Lawrence Livermore National Laboratory

Improved Solvers for Advanced Engine Combustion Simulation

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Project ID # ACE076

2015 DOE Vehicle Technologies Program
Annual Merit Review and Peer Evaluation Meeting
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LLNL-PRES-669834

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Overview

Timeline

- Ongoing project with yearly direction from DOE

Barriers

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

Budget

- FY13 funding: $340K
- FY14 funding: $475K
- FY15 funding: $460K
- GPU CRADA: $100K *pending Q4 start*

Partners

- Cummins, GM, Bosch, GE, Convergent Sciences & NVIDIA
- ANL, SNL, ORNL, NREL
- LSU, Indiana U., PSU, UC Berkeley, Caltech, U. Mich., RWTH Aachen
- AEC MOU, FACE working group, Combustion Inst., SAE, GPU Tech. Conf., and NFVSO Optima Team

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:

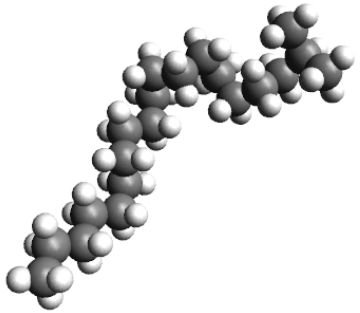
A. *Lack of fundamental knowledge of advanced engine combustion regimes*

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

D. *Lack of effective engine controls*

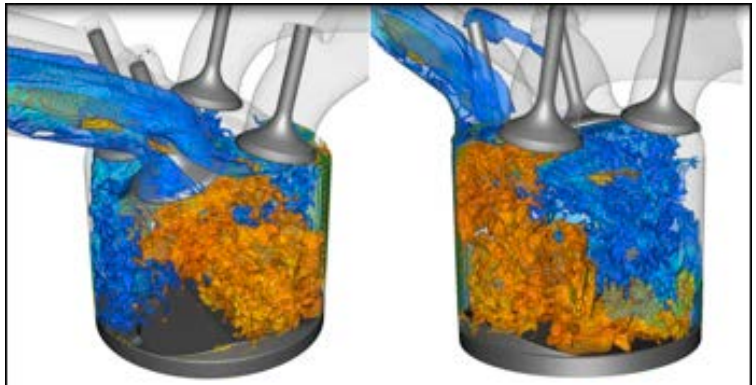
We want to use…

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

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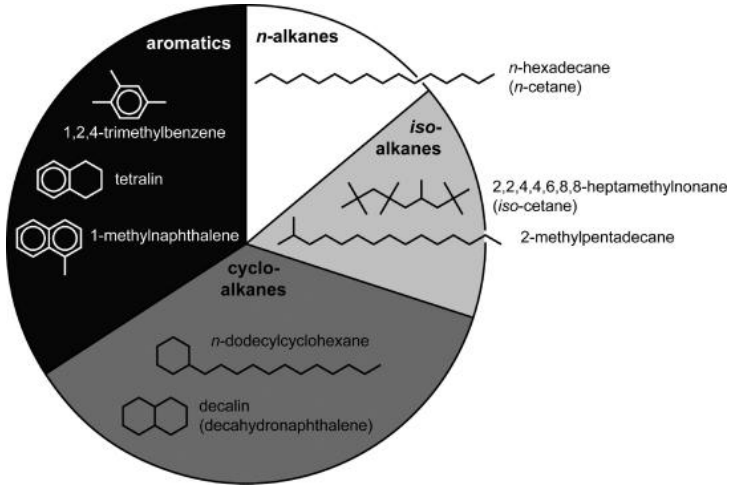
Now we want to use…

Detailed chemistry



Ex. 9-component diesel surrogate (AVFL18)
C. Mueller et al. Energy Fuels, 2012.
+10K species
+75K reaction steps

in highly resolved 3D simulations

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

Objective

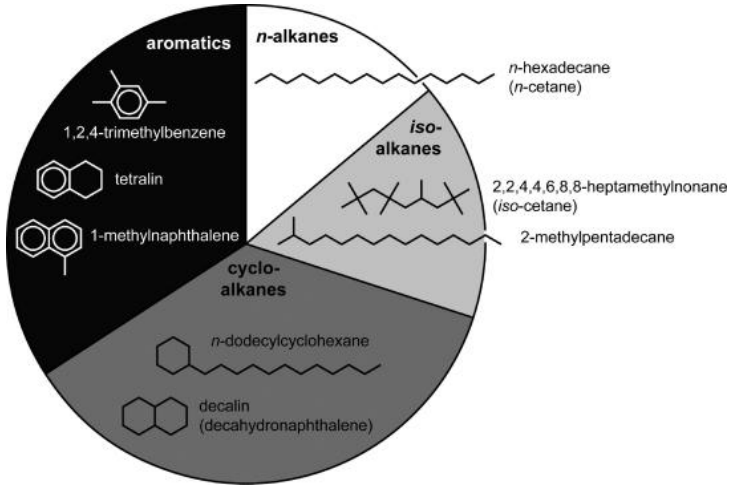
Create faster and more accurate combustion solvers.

AMR15 achievements:

- Completed chemistry mechanism diagnostic and debugging toolkit (ver. 1)
- Improved hybrid CPU-GPU chemistry
- Completed thermo repair utility (ver. 1)
- Completed variable volume reactor model for engines and RCMs:
  - *reduces ANL wait from days to minutes*
  - *reaction rate global sensitivity analysis for RCM now possible in hours*
- New GPU partnership with Cummins, CSI, IU, and ORNL (2 CRADAs pending)

Now we want to use…

Detailed chemistry



Ex. 9-component diesel surrogate (AVFL18)
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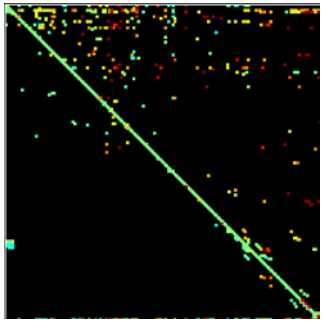
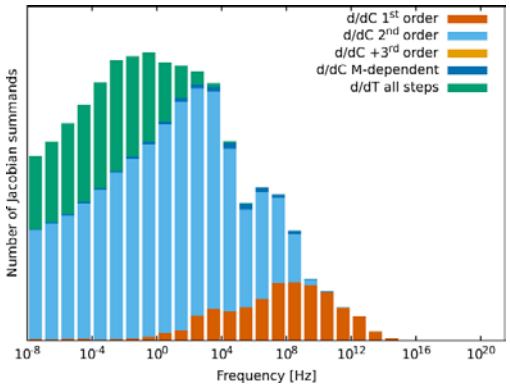
Approach – Accelerate research in advanced combustion regimes by developing faster and more predictive engine models



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)

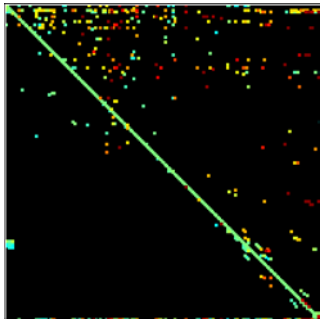


3. Improved physical models
   – more accuracy, better error control

Approach – FY14-FY15 milestones

Due	Type	Milestones	Status
6/30/2014	reg.	Create chemistry tool for reaction pathway analysis and error detection using LLNL's advanced combustion algortithms	complete
9/30/2014	reg.	Improve every-cell chemistry on the GPU	complete
12/31/2014	reg.	Further improve mechanism reliability software	complete
3/31/2015	reg.	Extend accelerated chemistry sensitivity tools to engine/rapid compression machine models	complete
6/30/2015	reg.	Develop an adaptive preconditioner framework to accelerate fully coupled transport/chemistry.	on schedule
9/30/2015	reg.	Develop an opposed diffusion model using the new adaptive preconditioner framework	on schedule
9/30/2015	reg.	Benchmark computational performance of the fully coupled transport/chemistry preconditioner versus the widely used operator splitting	on schedule

Accomplishment Outline



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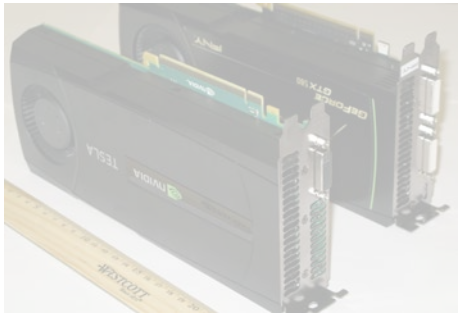

