Improved Solvers for Advanced Engine Combustion Simulation


2014 DOE Vehicle Technologies Program
Annual Merit Review and Peer Evaluation Meeting
June 17, 2014 - Washington, DC

This presentation does not contain any proprietary, confidential or otherwise restricted information
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
- 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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Now we want to use…
Detailed chemistry

Ex. 9-component diesel surrogate (AVFL18)
+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.

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

Ex. 9-component diesel surrogate (AVFL18)
+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

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

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

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   – more flops per second, per dollar, per watt

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

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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

- 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

- 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 ($\phi = 0.4$)
- High EGR (50%)
- Initial temperature set to match ignition time

4.8x speedup high fidelity multizone (35 fluid cells/reactor)

HCCI Engine (J. Dec)
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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- Analysis provides crucial guide for future algorithm research.
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:

\[ \text{C}_{20}\text{H}_{42} \text{ (LLNL)} \]
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 \textit{combustion textbooks} with zero typos.

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

\[ k = AT^n \exp\left(-\frac{E_a}{RT}\right) \]

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

* equivalent length of Warnatz, Maas & Dibble, \textit{Combustion. Lawrence Livermore National Laboratory}
AMR14 Accomplishment: Single-core version of A-factor sensitivity is an order of magnitude improvement over current commercial tools

Multiple IDT definitions analyzed simultaneously

\[ \Delta T = 400 \text{ K} \]
\[ \Delta T = 100 \text{ K} \]

n-heptane (LLNL):
654 species
2827 reactions
64 seconds (96 CPU cores)

Previously required days to weeks of waiting

Lawrence Livermore National Laboratory

McNenly, et al. LLNL-PRES-653560
AMR14 Accomplishment: Multi-core version of the A-factor sensitivity delivers seamless scalability to the available computing resources

$\Delta T = 400 \text{ K}$

$\Delta T = 100 \text{ K}$

**iso-octane (LLNL):**
- 874 species
- 3796 reactions
- 104 seconds (96 CPU cores)

Previously required days to weeks of waiting
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   Accomplishments discussed in more detail in Whitesides’ presentation (ACE012)

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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

Accomplishments discussed in more detail in Whitesides’ presentation (ACE012)
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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**
- **Detailed Jacobian data**
- **Reaction probability**
- **Connectivity analysis**
  - Initial: H₂, O₂, N₂
  - Gen-1: H, OH, HO₂, H₂O₂
  - Gen-2: Ar
  - Gen-3: Inactive

**Unimolecular rates**

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Lawrence Livermore National Laboratory

McNenly, et al. LLNL-PRES-653560
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

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<tr>
<th>Ongoing</th>
<th>Proposed</th>
<th>Planned</th>
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| FY14 – [Q3 Milestone] Complete the mechanism diagnostic and debugging suite of tools | FY15 – Accelerate multispecies diffusion and advection algorithms  
- Direct algorithm improvements  
- New GPU transport algorithms  
- Reduced order models with error control | FY15/16 – Rigorous error analysis of the multizone combustion solver for direct user control |
| FY14 – [Q4 Milestone] Improve high fidelity multizone chemistry on the GPU for engine CFD simulations | | FY15/16 – Accelerate detailed spray dynamics algorithms |
| FY14 – Continue to improve availability within the MOU for the new solvers – pursue online version of mechanism diagnostic tools | | |
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

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

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

Ex. Network Connectivity Tool
Technical Back-Up Slides (limit 5)
Implicit methods are necessary to integrate the chemical time scales over an engine cycle.

During ignition:

\[ \Delta t \text{ (explicit)} = 10^{-12} \text{ to } 10^{-15} \text{ s} \]
\[ \Delta t \text{ (implicit)} = 10^{-6} \text{ to } 10^{-8} \text{ s} \]

**Explicit Update**

(lower cpu/step)

\[
\begin{align*}
\frac{\partial x_1}{\partial t} &= f_1(t, x_1, \ldots, x_N) \\
\frac{\partial x_2}{\partial t} &= f_2(t, x_1, \ldots, x_N) \\
&\vdots \\
\frac{\partial x_N}{\partial t} &= f_N(t, x_1, \ldots, x_N).
\end{align*}
\]

**Implicit Update**

(more trajectory data)

\[
\begin{pmatrix}
\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\
\frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_N} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_N}{\partial x_1} & \frac{\partial f_N}{\partial x_2} & \cdots & \frac{\partial f_N}{\partial x_N}
\end{pmatrix}
\]
What is the physical meaning of the Jacobian?

The Jacobian matrix is given by:

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

Element: 

\[
J_{i,j} = \frac{dw_i}{dC_j}, \quad w_i = \frac{dC_i}{dt}
\]

Non-zero if both species \(i\) and \(j\) appear in the same reaction.

Magnitude represents the characteristic frequency at which the two species are coupled.
Approximate Jacobians can be used to precondition iterative linear system solvers like GMRES.

**Generalized Minimal RESiduals**

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

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

**Eigenvalue Spectra (200 x 200)**

- **A₁**: fast convergence
- **A₂**: slow convergence

**GMRES Error**

![GMRES Error Graph](image)
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

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

Our solver is as fast as the reduced mechanism without any loss of accuracy
LLNL’s solver delivers near linear scaling for mechanisms using the new PLOG reactions.