Lawrence Livermore National Laboratory

Improved Solvers for Advanced Engine Combustion Simulation

M. J. McNenly (PI), S. M. Aceves, N. J. Killingsworth,
G. Petitpas and R. A. Whitesides

Project ID # ACE076

2016 DOE Vehicle Technologies Program
Annual Merit Review and Peer Evaluation Meeting
June 5-9, 2016 - Washington, DC

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

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

Overview

Timeline

- Ongoing project with yearly direction from DOE
- FY17-FY20 program plan under review

Budget

- FY15 funding: $460K
- FY16 funding: $460K

Barriers

- Lack of fundamental knowledge of advanced engine combustion regimes
- Lack of modeling capability for combustion and emission control
- Lack of effective engine controls

Partners

- Cummins, GM, Convergent Sciences Inc. & NVIDIA
- ANL, LANL, NREL, SNL & ORNL
- LSU, PSU, Caltech & WVU
- AEC MOU, FACE working group, Combustion Inst., SAE, GPU Tech. Conf., and Co-Optima Program

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

Objective

Create faster and more accurate combustion solvers.

Accelerates R&D on three major challenges identified in the VT multi-year program plan:

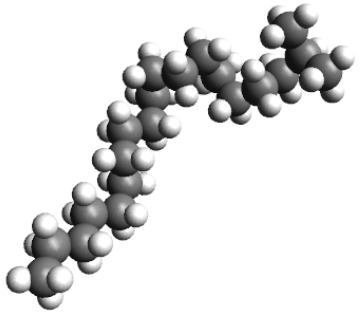
A. *Lack of fundamental knowledge of advanced engine combustion regimes*

C. *Lack of modeling capability for combustion and emission control*

D. *Lack of effective engine controls*

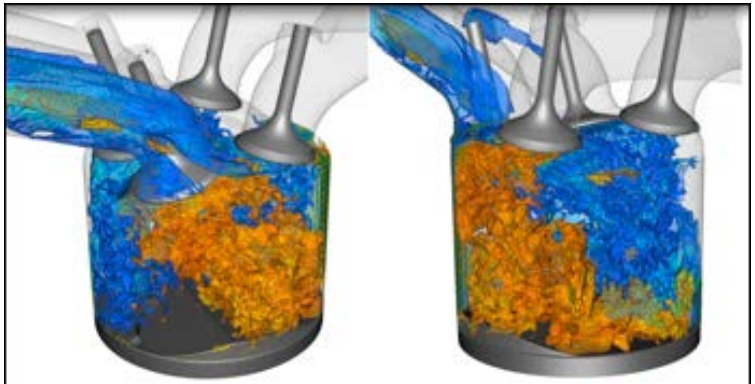
We wanted to use…

Detailed chemistry



Ex. Biodiesel component $C_{20}H_{42}$ (LLNL)
7.2K species
53K reaction steps

in highly resolved 3D simulations



Ex. SI/HCCI transition ~30M cells for Bosch in LLNL's hpc4energy incubator

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

Objective

Create faster and more accurate combustion solvers.

Accelerates R&D on three major challenges identified in the VT multi-year program plan:

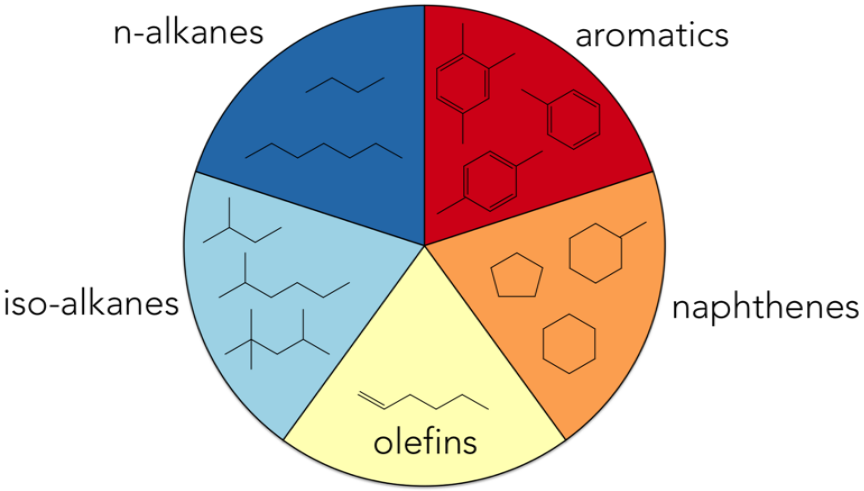
A. *Lack of fundamental knowledge of advanced engine combustion regimes*

C. *Lack of modeling capability for combustion and emission control*

D. *Lack of effective engine controls*

Now we want to use…

Detailed chemistry



Ex. 12-component gasoline surrogate (see Pitz, ACE013)

+2.7K species

+22K reactions, including

+11K soot reactions

in highly resolved 3D simulations

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

Objective

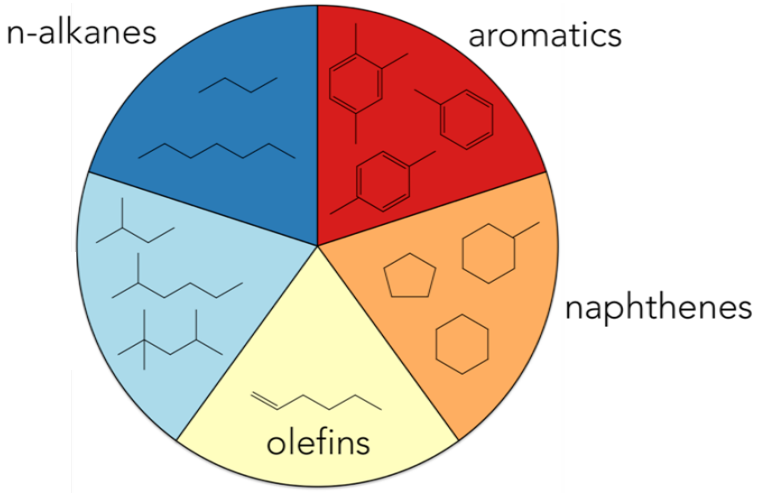
Create faster and more accurate combustion solvers.

AMR16 achievements:

- Zero-RK won a 2015 R&D100 award - LLNL's fast chemistry solver library
- Added capability to capture more complex pressure dependent reactions in Zero-RK
- Added detailed soot modeling capability in Zero-RK
- Added new reaction forms to decouple reaction order from stoichiometry for global or phenomenological models
- Created deeper tests for the ignition diagnostic and mechanism debugging tool

Now we want to use…

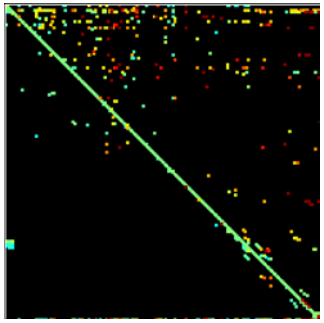
Detailed chemistry



Ex. 12-component gasoline surrogate (see Pitz, ACE013)

+2.7K species
+22K reactions, including
+11K soot reactions

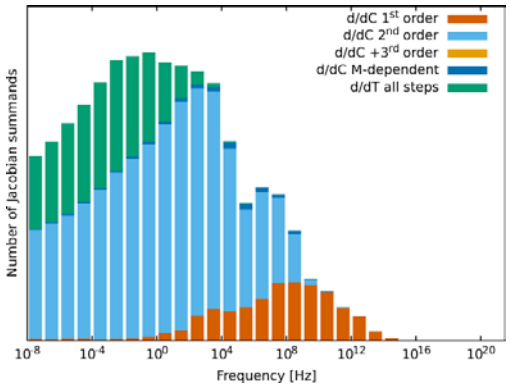
Approach – Accelerate research in advanced combustion regimes by developing faster and more predictive engine models



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 (ACE012)

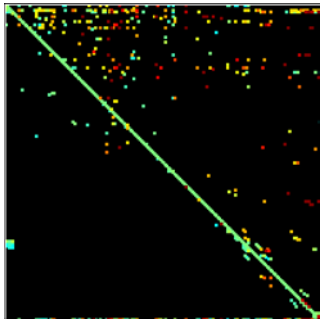


3. Improved physical models
   – more accuracy, better error control

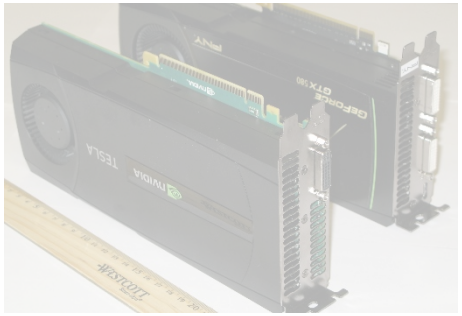
Approach – FY16 AOP milestones for all LLNL ACE projects

Due	Type	Milestones	Status
12/31/2015	reg.	Improved iso-cetane mechanism	complete
3/31/2016	reg.	Evaluate research progress and impact	complete
3/31/2016	Go/No-Go	Pursue higher-accuracy CRC AVFL 18a diesel surrogate with more than 9-components? *No-Go, the continued research of the 9-component surrogate palette (and smaller subsets) is expected to have a higher impact on the development of improved diesel surrogate kinetic models in the next 1-2 years than work on the 13-component palette.*	complete
6/30/2015	reg.	[Specific for ACE076] Create a technical report on mechanism repair and user guide for the LLNL inspection and repair utility.	on schedule
9/30/2015	reg.	Evaluate different load-balancing schemes for chemical kinetics in parallel CFD simulations and implement most promising technique.	on schedule

Accomplishment Outline

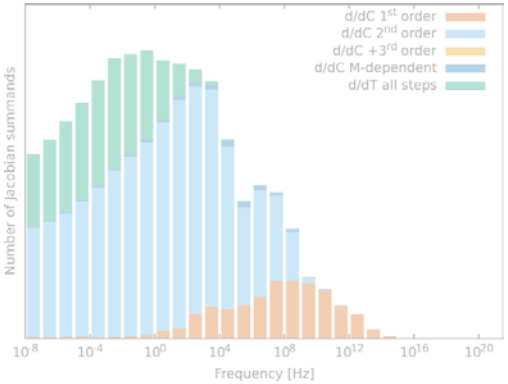


1. Better algorithms and applied mathematics
   – same solution only faster



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

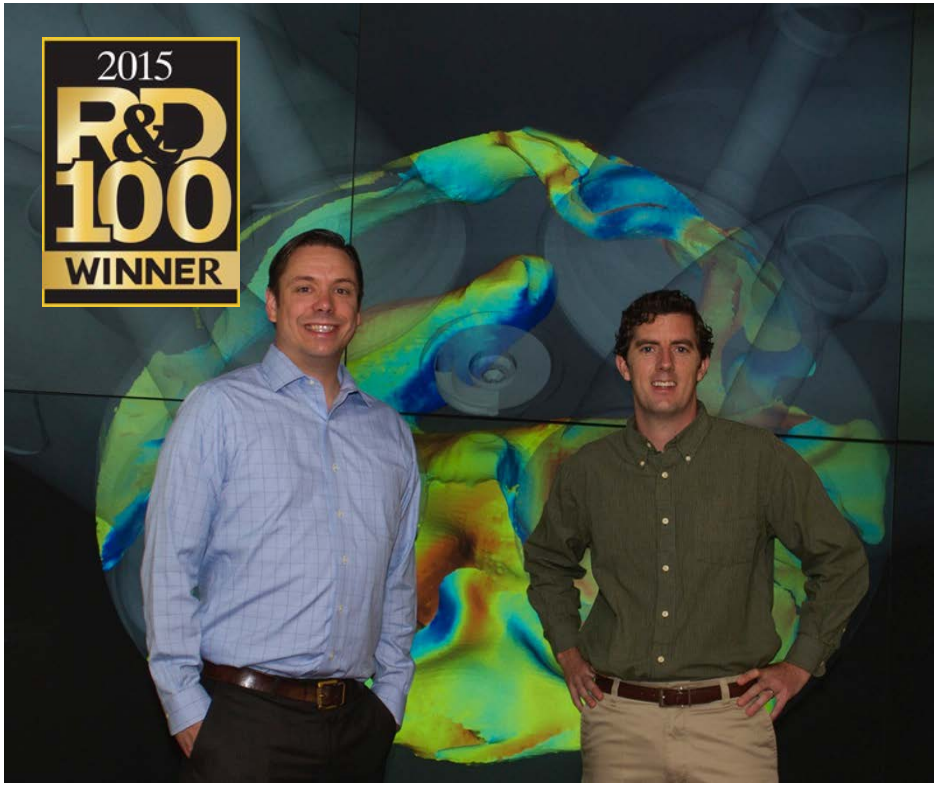
Accomplishments discussed in more detail in Whitesides' presentation (ACE012)