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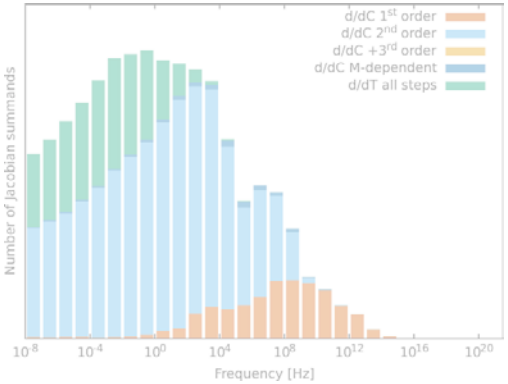
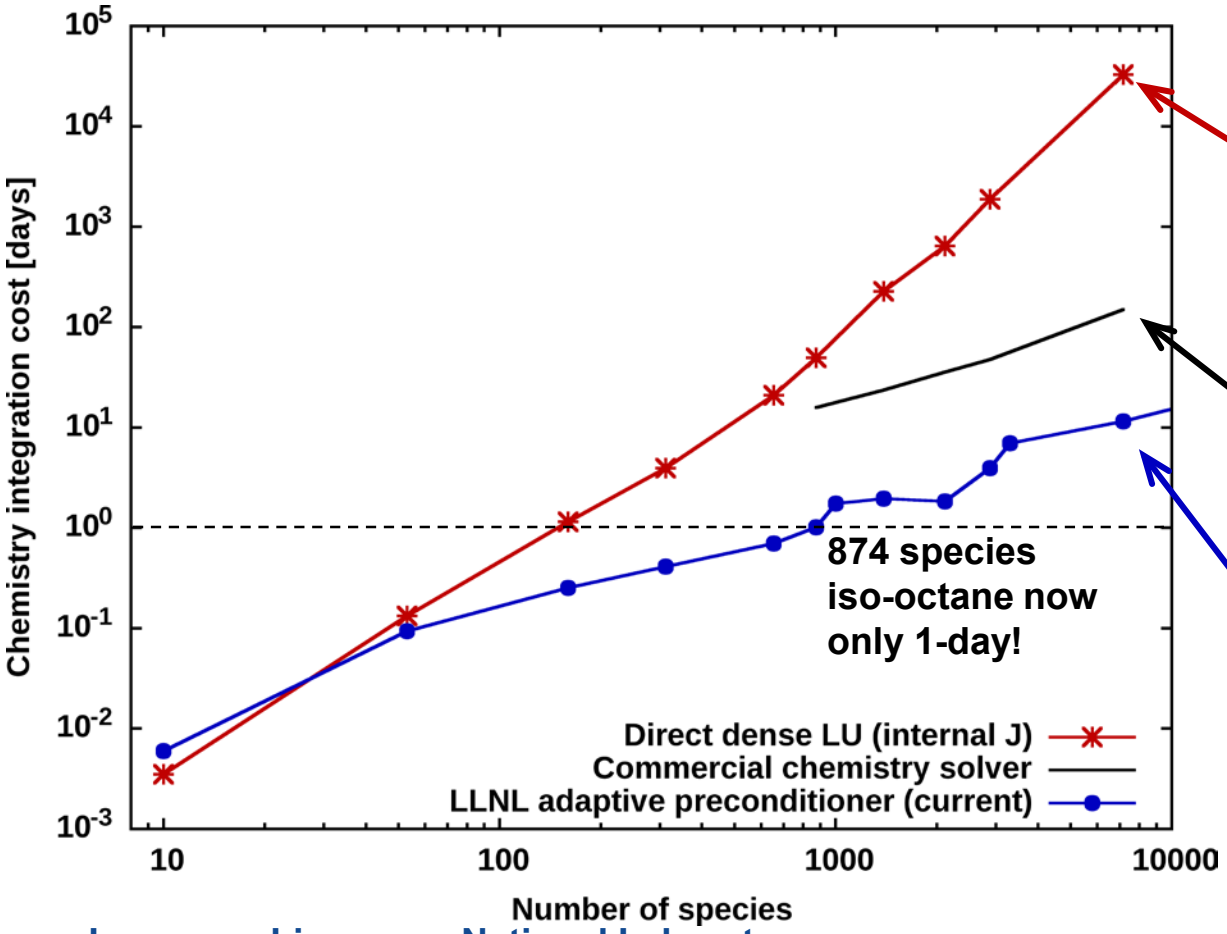
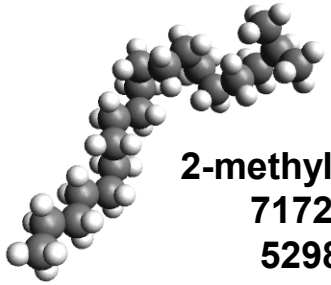


3. Improved physical models
   – more accuracy, better error control

AMR13 Accomplishment: LLNL's new solver brings well-resolved chemistry and 3D CFD to 1-day engine design iterations

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

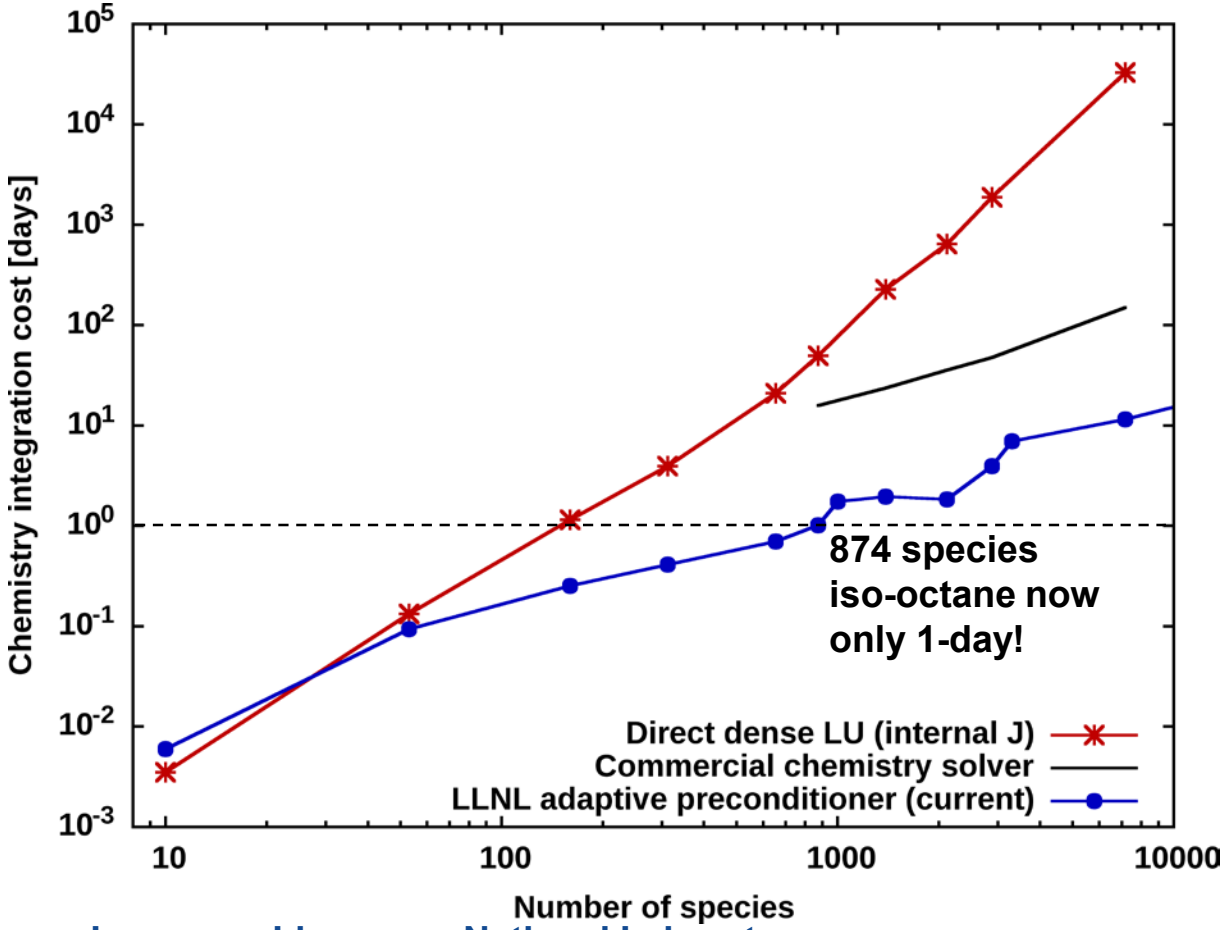
New LLNL solvers created for ACE program FY13

- 11 days

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

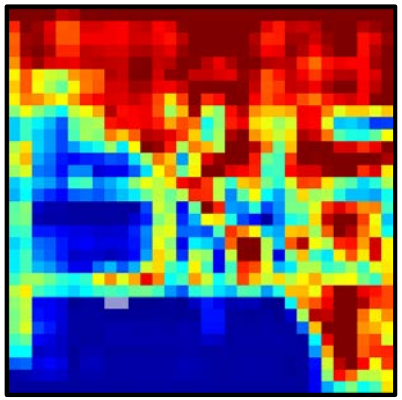
Approach: Extend the high performance chemistry solvers to more applications impacting the ACE R&D workflow

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



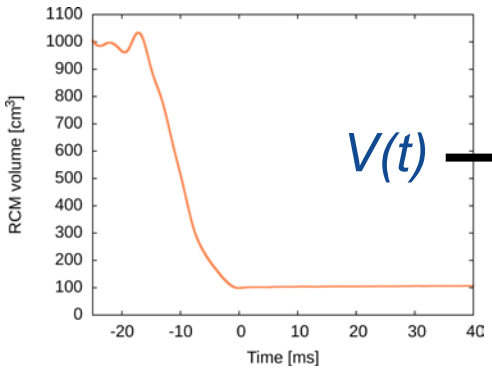
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

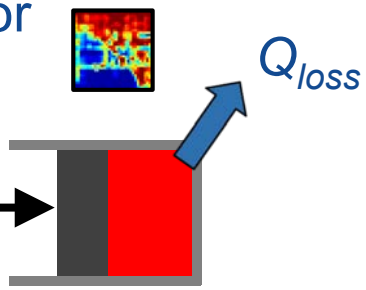
$J =$



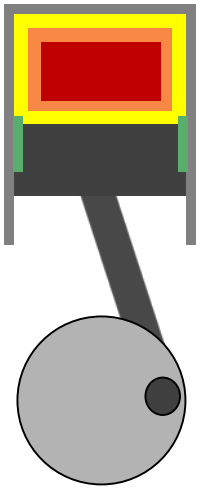
Approach: Create a flexible framework for the reactor Jacobians to easily build many applications on LLNL's chemistry algorithms

