Lawrence Livermore National Laboratory

Computationally Efficient Modeling of High-Efficiency Clean Combustion Engines

Daniel Flowers (PI), Salvador Aceves, Nick Killingsworth, Matt McNenly, Guillaume Petitpas, Tom Piggott, Mark Havstad, Russell Whitesides, Randy Hessel (U Wisc), J.Y. Chen (UCB)

Project ID # ACE012

2012 DOE Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting

May 15, 2012 - Washington, DC

This presentation does not contain any proprietary or confidential information

Overview

Timeline

- Ongoing project with yearly direction from DOE

Budget

- FY10 funding: $700K
- FY11 funding: $740K

Barriers

- Inadequate understanding of the fundamentals of HECC
- Inadequate understanding of the fundamentals of mixed mode operation
- Computational expense of HECC simulations

Partners

- Sandia, Oak Ridge, Los Alamos
- Ford, GM, Bosch, Delphi, Volvo
- UC Berkeley, University of Wisconsin, University of Michigan, Lund Institute of Technology, Chalmers University, Tianjin University
- FACE working group, AEC MOU, SAE

Relevance to DOE objectives

- By 2015, improve the fuel economy of light-duty gasoline vehicles by 25 percent and of light-duty diesel vehicles by 40 percent, compared to the baseline 2009 gasoline vehicle.

  - **Light-duty research focuses on reducing fuel consumption through investigating HCCI and PCCI part load, and transition to SI or CIDI for full load operation**

- By 2015, improve heavy truck efficiency to 50 percent with demonstration in commercial vehicle platforms. This represents about a 20 percent improvement over current engine efficiency.

  - **Heavy-duty engine research directed towards high efficiency strategies, such as PPC, HCCI, RCCI and Low-temperature Diesel**

- By 2018, further increase the thermal efficiency of a heavy truck engine to 55 percent which represents about a 30 percent improvement over current engines.

  - **We continue to provide the engine research community with insight and simulation tools for advanced combustion concepts**

Objective: Enhance understanding of clean and efficient engine operation through detailed numerical modeling
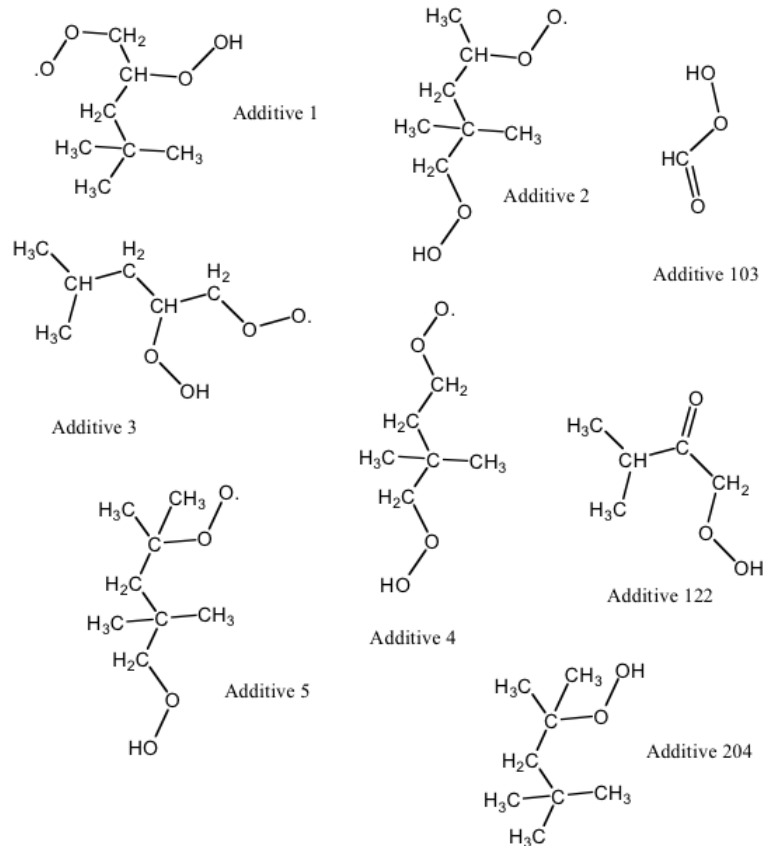

