Lawrence Livermore National Laboratory

Improved Solvers for Advanced Engine Combustion Simulation

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Project ID # ACE076

2014 DOE Vehicle Technologies Program
Annual Merit Review and Peer Evaluation Meeting
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LLNL-PRES-653560

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Overview

Timeline

- Ongoing project with yearly direction from DOE

Budget

- FY12 funding: $340K
- FY13 funding: $340K
- FY14 funding: $475K

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

- Ford, GM, Bosch, Volvo, Cummins, Convergent Sciences & NVIDIA
- Argonne NL, Sandia NL, Oak Ridge NL
- UC Berkeley, U. Wisc., U. Mich., LSU, Indiana U. & RWTH Aachen
- FACE working group, AEC MOU, SAE, Combustion Inst., GPU Tech. Conf. & NSF HPC software planning

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:

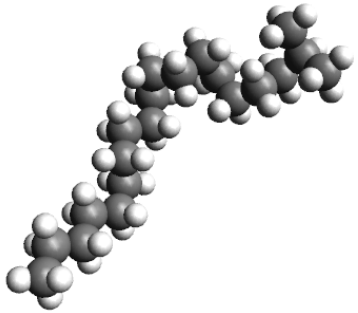
A. *Lack of fundamental knowledge of advanced engine combustion regimes*

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

D. *Lack of effective engine controls*

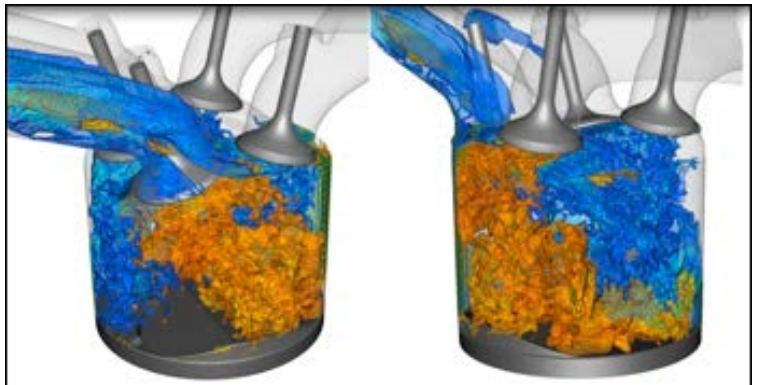
We want to use…

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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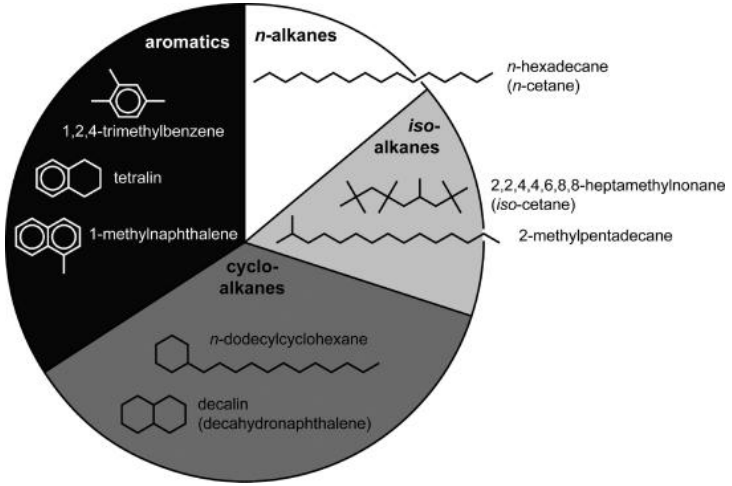

Ex. 9-component diesel surrogate (AVFL18)
C. Mueller et al. Energy Fuels, 2012.
+10K species
+75K reaction steps

in highly resolved 3D simulations

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

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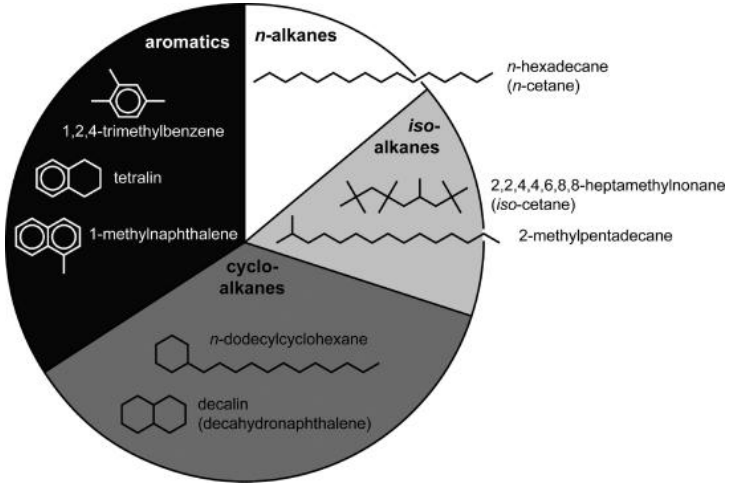
Create faster and more accurate combustion solvers.

AMR14 achievements:

- Completed initial scaling analysis of chemistry/transport in engine CFD
- Completed multiprocessor reaction sensitivity tool for fuel researchers
  – *reduces wait from days to under an hour*
- Established new partnership with NVIDIA for support and hardware developing engine simulations on GPUs
- Demonstrated beta version of mechanism diagnostic/debugging tool

Now we want to use…

Detailed chemistry



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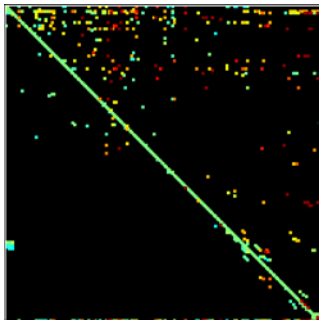
+10K species
+75K reaction steps

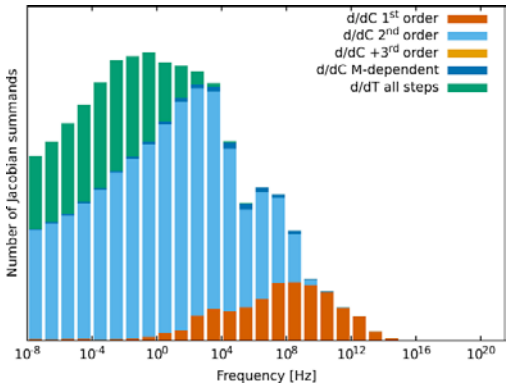
Approach – Accelerate research in advanced combustion regimes by developing faster and more predictive engine models



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)

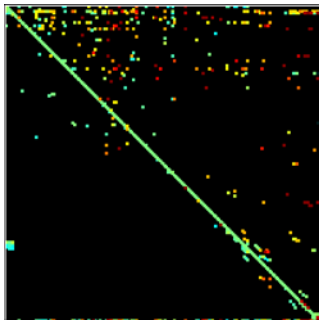


3. **Improved physical models**
   – more accuracy, better error control

Approach – FY14 milestones

Qtr	Due Date	Type	Milestones	Status
Q1	12/31/2013	Regular	Detailed algorithm analysis and profiling for multi-species transport	Completed
Q2	3/31/2014	Regular	Create a chemistry tool for the reaction rate sensitivity analysis using LLNL's adaptive preconditioners	Completed
Q3	6/30/2014	Regular	Create a chemistry tool for reaction pathway analysis and error detection using LLNL's advanced combustion algorithms	Beta Version Running
Q4	9/30/2014	Regular	Improve every-cell chemistry calculation on the GPU	On Schedule

Accomplishment Outline



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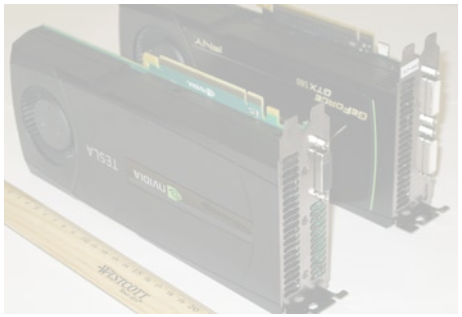

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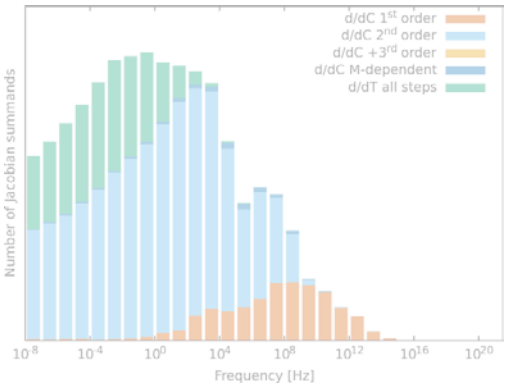