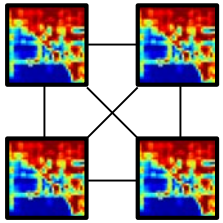
Variable Volume Reactor



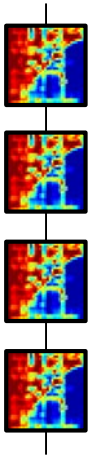


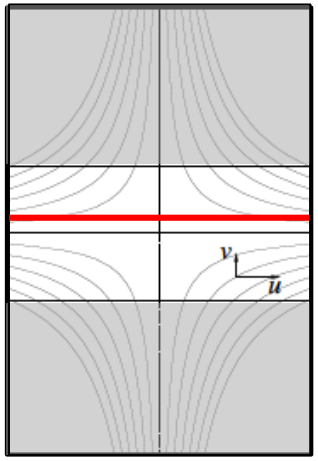
Quasi-Dimensional Multizone



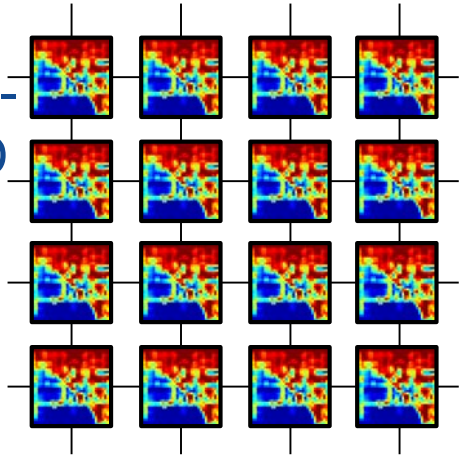


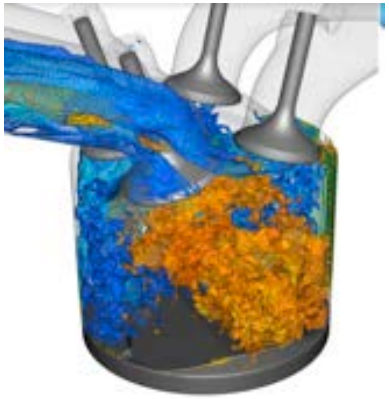
1D Flame Models





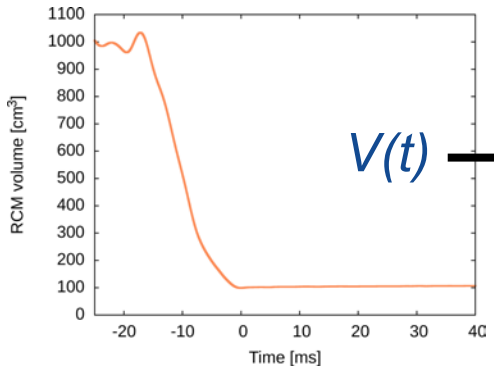
Detailed Fully-Coupled CFD

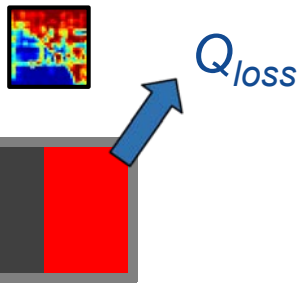


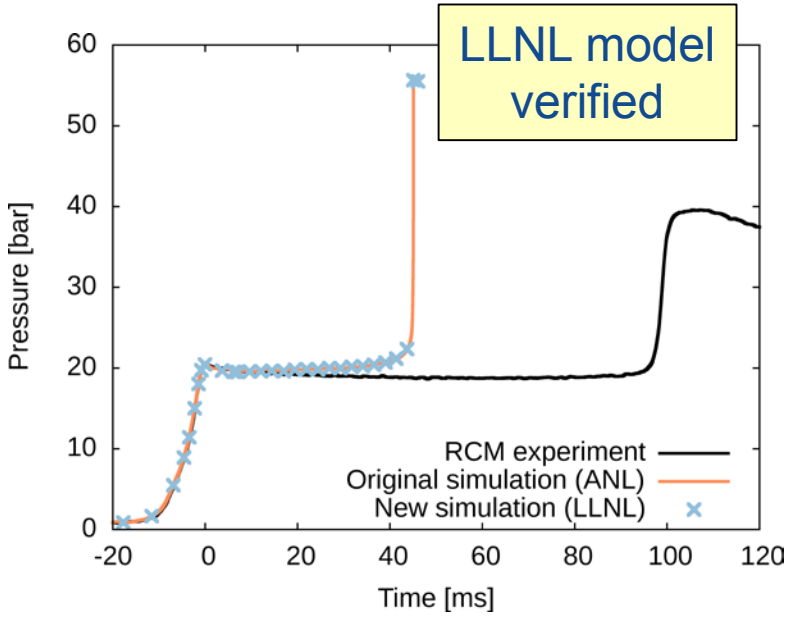


AMR15 Accomplishment: Accelerated the rapid compression machine model – realistic gasoline (1,700 species) from a day to minutes

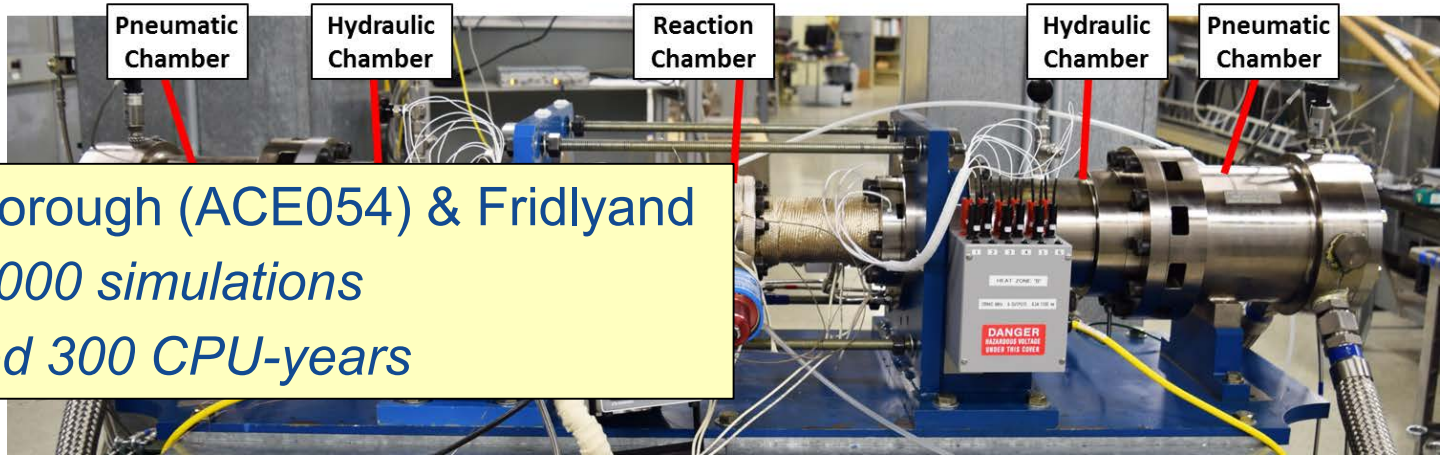
Variable Volume Reactor







ANL Rapid Compression Machine:

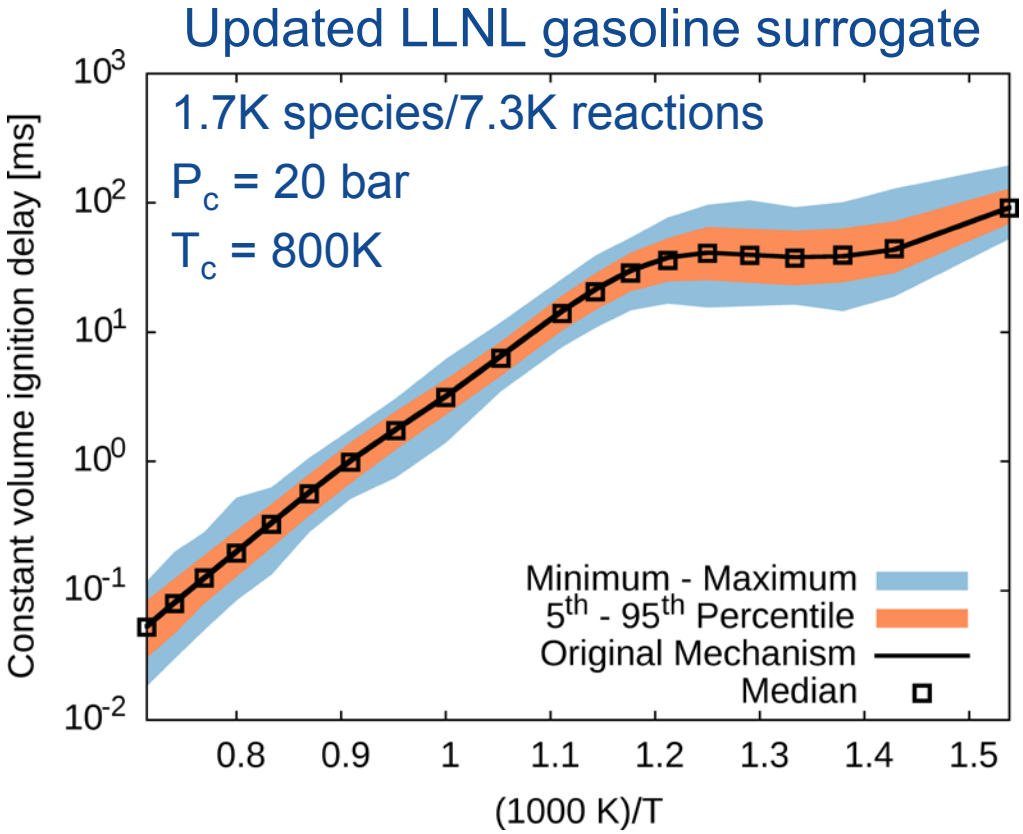


Goldsborough (ACE054) & Fridlyand

100,000 simulations

saved 300 CPU-years

AMR15 Accomplishment: Local sensitivity software updated for user-defined A-Factor distributions for global sensitivity analysis (GSA)



