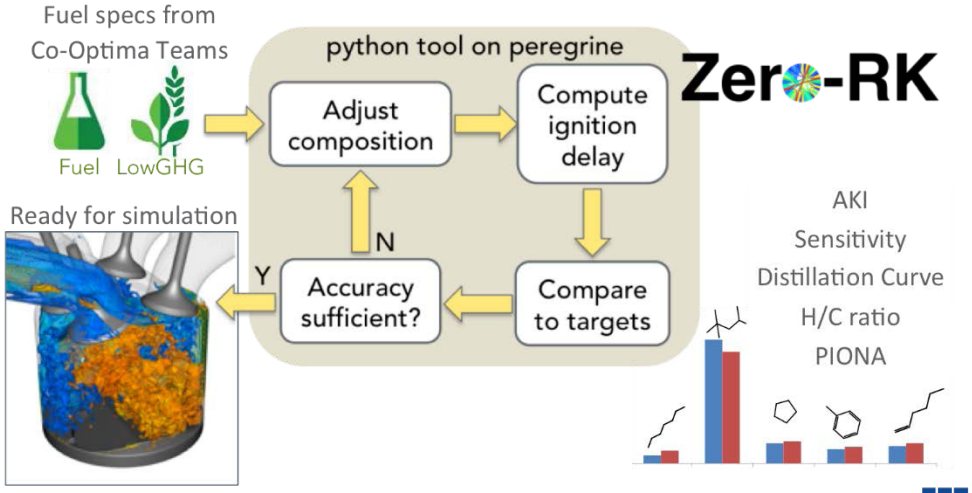
AMR16 comments were generally positive (3.50/4 overall) with the reviewers posing the following questions and making some key suggestions:



1. What is the relevance of the homogenous reactor models and flame models shown to engine research?
2. How accurate is the model for multi-component fuels? for heterogeneous reactors? How is it validated?
3. What is the rationale behind the choice of fuels studied? the surrogate components included in the mechanisms?
4. A multi-code strategy is recommended in the future to ensure the greatest impact on the industry.

Collaborations include engagement with industry, national laboratories, and universities

- **Industry:** Convergent Sciences Inc. (licensee of solvers), GM (testing Zero-RK in ConvergeCFD on Titan Supercomputer), NVIDIA (new matrix library help), and solvers used by CRC and FACE working group participants
- **Academia:** LSU (funded - μFIT & LLNL sabbatical visit), PSU (unfunded - chemistry solver consultation), Caltech (unfunded - hosted by turbulent-combustion group); and WVU (presently unfunded - molecular dynamics soot pathway discovery)
- **National Laboratories:** leading the Simulation Toolkit Team in Co-Optima program (see FT052); coordinating Co-Optima simulation efforts between ANL, LLNL, NREL, ORNL, and SNL; and sharing Zero-RK tools on Peregrine cluster:



Remaining challenges and barriers to Advanced Combustion Systems research

The following areas are challenges facing the creation of a truly predictive simulation tool for use in the engine design community:

- Robust detailed mechanism usage in engine CFD
  - more automated mechanism debugging tools
  - greater user control of chemistry errors
- Reduced computational cost for multispecies transport in engine CFD
- More accurate coupling between chemistry and transport models
- Detailed (predictive) spray dynamics with reduced computational cost
- More development for future engine simulations including massively parallel, non-uniform architectures
- Understanding incipient soot reaction pathways
- Understanding nonlinear fuel component interactions

Future Work: LLNL will continue to explore strategies to increase speed and accuracy

Ongoing ACS076

FY17 – Q4 Milestone report on Zero-RK's performance using more sophisticated soot formation with detailed kinetics for real transportation fuels

FY17 – Deploy public web tools to help inspect and repair detailed chemistry mechanisms

FY17 – Complete adjoint sensitivity and steady-state solver extensions for Zero-RK