3. **Improved physical models**
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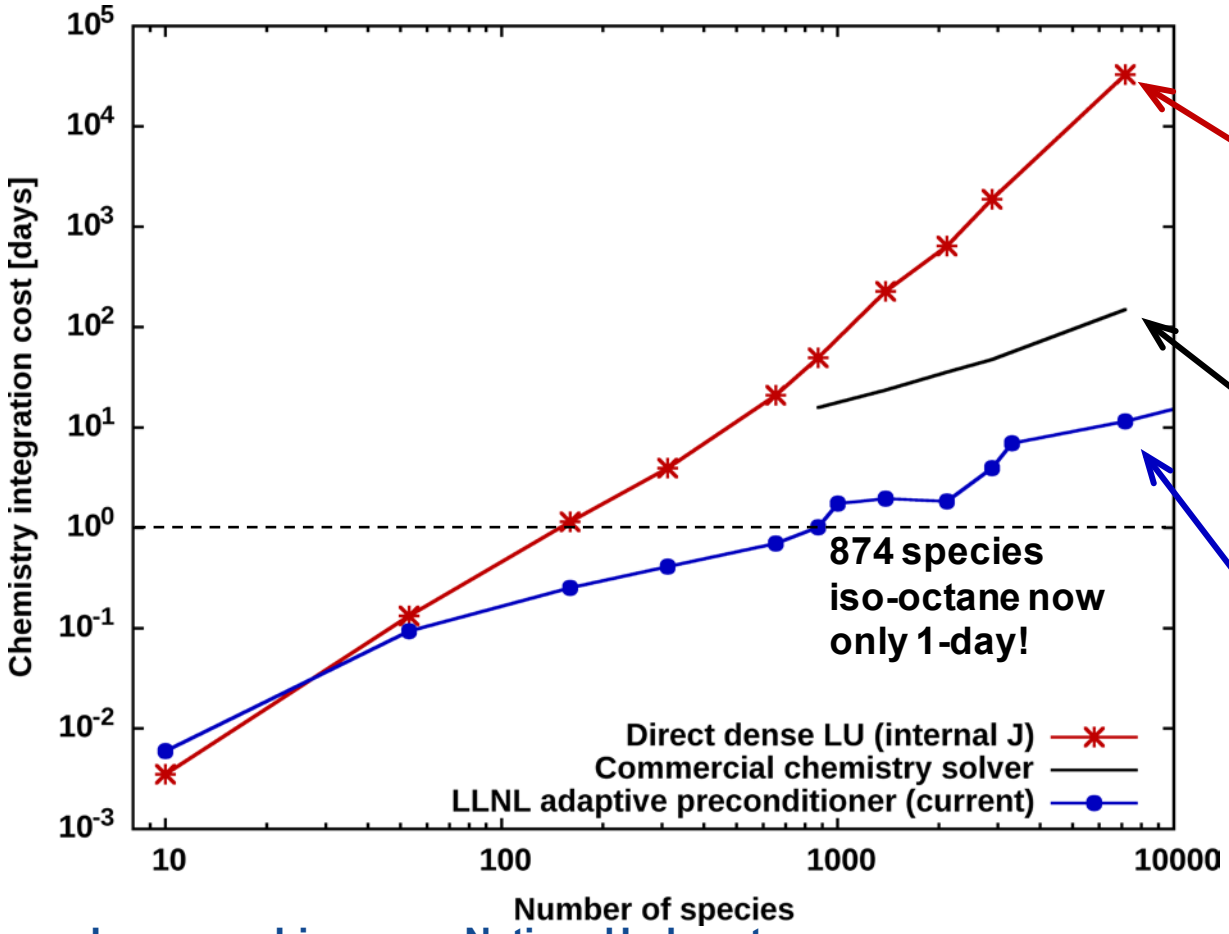
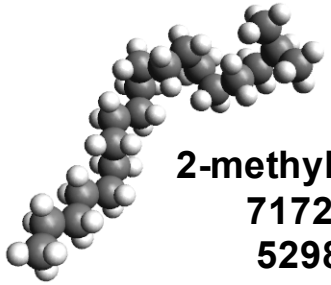
AMR13 Accomplishment: LLNL's new solver brings well-resolved chemistry and 3D CFD to 1-day engine design iterations

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

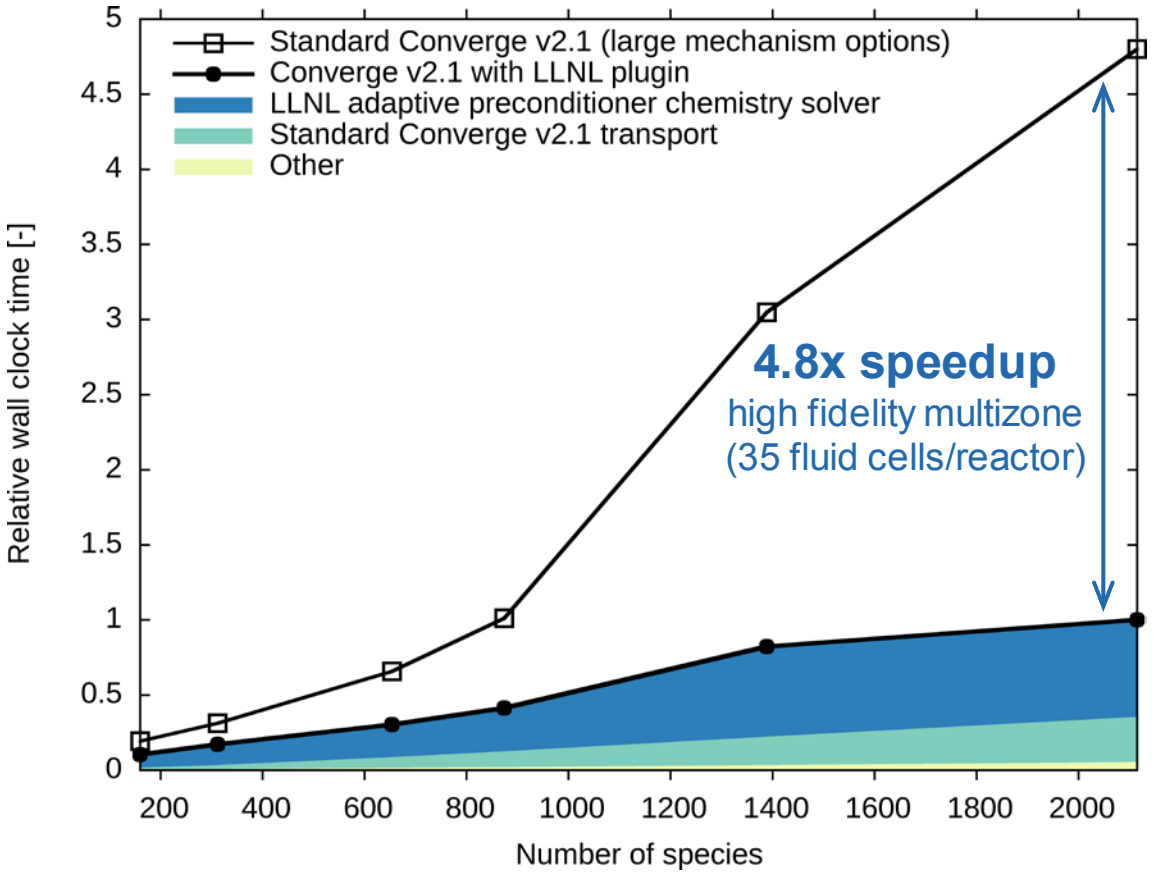
- 150 days

New LLNL solvers created for ACE program FY13

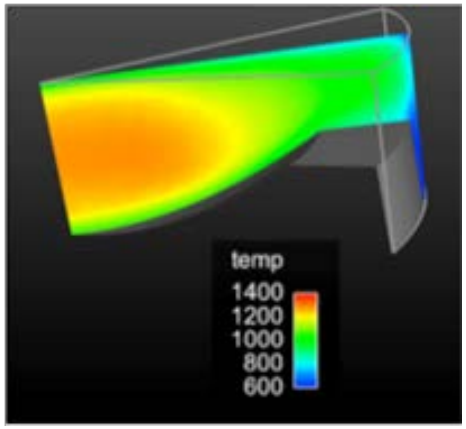
- 11 days

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

AMR14 Accomplishment: analysis of multispecies transport algorithms in engine CFD using accurate fuel chemistry