- 0.05% n-heptane
- 0.60% iso-octane
- 0.09% toluene
- 0.09% methylcyclohexane
- 0.15% 2-hexene
- 12.2% oxygen
- 86.8% nitrogen

New tool features:

- Generalized matrix input to control individual A-Factor distributions
- Automatic task allocation and data collection on parallel systems

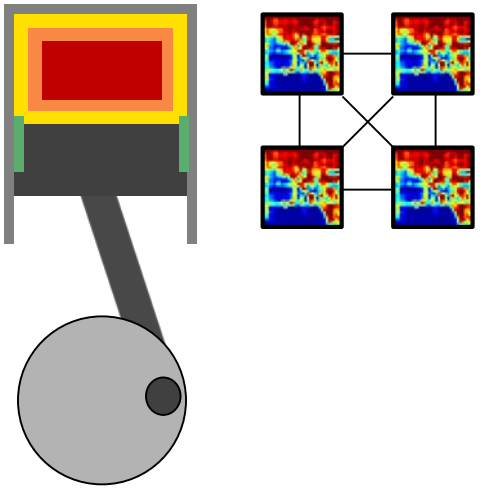
1,000,000 GSA simulations for detailed gasoline chemistry performed for ACE054:

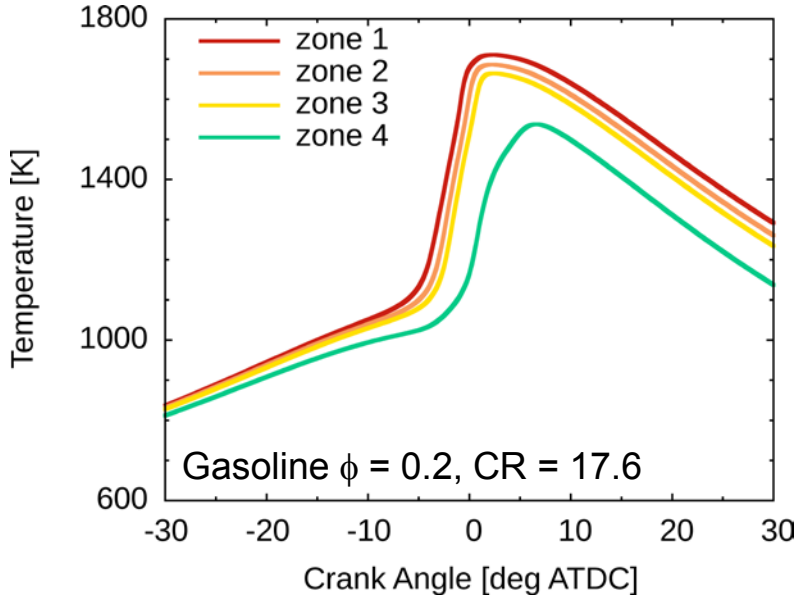
A. Fridlyand, *et al.*, in 9th *US Nat Combust Meet,* 2015.

R. West, *et al.*, in 15th *Intl Conf Numer Combust*, 2015.

AMR15 Accomplishment: Accelerated the fully-coupled multizone model – 35x speedup for realistic gasoline (1,400 species)

Quasi-Dimensional Multizone





- Tested fully coupled multizone model of an HCCI engine
- Heat transfer model – J. Kodavasal *et al.*, *Int J Engine Res*, 2013
- Improved block diagonal preconditioner – M. McNenly, *et al.*, SAE *Int J Fuels Lubricants*, 2010

- Uniform pressure couples all zones
- Energy coupled with walls
- Mass, energy, and species may also be transferred between zones
- More accurate burn duration
- LLNL advanced preconditioner now applied to each sub-block

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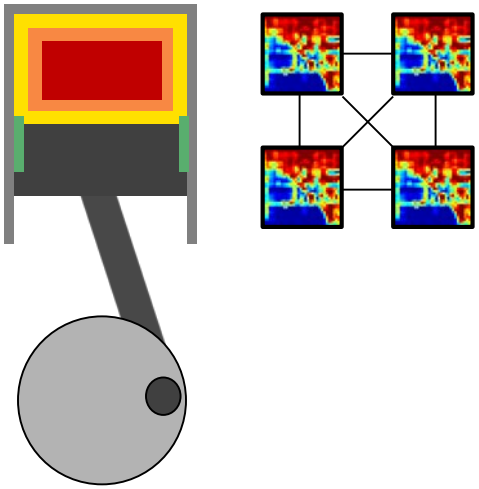
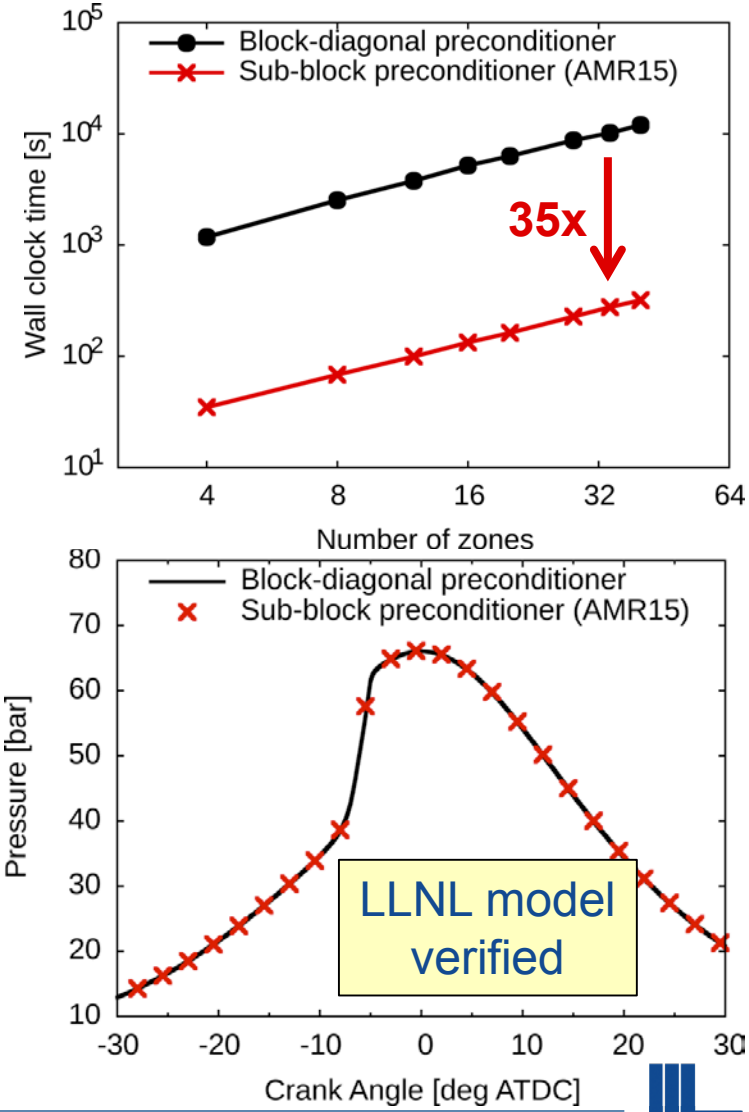
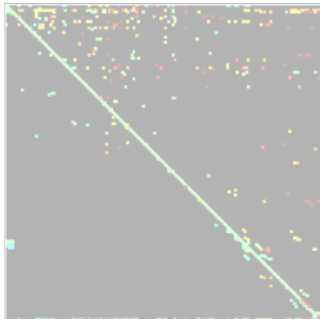




- Timescales coupling the pressure between zones much faster than zones linked by transport – more demanding
- Approach expected to work well for other fully-coupled models (1D flames & CFD)
- Improvements to sub-block preconditioner could yield another 2-5x