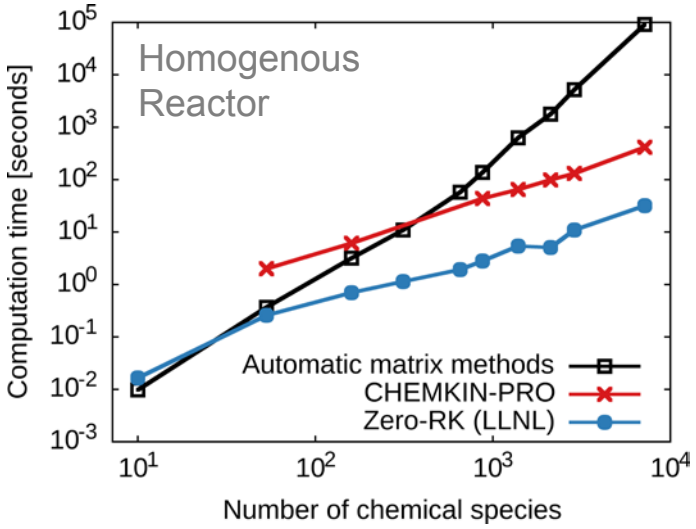


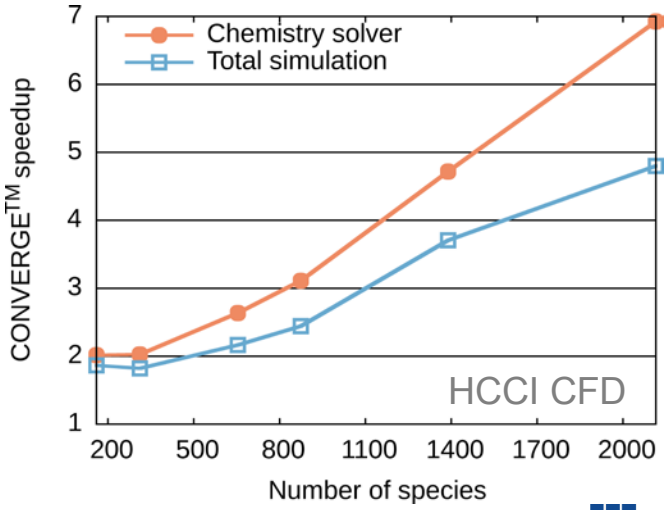
3. Improved physical models
   – more accuracy, better error control

AMR16 Accomplishment: LLNL's Zero-RK chemistry software earns a 2015 R&D 100 award in the software & services category

Zero-RK







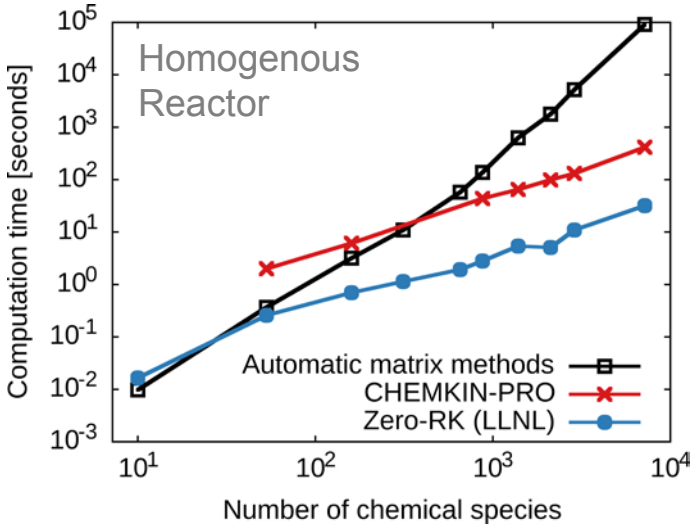
Approach: Extend the high performance chemistry solvers to more applications impacting the ACE R&D workflow

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

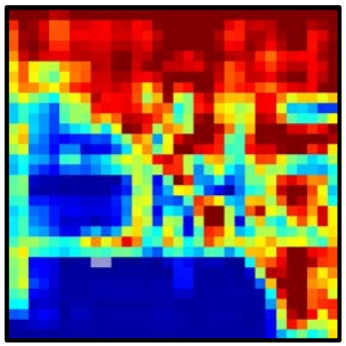
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

Slow/No reaction coupling

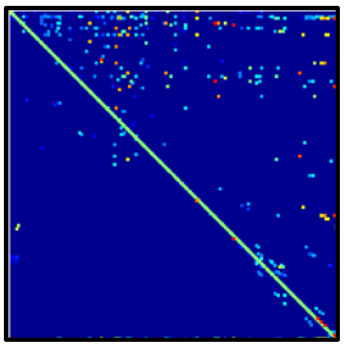
Fast reaction coupling



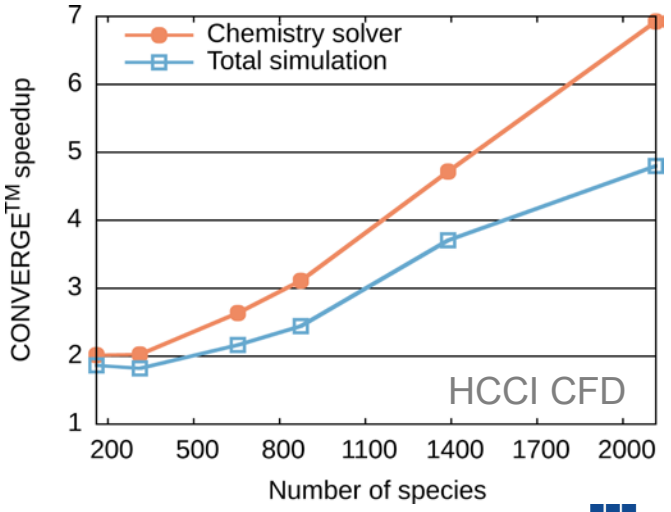
$J =$



Reduced *i*-C_8H_{18}
63 species

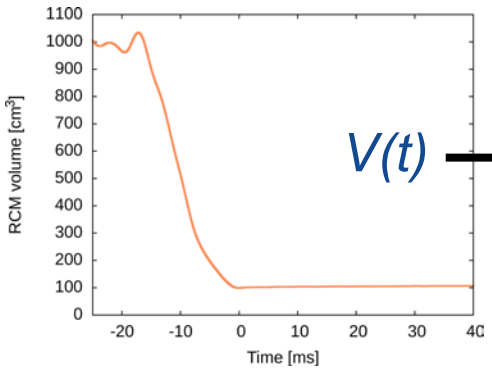


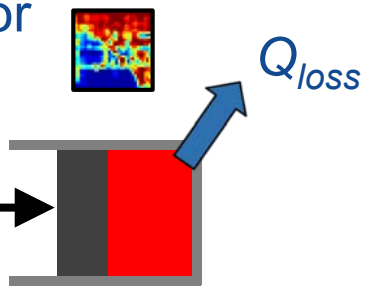
Detailed *i*-C_8H_{18}
874 species



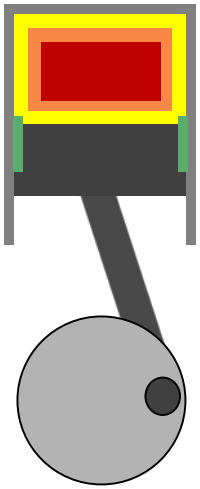
Approach: Create a flexible framework for the reactor Jacobians to easily build many applications on LLNL's chemistry algorithms

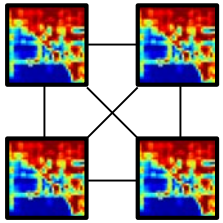
Variable Volume Reactor



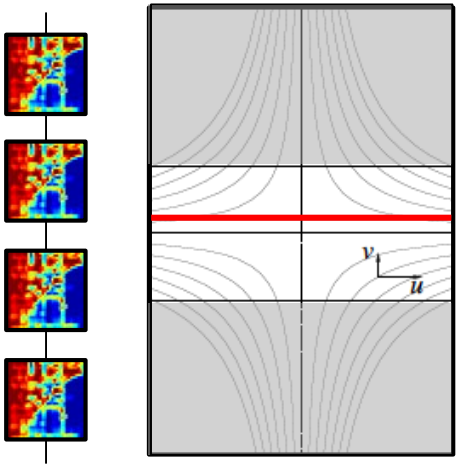


Quasi-Dimensional Multizone

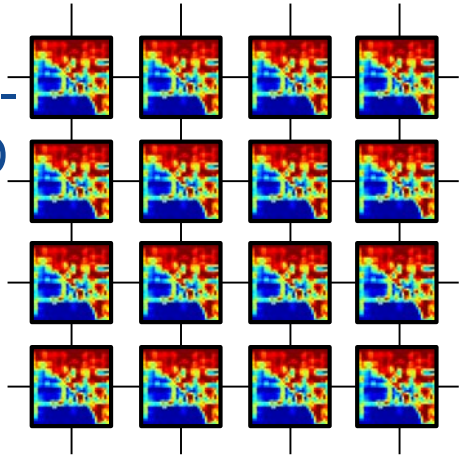


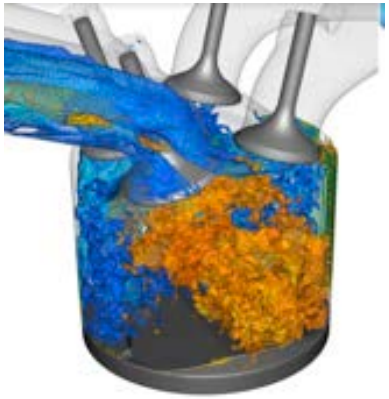


1D Flame Models



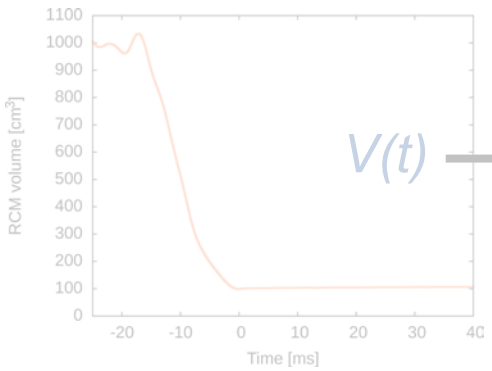
Detailed Fully-Coupled CFD



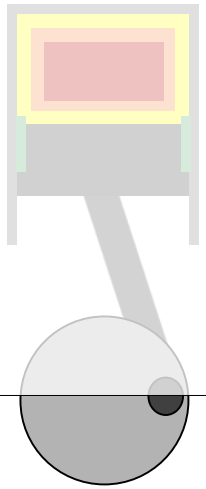


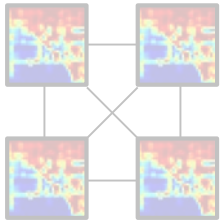
Approach: Create a flexible framework for the reactor Jacobians to easily build many applications on LLNL's chemistry algorithms