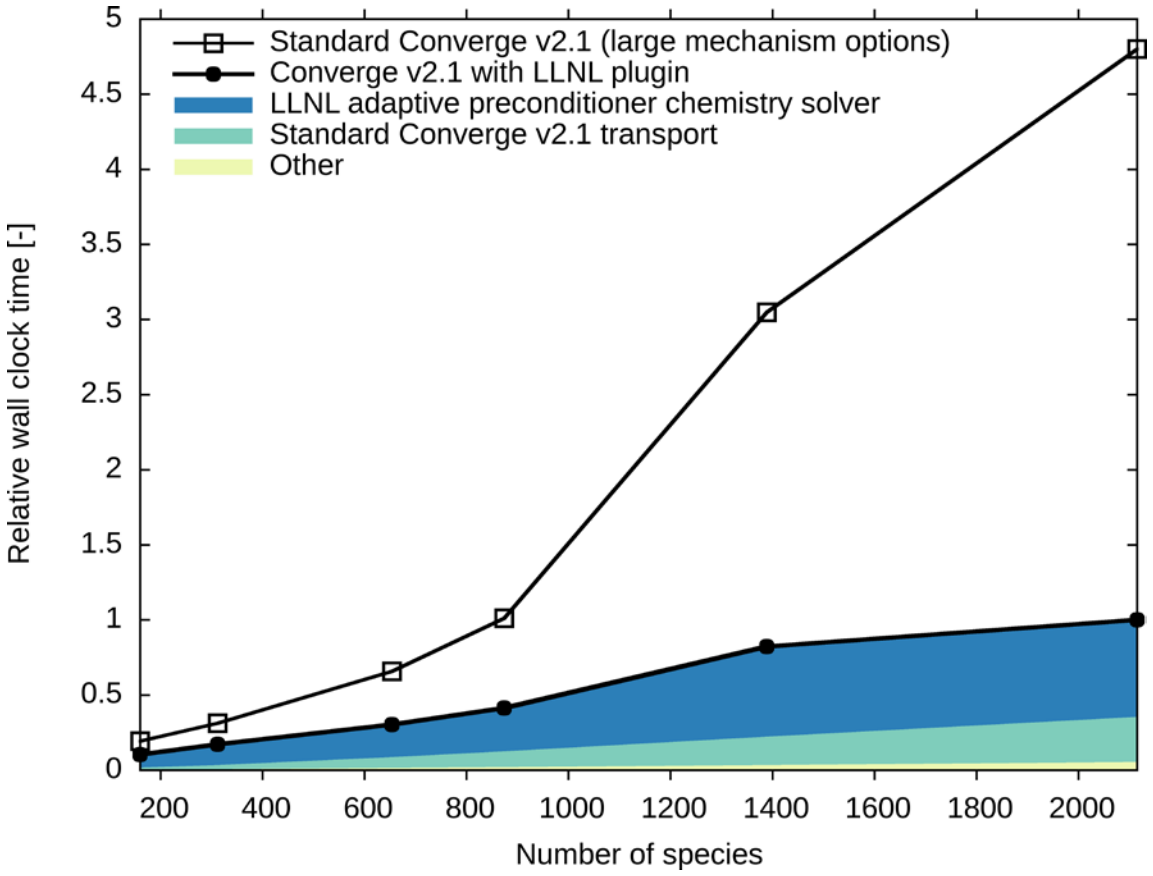


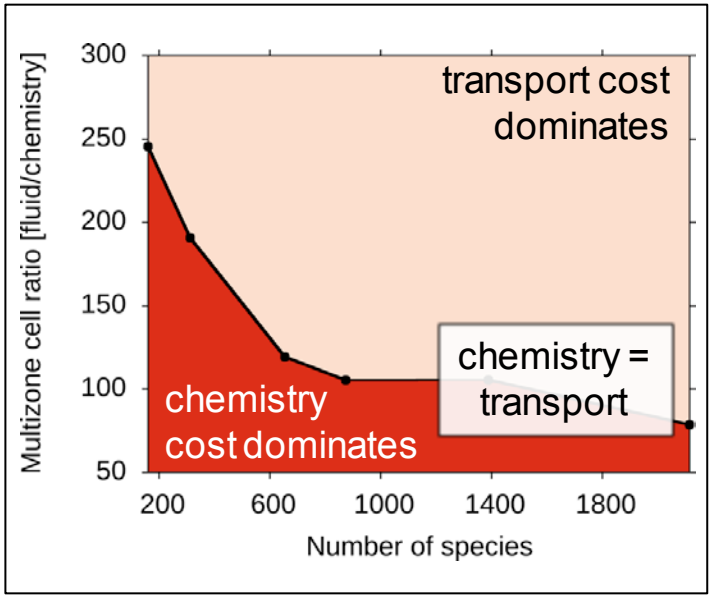
HCCI Engine (J. Dec)



- Detailed fuel mechanisms:
  - n-heptane (160/654 species)
  - iso-octane (874 species)
  - n-hexadecane (2115 species)
  - E85 surrogate (312 species)
  - Gasoline surrogate (1389 species)
- Lean burn (ϕ = 0.4)
- High EGR (50%)
- Initial temperature set to match ignition time

AMR14 Accomplishment: detailed algorithm analysis reveals when the chemistry and transport calculation costs are dominant





Detailed algorithm costs found using HPCToolkit (Mellor-Crummey, Rice):

- The transport and chemistry cost the same when there are 100-250 fluid cells per multizone reactor (+150 species).
- Saved considerable development time because HPCToolkit can measure optimized and precompiled software.
- Analysis provides crucial guide for future algorithm research.

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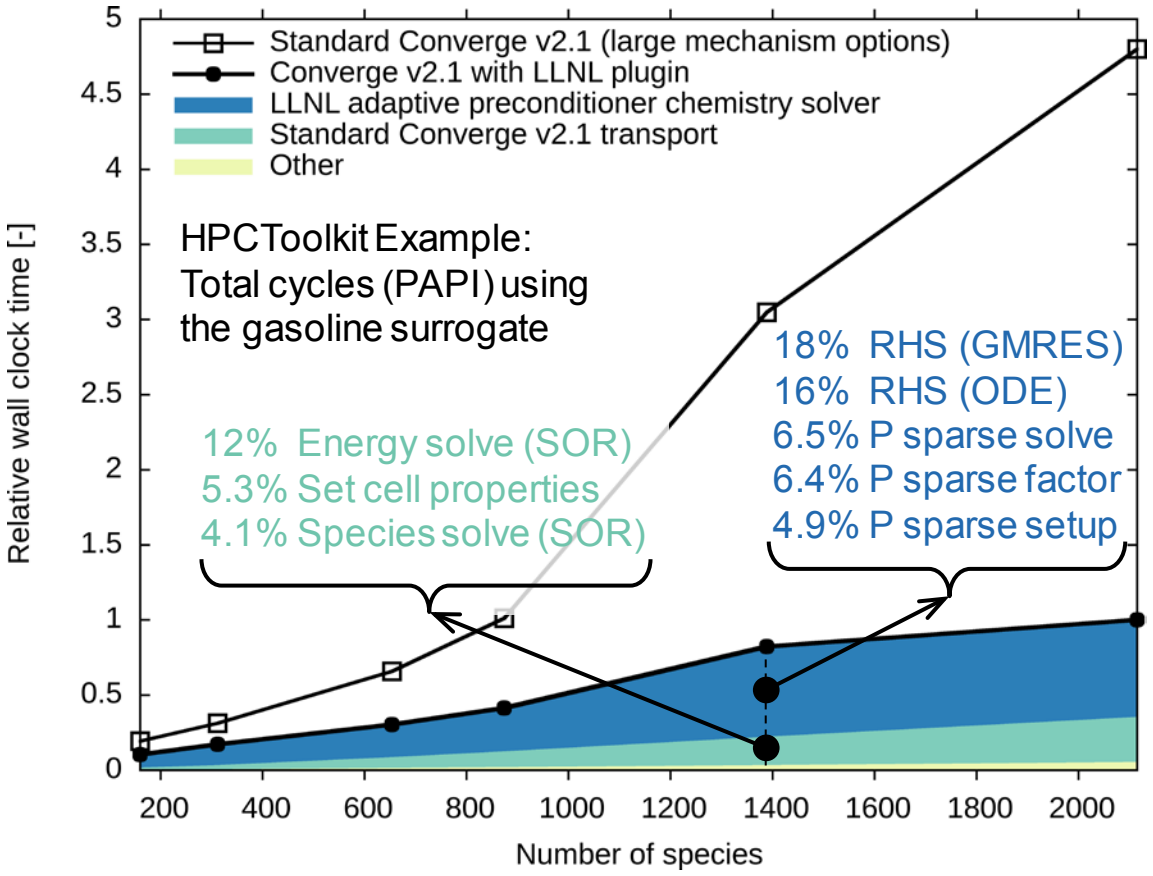

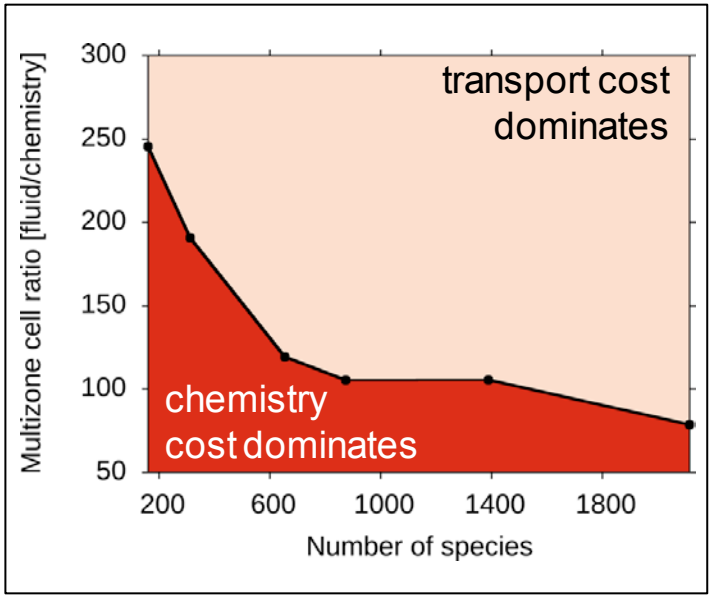

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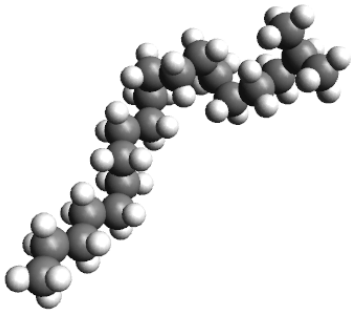
The concepts advanced in this project are applied to mechanism development tools to eliminate other bottlenecks in HECC R&D

State-of-the-art mechanisms must be developed and maintained with considerable care:

$C_{20}H_{42}$ (LLNL)

7.2K species

53K reaction steps



How much data?

- mechanism file 4MB (64K lines)
- thermodynamics file 8MB (104K lines)

The challenge from a publishing standpoint is equivalent to printing *9.5 combustion textbooks** with zero typos.

* equivalent length of Warnatz, Maas & Dibble, *Combustion*.

How can the advanced combustion numerics project help?