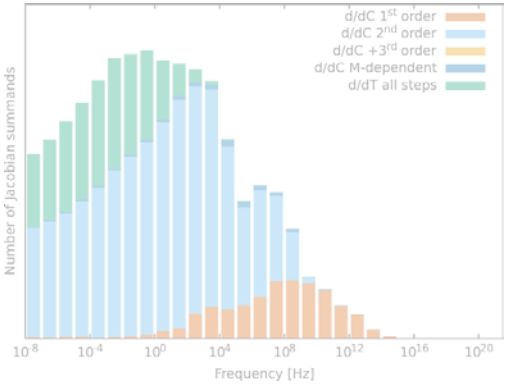
Accomplishment Outline



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
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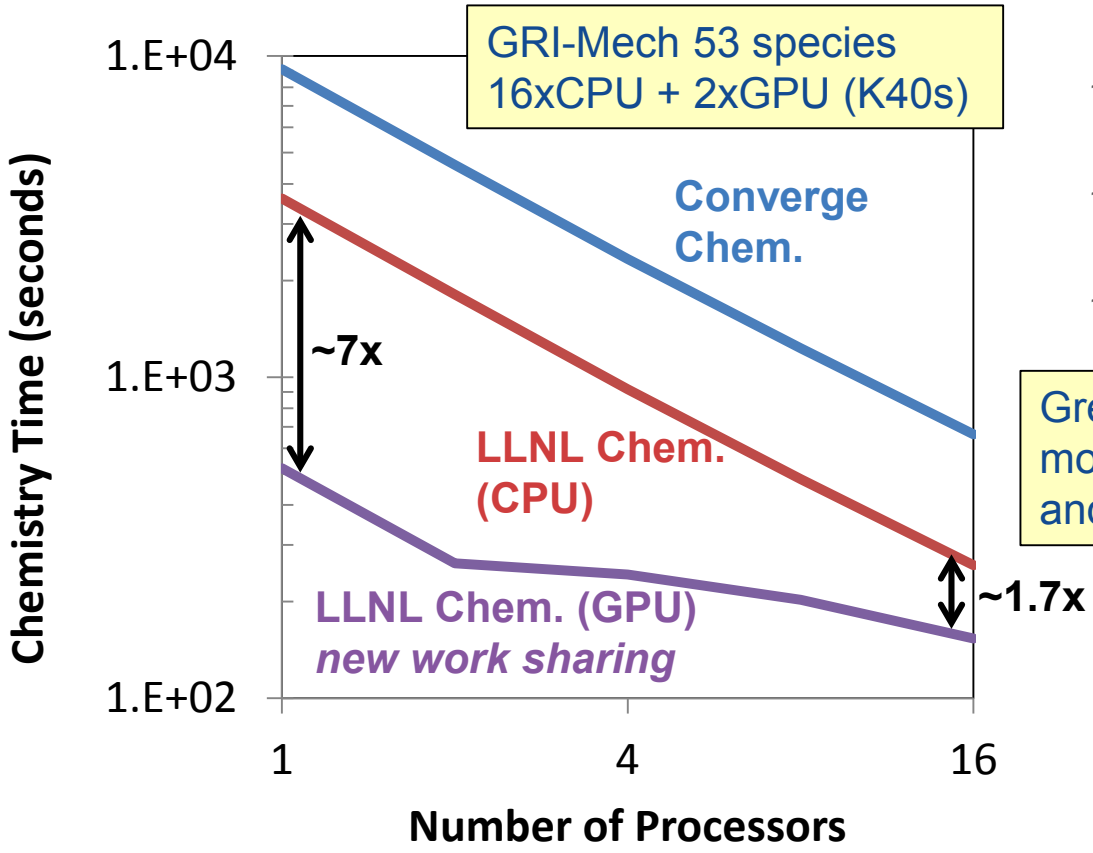
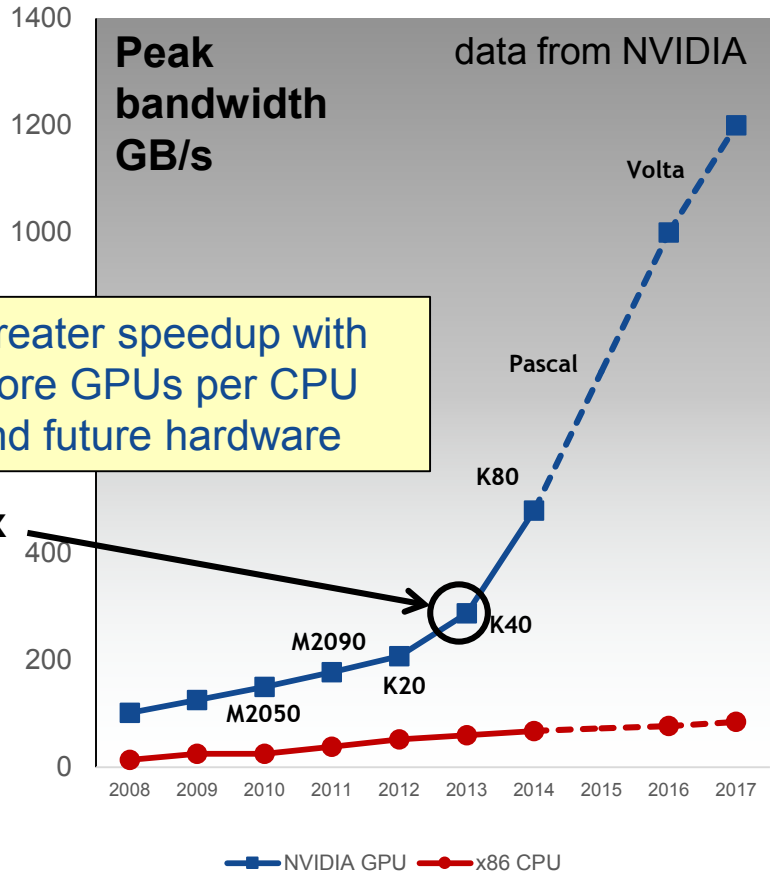
AMR15 Accomplishment: LLNL's GPU chemistry solver has improved CPU/GPU cooperation and large mechanism performance





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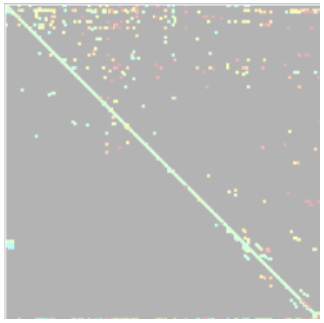

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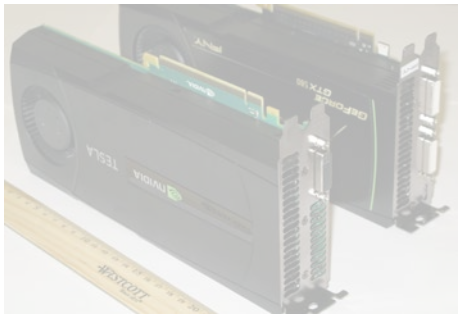

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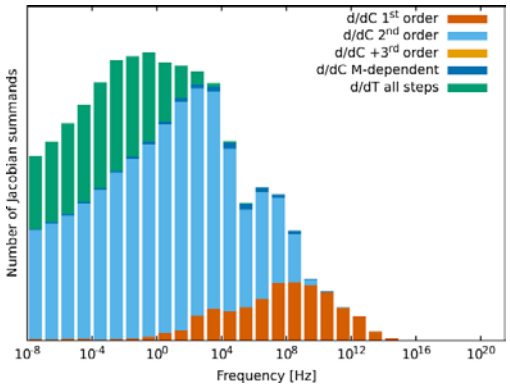

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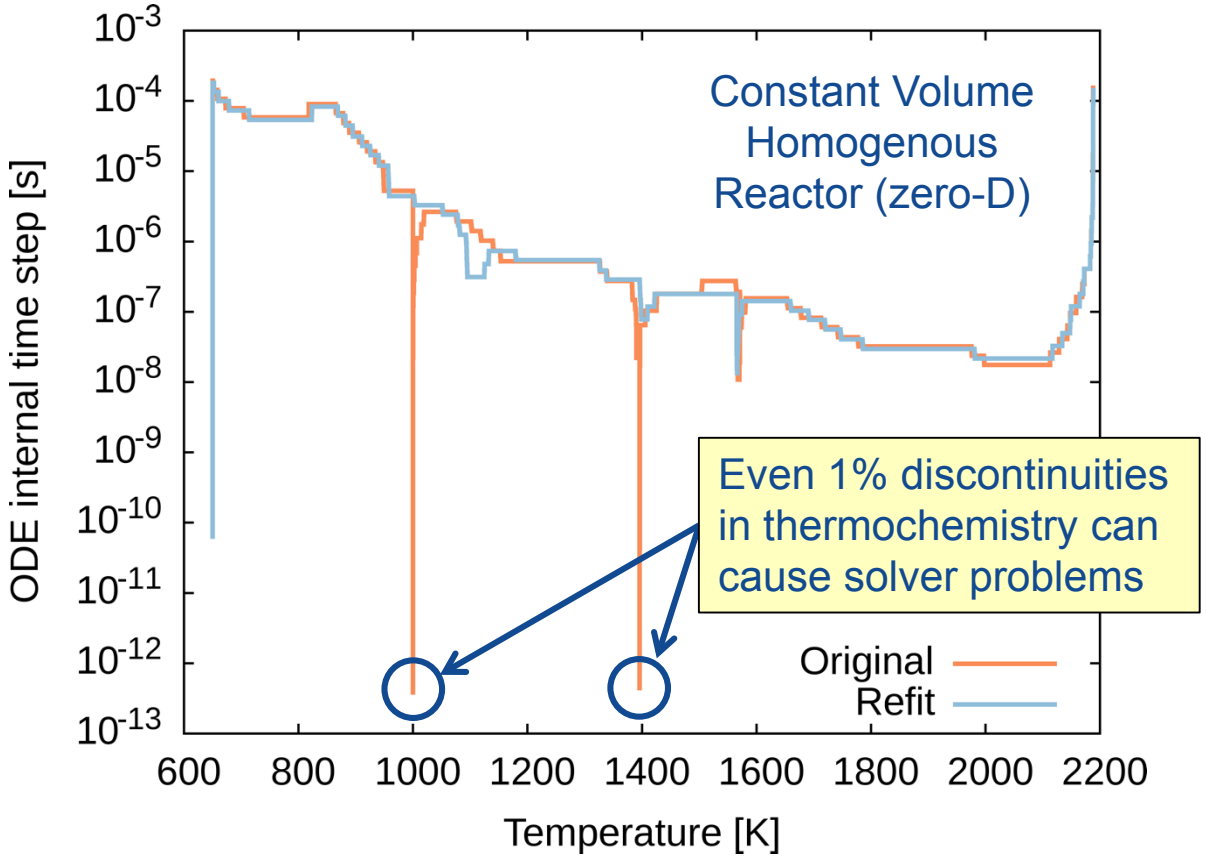
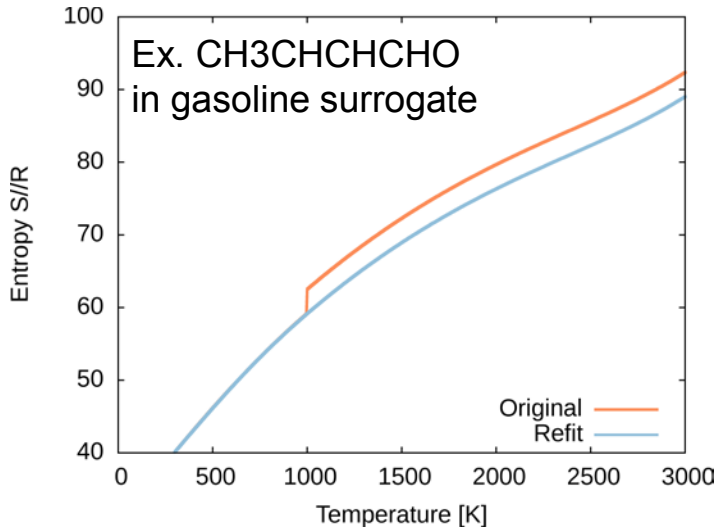
AMR15 Accomplishment: Improved gasoline surrogate chemistry with the LLNL ignition delay diagnostic tool for ANL RCM models