Variable Volume Reactor



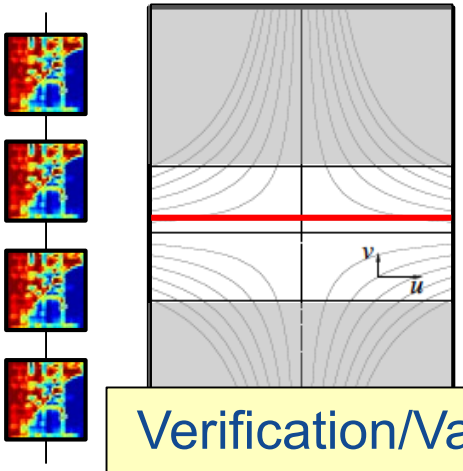
Quasi-Dimensional Multizone





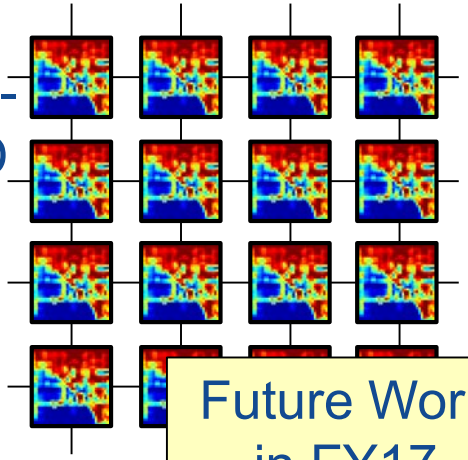
AMR 2015 Accomplishments

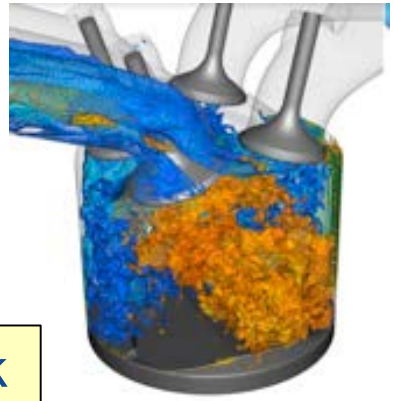
1D Flame Models



Verification/Validation end of FY16

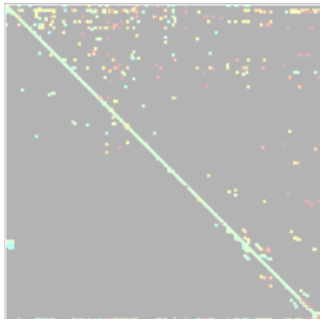
Detailed Fully-Coupled CFD



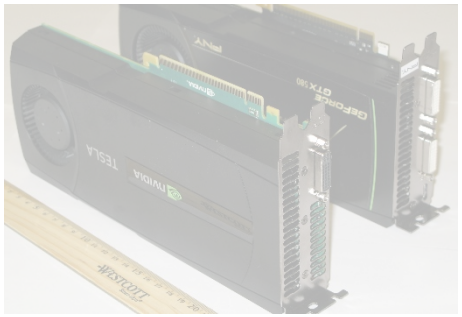


Future Work in FY17

Accomplishment Outline

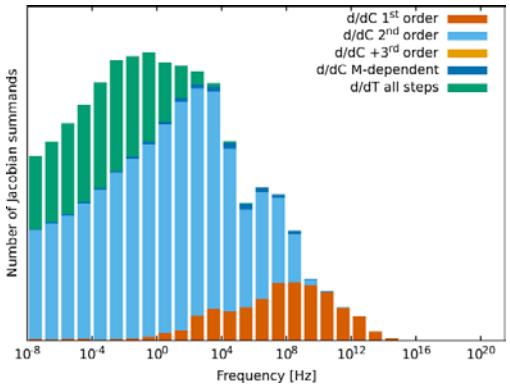


1. Better algorithms and applied mathematics
   – same solution only faster



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

Accomplishments discussed in more detail in Whitesides' presentation (ACE012)

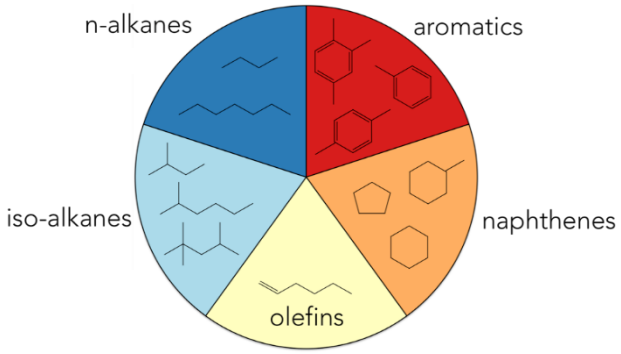


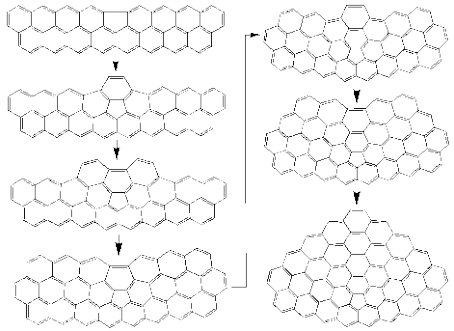
3. Improved physical models
   – more accuracy, better error control

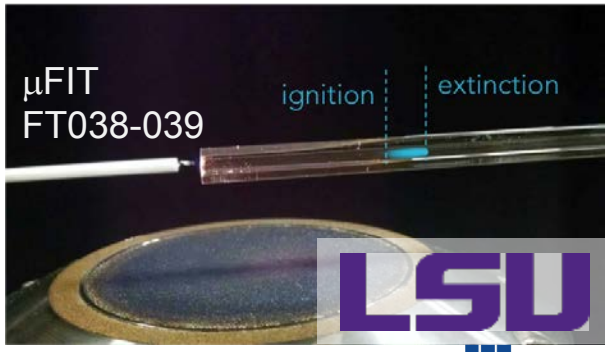
Relevance: Several DOE projects and AEC industry partners are demanding fast solvers for more accurate gasoline surrogates

Zero-RK must add the following updates to support user demands:

- more complex pressure dependent reaction rate tables
- fractional species
- large molecules (more than 999 atoms)
- decoupled reaction order & stoichiometry





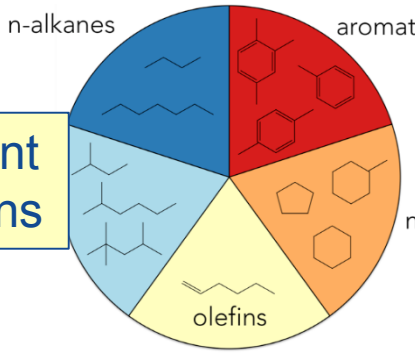


Relevance: Several DOE projects and AEC industry partners are demanding fast solvers for more accurate gasoline surrogates

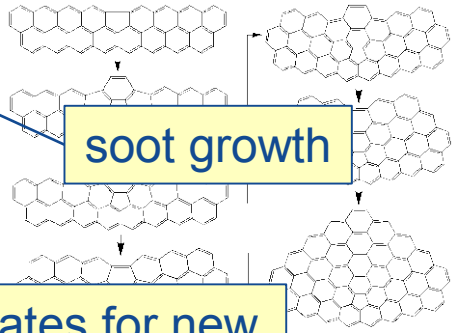
Zero-RK must add the following updates to support user demands:

- more complex pressure dependent reaction rate tables
- fractional species
- large molecules (more than 999 atoms)
- decoupled reaction order & stoichiometry

component interactions

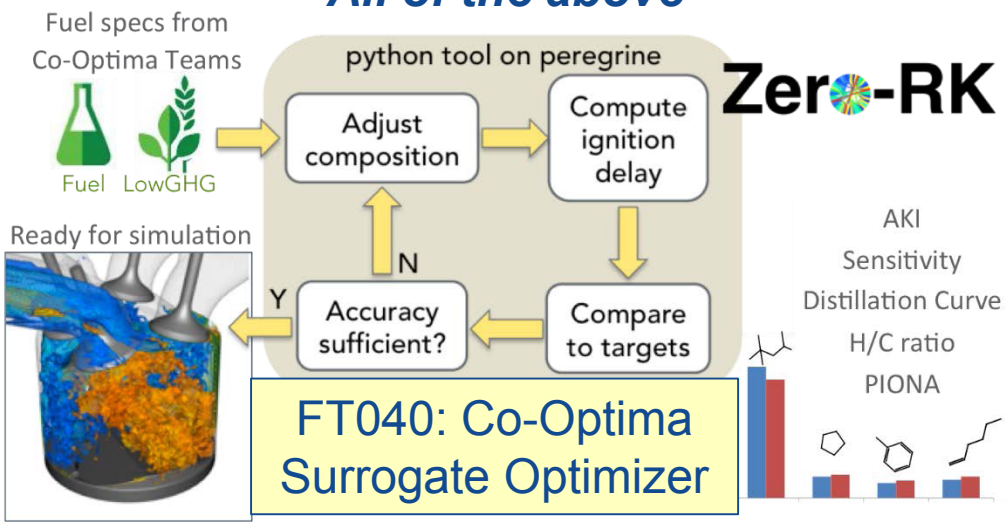


soot growth

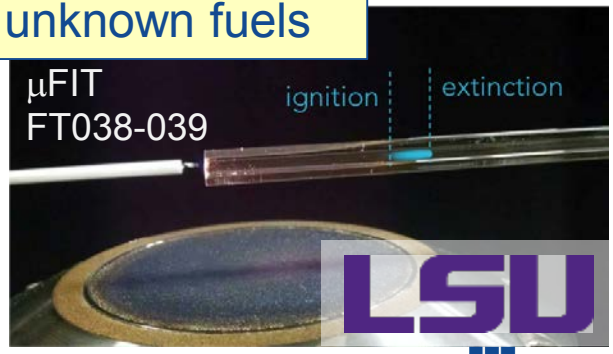


global rates for new or unknown fuels

All of the above



FT040: Co-Optima Surrogate Optimizer



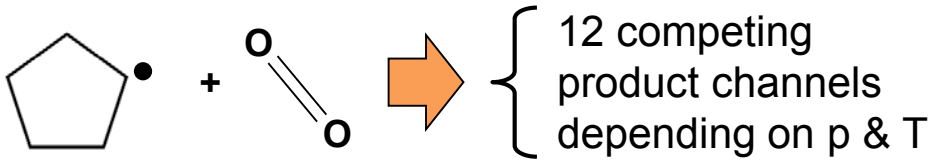
AMR16 Accomplishment: Enhanced Zero-RK capabilities for complex pressure dependent reaction rate tables

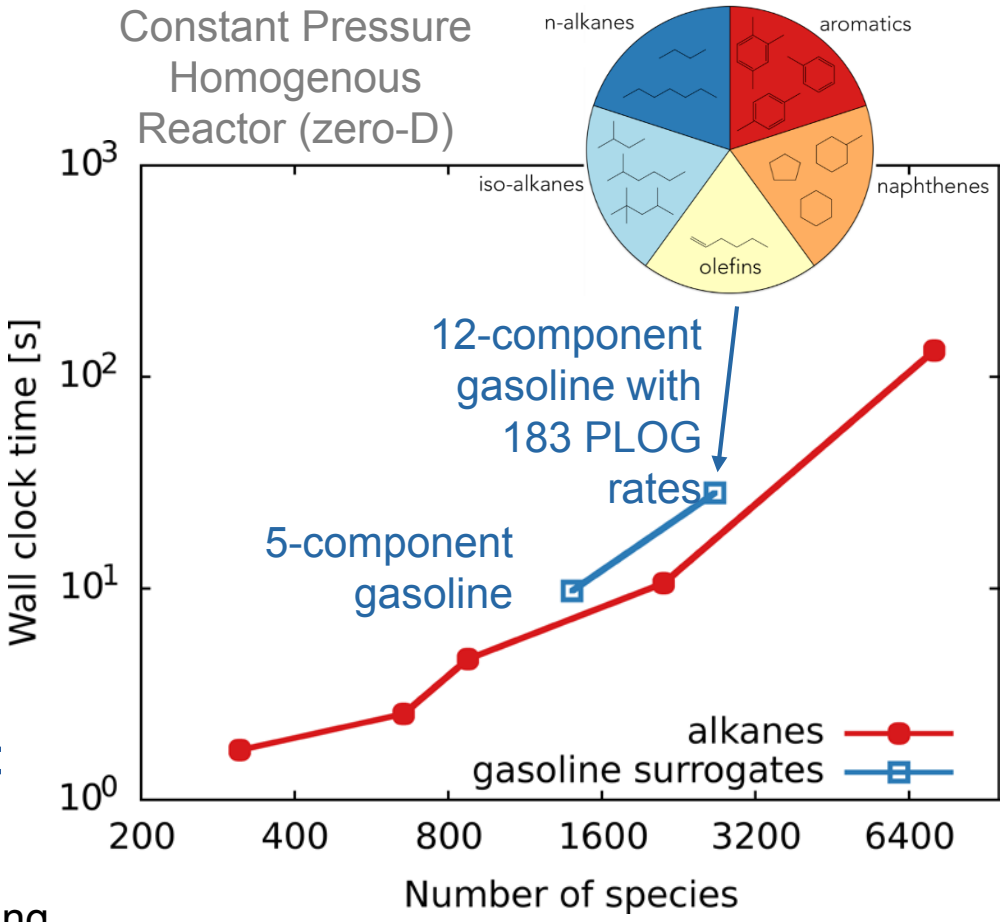
New tables using logarithmic pressure interpolations (PLOG) can handle:

