Lawrence Livermore National Laboratory

Improved Solvers for Advanced Engine Combustion Simulation

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Project ID # ACE076

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Overview

Timeline

- Ongoing project with yearly direction from DOE

Budget

- FY11 funding: $300K
- FY12 funding: $340K
- FY13 funding: $340K

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 Inc. (CSI)
- Sandia NL, Oak Ridge NL
- UC Berkeley, Univ. of Wisconsin, Univ. of Michigan, Lund Institute of Tech., Chalmers Univ. and UC Merced
- FACE working group, AEC MOU, SAE, Combustion Inst.

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:

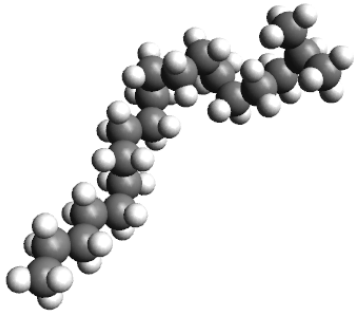
  A. *Lack of fundamental knowledge of advanced engine combustion regimes*

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

  D. *Lack of effective engine controls*

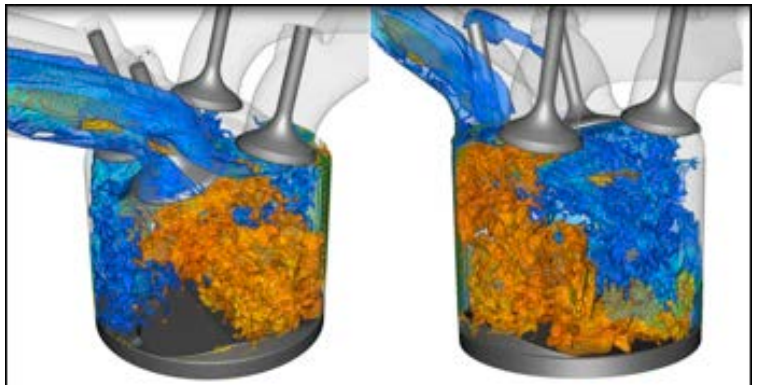
We want to use…

Detailed chemistry



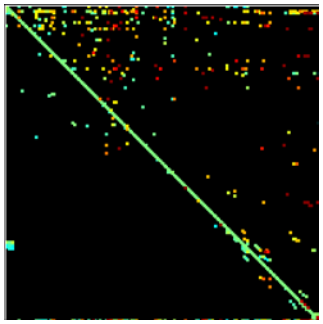
Ex. Biodiesel component $C_{20}H_{42}$ (LLNL)
7.2K species
53K reaction steps

in highly resolved 3D simulations



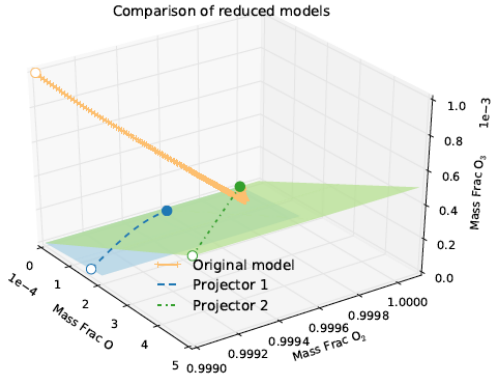
Ex. SI/HCCI transition ~30M cells for Bosch in LLNL's hpc4energy incubator

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

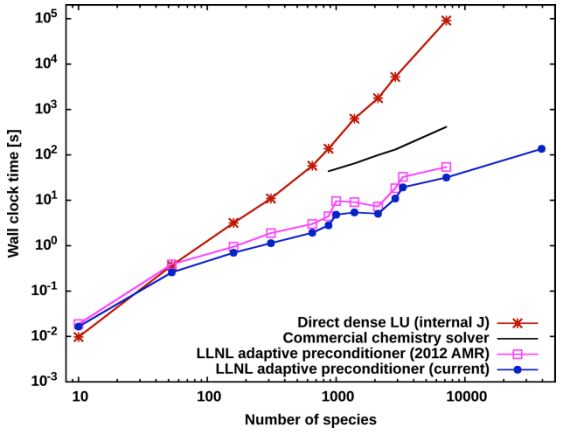


3. **Improved physical models**
   – more accuracy, better error control

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

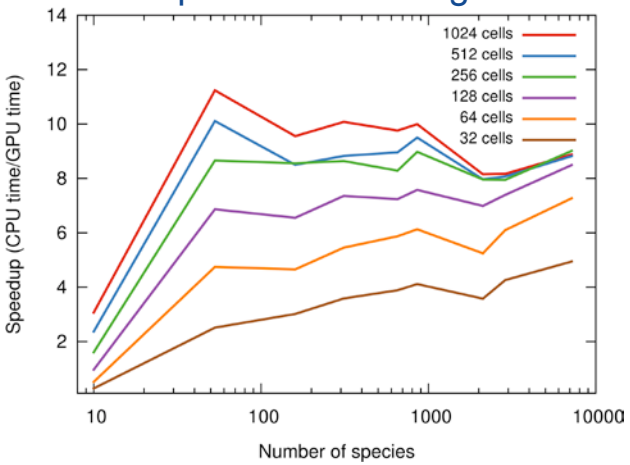
Milestones – Advanced Combustion Numerics project

1. **Better Algorithms**: Adaptive Preconditioners



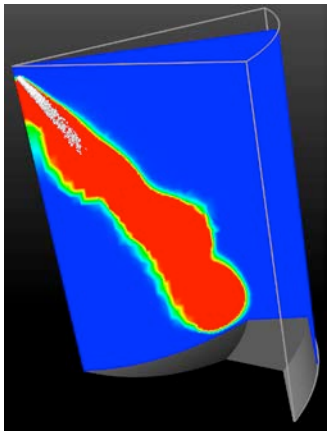
- FY12 – Refined LLNL solver settings for extra 2x speedup.
- FY13 – Verified solver performance on new fuel classes and 39K species (C9) automatic mech. generator.
- FY13 – Identified new pre-conditioners for further gains.
- End of FY13 – Identify bottlenecks in multispecies transport algorithms.

2. **New Architecture**: Graphical Processing Units



- FY13 – Created new GPU algorithms for multiple cell thermo-chemical functions that are up to 8x faster.
- FY13 – Ported ODE vector operations to the GPU.
- End of FY13 – Create new GPU algorithms for multiple cell matrix functions – overall speedup possible 8x or more.

3. **Improved Physics**: Detailed Chemistry in 3D CFD



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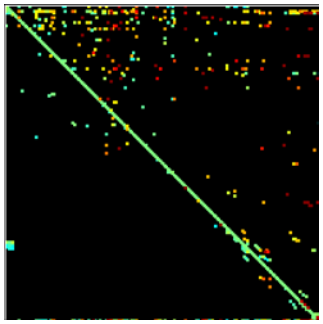
Technical Accomplishments – Outline



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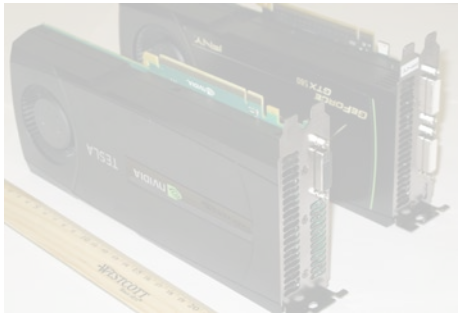

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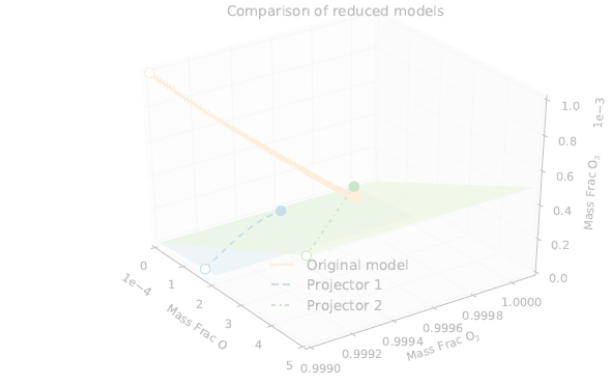


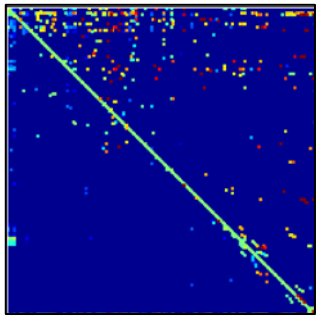
3. **Improved physical models – more accuracy, better error control**

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

FY12 Accomplishment – Adaptive preconditioner using on-the-fly reduction produces the same solution significantly faster

Two approaches to faster chemistry solutions

Ex. iso-octane
874 species
3796 reactions



Jacobian Matrix
(species coupling freq.)