Chemical kinetics
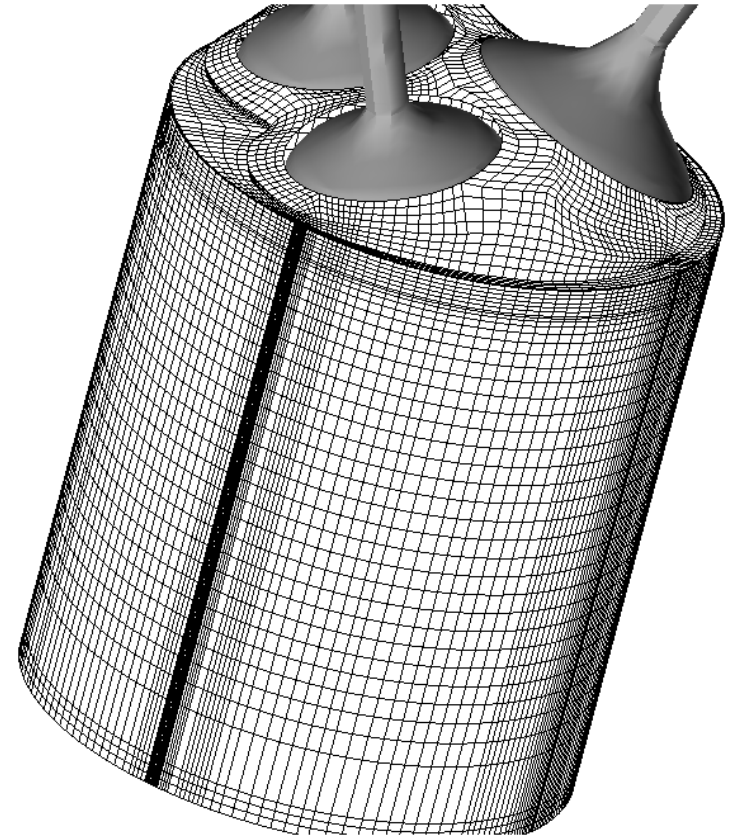
Fluid mechanics

Approach: Collaborate with industry, academia and national labs in the development of analysis tools leading to clean, efficient engines

- Gain fundamental and practical insight into HECC regimes through numerical simulations and experiments

- Develop and apply numerical tools to simulate HECC by combining multidimensional fluid mechanics with chemical kinetics

- Reduce computational expense for HECC simulations

- Democratize simulation: bring chemical kinetics-fluid mechanics computational tools to the desktop PC

Milestones: We have developed and experimentally validated detailed engine modeling tools
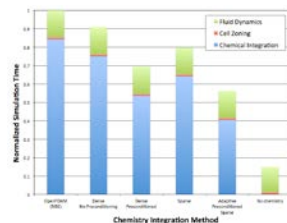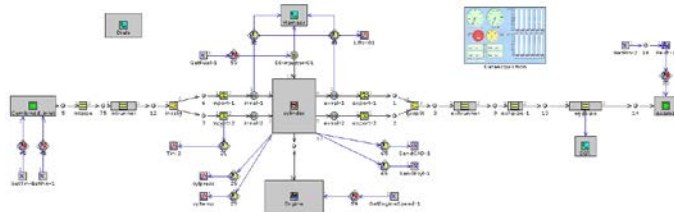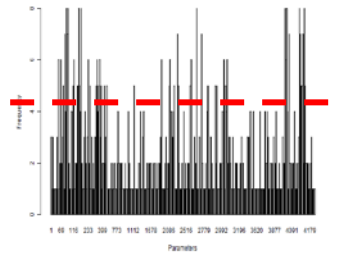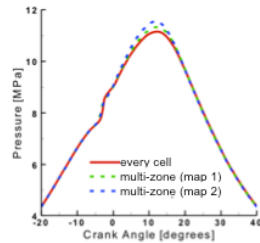

- Validated CONVERGE multi-zone for DI engine simulations (8/11)

- Tuned LTHR parameters for gasoline mechanism based on engine data (11/11)

- Multi-zone integrated into GT-power (12/11)