- multiple additive Arrhenius functions
- unequal number of Arrhenius functions per pressure
- negative A-Factors

Complexity needed to resolve component interactions – especially toluene & cyclopentane:

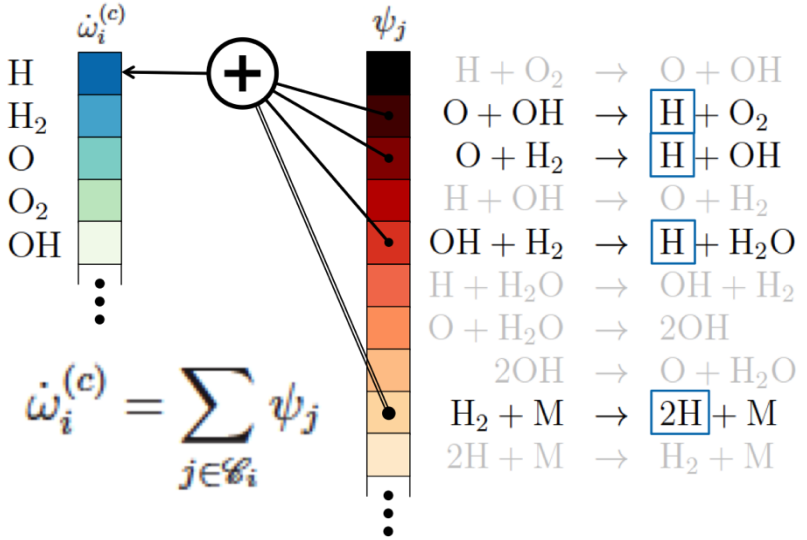
Ex.

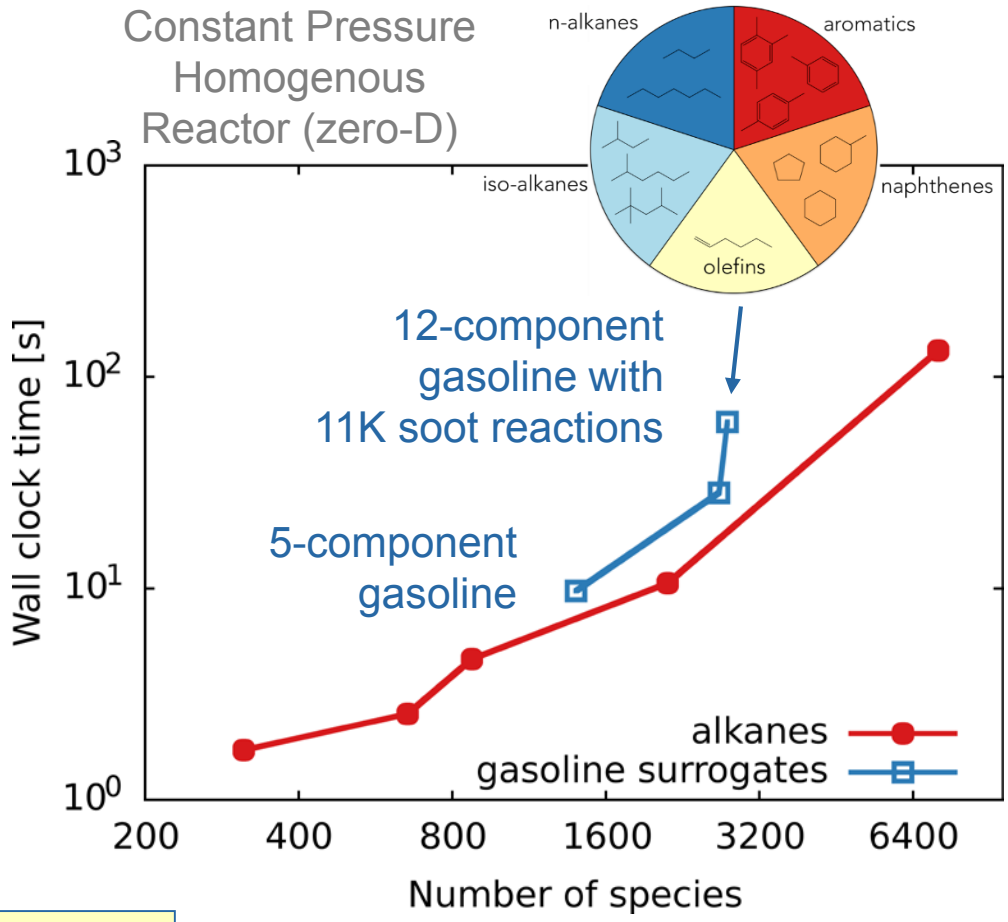




AMR16 Accomplishment: Enhanced Zero-RK capabilities for detailed soot mechanisms and phenomenological global rates

Upgrades challenging because they affect the sparse operator lists used to compute the reaction rates and Jacobian terms:





Implemented special non-integer stoichiometry classes to handle soot models without losing performance.

McNenly, *et al.*

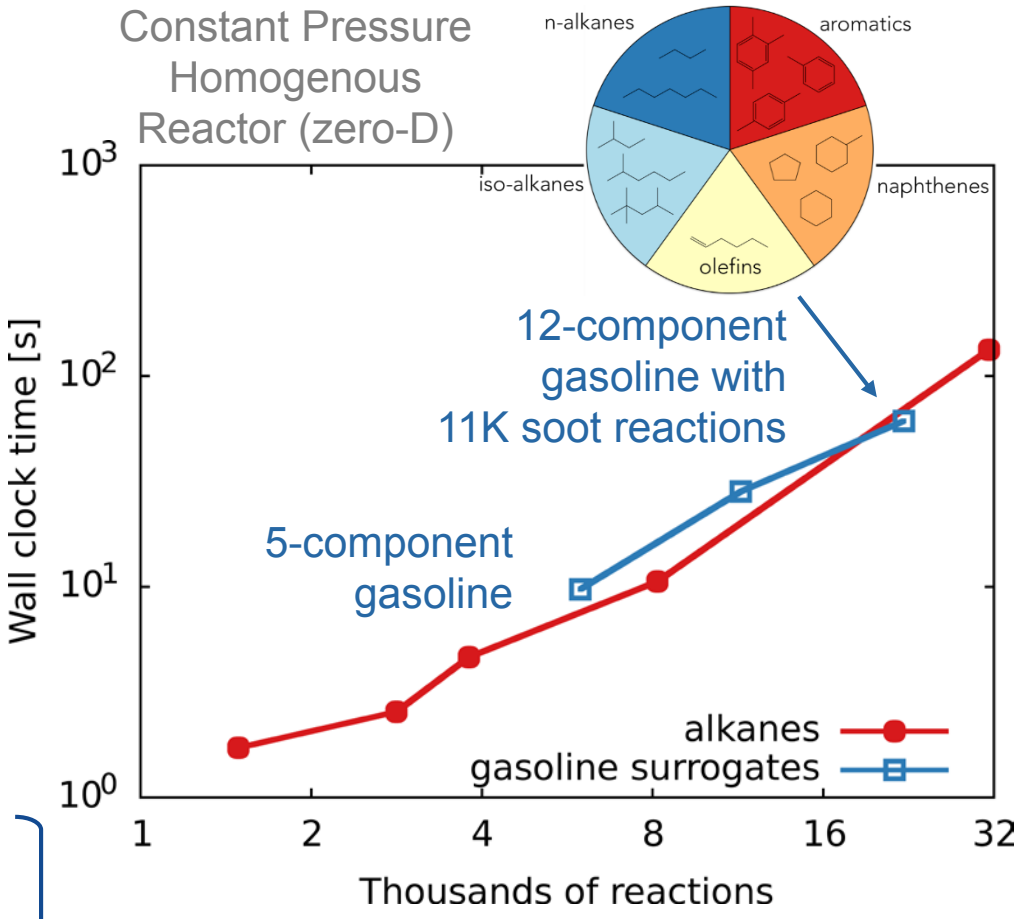
AMR16 Accomplishment: New features for complex and non-elementary reactions retain Zero-RK performance per reaction

Unit tests were created in the Google Test framework to identify errors quickly for the following:

- complex PLOG pressure dependencies
- non-integer stoichiometry reactions
- associated Jacobian terms

Future work:

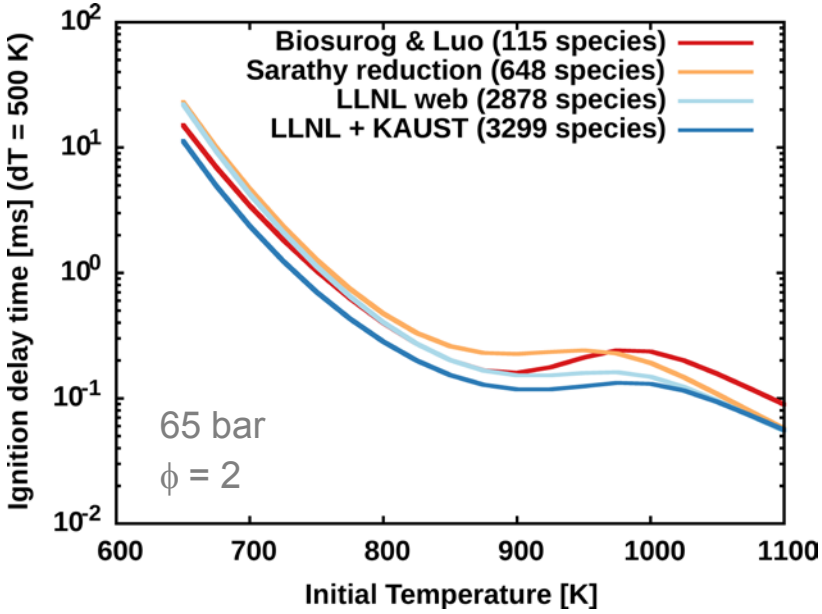
- include all reactions classes in the unit tests
- automated regression testing for all repo commits
- re-factor Zero-RK to have a more expandable & documented API



Whitesides (ACE012) applied for LLNL & DOE tech maturation funding to speed transfer to industry and software vendors.

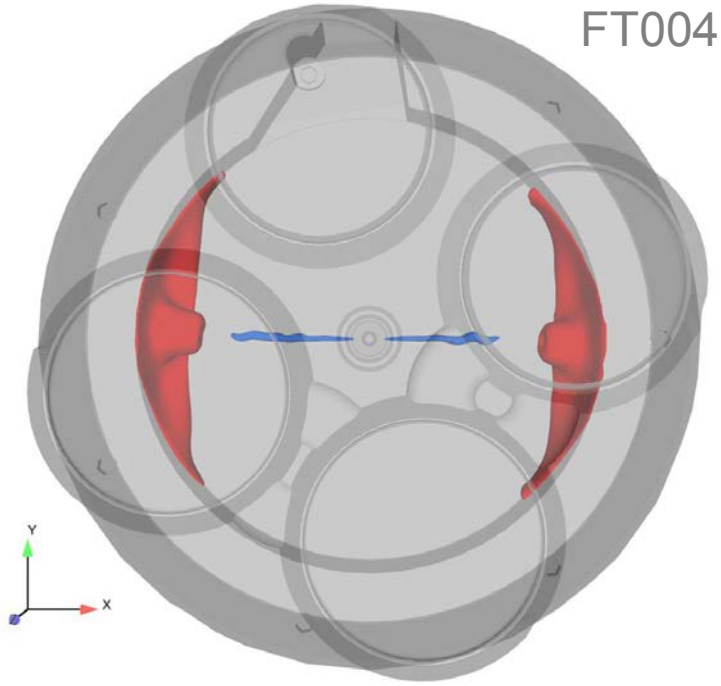
Challenge: Updated methyldecanoate mechanism crashes the diesel engine CFD simulations in the chemistry solver

CFD validation indicates a more reactive mechanism would have greater agreement:

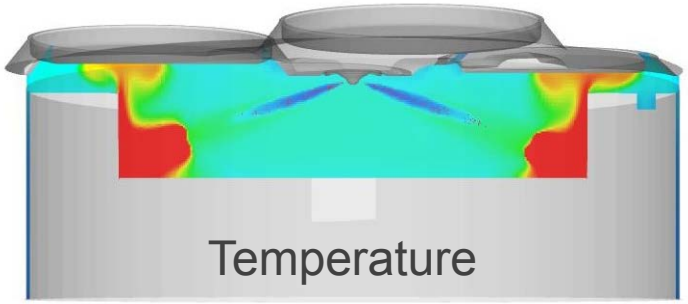


KAUST update to LLNL mechanism good candidate, but crashes during ignition!