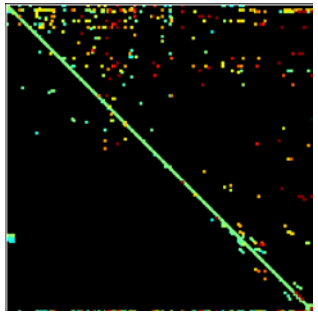
slower ⟷ faster

1. Classic mechanism reduction:

Ex.197 species 

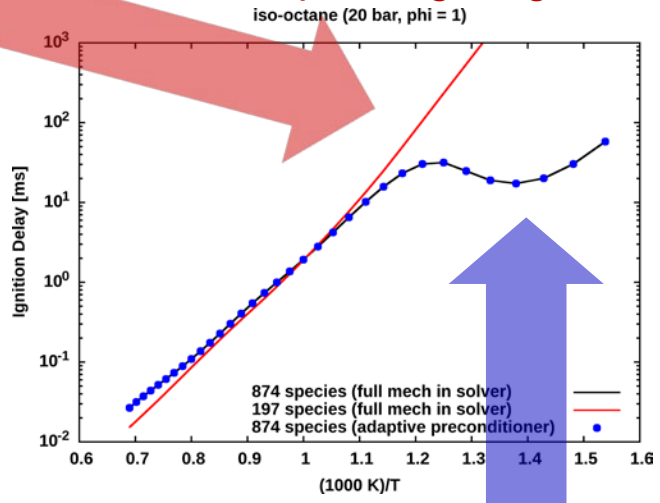
- Smaller ODE size
- Smaller Jacobian matrix

2. LLNL's adaptive preconditioner:



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

Solution is faster but is not accurate over the entire operating range



Filter out 50-75% of the least important reactions

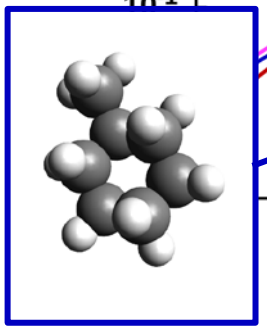
Our solver is as fast as the reduced mechanism without any loss of accuracy
- more than 10x speedup

FY13 Accomplishment – Adaptive preconditioner achieves additional 2x speedup and its verification is extended to new mechanism classes

Automatic Mechanism Generator – up to C9 (MIT – Green group)
39K species
150K steps

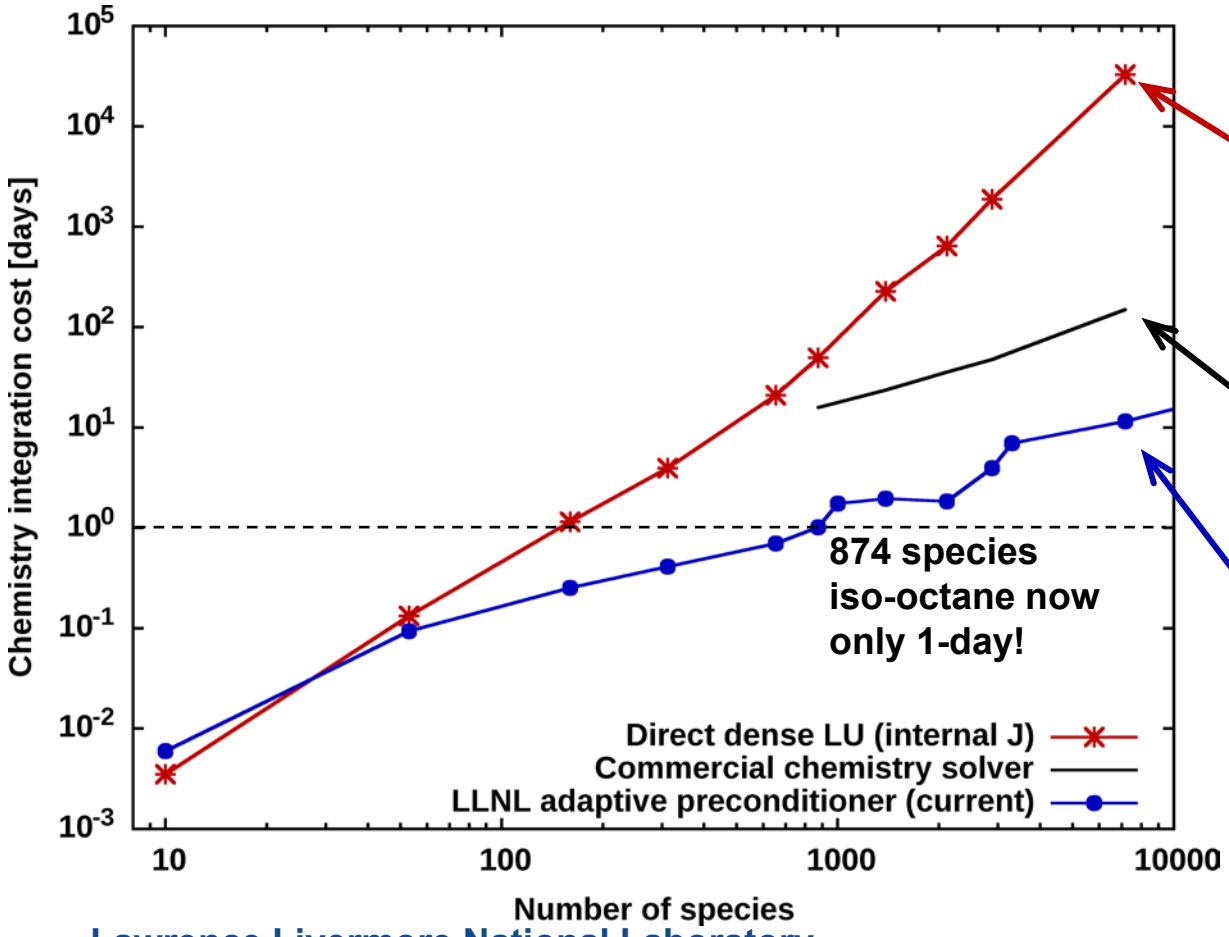
3-component biodiesel (LLNL – Herbinet *et al.*)
3.3K species
21K steps

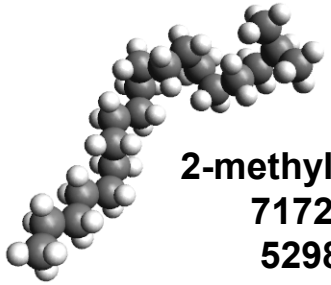
methylcyclohexane (LLNL – Pitz *et al.*)
1.0K species
8.7K steps



LLNL's new solver brings well-resolved chemistry and 3D CFD to 1-day engine design iterations using iso-octane (874 species)