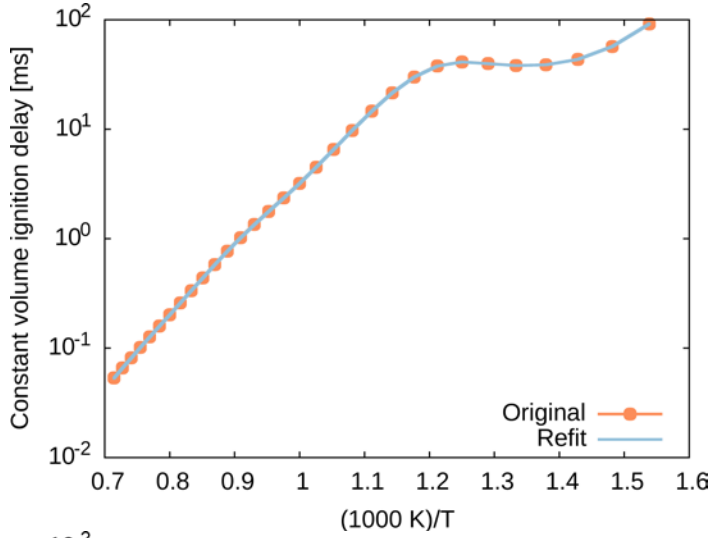
ANL RCM gasoline surrogate conditions

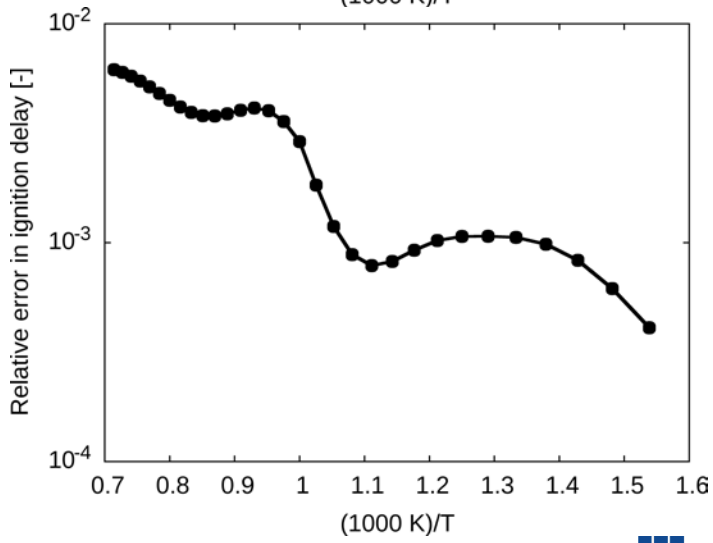
- P_c = 20 bar
- T_c = 800 K
- 0.05% n-heptane
- 0.60% iso-octane
- 0.09% toluene
- 0.09% MCH
- 0.15% 2-hexene
- 12.2% oxygen
- 86.8% nitrogen



AMR15 Accomplishment: Developed an automatic repair utility for the thermodynamic properties to speedup ACE R&D workflow

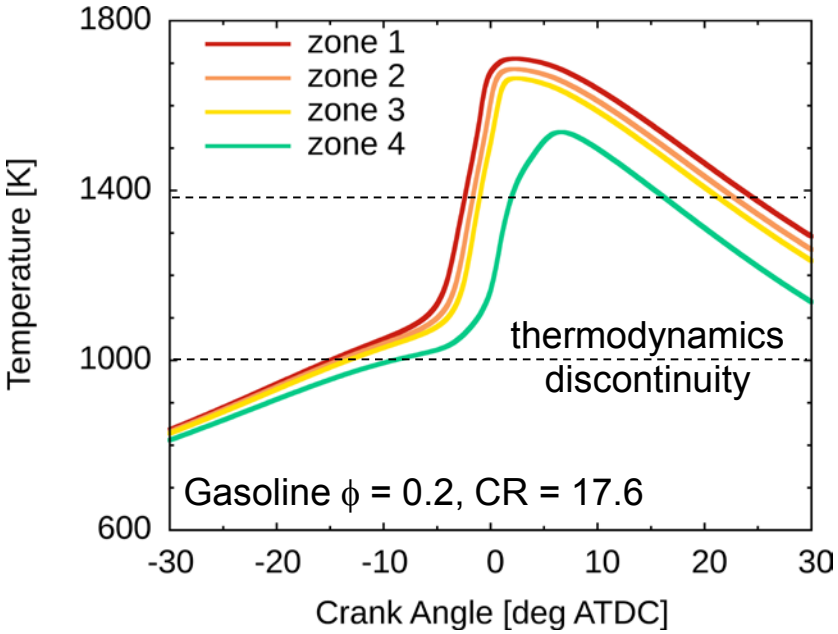


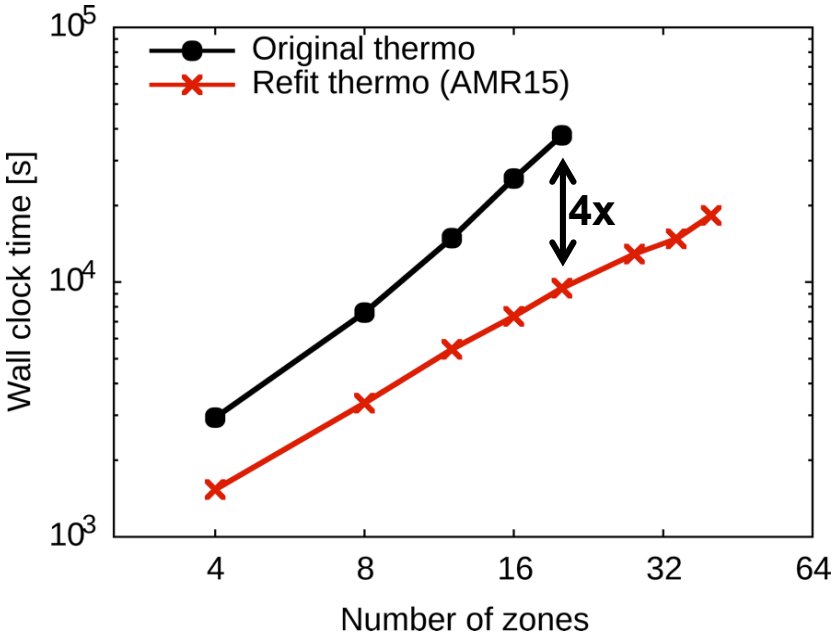




- Human inspection of any large changes still recommended
- Ignition delay calculations are also recommended to detect unusually high sensitivity to species thermodynamics
- Improved visual interface needed to speedup the human side of the workflow

AMR15 Accomplishment: Repaired thermodynamic properties accelerate coupled reactor models for the gasoline surrogate





- Every time a fluid dynamic cell or reactor zone crosses a discontinuity the solver time step can drop from 10^{-7} s to 10^{-13} s or smaller
- Independent reactors (*e.g.* CFD with operator splitting) with discontinuities add 25% in the computational cost where ignition occurs
- Stronger inter-zone coupling between dependent reactors with discontinuities results in much greater computational cost (up to 4x slowdown observed)

Response to AMR14 reviewers comments

AMR14 comments were generally positive (3.48/4 overall) with the reviewers posing the following questions:

1. *How does industry get access (and how much extra will it cost)?*

   We have 3 automotive users that are beta testing the ConvergeCFD interface (Cummins, GM & NVIDIA/JAMA). The engagements started by the industrial collaborators contacting us with problems that need faster detailed chemistry. LLNL's Industrial Partnerships Office is also updating its pathways for licensing to increase industry engagement (cost TBD).

2. *More HECC engine validation, please.*

   Validation studies were performed using experimental data from Mueller and Sjoberg's engine labs at SNL as part of the Whitesides ACE012 project. Validation was also performed using the RCM data in support of the Goldsborough ACE054 project. More validation is planned for FY16.

3. *Can it work with other codes like KIVA?*

   Yes, discussions with Carrington (LANL) have started, and we are in the process of defining the use cases and interface requirements for an efficient implementation. The chemistry solver also has an OpenFOAM interface.

4. *Will you have the necessary source code access to improve the species transport?*

   Yes, Convergent Sciences Inc (CSI) has agreed to provide source code access for the species transport algorithm as part of the negotiations for the pending Cummins/CSI/IU CRADA. The species transport algorithms will have a general interface to facilitate linking with other CFD software

5. *Have you made comparisons to tabulated flamelets?*

   Not yet, assessing the necessary number of chemical species for kinetically controlled engine design is an open question that we want our fast chemistry solvers to address. Prior exploration has been limited by the prohibitive cost of detailed chemistry and fluid dynamics. The new framework for accelerating fully-coupled chemistry and transport solvers will also speedup and simplify the process of generating flamelet tables for large fuel mechanisms.