- Implemented and tested advanced solvers in LLNL parallel CFD multi-zone (2/12)
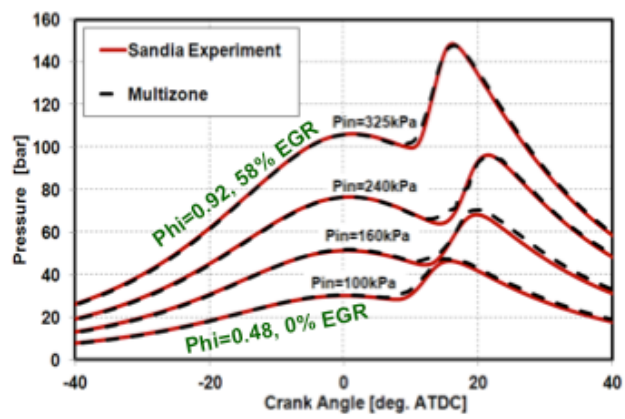
Technical Accomplishments: We have made significant progress in improving and applying our advanced simulation tools to HECC
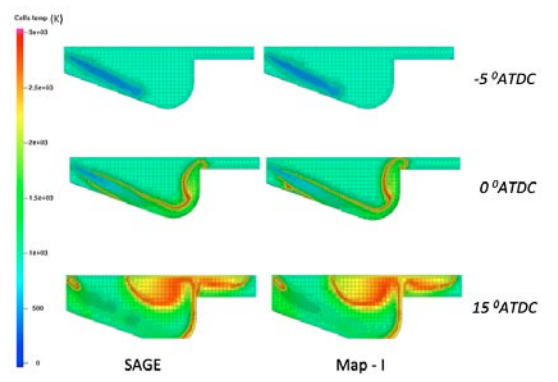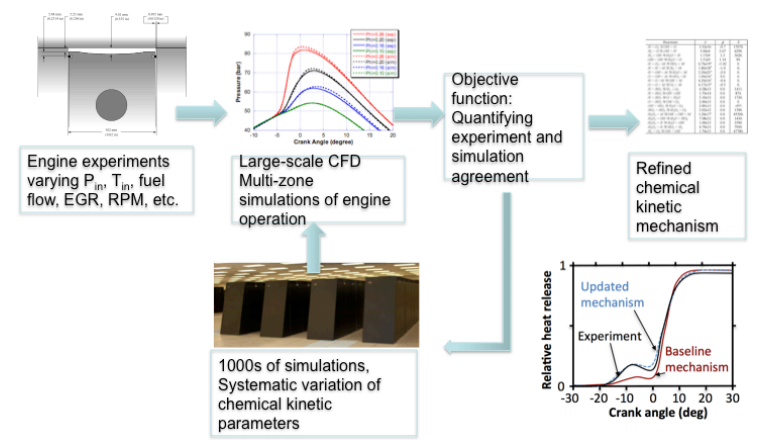

CFD-Multi-zone with CONVERGE
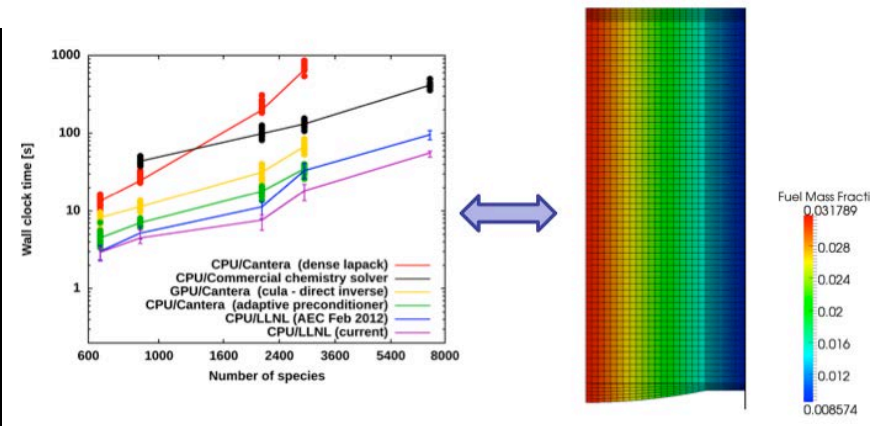
Parallel CFD+MZ with advanced kinetics solvers