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

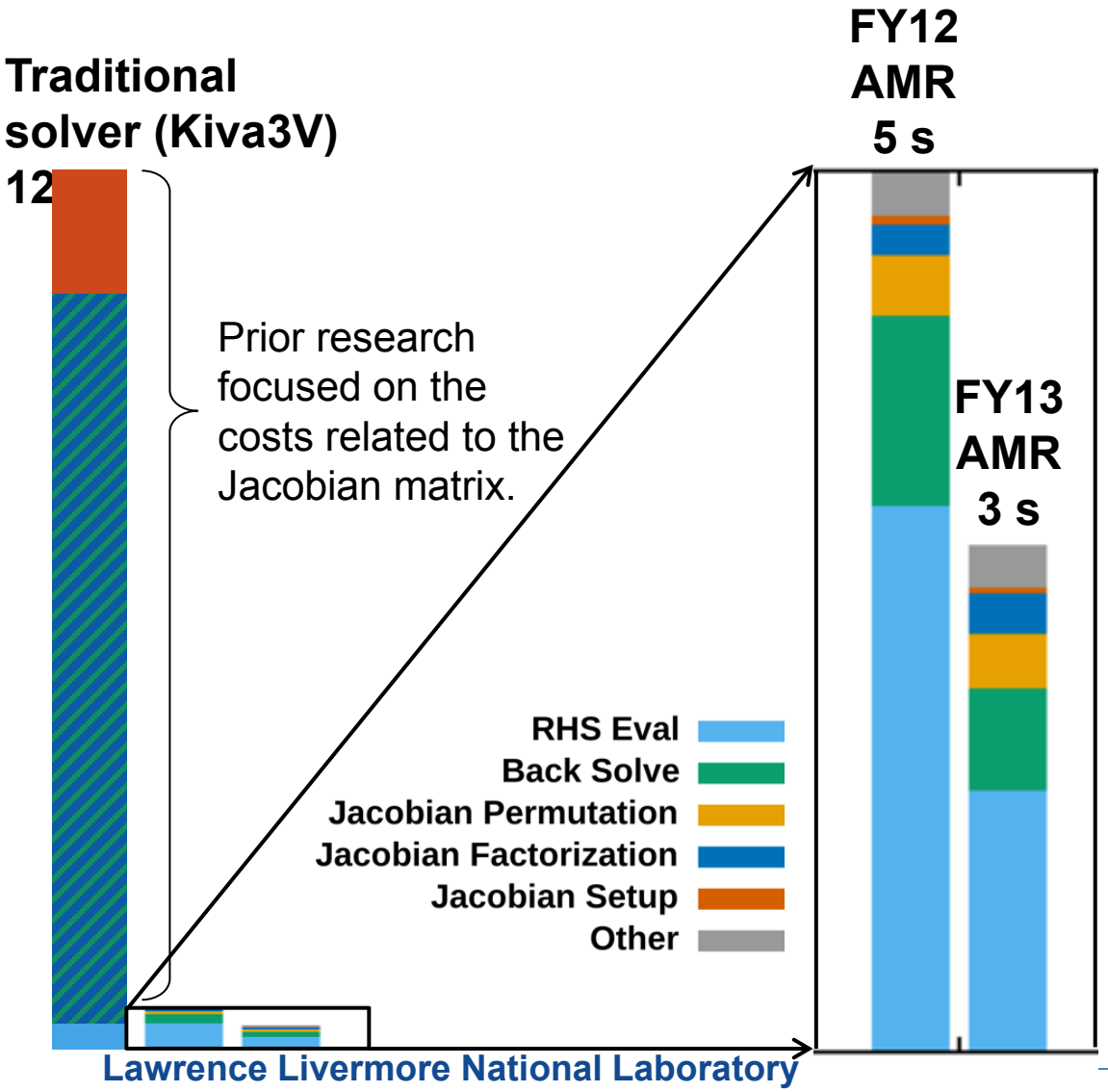
- 150 days

New LLNL solvers created for ACE program FY13

- 11 days

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

Recent factor of two speedup is the last low hanging fruit for improving the chemistry solver in a single CFD cell



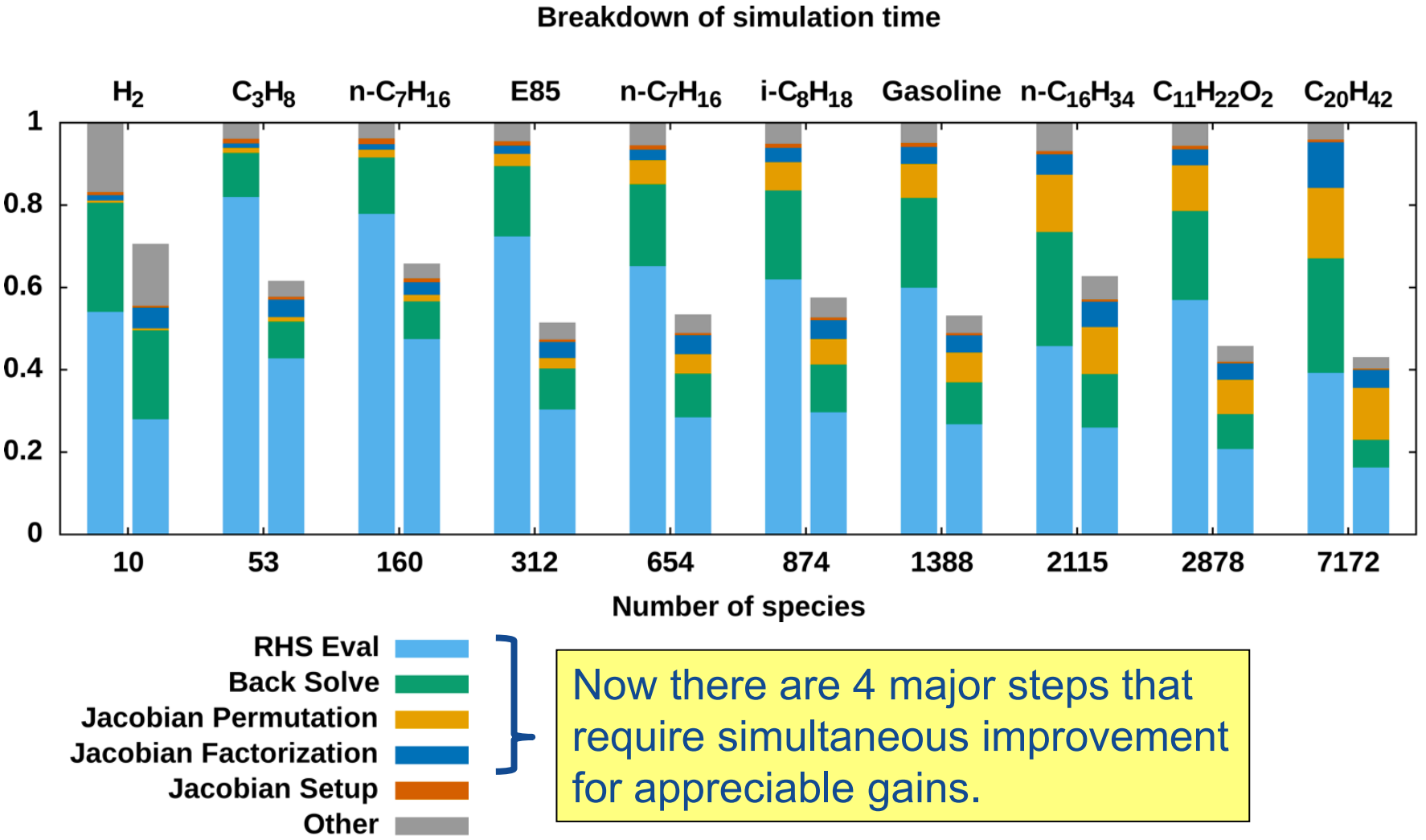
Jacobian matrix

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

Right-hand side evaluation

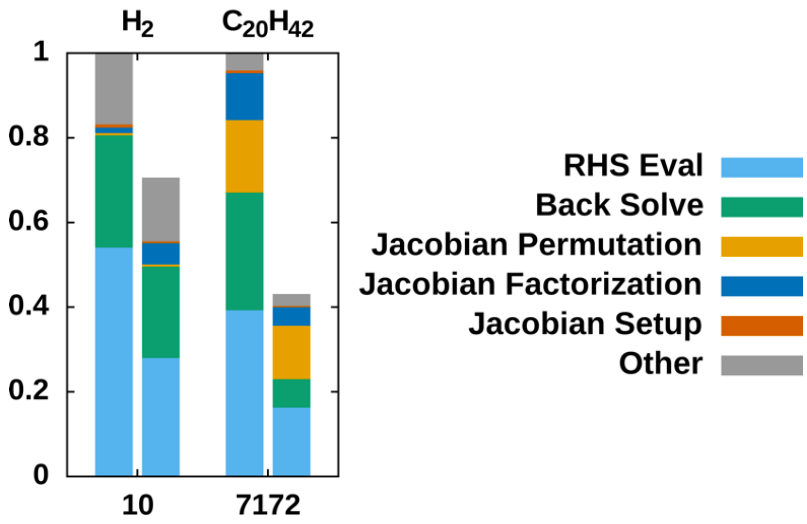
$$\begin{pmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \\ \vdots \\ \frac{\partial x_N}{\partial t} \end{pmatrix} = \begin{pmatrix} f_1(x_1, \square, x_N, t) \\ f_2(x_1, \square, x_N, t) \\ \vdots \\ f_N(x_1, \square, x_N, t) \end{pmatrix}$$