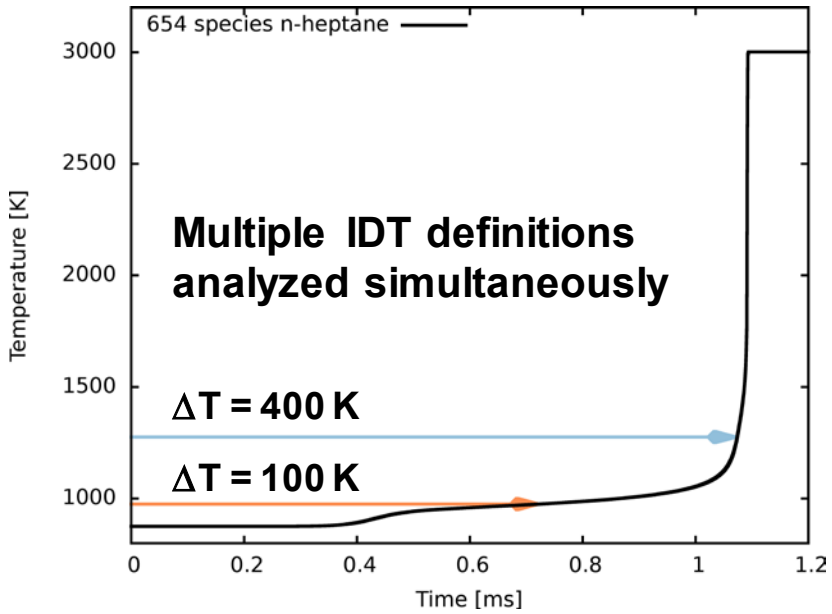
- Accelerate fuel development models using LLNL's adaptive preconditioner approach (*e.g.*, flame speed, 1D diffusion, piston model, RCM model, *etc.*)
- Create mechanism debugging tools by leveraging the analysis used to speedup the combustion algorithms

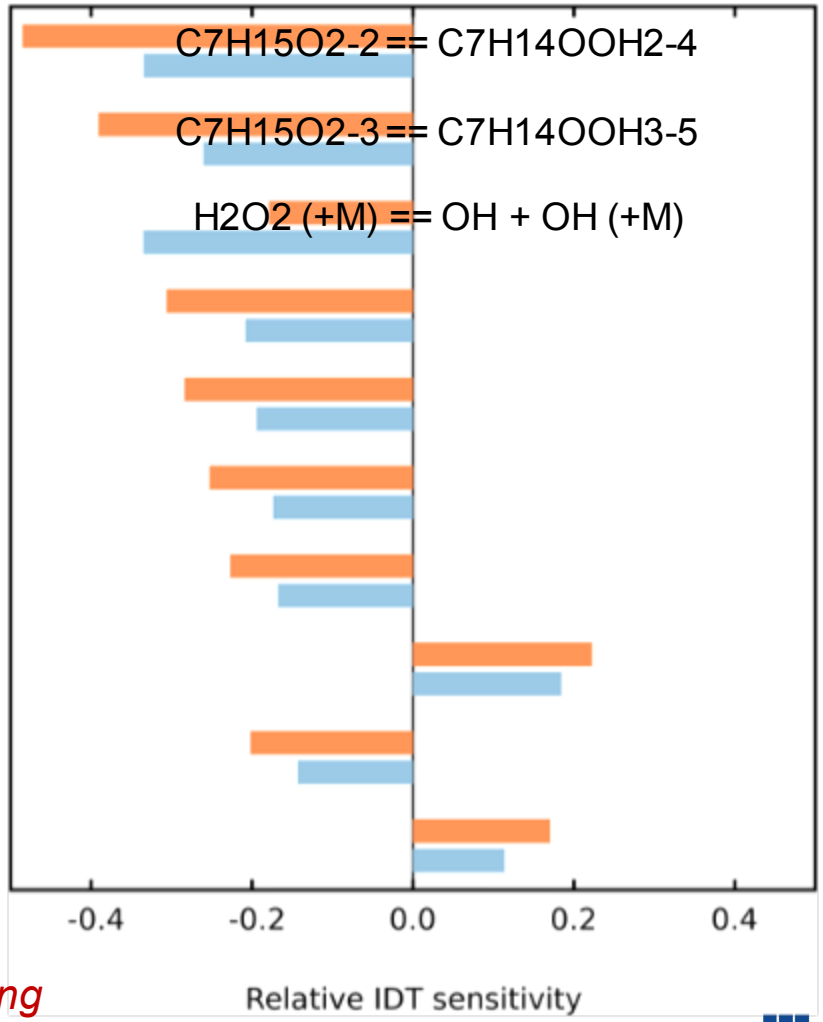
Top priority (Pitz): A-Factor sensitivity

$$k = AT^n \exp(-E_a / RT)$$

Brute force ignition delay calculation perturbing each reaction's A-factor independently

AMR14 Accomplishment: Single-core version of A-factor sensitivity is an order of magnitude improvement over current commercial tools





n-heptane (LLNL):

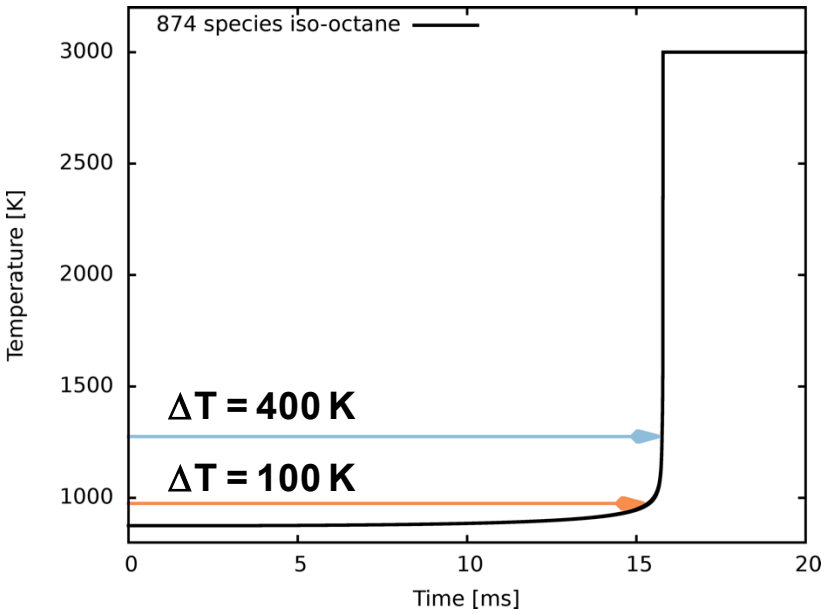
654 species

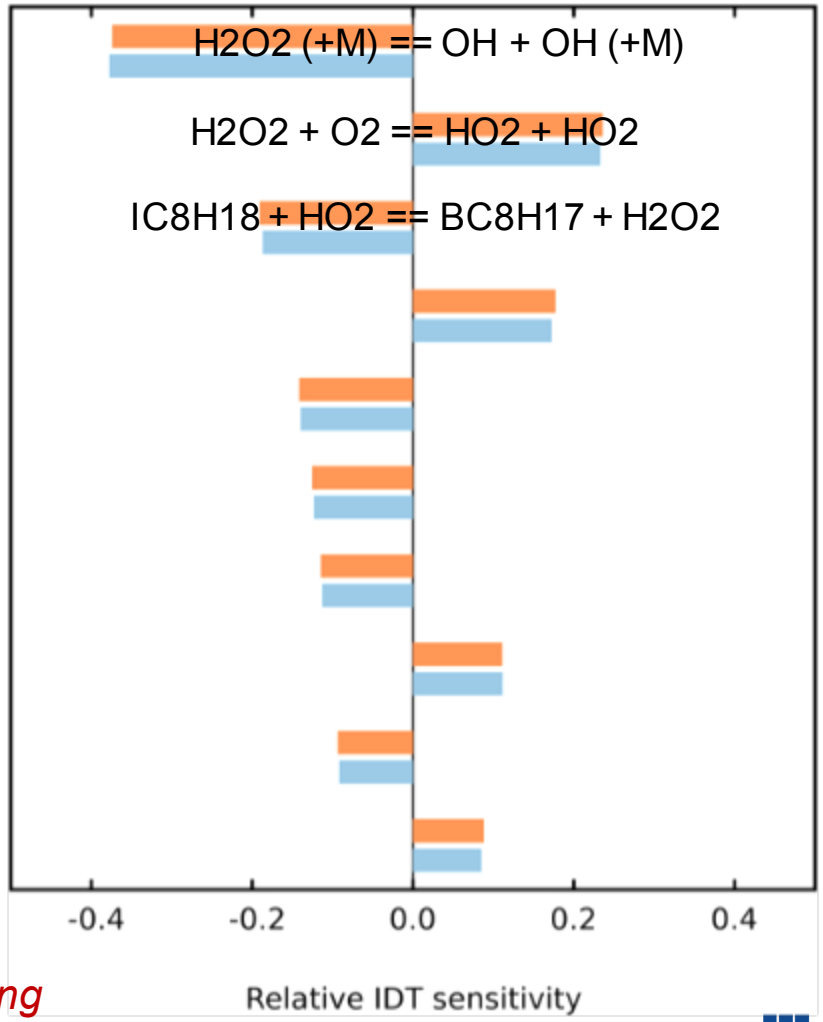
2827 reactions

64 seconds (96 CPU cores)

Previously required days to weeks of waiting

AMR14 Accomplishment: Multi-core version of the A-factor sensitivity delivers seamless scalability to the available computing resources





iso-octane (LLNL):

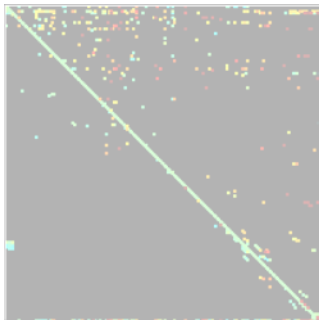
874 species

3796 reactions

104 seconds (96 CPU cores)