Proposed supports multiple VTO R&D efforts

FY18-20 – Accelerate new soot model algorithms

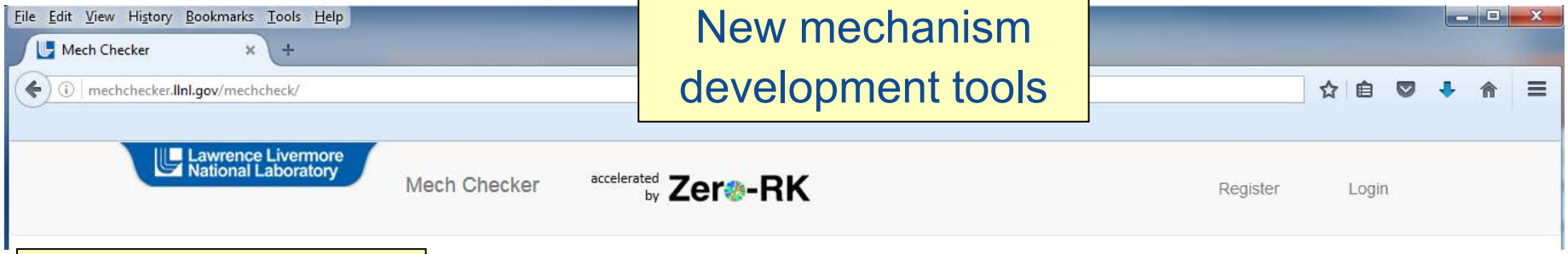
FY18-20 – Couple chemistry-turbulence models with detailed kinetic mechanisms for transportation fuels

FY18-20 – Accelerate detailed spray dynamics algorithms

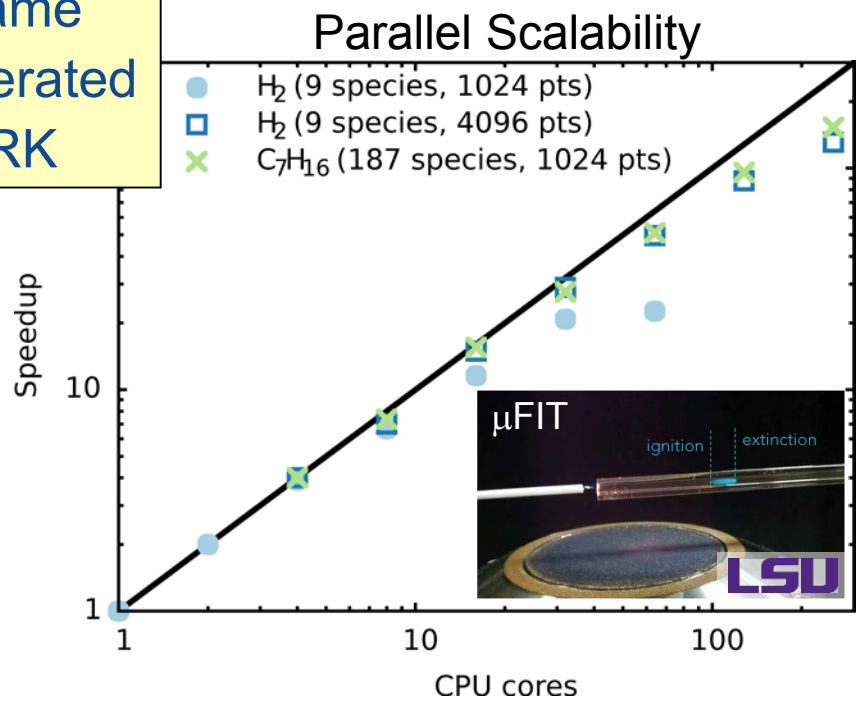
**Any proposed future work is subject to change based on funding levels.*

Summary: LLNL's research increases the speed, accuracy, and impact of the larger R&D effort in VTO and beyond