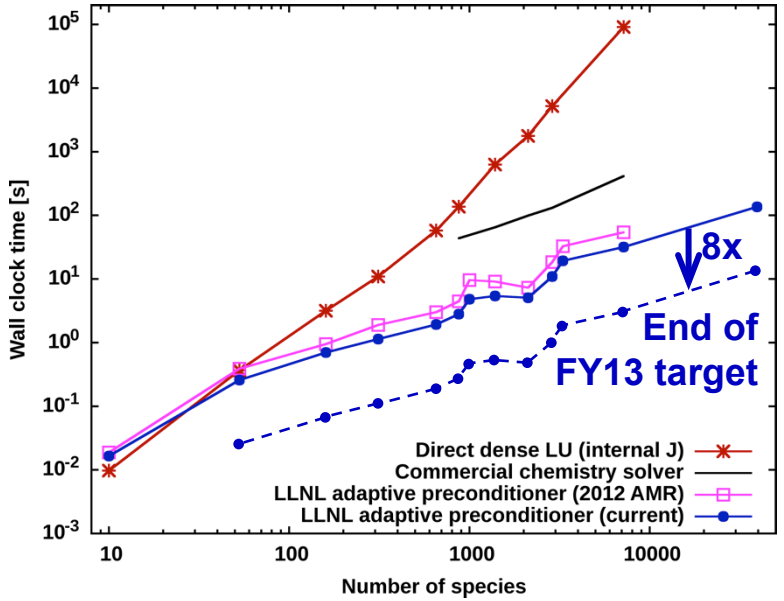
Additional 1.5-2x speedup achieved through vectorized exponentials and improved sparse solver settings



Now there are 4 major steps that require simultaneous improvement for appreciable gains.

Future improvements to the chemistry solver must combine the adaptive preconditioners with new solver algorithms and hardware





1. Larger timesteps:
   - new non-linear solvers (e.g multi-step solve, QSS predictor)
   - exponential integrators
   - more robust ODE error control schemes
   - global error theory

2. Graphics Processing Units (GPUs):
   - simultaneous fluid cell solution shows promise of 8x speedup
   - thermo-chemical functions already demonstrate 8x speedup
   - more GPU-friendly solvers for the preconditioners currently under development

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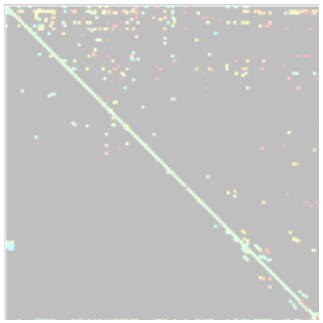

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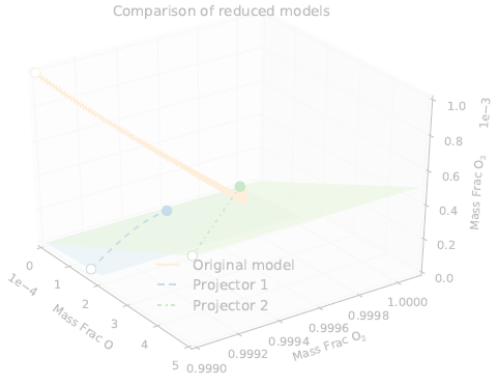

3. Improved physical models
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Accomplishments discussed in more detail in Flowers' presentation (ACE012)

FY13 Accomplishment – GPU algorithms speedup thermo-chemical functions by 8x after resolving the production rate bottleneck

The net species production rate is the difference of the creation and destruction rates, which have the form:

Creation rate of species i

$$\dot{\omega}_i^{(c)} = \sum_{j \in \mathscr{C}_i} \psi_j$$

Rate of progress of reaction step j

Summation over all reactions containing species i as a product

Example: hydrogen mechanism

$$\dot{\omega}_H^{(c)} = \psi_2 + \psi_3 + \cdots$$
$$\dot{\omega}_{OH}^{(c)} = \psi_1 + \psi_3 + \cdots$$
$$\vdots$$

$$\psi_1 = k_1(T) C_H C_{O_2}$$
$$\psi_2 = k_2(T) C_O C_{OH}$$
$$\psi_3 = k_3(T) C_O C_{H_2}$$
$$\vdots$$

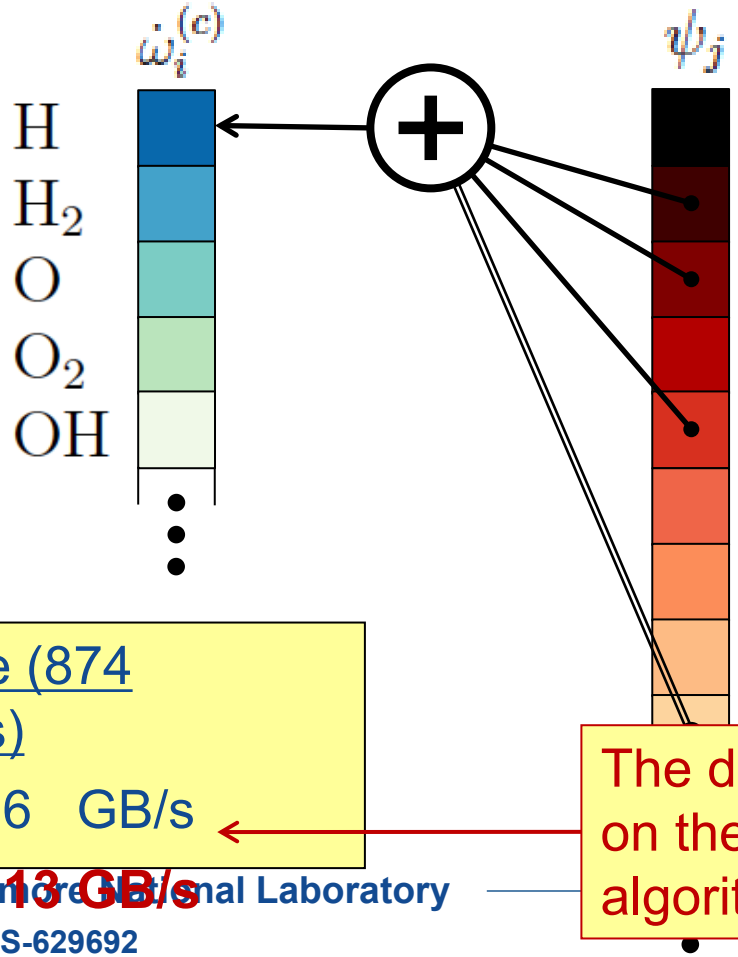
$$\mathrm{H} + \mathrm{O_2} \rightarrow \mathrm{O} + \mathrm{OH}$$
$$\mathrm{O} + \mathrm{OH} \rightarrow \mathrm{H} + \mathrm{O_2}$$
$$\mathrm{O} + \mathrm{H_2} \rightarrow \mathrm{H} + \mathrm{OH}$$
$$\vdots$$

Directly translating the CPU algorithm for the creation and destruction rates actually makes the GPU solution slower

Scatter-add for the species production rates

$$\dot{\omega}_i^{(c)} = \sum_{j \in \mathscr{C}_i} \psi_j$$

Unstructured read or write operations very costly on GPU



$$\begin{aligned}
H + O_2 &\rightarrow O + OH \\
O + OH &\rightarrow \boxed{H} + O_2 \\
O + H_2 &\rightarrow \boxed{H} + OH \\
H + OH &\rightarrow O + H_2 \\
OH + H_2 &\rightarrow \boxed{H} + H_2O \\
H + H_2O &\rightarrow OH + H_2 \\
O + H_2O &\rightarrow 2OH \\
2OH &\rightarrow O + H_2O
\end{aligned}$$

iso-octane (874 species)