Previously required days to weeks of waiting

Accomplishment Outline



1. Better algorithms and applied mathematics
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2. **New computing architecture**
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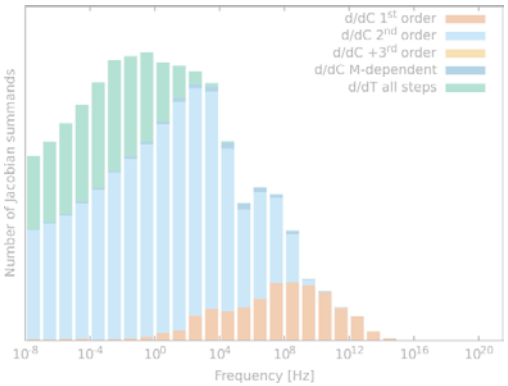
Accomplishments discussed in more detail in Whitesides' presentation (ACE012)



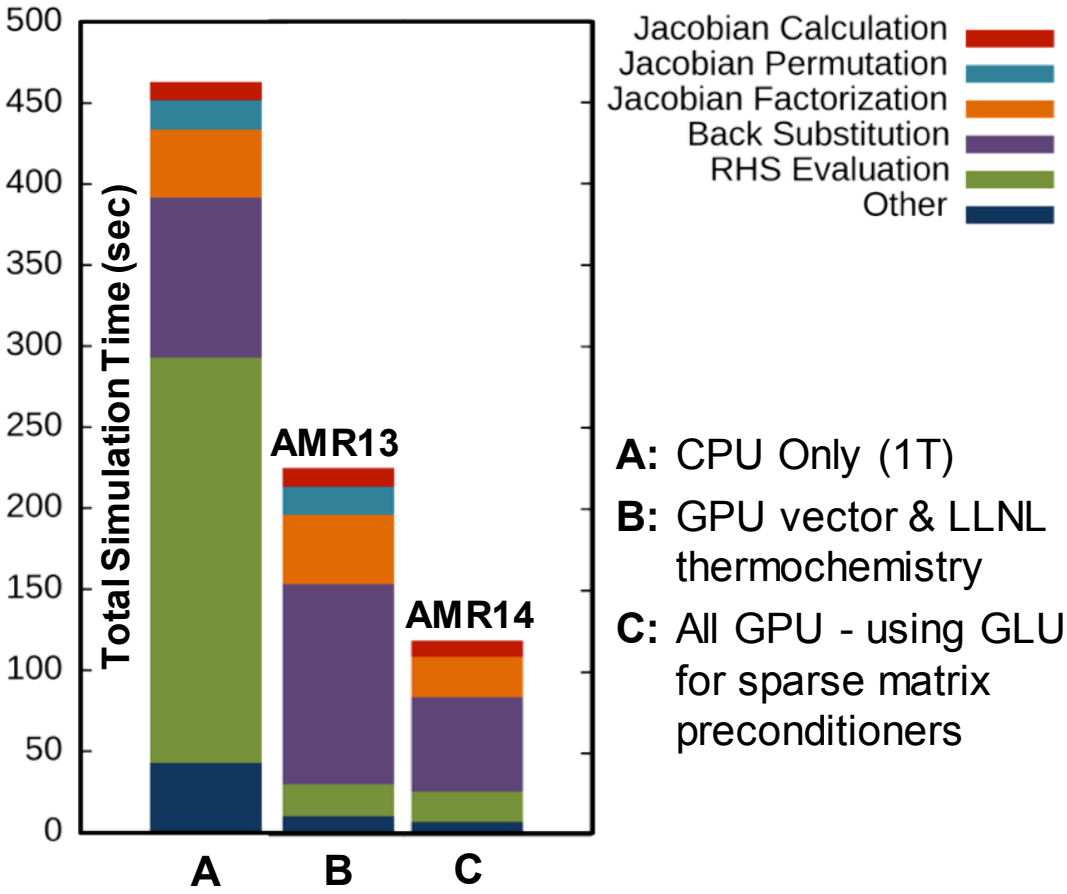
3. Improved physical models
   – more accuracy, better error control

AMR14 Accomplishment: Established a new partnership with NVIDIA for support and hardware developing engine simulations on GPUs

New Tesla K20 GPUs w/2,496 CUDA cores provided for testing

LLNL used NVIDIA's GLU sparse matrix solver to create a 100% GPU-based multizone solver:

- GLU developed internally at NVIDIA by Naumov & Chetlur
- original application is for circuit simulations (SPICE)
- contains direct sparse solvers for non-symmetric matrices
- LLNL given early access (beta tester)
- latest update includes recommended features to speedup *engine CFD simulations*



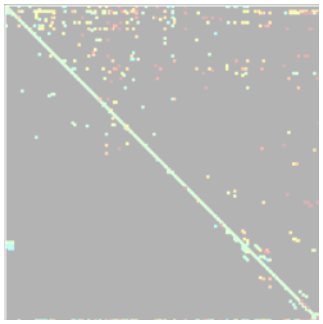
A: CPU Only (1T)

B: GPU vector & LLNL thermochemistry

C: All GPU - using GLU for sparse matrix preconditioners

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

Accomplishment Outline



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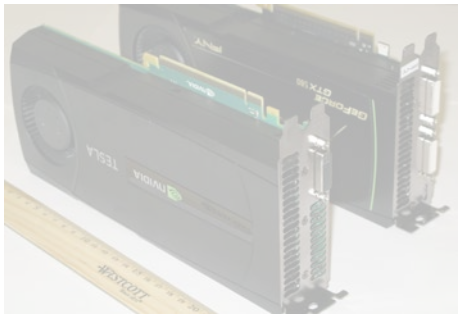

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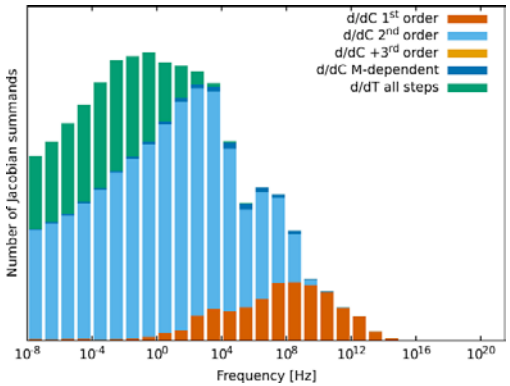


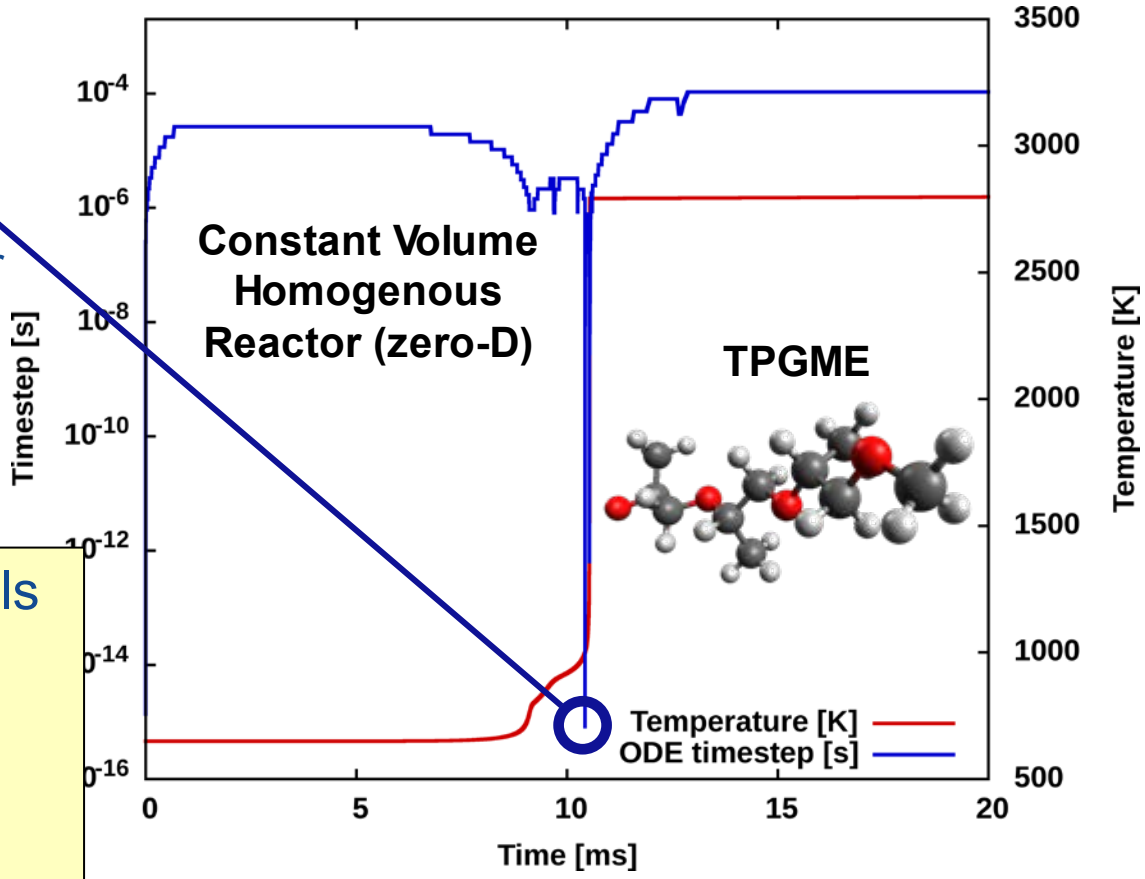
3. **Improved physical models**
   – more accuracy, better error control

Ignition delay solver is augmented to provide a detailed report of the system state when the ODE integrator issues any warning or error

Report includes:

- thermodynamic state
- thermodynamic derivatives
- ODE state convergence error
- Jacobian terms (every rate-of-progress derivative)

Setting tight accuracy controls can reveal species and reactions that impact solver performance in even well-behaved mechanisms