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

- **Cummins**; CPU/GPU solvers for Converge CFD to run biodiesel engine simulations on new Indiana Univ. GPU supercomputer.
- **Ford**; gaseous direct injection, chemistry solver/mechanism assistance
- **Volvo**; multi-zone cycle simulation, OpenFOAM model development
- **Bosch**; High Performance Computing of HCCI/SI transition
- **GE Research**; new solvers applied to combustor turbine systems
- **Convergent Science Inc. (CSI)**; Multi-zone model development, thermo-chemical functions (CPU/GPU), adaptive preconditioners (CPU)
- **NVIDIA;** new GPU hardware, new GPU software & support for HECC simulations
- **Argonne National Laboratory**; mechanism debugging and sensitivity analysis
- **National Renewable Energy Laboratory;** microliter fuel ignition tester
- **Sandia National Laboratory**; experiment simulations for HECC validation
- **Universities**; UC Berkeley, Univ. Wisconsin, Univ. Michigan, UC Merced, Univ. Indiana, Louisiana St. Univ. Penn State Univ. and RWTH Aachen
- **Fuels for Advanced Combustion Engines (FACE);** working group
- **Advanced Engine Combustion (AEC);** working group (Industry, National labs, Univ. of Wisc., Univ of Mich., MIT, UC Berkeley); semiannual presentations

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

FY15 – [Q3 Milestone] Complete framework to accelerate a fully coupled transport and chemistry solver

FY15 – [Q4 Milestone] Apply the accelerated framework to the opposed diffusion flame model used in mechanism design

FY15 – [Q4 Milestone] Benchmark the fully coupled framework against operator splitting techniques used in design simulations

Proposed supports multiple VTO R&D efforts

FY16 – Accelerate multispecies diffusion and advection algorithms

- Direct algorithm improvements
- New GPU transport algorithms
- Reduced order models with error control

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

Planned future solvers for CFD

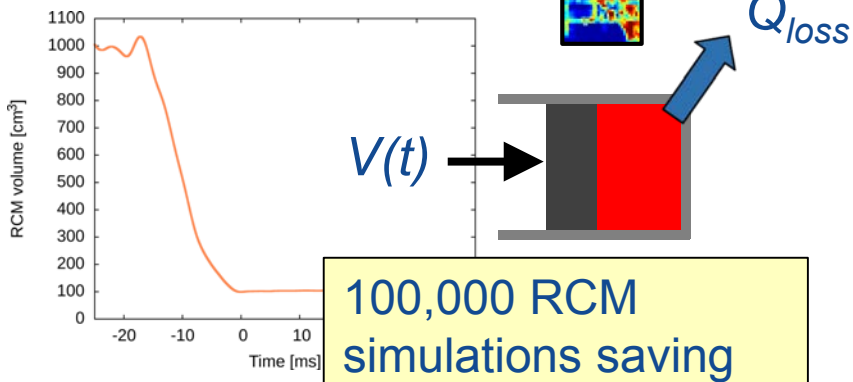
FY16/17 – Accelerate detailed spray dynamics algorithms

FY16/17 – Accelerate soot model algorithms

FY16/17 – Chemistry-turbulence models for detailed fuel chemistry

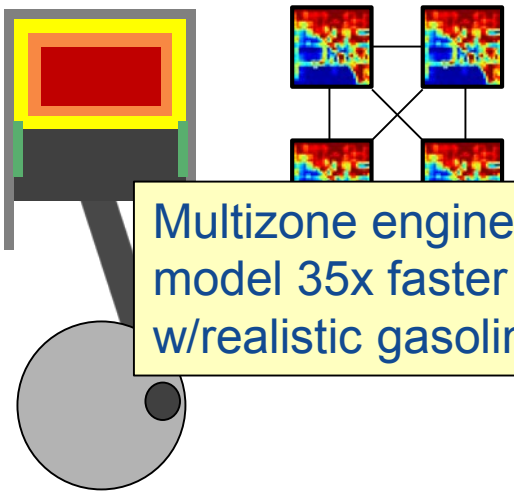
Summary: LLNL has extended the high performance chemistry solvers to several applications impacting the ACE R&D workflow

Variable Volume Reactor



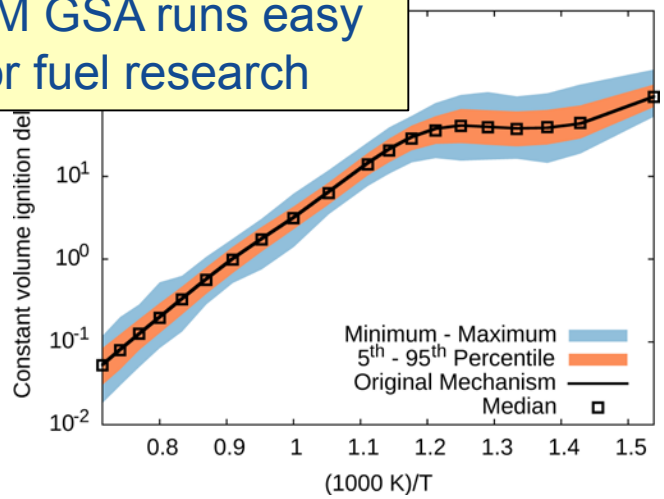
100,000 RCM simulations saving ANL 300 CPU-years

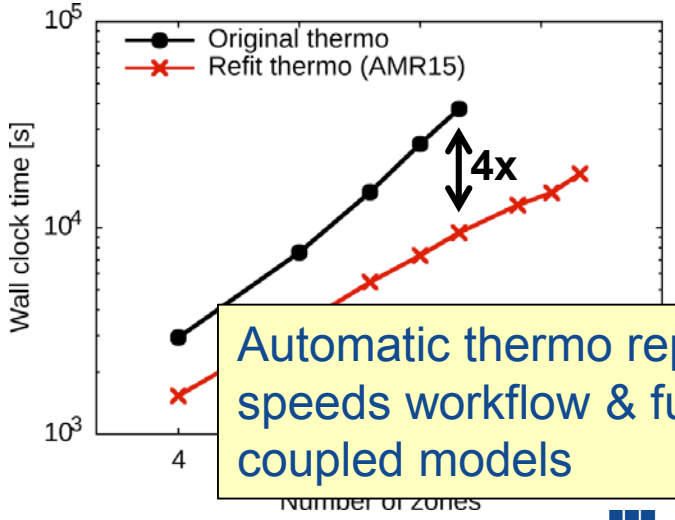
Quasi-Dimensional Multizone



Multizone engine model 35x faster w/realistic gasoline

1M GSA runs easy for fuel research

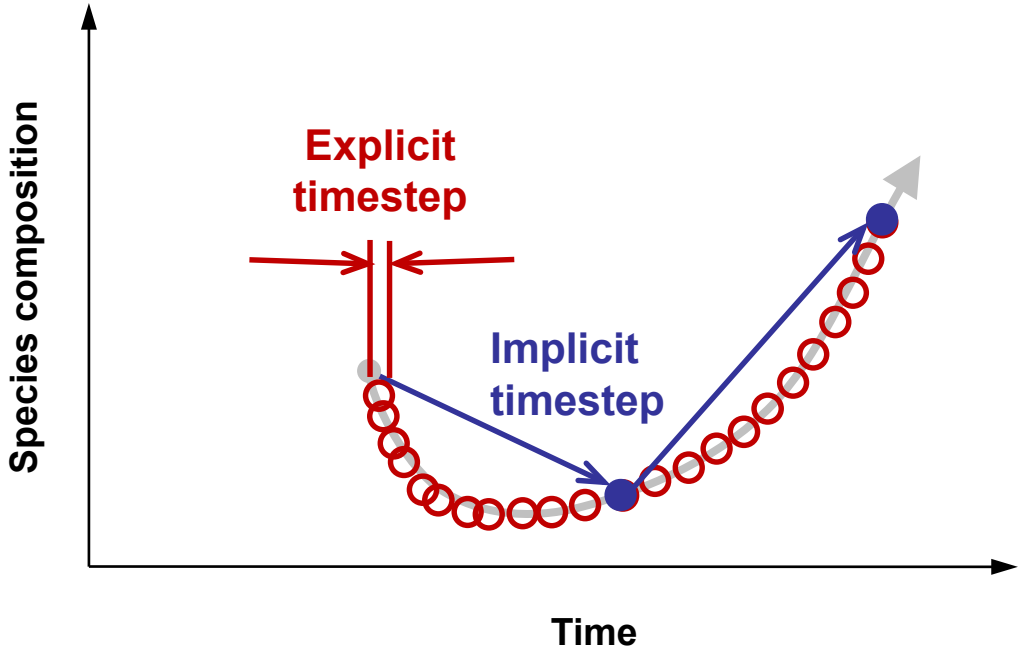




Automatic thermo repair speeds workflow & fully coupled models

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?