CPU: 6.6 GB/s

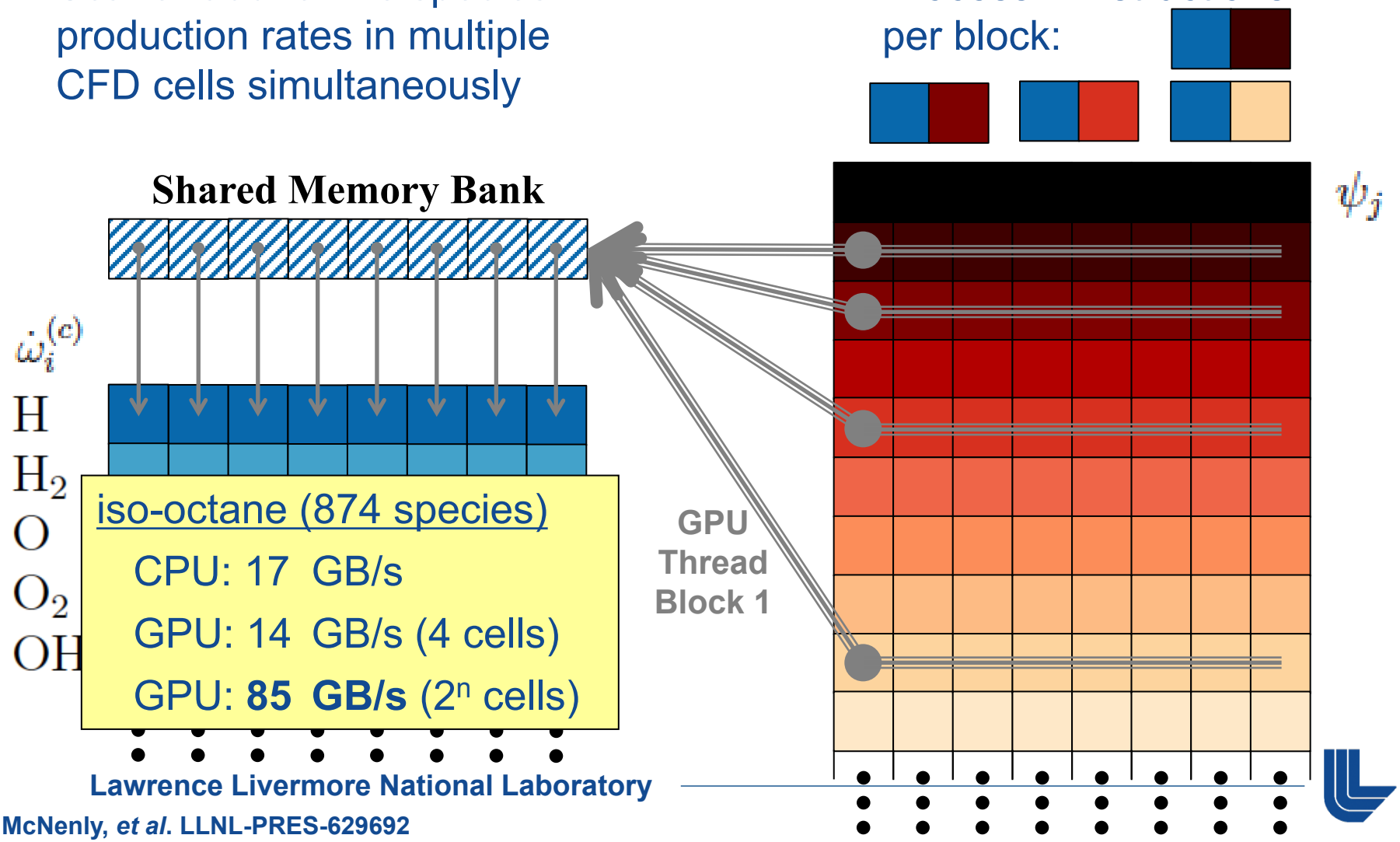
GPU: 0.13 GB/s

The data throughput is 50x slower on the GPU using the naïve algorithm. We must do better.

Reorganizing the data structures to calculate the species production rate in multiple CFD cells simultaneously on the GPU is 5x faster

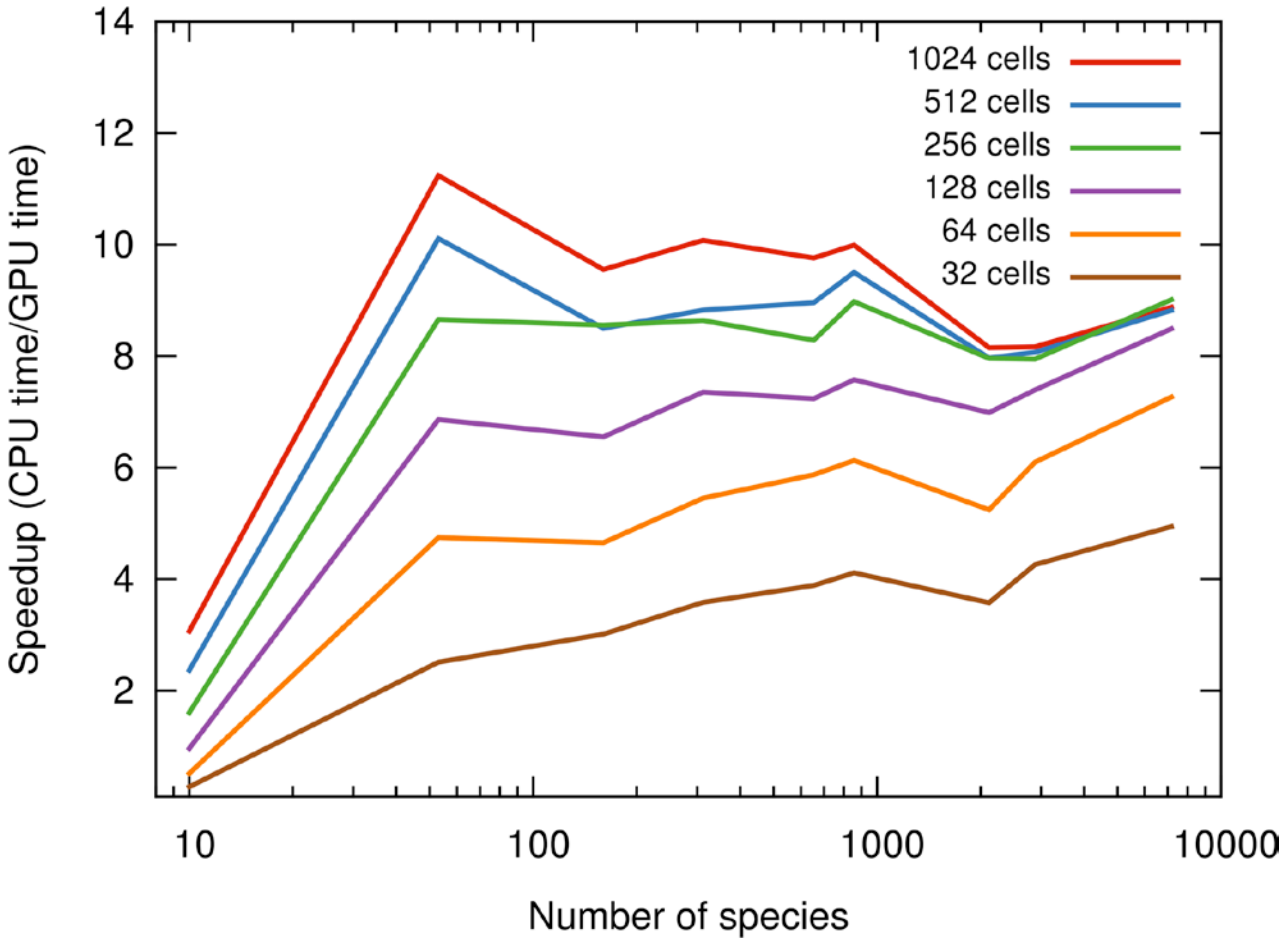
Scatter-add for the species production rates in multiple CFD cells simultaneously

Process 4 instructions per block:



Similar algorithm improvements produce an order of magnitude speedup calculating the system derivatives on the GPU