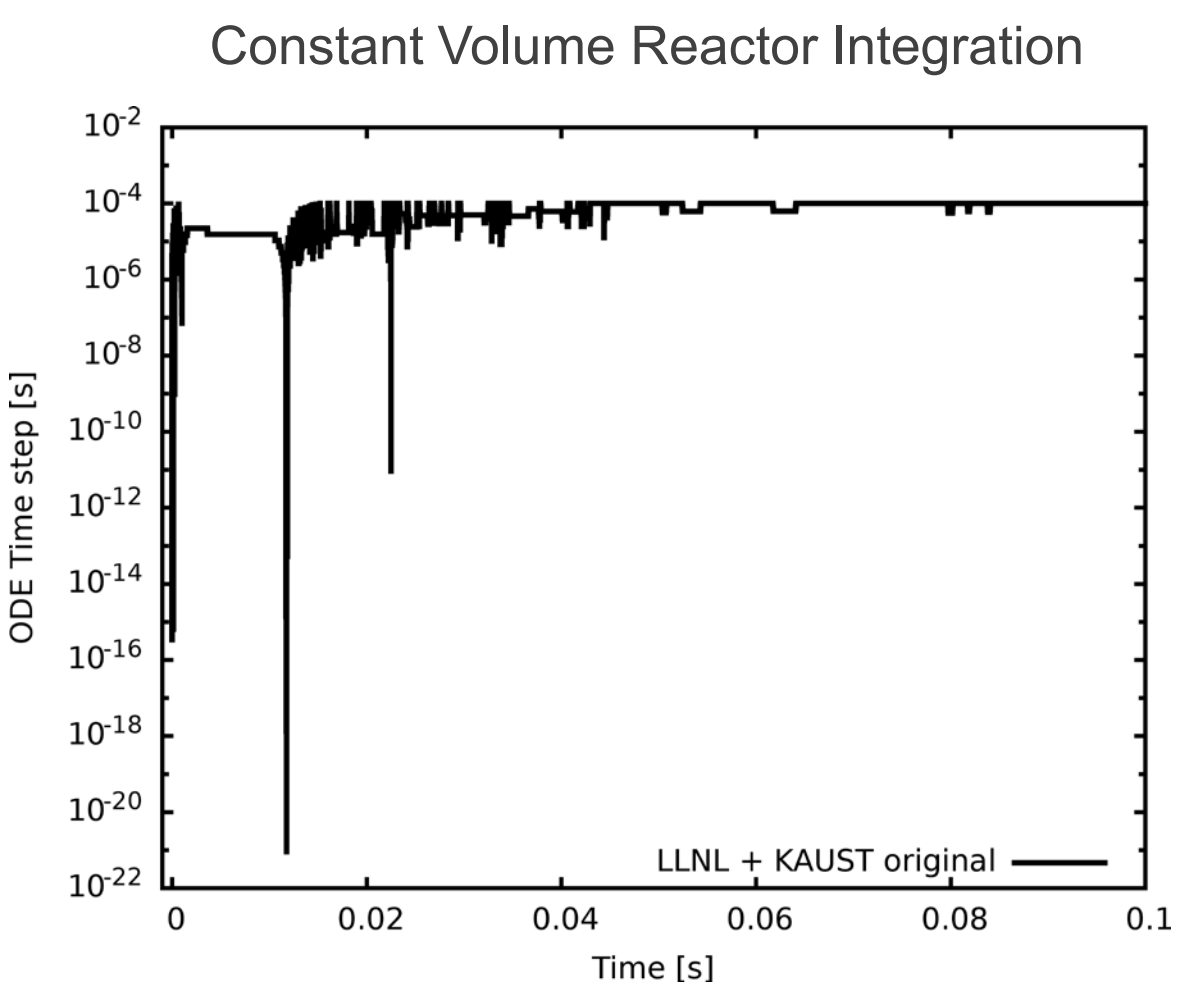
C. Mueller Diesel Engine (SNL)
FT004



N. Killingsworth
ConvergeCFD
ACE012

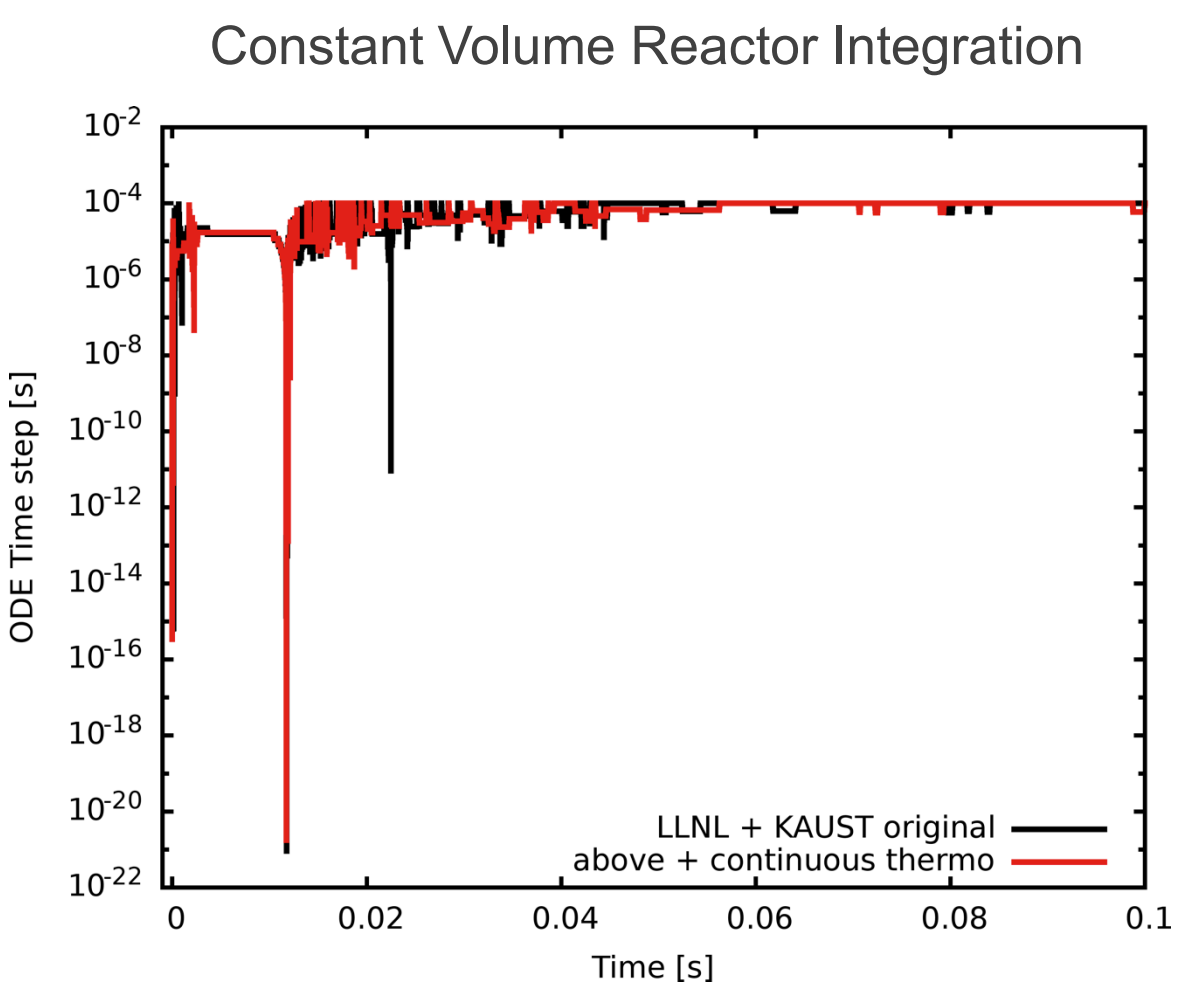


AMR16 Accomplishment: New mechanism diagnostics created to help debug the biodiesel simulations



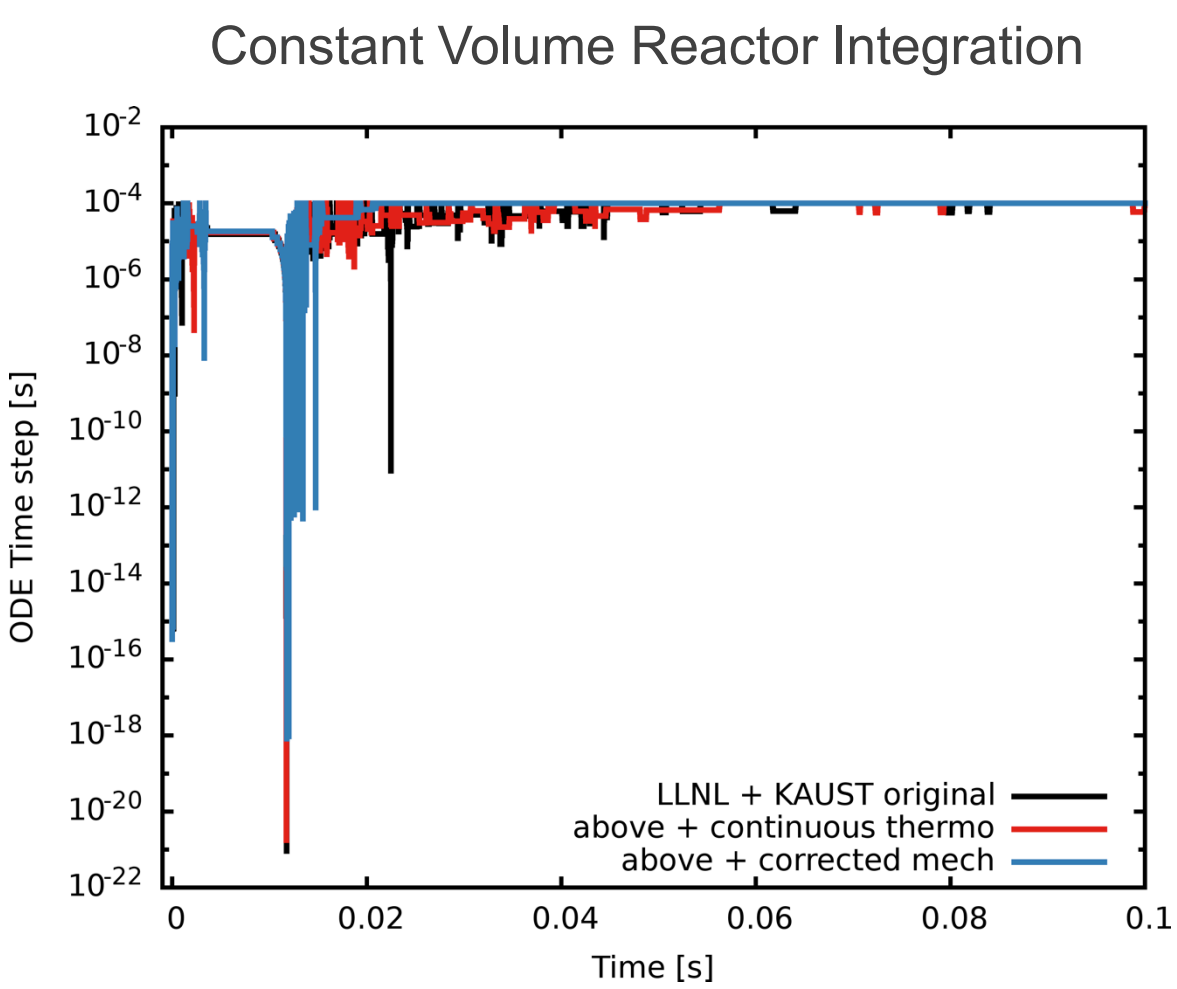
1. Original mechanism & thermodynamics data
   - 754 steps dt < 10^{-14} s

AMR16 Accomplishment: New mechanism diagnostics created to help debug the biodiesel simulations