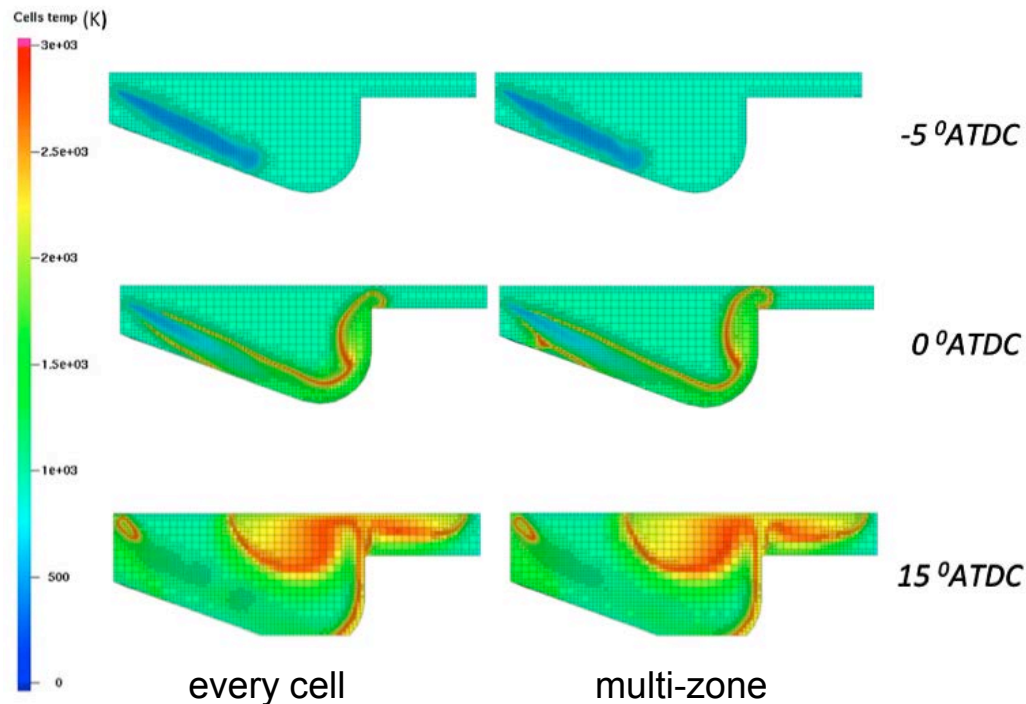**Standalone multi-zone for cycle simulation**

**Improving chemical kinetic mechanisms at engine conditions**

Convergent Sciences Inc. licensed LLNL multi-zone model for their CONVERGE engine CFD simulation software

- Converge is widely used in industry for engine simulation (GM, Ford, Cummins, Caterpillar, etc)
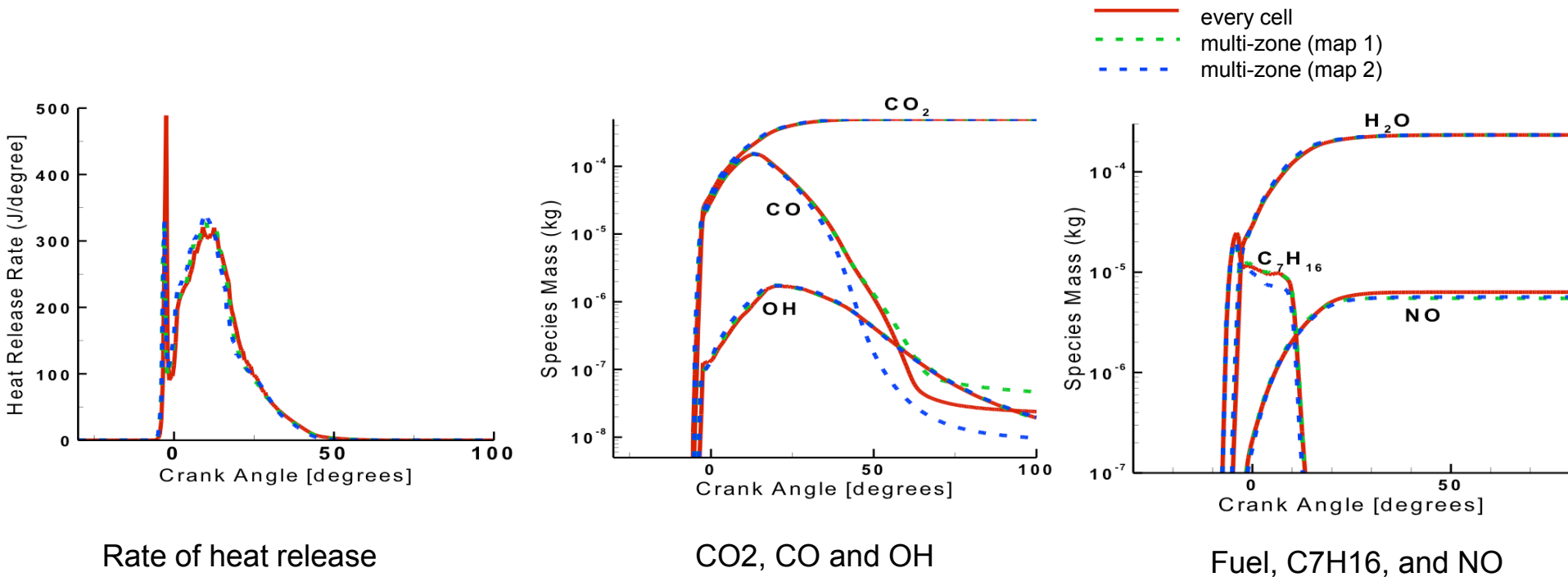