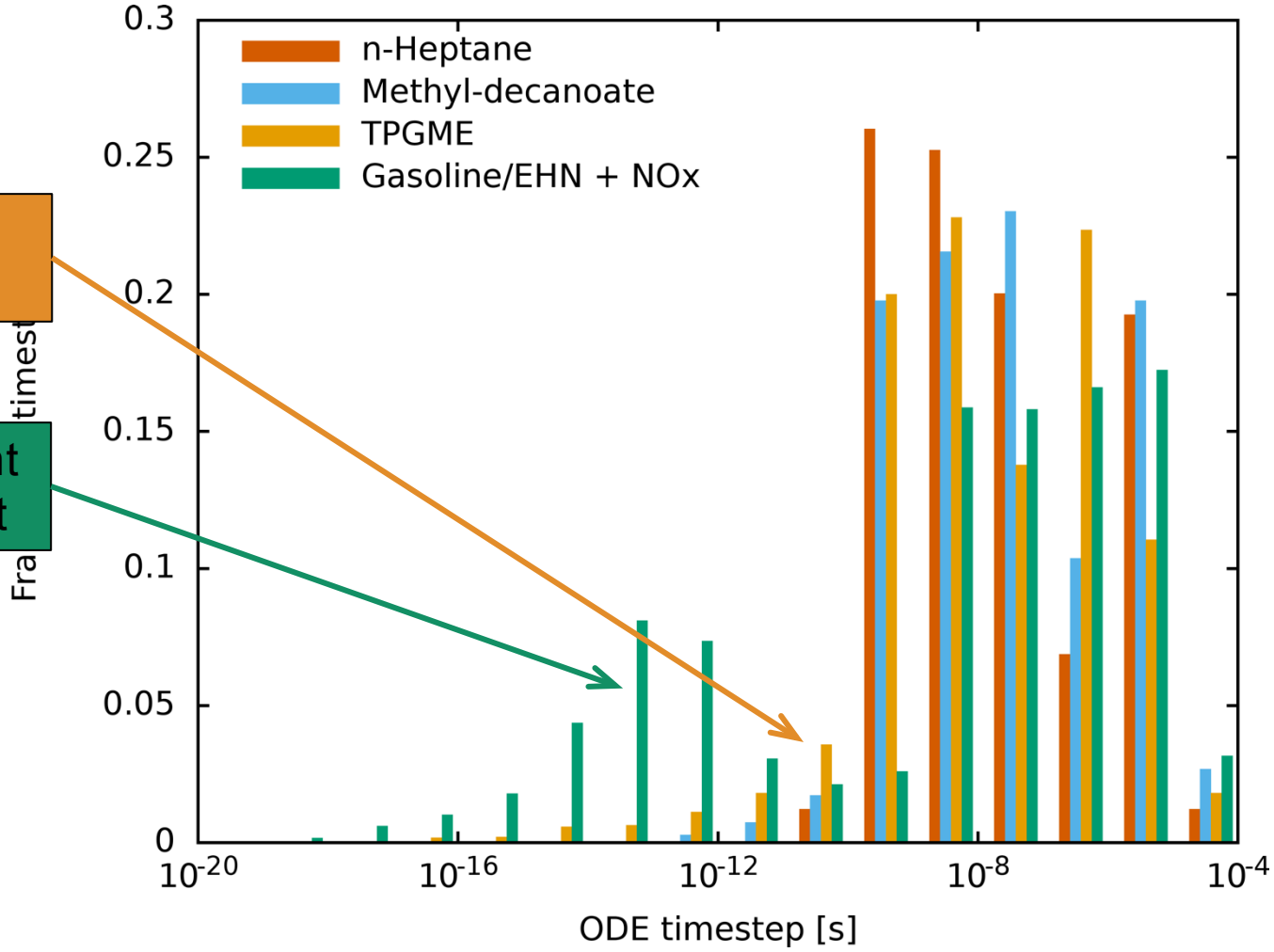


Analyzing the computational workload for the ODE solver can detect mechanism problems affecting accuracy and robustness

Examples:

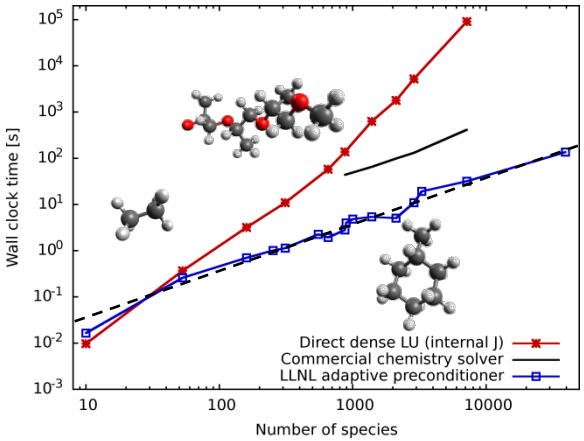
Thermodynamic discontinuities

Reverse rate constant (bimolecular) too fast

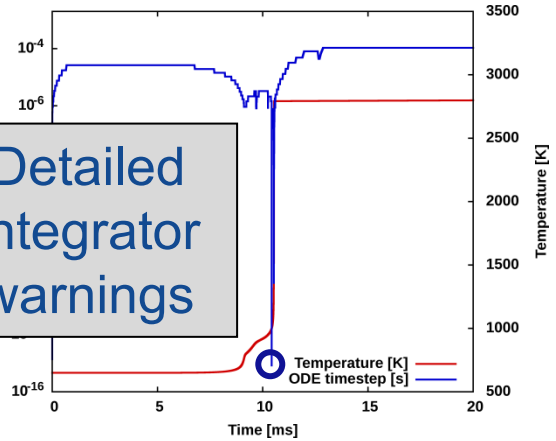


AMR14 Accomplishment: we have created a suite of new tools using our high performance chemistry solver to aid in fuel mechanism design