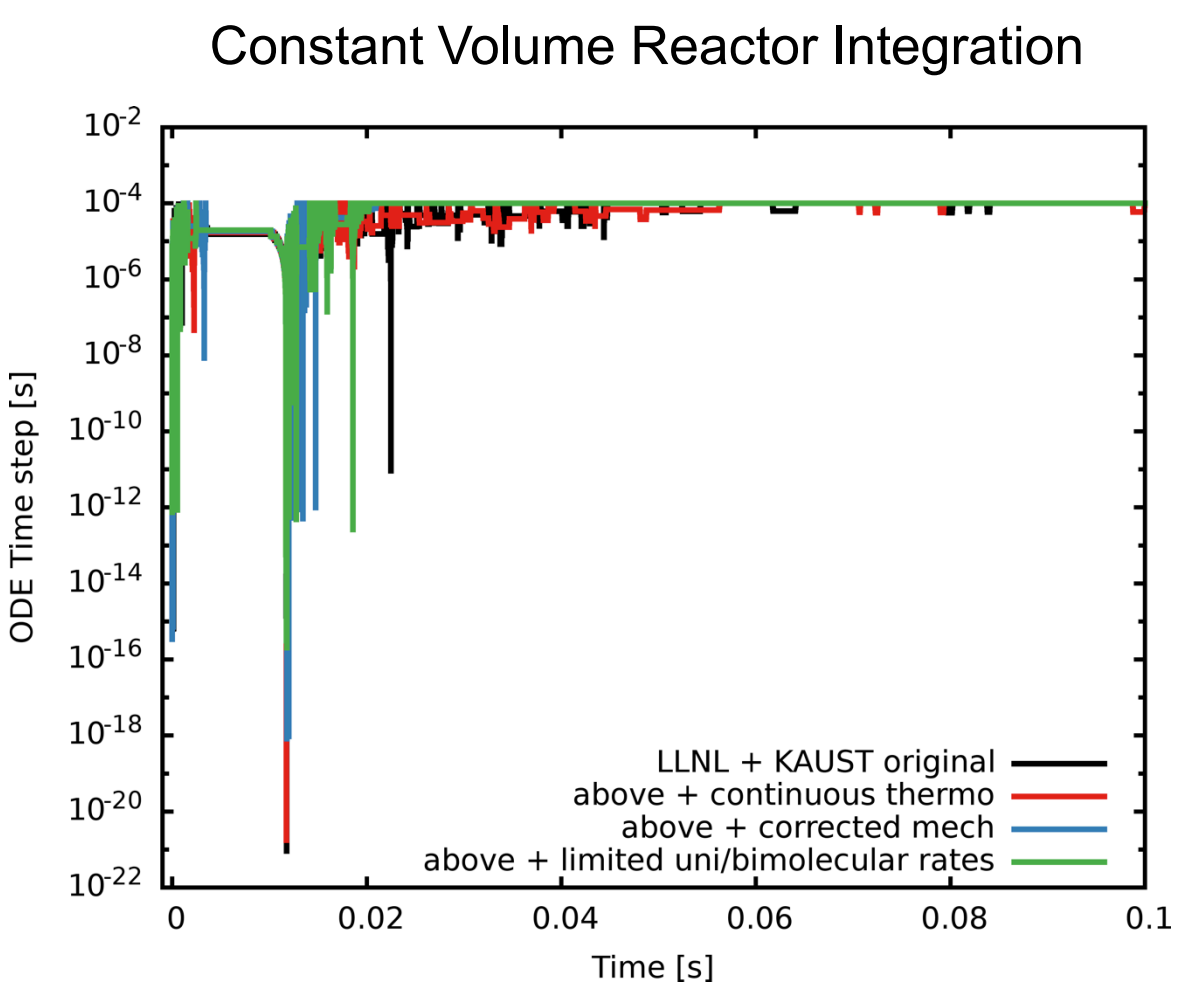
1. Original mechanism & thermodynamics data
   - 754 steps dt < 10^{-14} s
2. Enforce continuous thermodynamics
   - repaired 36 species with Cp/R, H/RT, or S/R > 0.1
   - 935 steps dt < 10^{-14} s

AMR16 Accomplishment: New mechanism diagnostics created to help debug the biodiesel simulations



1. Original mechanism & thermodynamics data
   - 754 steps dt < 10^{-14} s
2. Enforce continuous thermodynamics
   - repaired 36 species with Cp/R, H/RT, or S/R > 0.1
   - 935 steps dt < 10^{-14} s
3. Correct mechanism errors
   - no +4-body reactions
   - fix cyclic ether paths
   - 405 steps dt < 10^{-14} s

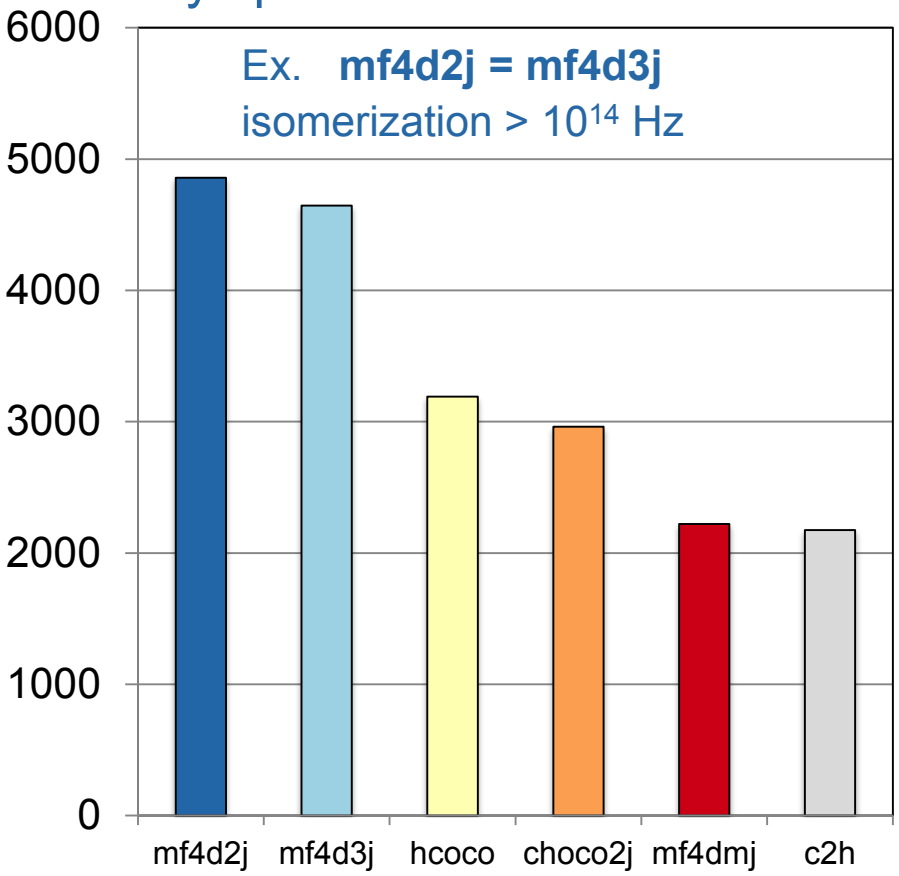
AMR16 Accomplishment: New mechanism diagnostics created to help debug the biodiesel simulations



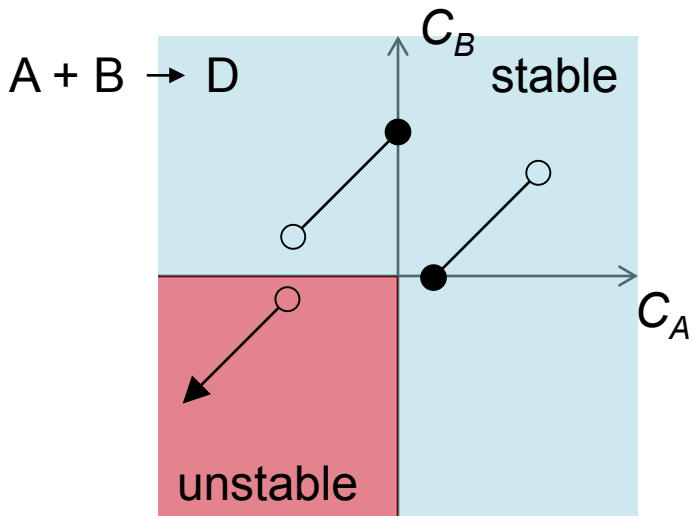
1. Original mechanism & thermodynamics data
   - 754 steps dt < 10^{-14} s
2. Enforce continuous thermodynamics
   - repaired 36 species with Cp/R, H/RT, or S/R > 0.1
   - 935 steps dt < 10^{-14} s
3. Correct mechanism errors
   - no +4-body reactions
   - fix cyclic ether paths
   - 405 steps dt < 10^{-14} s
4. Enforce uni/bimolecular limits (artificial)
   - 307 steps dt < 10^{-14} s

AMR16 Accomplishment: New mechanism diagnostics created to help debug the biodiesel simulations

Frequency of integrator errors by species and reaction

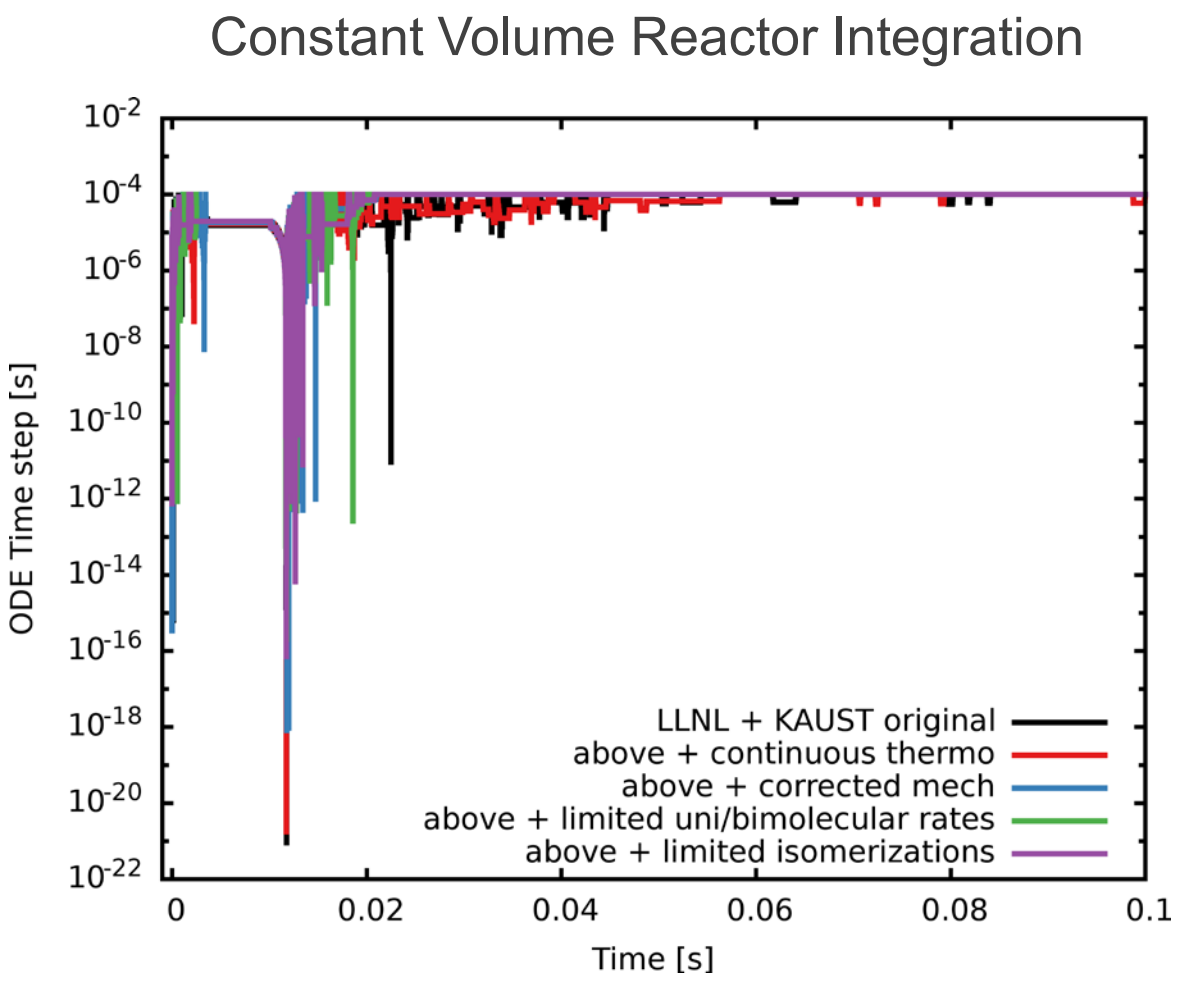


Negative Concentrations



- New diagnostic integrator can strictly enforce non-negativity
- Must be careful not to introduce discontinuities
- No unstable negative modes found in practice at recommend absolute tolerance 10^{-20}

AMR16 Accomplishment: New mechanism diagnostics created to help debug the biodiesel simulations



5. Limit the problematic isomerizations found by the new diagnostics
   - 169 steps dt < 10^{-14} s

Future Work

- Check thermo against isomers & other databases
- Compute "best-fit" reverse Arrhenius rate expressions for problematic reactions using equilibrium
- Compute the minimum thermodynamic perturbations to satisfy physical limits on unimolecular and bimolecular rates

Response to AMR15 reviewers comments

AMR15 comments were generally positive (3.64/4 overall) with the reviewers posing the following questions and making some key suggestions:

1. *"... the project team may want to explicitly state the differences between this project and Russell Whiteside's project (ACE012)"*

   Project ACE076, led by McNenly, is focused on fundamental algorithm development using applied mathematics research and new computing hardware to increase computational efficiency and physical accuracy. Computational efficiency refers to both the human and electronic computer, as recent work has looked more broadly at the bottlenecks facing the ACE research community. Project ACE012, led by Whitesides, applies the fundamental research results from ACE076 to multi-dimensional modeling simulations. This also includes algorithm development to get the new solvers running inside the CFD tools used by industry.