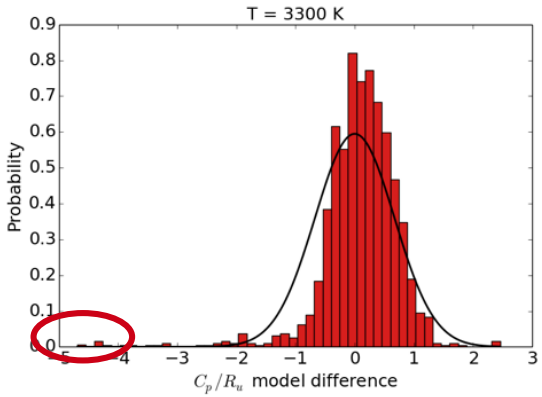
New mechanism development tools



Parallel flame solver accelerated by Zero-RK

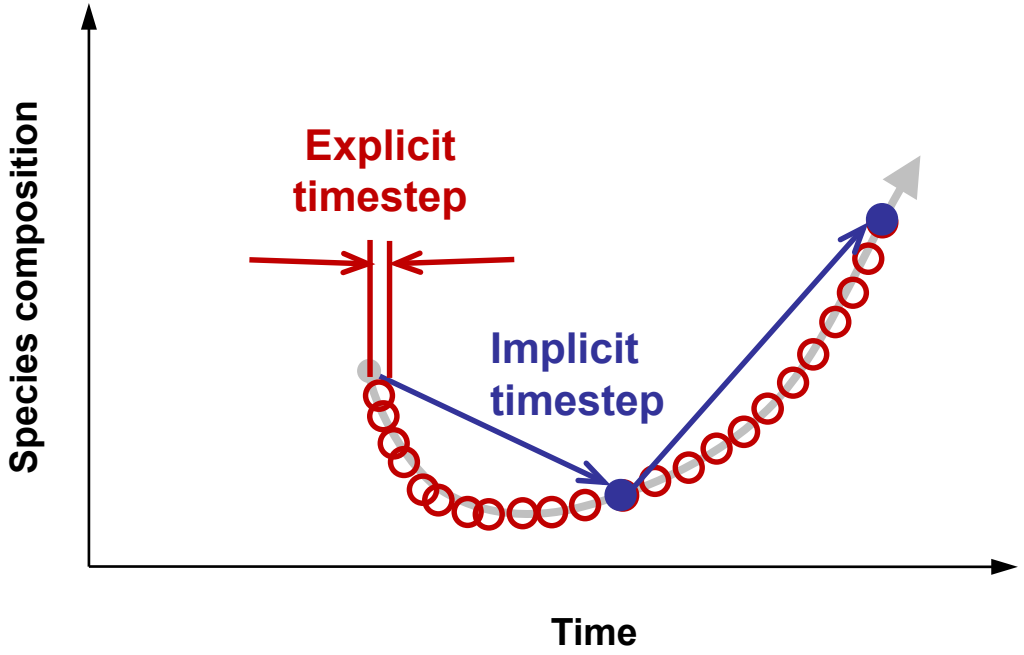


Anomaly detection to rank & organize for human review



Technical Back-Up Slides (limit 5)

Implicit methods are necessary to integrate the chemical time scales over an engine cycle



Explicit Update
(lower cpu/step)

$$\frac{\partial x_1}{\partial t} = f_1(t, x_1, \ldots, x_N)$$
$$\frac{\partial x_2}{\partial t} = f_2(t, x_1, \ldots, x_N)$$
$$\vdots$$
$$\frac{\partial x_N}{\partial t} = f_N(t, x_1, \ldots, x_N).$$

Implicit Update
(more trajectory data)

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

During ignition:

Δt (explicit) = 10^{-12} to 10^{-15} s

Δt (implicit) = 10^{-6} to 10^{-8} s

What is the physical meaning of the Jacobian?