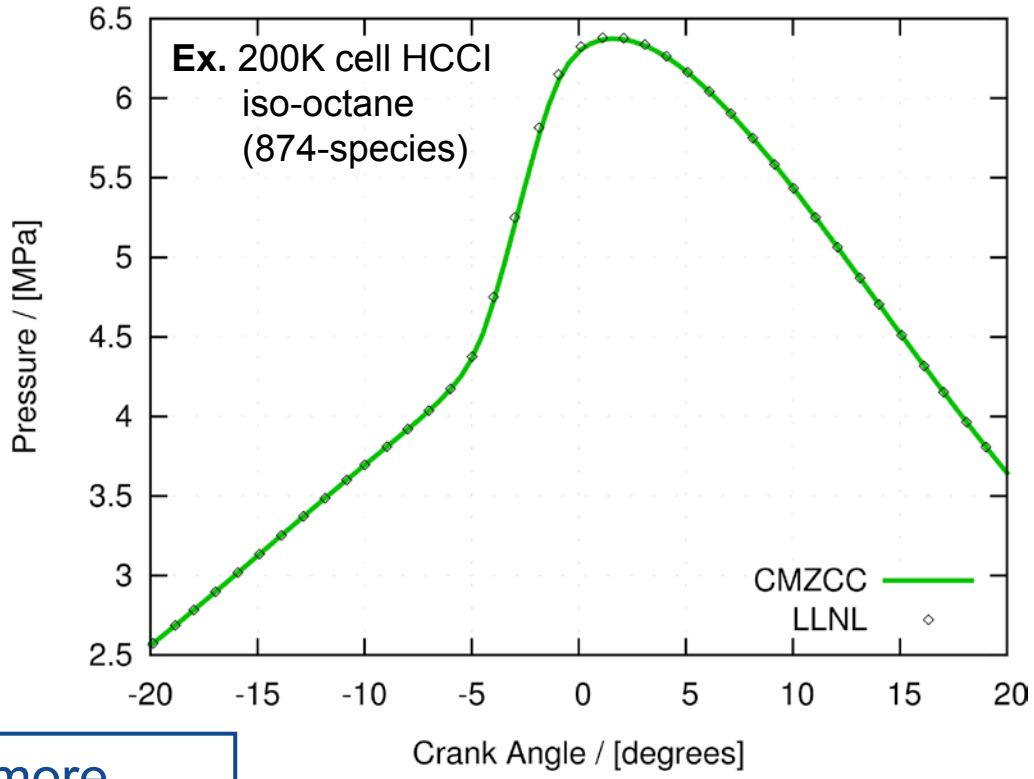
- Processing 256 CFD cells simultaneously provides an 8x speedup for the system derivatives of mechanisms larger than 50 species.
- The GPU algorithm for derivatives also includes new functions for
  - rate constants
  - thermodynamic props.
  - rate of progress (scatter-multiplication)
- The vector operations for the ODE solver are now on the GPU for even further speedup.
- End of FY13 goal is to get all the preconditioner operations on the GPU for at least 8x total speedup.



FY13 Accomplishment – CFD interface created for LLNL's new solvers to be used in CONVERGE™

License agreement with Convergent Sciences Inc. (CSI) and LLNL code release paperwork completed FY13 Q2.

- New LLNL solver delivers the same solution as CONVERGE™.
- Chemistry solution time is reduced by an order of magnitude for iso-octane (874 species).
- Combined with earlier LLNL multizone license, the chemistry time for 200K cell HCCI simulation is less than 20 min.



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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
- **Delphi**; direct injection
- **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)
- **Fuels for Advanced Combustion Engines (FACE)** working group
- **Sandia National Laboratory**; researchers on HCCI and PCCI, gaseous injection simulations
- **Oak Ridge National Laboratory**; SI-HCCI transition and ^{14}C exhaust analysis for HCCI and Diesel engines
- **Universities**: UC Berkeley, Univ. Wisconsin, Univ. Michigan, Lund Institute, Chalmers Univ., Tianjin Univ. and UC Merced
- **Advanced Engine Combustion (AEC)** working group (Industry, National labs, Univ. of Wisc., Univ of Mich., MIT, UC Berkeley); semiannual presentations

Collaboration – We support many avenues for partnership growth

- Chemistry solver support for MOU partners (email mcnenly1@llnl.gov)
  - Oct. 2012, Ford/Convergent Sciences Inc. (CSI): code changes for greater integrator stability and enhanced CONVERGE™ capabilities for big mechanisms.
- Licensing solvers for use in commercial CFD
  - FY Q2, CSI: completed license agreement and code release paperwork for latest adaptive preconditioner solver for the CPU and GPU.
- Providing applications for the new solvers, guiding research plan
  - FY13 Q1-2, Cummins/CSI: developed UDF to use fast LLNL CPU and GPU solvers in CONVERGE™ v2.1 to run biodiesel engine simulations on new Indiana Univ. GPU supercomputer.
- Hosting industrial collaborators
  - FY12-13, Robert Bosch: providing access to high performance computing through hpc4energy incubator for HCCI/SI transient simulations.
  - FY13 Q3-4, GE Research: providing access to computing resources (remote/on-site) to support a visiting research testing the new solvers.

Future Work – We will continue to explore strategies for improving efficiency of CFD and chemistry simulations

Ongoing

FY13 – Create new GPU algorithms for multiple cell matrix functions.

FY13 – Identify CFD bottlenecks in multispecies diffusion and advection with large kinetic mechanisms.

FY13/14 – Develop turnkey package of the chemistry solvers and common applications (ignition delay, flame speed, *etc*.) for testing by the MOU partners.

Proposed supports diesel research in ACE012, ACE013

FY14 – Accelerate multispecies diffusion and advection algorithms

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

FY14 – Add more applications to the turnkey package of the chemistry solvers (diffusion flames, extinction, sensitivity, *etc*.).

Planned future solvers for use in CFD packages

FY14/15 – Develop new chemistry solvers capable of larger and lower cost timesteps to speedup all mechanism sizes.

- Continued migration of solver components to the GPU.
- New Krylov iterations and hybrid time-stepping schemes

Summary – Advanced Combustion Numerics project

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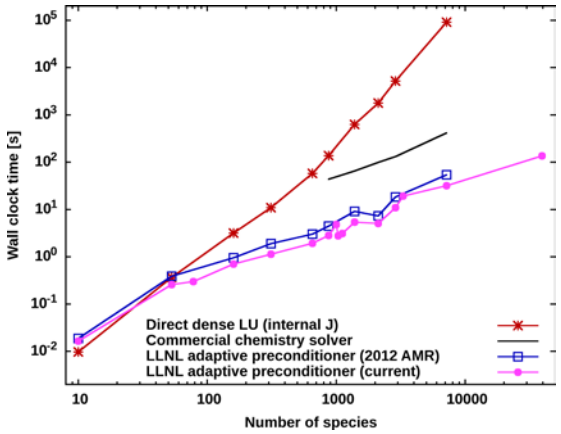

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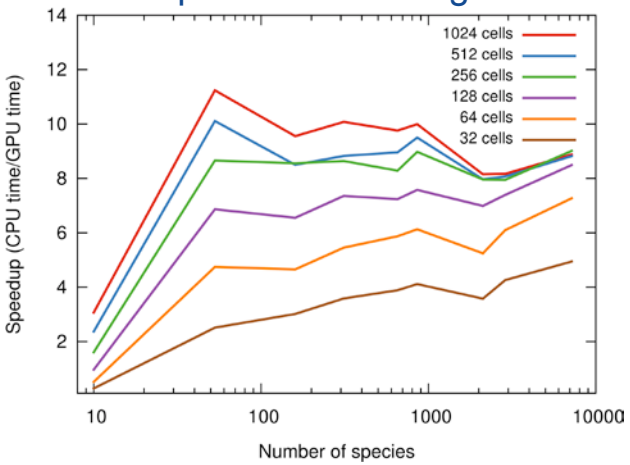

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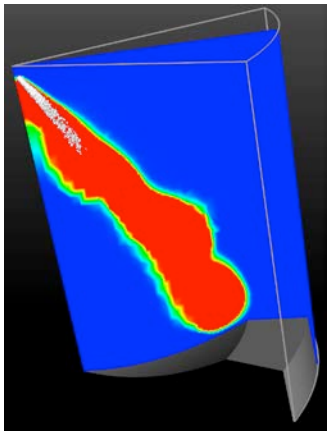