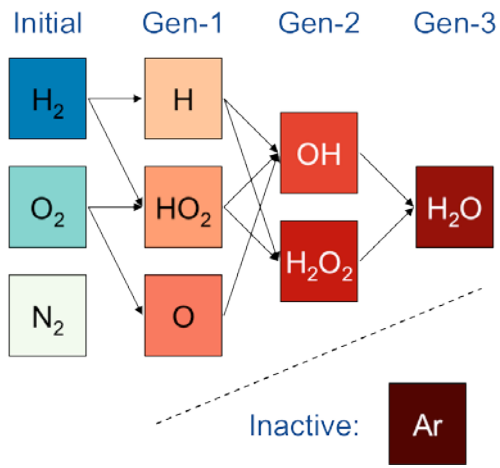
PLOG reactions



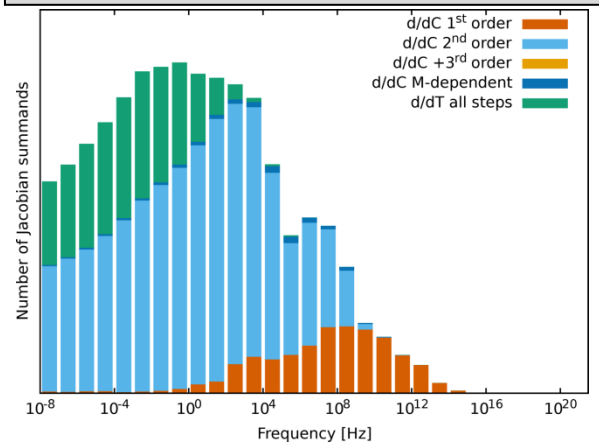
Detailed integrator warnings



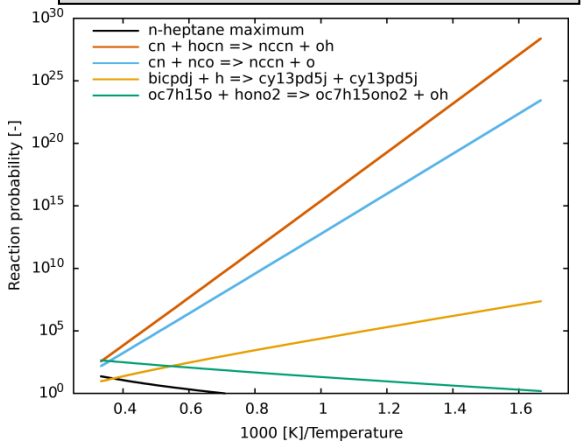
Connectivity analysis



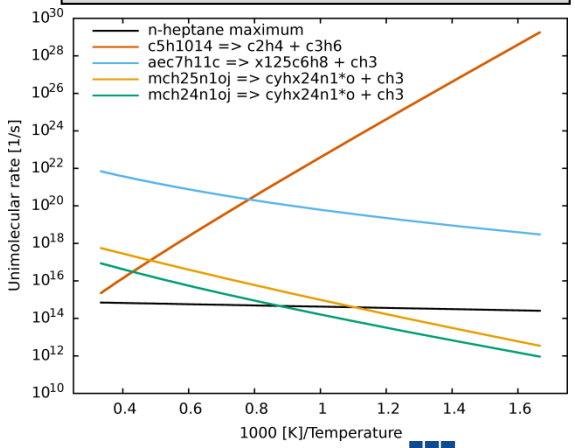
Detailed Jacobian data



Reaction probability



Unimolecular rates



Response to reviewers comments

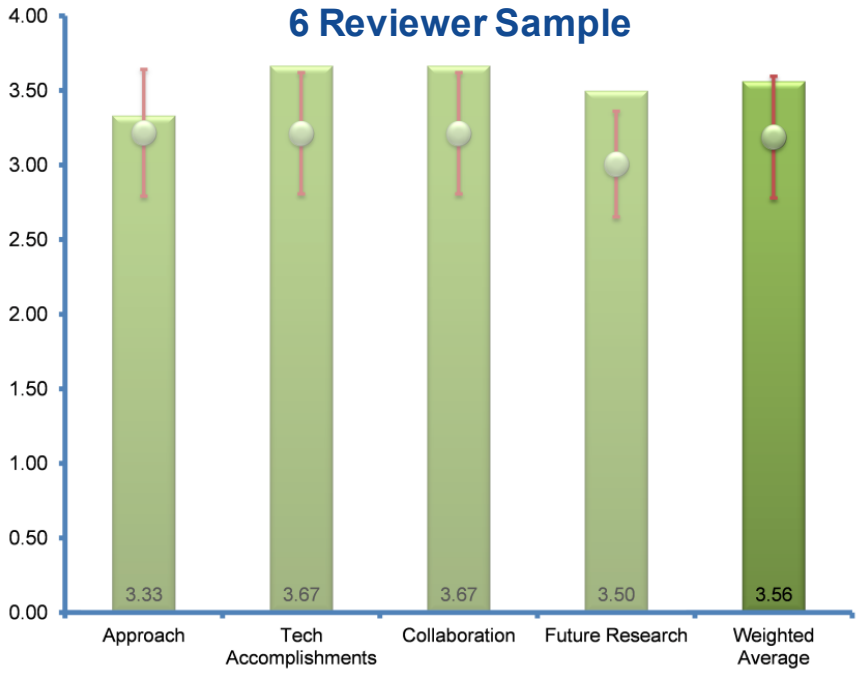
AMR13 comments were generally positive with the reviewers posing three basic questions:

1. *Is it correct?*

The LLNL thermochemistry library has been verified against other available solvers (Cantera, Chemkin & TChem) and is found to agree to within a relative tolerance of $O(10^{-4})$ – corresponding to the difference in molecular weights and physical constants. The adaptive preconditioner solver has been verified against traditional direct approaches. The ignition delay times and major species concentrations have a relative accuracy within an order of magnitude of the integrator tolerance and typically achieve an accuracy of $O(10^{-7})$.

2. *Has it been validated for HECC engines?*

The simulation validation for HECC engines is led by the ACE-012 project at LLNL, and is featured in Whitesides presentation at AMR14. We actively collaborate to ensure that the new solvers are applicable to engine CFD simulation, with this project leading the verification effort.



3. *Do you still need to speedup chemistry?*

Depends on the number of multizones needed to accurately resolve combustion (see slide11). While this remains an open question, there are a number of simulations used in industry where the CFD transport is the dominant cost. This project is shifting its focus to accelerate other bottlenecks in HECC research: multispecies transport in CFD; mechanism development and debugging; and detailed spray dynamics.

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 HCCI and PCCI
- **Universities**; UC Berkeley, Univ. Wisconsin, Univ. Michigan, UC Merced, Univ. Indiana, Louisiana St. 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 – We will continue to explore strategies for improving efficiency and accuracy of chemistry and engine CFD

Ongoing

FY14 – [Q3 Milestone] Complete the mechanism diagnostic and debugging suite of tools

FY14 – [Q4 Milestone] Improve high fidelity multizone chemistry on the GPU for engine CFD simulations

FY14 – Continue to improve availability within the MOU for the new solvers – pursue online version of mechanism diagnostic tools

Proposed supports diesel research in ACE012, ACE013

FY15 – Accelerate multispecies diffusion and advection algorithms

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

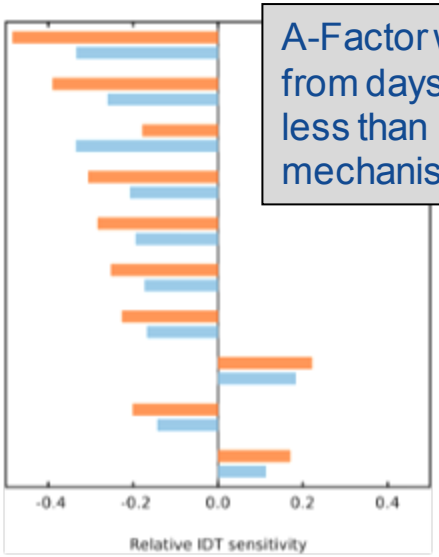
FY15 – Add more applications to the turnkey package of the chemistry solvers (diffusion flames, extinction, sensitivity, *etc.*)

Planned future solvers for use in CFD packages

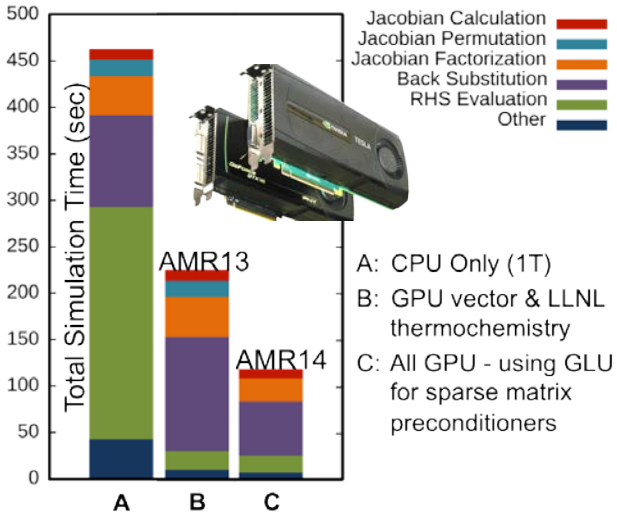
FY15/16 – Rigorous error analysis of the multizone combustion solver for direct user control

FY15/16 – Accelerate detailed spray dynamics algorithms

Summary: The advanced combustion numerics project completed several key tasks toward the program's objectives for HECC R&D

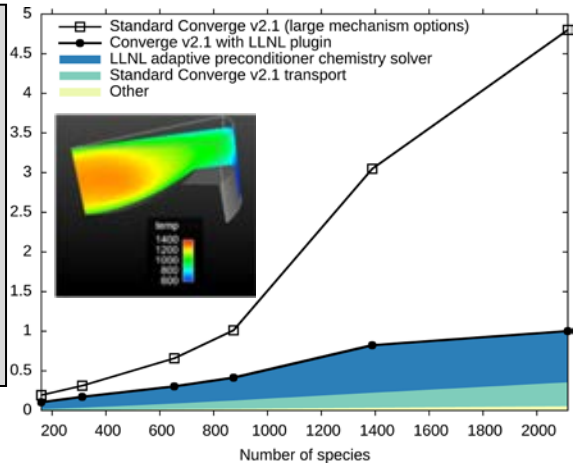


A-Factor wait time reduced from days (even weeks) to less than an hour for fuel mechanism developers



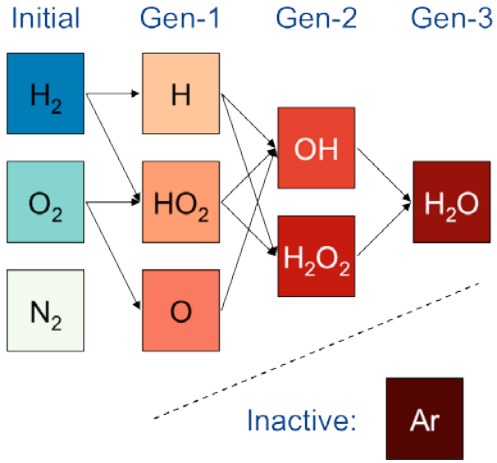
100% GPU version of the multizone chemistry solver completed with new collaboration with NVIDIA

Detailed algorithm analysis completed for key chemistry and species transport algorithms using detailed fuel mechanisms in an HCCI engine



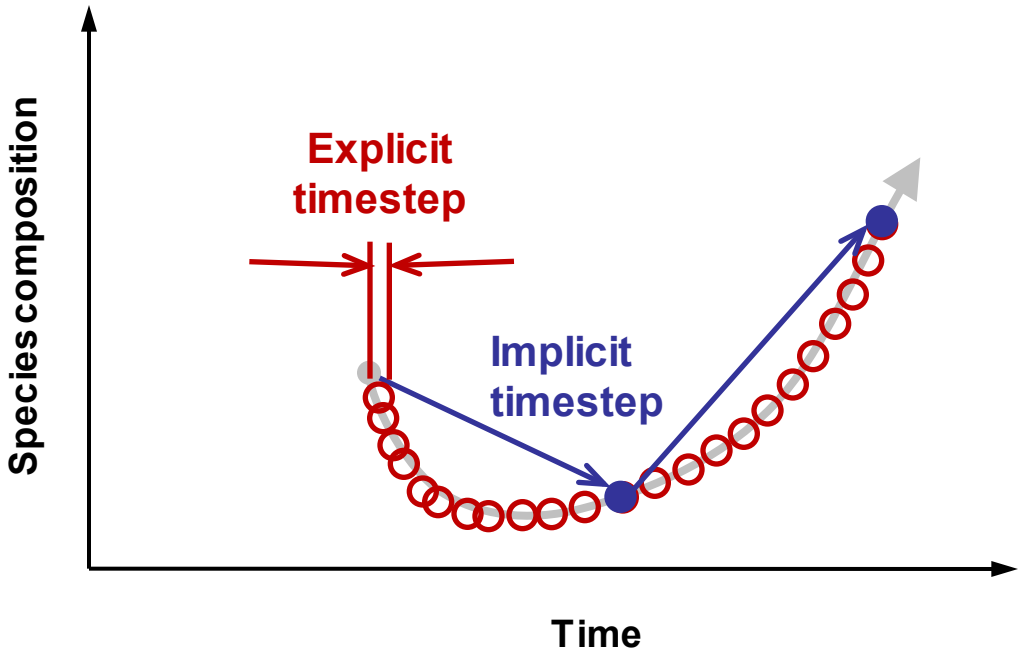
Mechanism debugging and diagnostic suite (beta) is already helping fuel researchers create more robust and accurate mechanisms

Ex. Network Connectivity Tool



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?