2. *"… why this project could not be folded into ace012?"*

   ACE076 was spun-off from ACE012 when there was interest in having more granularity in the projects. If the VTO deems it appropriate to track one large simulation project at LLNL, then we will fold the projects back together.

3. *"The project should incorporate some sort of rationale for reducing the number of steps... The project does not appear to consider strategies for chemistry reduction "*

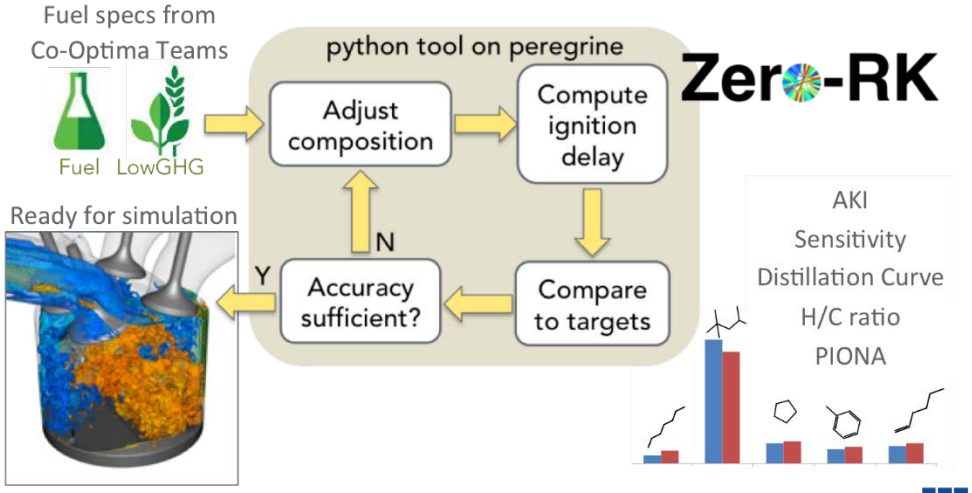
   Chemistry reduction is in fact the motivation behind the adaptive preconditioner approach developed for Zero-RK (see slide 33 or McNenly, PROCI, 2015). The precon-ditioners for the ODE system are reduced mechanisms, but the entire system is retained so there is no loss of accuracy. We see our unique role within DOE is to push the upper limits of chemistry fidelity in ACE simulations. Specifically, we focus on time savings that have either no loss of accuracy, or a measureable loss of accuracy that is user-controlled.

4. *"… a broader base touching more tools (KIVA, etc.) and even vendors (CD-Adapco, ANSYS, etc.) is encouraged."*

   The new Co-Optima program has enabled LLNL to field Zero-RK to a wider group of users. Several new applications have been built on Zero-RK for other national labs. We have also applied for LLNL and DOE tech maturation funding to produce an easier to use version of Zero-RK to increase the licensing opportunities.

Collaboration – We have ongoing interactions with industry, national laboratories, and universities

- **Industry:** Convergent Sciences Inc. (licensee of Zero-RK), Cummins (GPU development), GM (beta-testing Zero-RK in ConvergeCFD), and NVIDIA (new matrix library help)
- **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 FT040); coordinating Co-Optima simulation efforts between ANL, LANL, LLNL, NREL, ORNL, and SNL; and sharing Zero-RK tools on Peregrine cluster:



Remaining challenges and barriers to High Efficiency Clean Combustion (HECC) 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 for improving efficiency and accuracy of chemistry and engine CFD

Ongoing ACE076

FY16 – Create a report on mechanism debugging and a user guide for the LLNL inspection and repair utility.

FY16 – Develop a public web application to help inspect and repair detailed chemistry mechanisms

FY16 – Complete multispecies diffusion and chemistry validation for canonical flames (laminar flame speed & opposed diffusion)

Proposed supports multiple VTO R&D efforts

FY17-20 – Accelerate new soot model algorithms

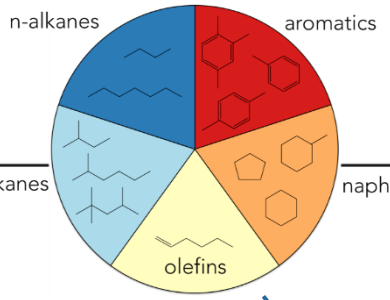
FY17-20 – Couple chemistry-turbulence models with detailed kinetic mechanisms for transportation fuels

FY17-20 – Accelerate detailed spray dynamics algorithms

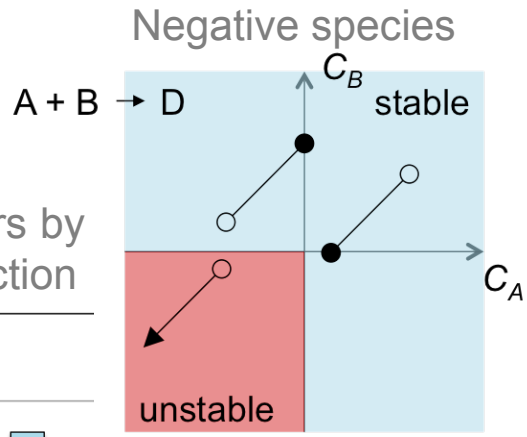
Summary: LLNL has increased the capabilities of Zero-RK for more reaction types and created more rigorous mechanism debugging tools

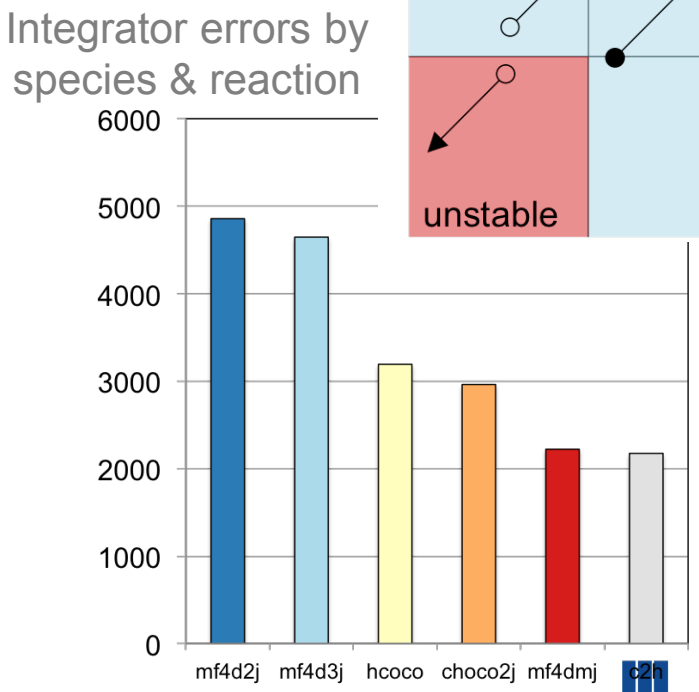
Zero-RK can efficiently solve detailed soot and complex pressure dependent reactions

Zero-RK



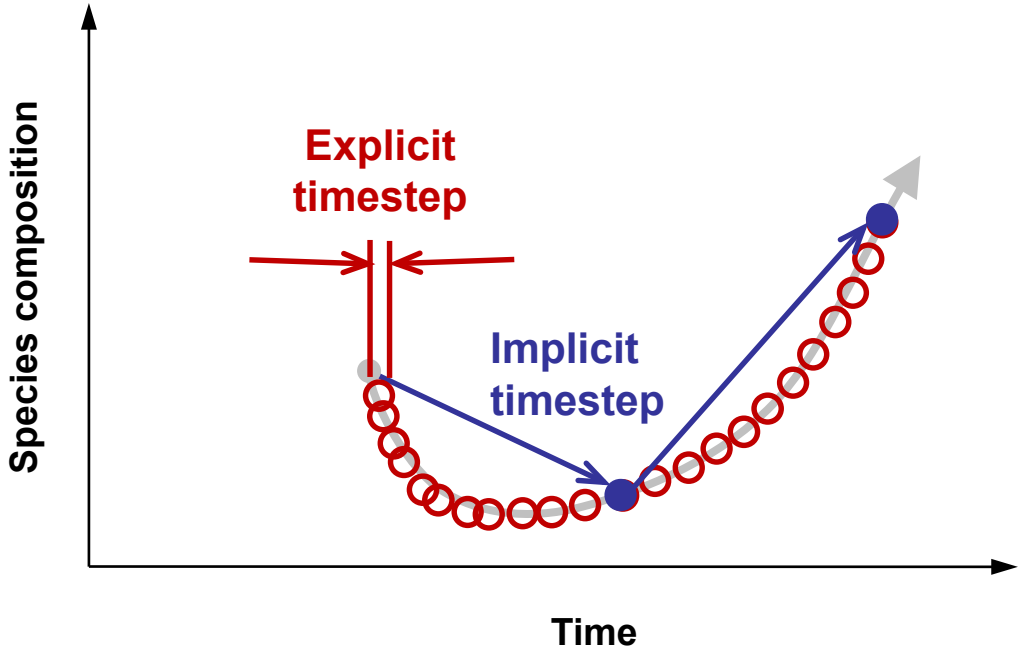
Mechanism debugging suite offers new checks





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?