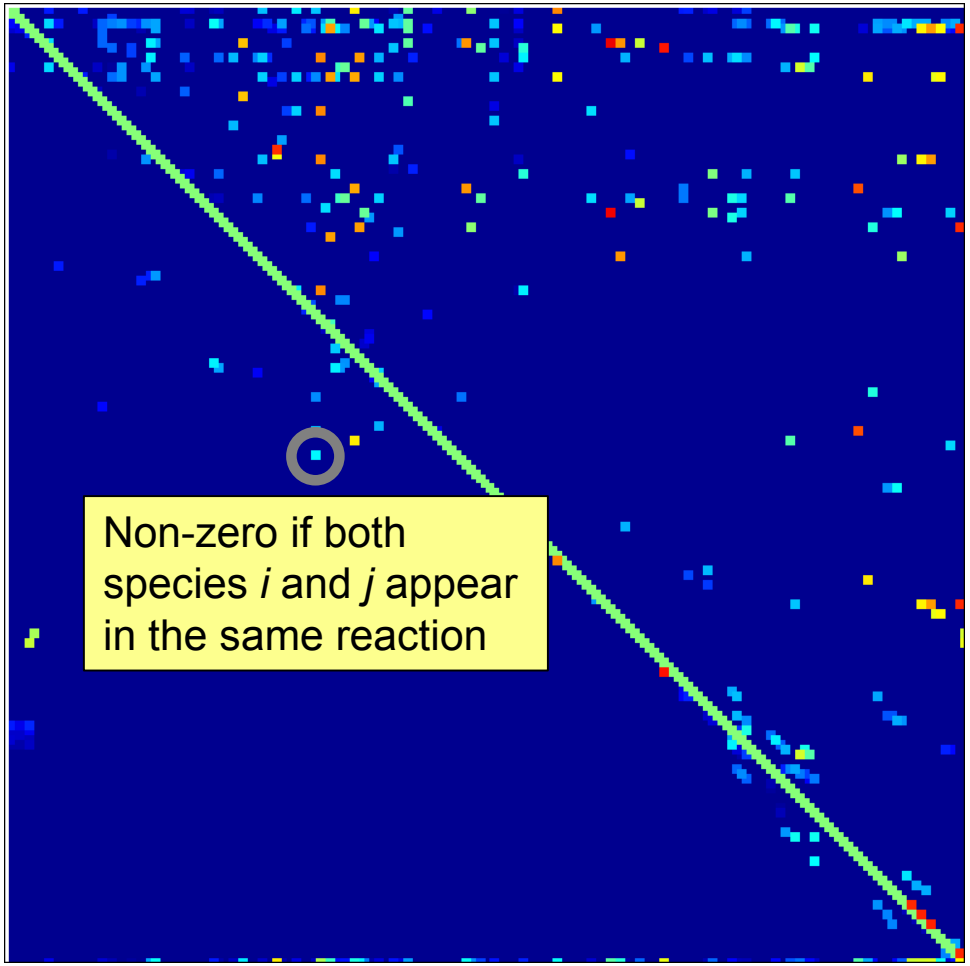
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

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

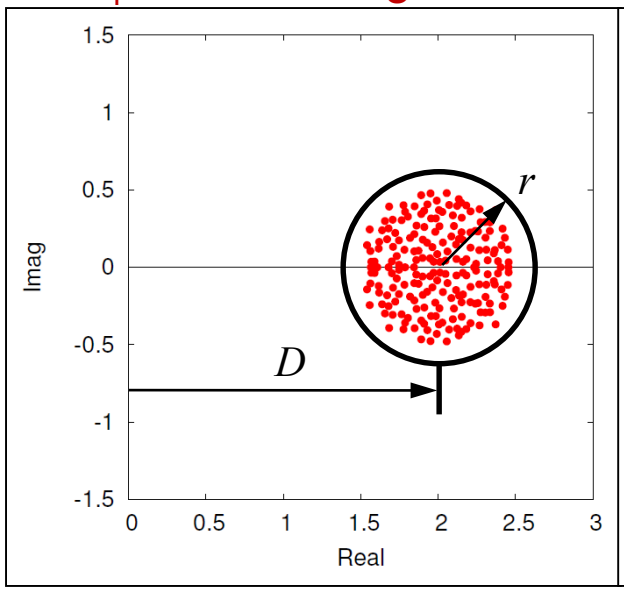
Generalized **M**inimal **RES**iduals

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

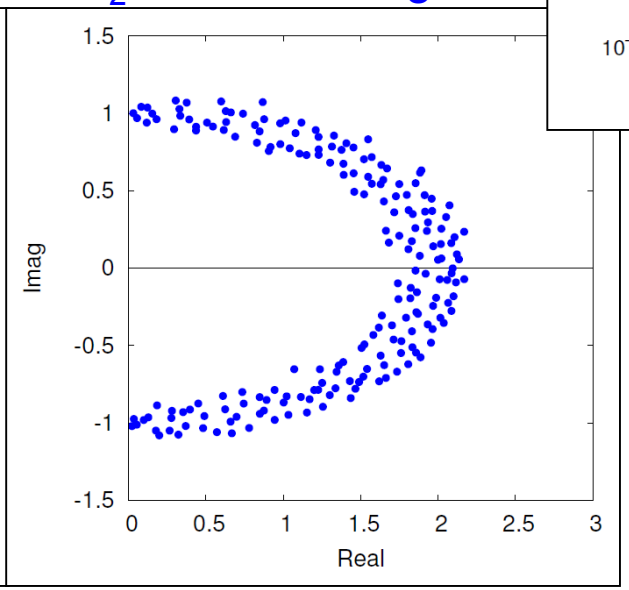
$$\Lambda \approx \frac{r}{D}$$

Eigenvalue Spectra (200 x 200)

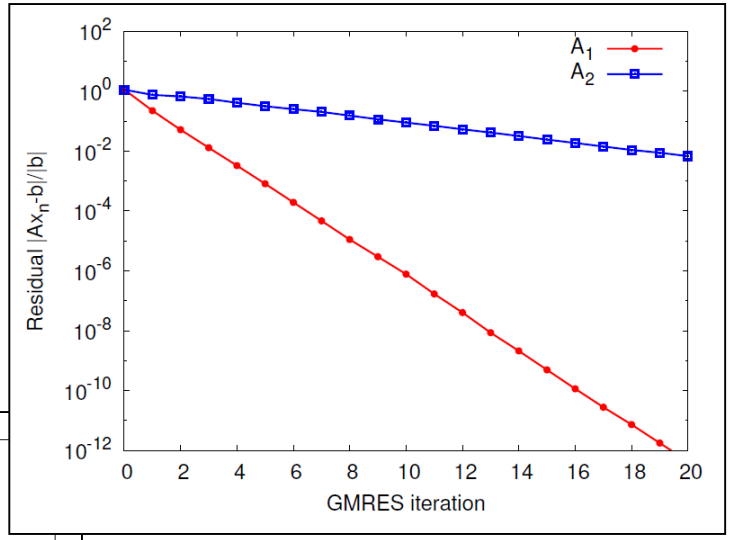
A_1: fast convergence



A_2: slow convergence



GMRES Error

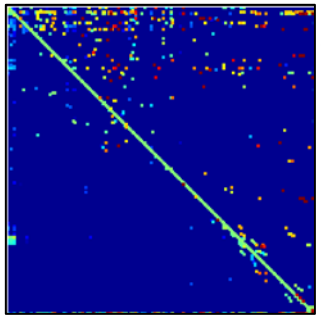


Adaptive preconditioner using on-the-fly reduction produces the same solution significantly faster

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.)

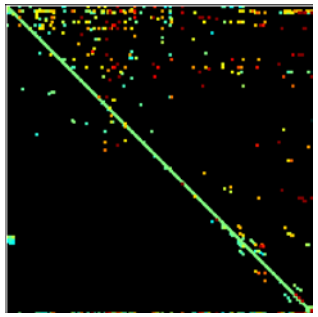
slower ⟷ faster

1. Classic mechanism reduction:

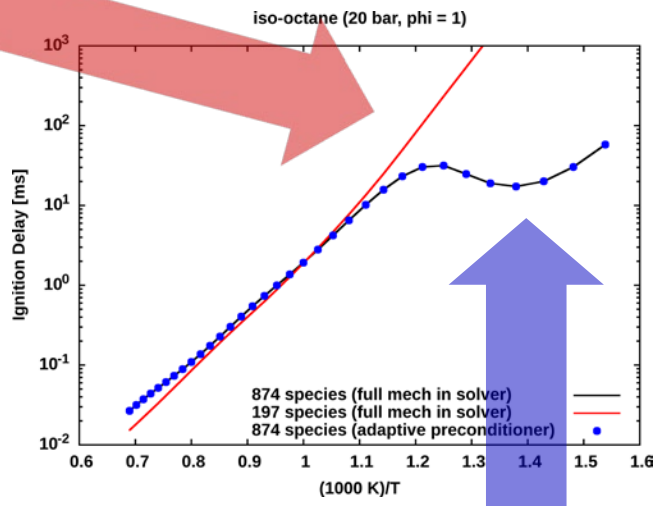
Ex.197 species 

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

2. LLNL's adaptive preconditioner:

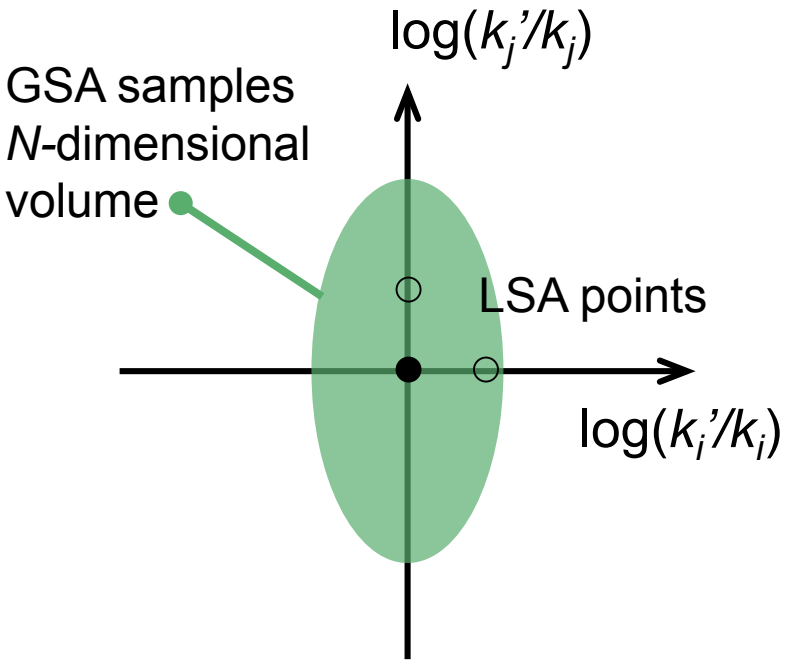


- *Identical ODE*
- Reduced mech *only* in preconditioner



Filter out 50-75% of the least important reactions

Global sensitivity analysis (GSA) allows the rate constant uncertainty and reaction coupling to be explored simultaneously



Brute force A-Factor provides local sensitivity (LSA)

Updated LLNL gasoline surrogate

p = 20 bar, T = 800 K