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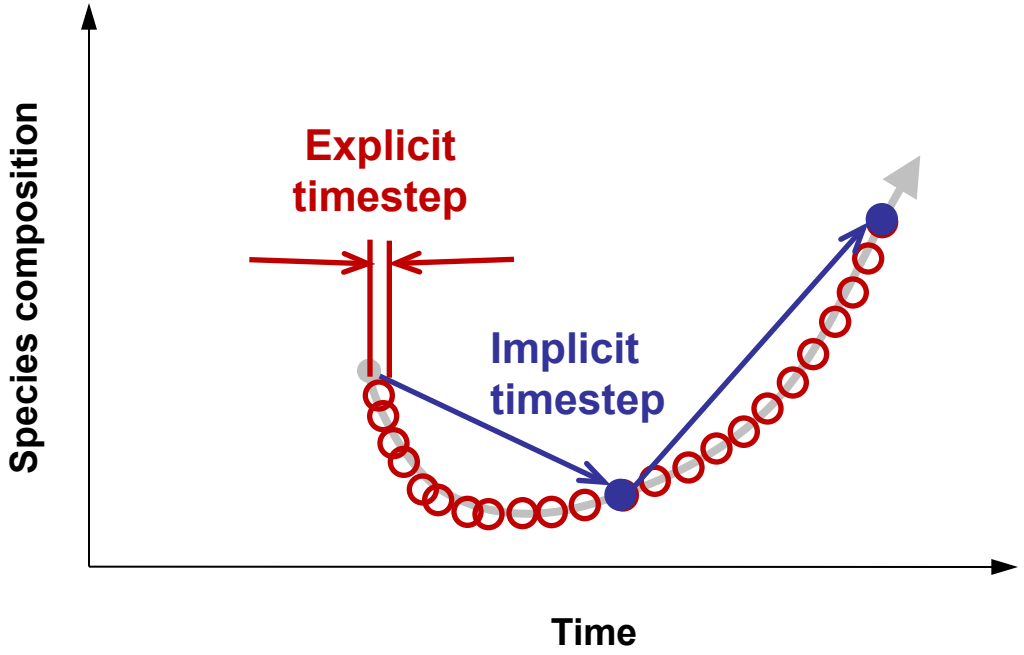
Technical Back-Up Slides (limit 5)

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?

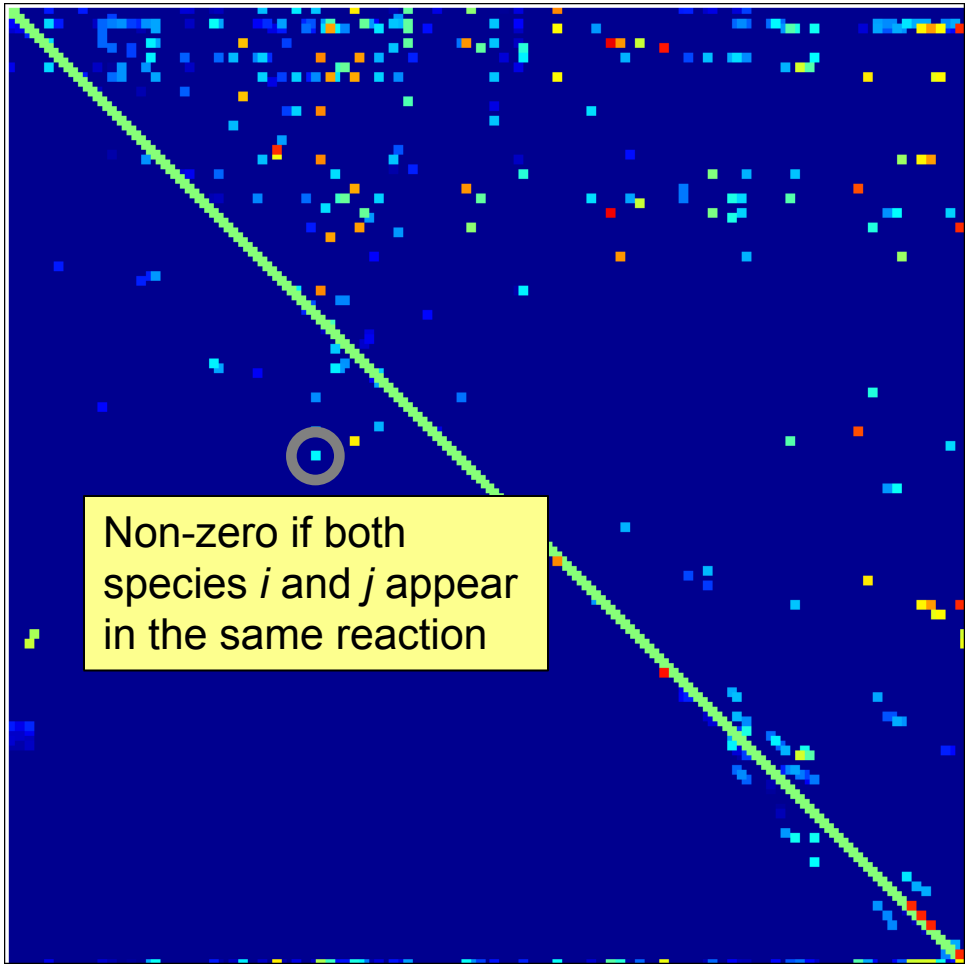
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

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)



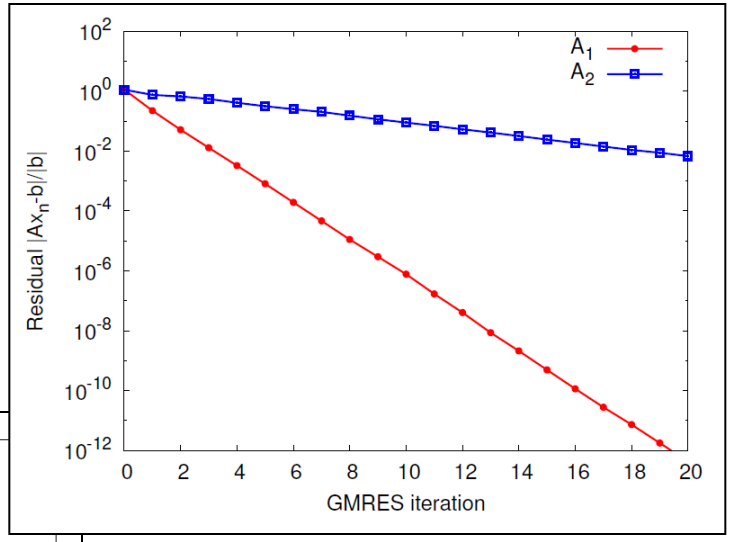
Approximate Jacobians can be used to precondition iterative linear system solvers like GMRES

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

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

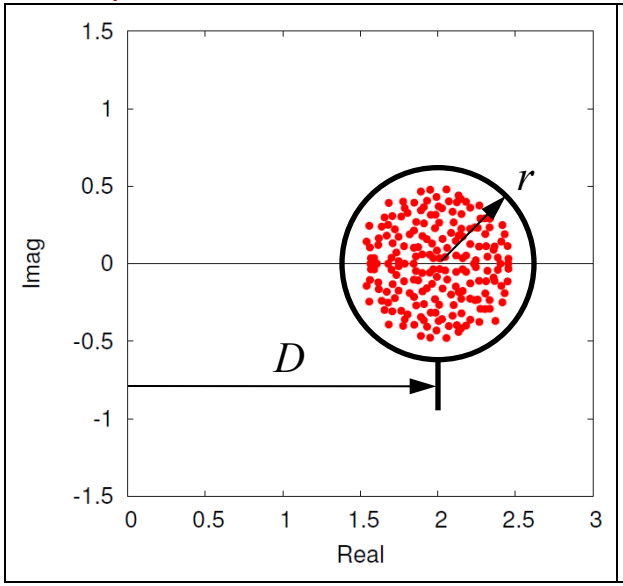
$$\Lambda \approx \frac{r}{D}$$

GMRES Error

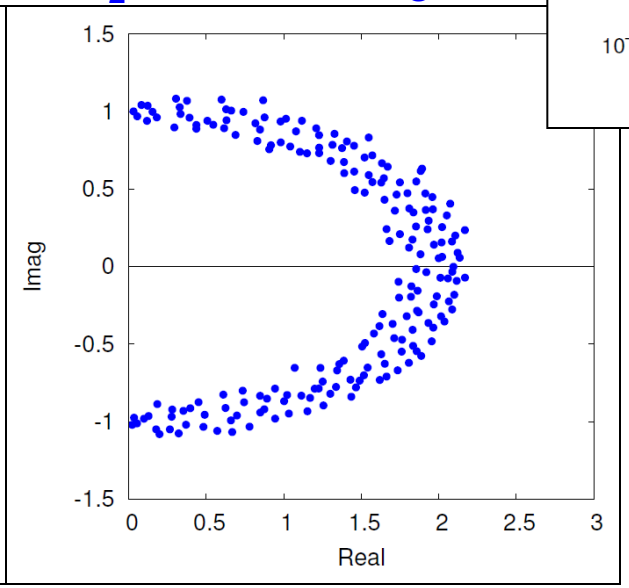


Eigenvalue Spectra (200 x 200)