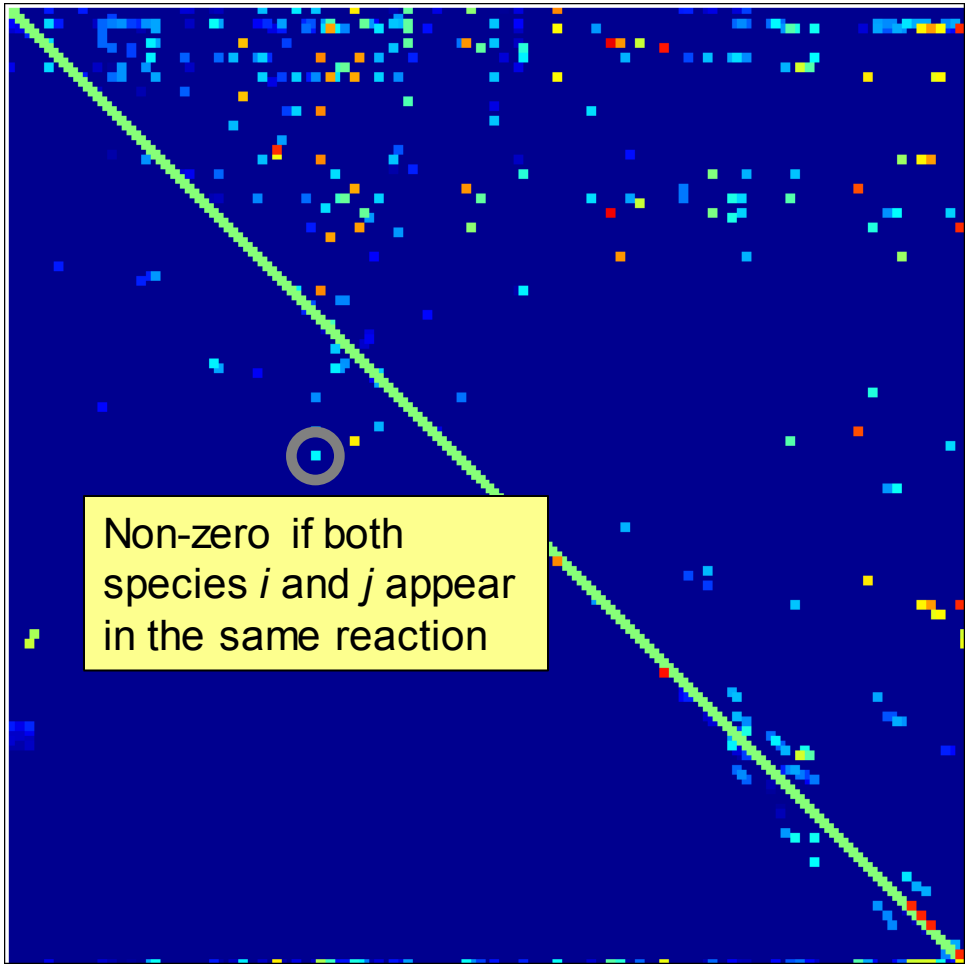
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

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)



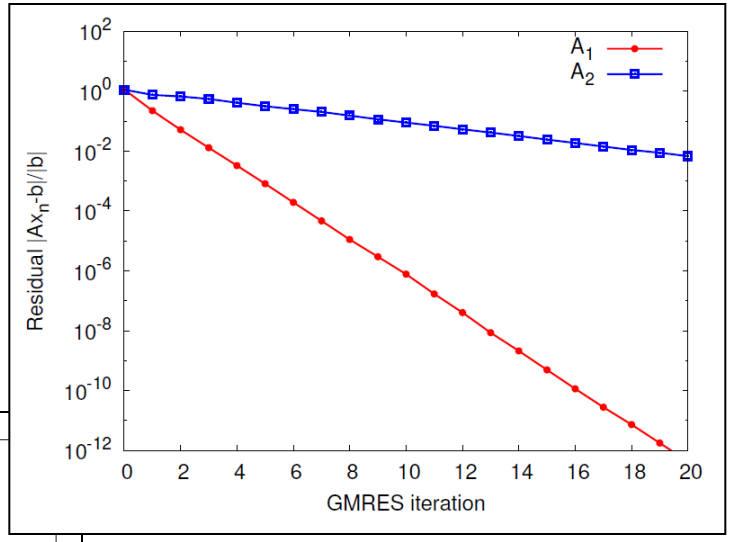
Approximate Jacobians can be used to precondition iterative linear system solvers like GMRES

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

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

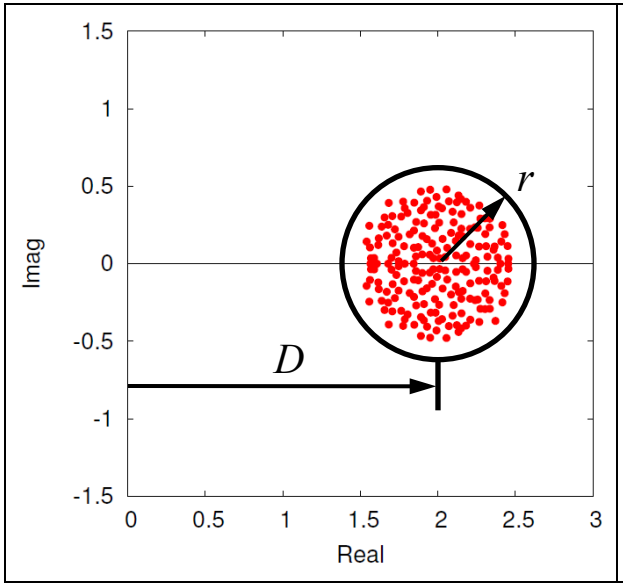
$$\Lambda \approx \frac{r}{D}$$

GMRES Error

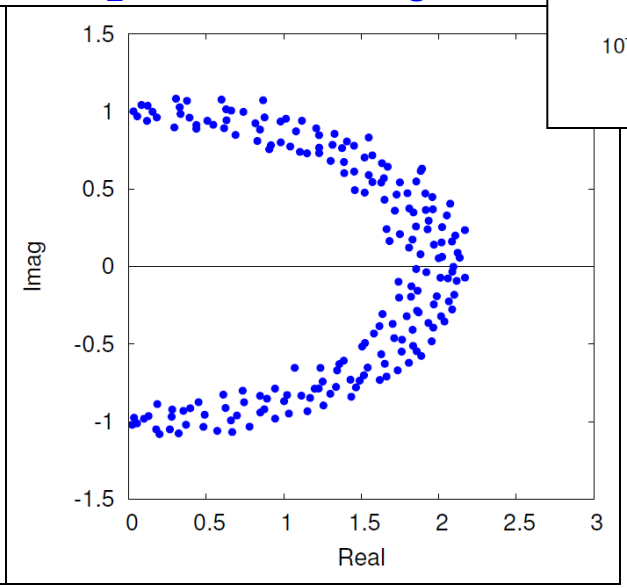


Eigenvalue Spectra (200 x 200)

A_1: fast convergence



A_2: slow convergence

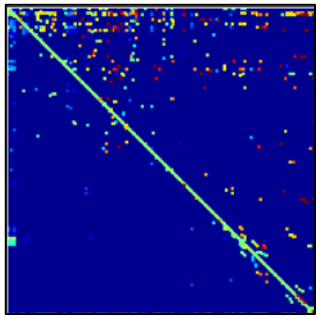


Adaptive preconditioner using on-the-fly reduction produces the same solution significantly faster

Our solver is as fast as the reduced mechanism without any loss of accuracy

Two approaches to faster chemistry solutions

Ex. iso-octane
874 species
3796 reactions



Jacobian Matrix
(species coupling freq.)

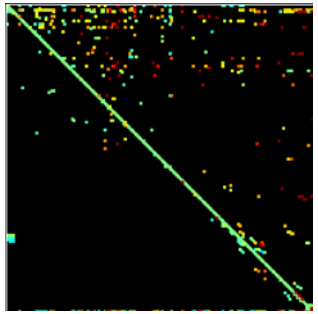
slower ⟷ faster

1. Classic mechanism reduction:

Ex.197 species 

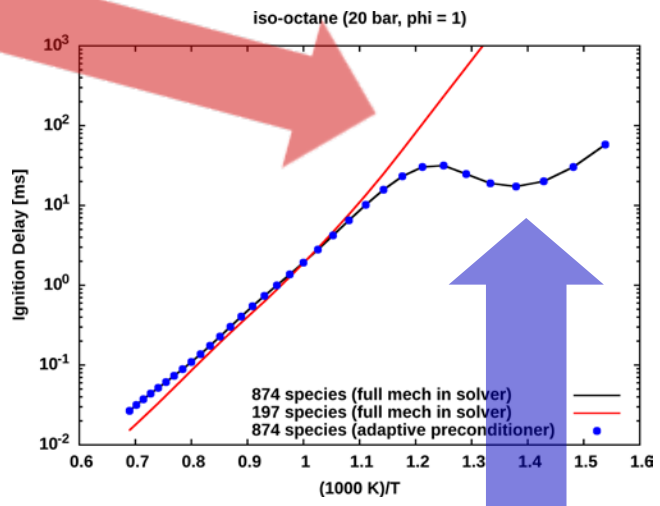
- Smaller ODE size
- Smaller Jacobian
- Poor low T accuracy

2. LLNL's adaptive preconditioner:



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

Filter out 50-75% of the least important reactions



LLNL's solver delivers near linear scaling for mechanisms using the new PLOG reactions