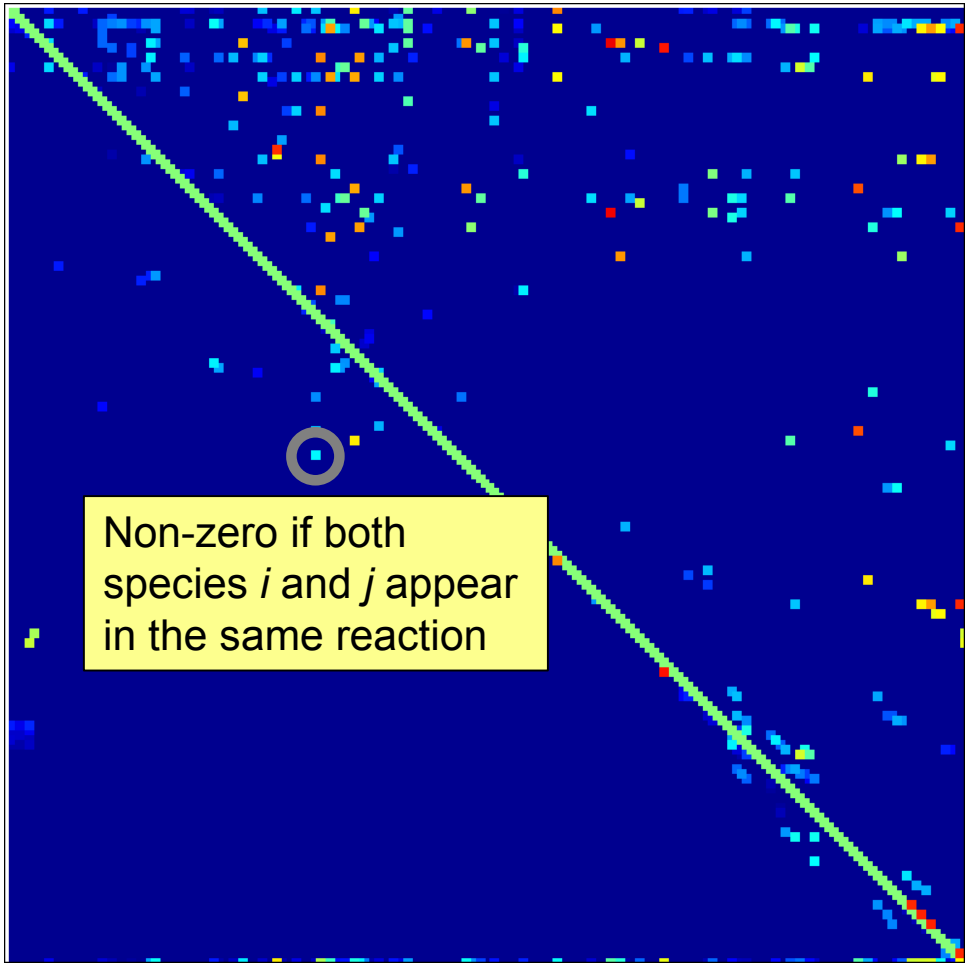
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

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)



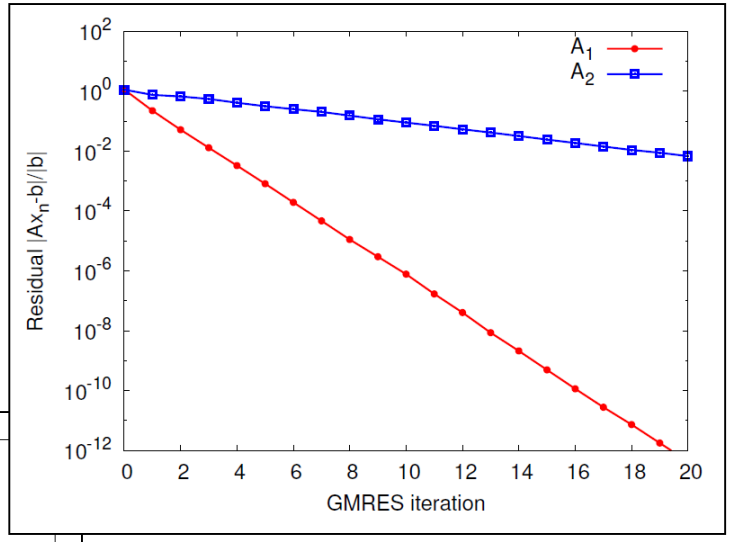
Approximate Jacobians can be used to precondition iterative linear system solvers like GMRES

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

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

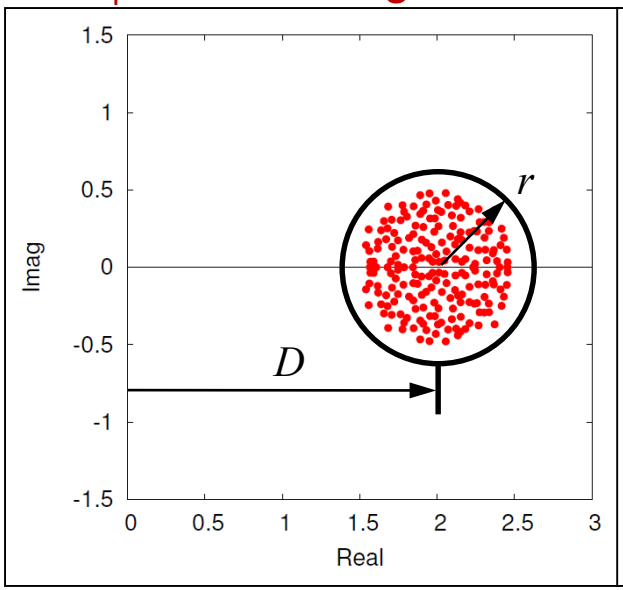
$$\Lambda \approx \frac{r}{D}$$

GMRES Error

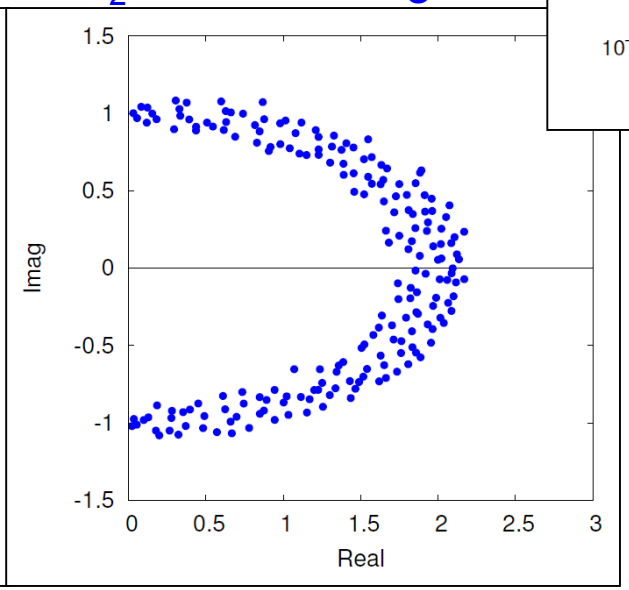


Eigenvalue Spectra (200 x 200)

A_1: fast convergence



A_2: slow convergence

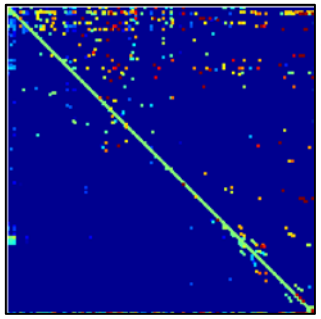


Adaptive preconditioner using on-the-fly reduction produces the same solution significantly faster

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.)

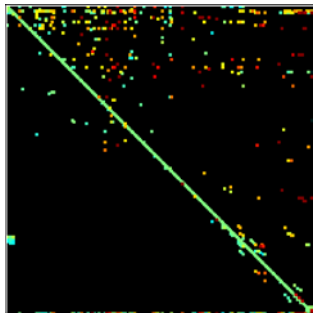
slower ⟷ faster

1. Classic mechanism reduction:

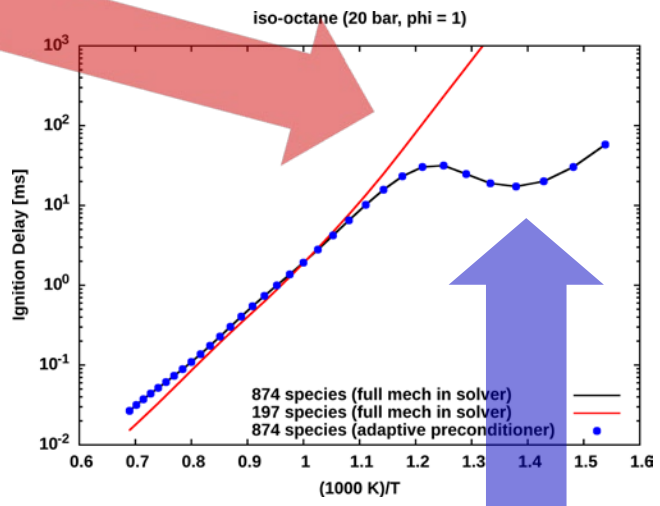
Ex.197 species 

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

2. LLNL's adaptive preconditioner:



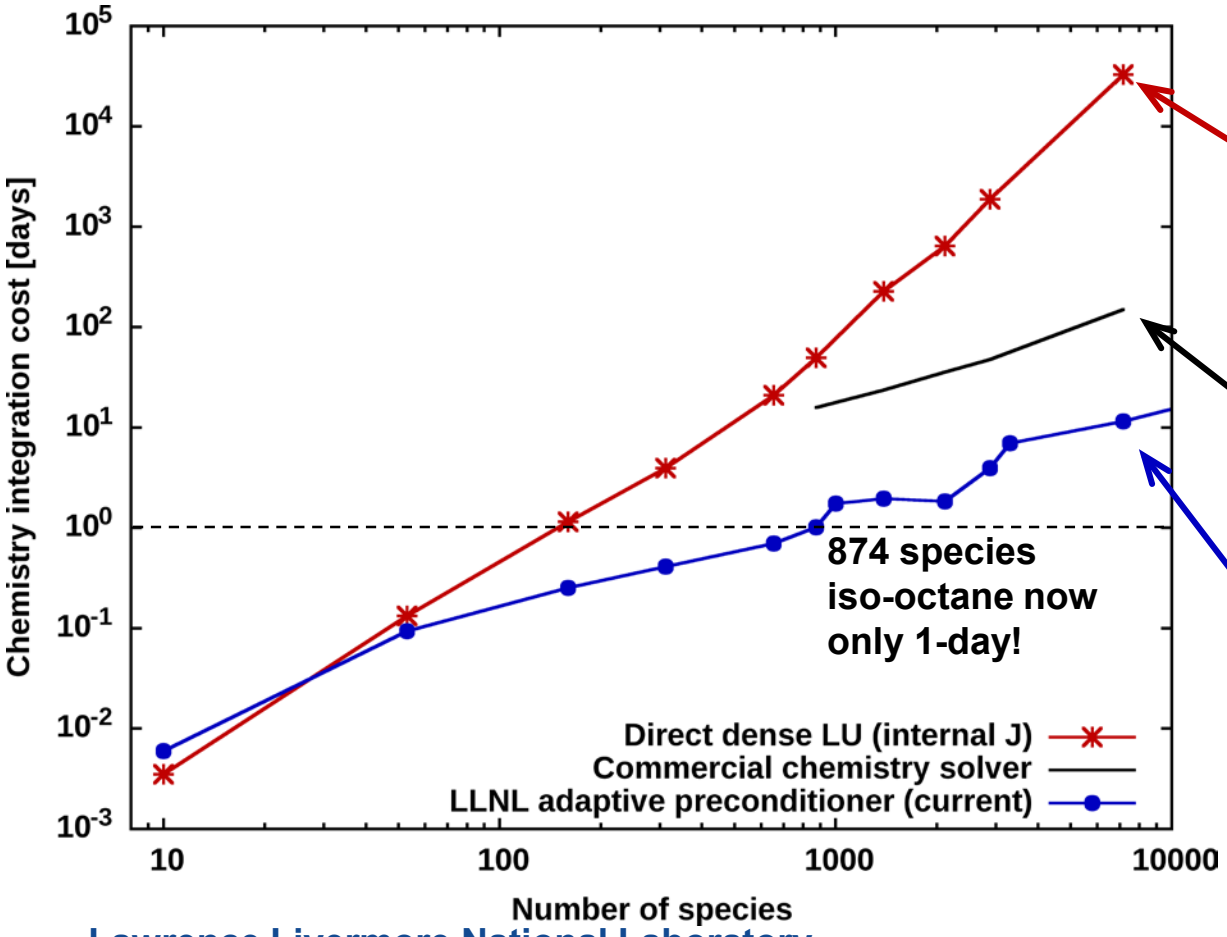
- *Identical ODE*
- Reduced mech *only* in preconditioner

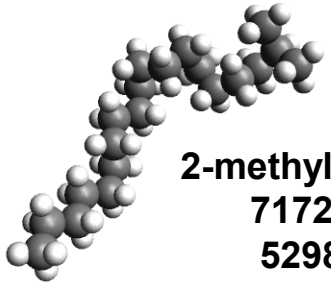


Filter out 50-75% of the least important reactions

AMR15 Accomplishment: LLNL's Zero-RK chemistry software earns a 2015 R&D 100 award in the software & services category

Simulation time (chemistry-only) for 10^6 cells on 32 processors





2-methylnonadecane
7172 species
52980 steps

Traditional dense matrix ODE solvers still found in KIVA and OpenFOAM

- 90 years

New commercial solvers using sparse systems

- 150 days

New LLNL solvers created for ACE program FY13

- 11 days

This project and ACE012 have coupled our solvers to CONVERGE™ CFD.