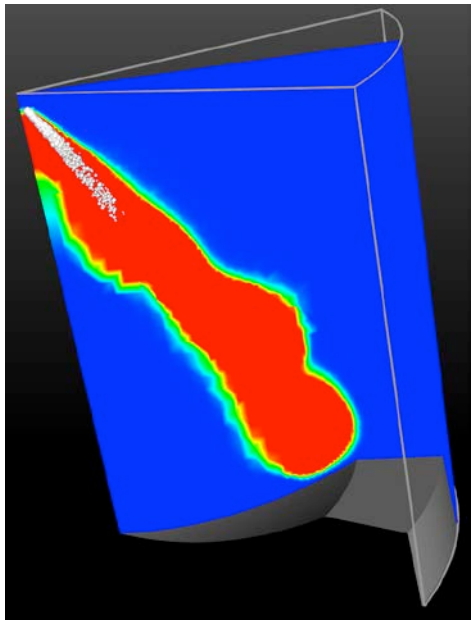
A_1: fast convergence

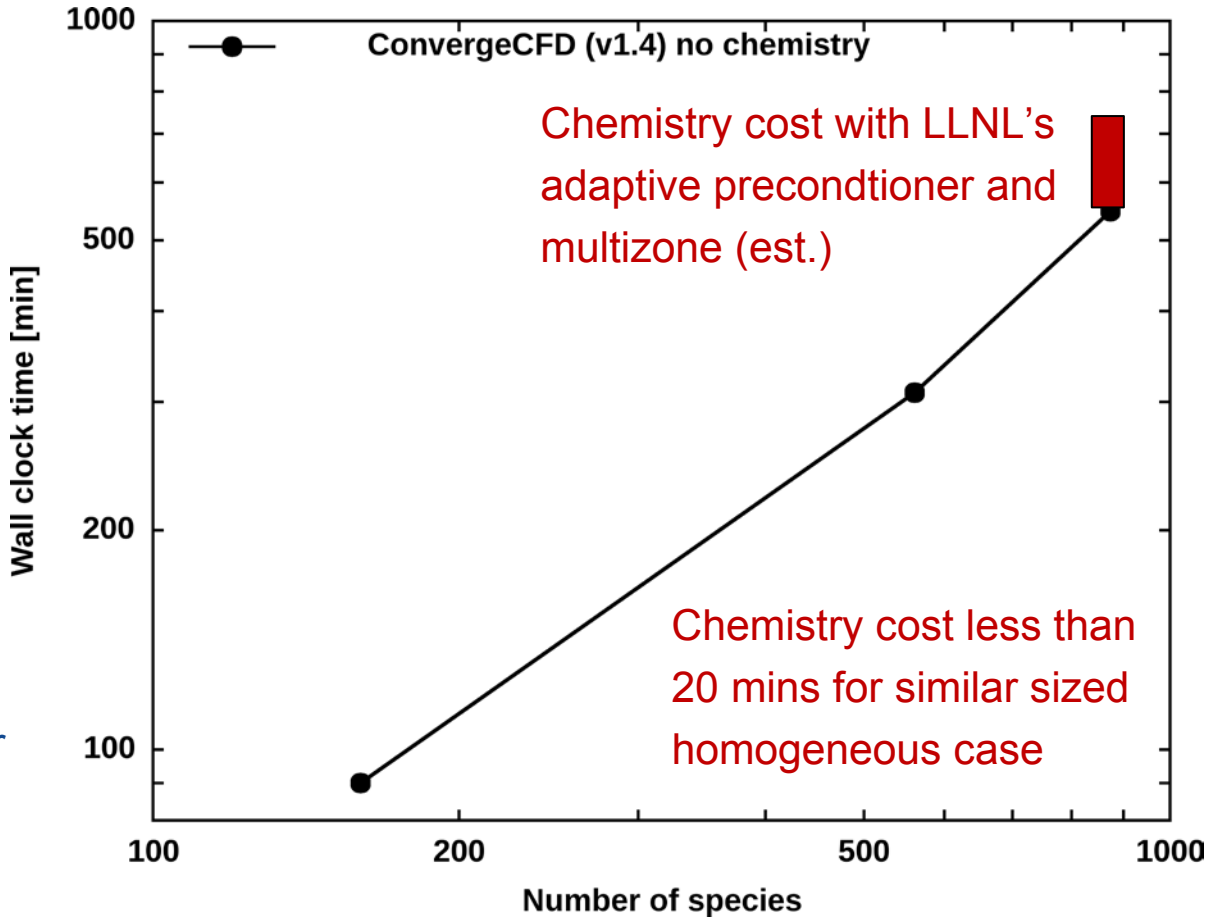


A_2: slow convergence



Successful reduction in chemistry cost reveals that multi-species transport now dominates simulation time

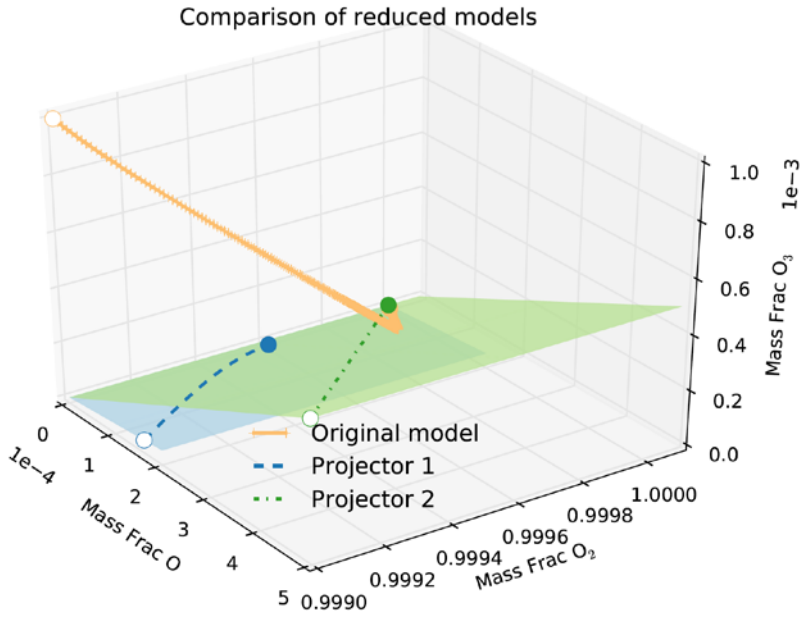


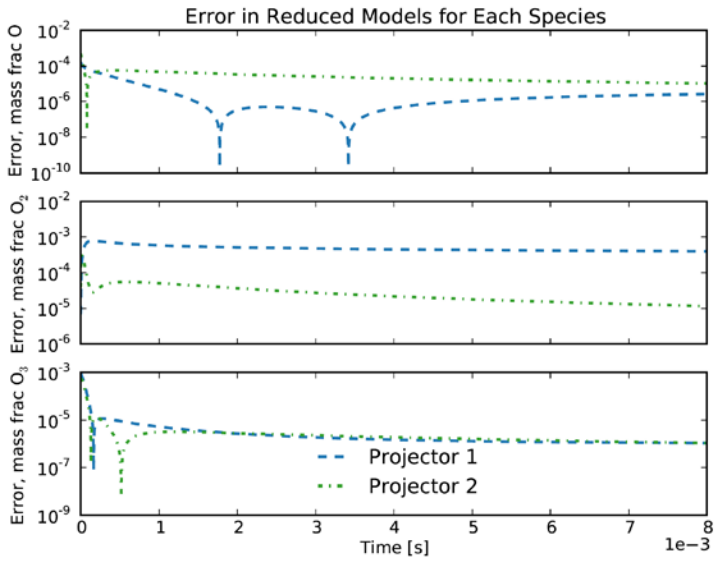


- Sandia (Dec) iso-octane data
- Converge spray models
- LLNL multi-zone and AP solver
- 874 species (Pitz/LLNL)
- 60 degree sector, closed cycle
- 200K cells (at BDC)
- Low load (phi=0.12 overall)

New error analysis framework can lead to robust reduced order models for reacting flow without a steep learning curve for users

Building on the thesis research of new team member Geoff Oxberry:





- Developed connection in solution space between quasi-steady state (QSS), lumped species and projection-based approximations.
- Derived the first error bounds:
  - oblique projectors – slow mode resolution (QSS) & fast-mode resolution
  - approximate ODE systems – multizone & mechanism reduction