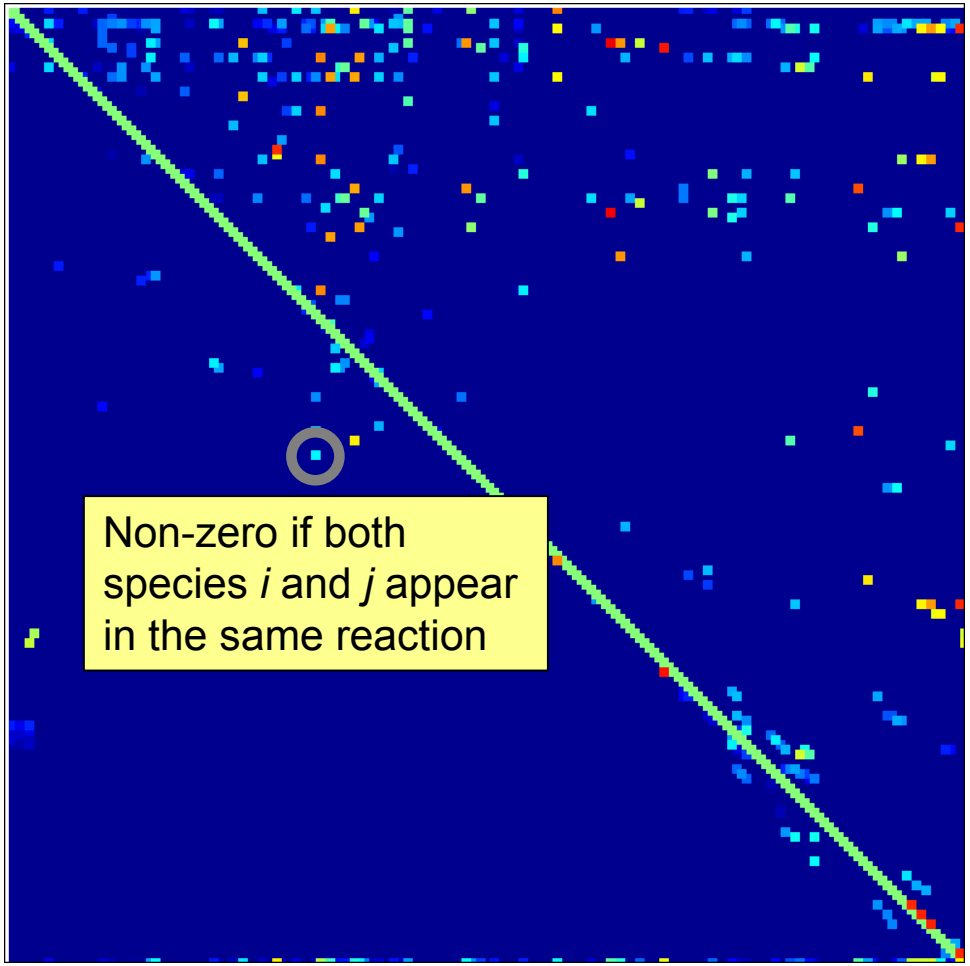
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

Element: $J_{i,j} = \frac{dw_i}{dC_j}, \quad w_i = \frac{dC_i}{dt}$

Magnitude represents the characteristic frequency at which the two species are coupled

10^{-4} 10^{0} 10^{4}

Matrix element magnitude (relative to diagonal)



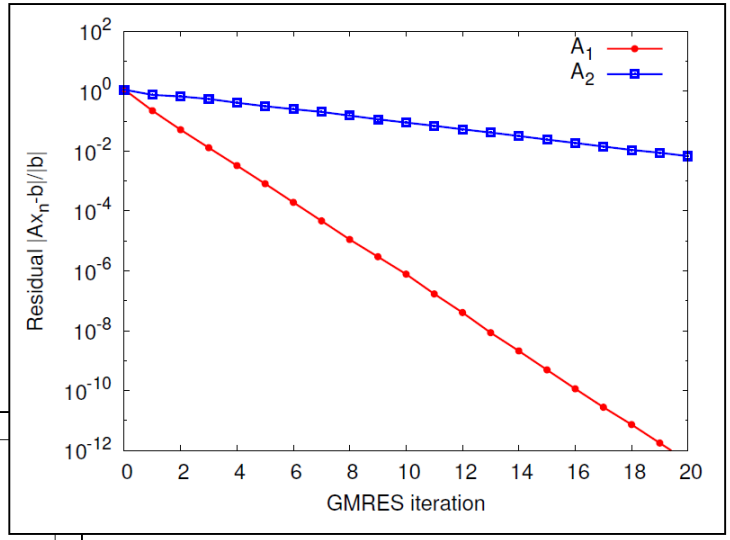
Approximate Jacobians can be used to precondition iterative linear system solvers like GMRES

Generalized **M**inimal **RES**iduals

$$E^{(n)} = \frac{\|Ax^{(n)} - b\|_2}{\|b\|_2} \leq \Lambda^n \mathrm{cond}(V)$$

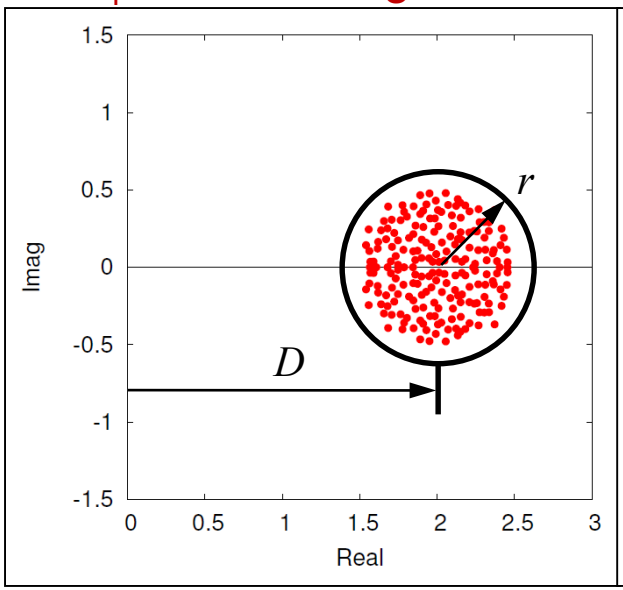
$$\Lambda \approx \frac{r}{D}$$

GMRES Error

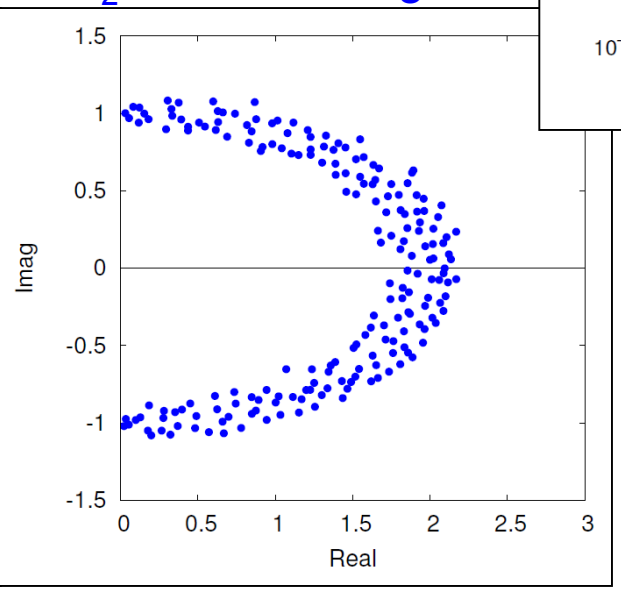


Eigenvalue Spectra (200 x 200)

A_1: fast convergence



A_2: slow convergence

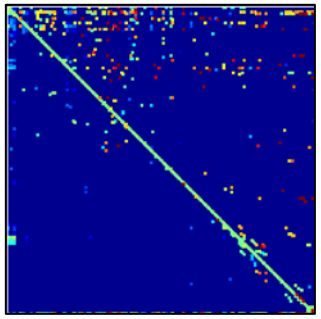


Adaptive preconditioner using on-the-fly reduction produces the same solution significantly faster

Our solver provides reduced mechanism speed without any loss of accuracy

Two approaches to faster chemistry solutions

Ex. iso-octane
874 species
3796 reactions



Jacobian Matrix
(species coupling freq.)

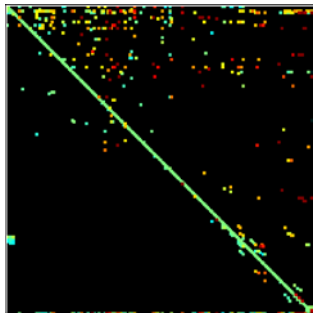
slower ⟷ faster

1. Classic mechanism reduction:

Ex.197 species 

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

2. LLNL's adaptive preconditioner:



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

Filter out 50-75% of the least important reactions