every cell   multi-zone

Temperature contours for CONVERGE with every-cell and multi-zone chemistry for DI diesel
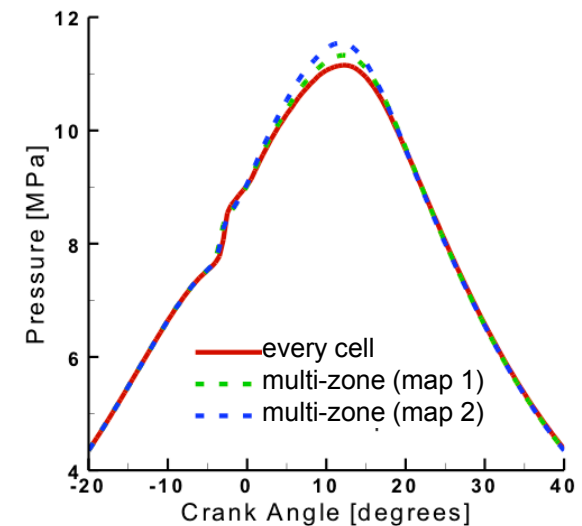
In-cylinder pressure predicted by CONVERGE for every-cell and multi-zone model

Predictions are very consistent between CONVERGE every-cell and multi-zone simulations

Legend:
— every cell
- - - multi-zone (map 1)
- - - multi-zone (map 2)

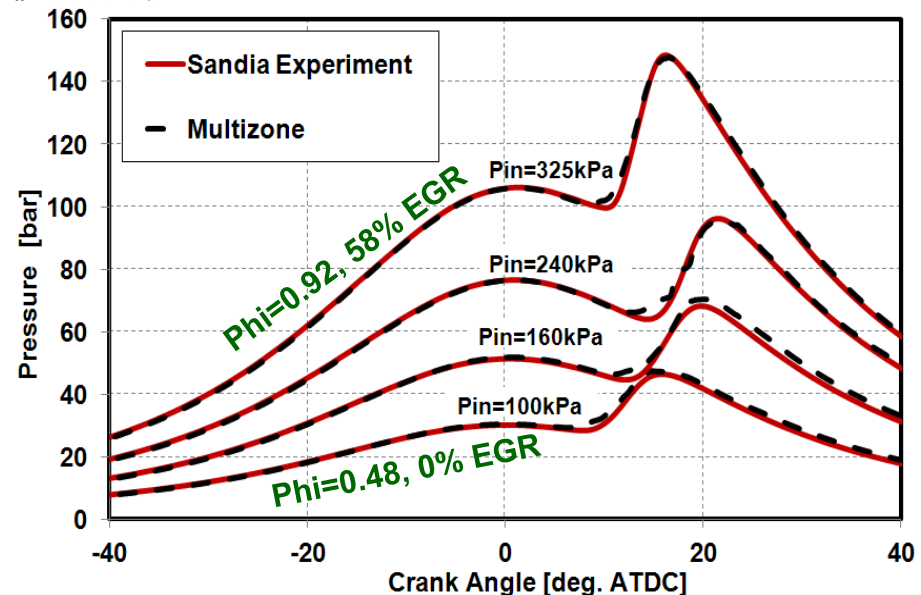Rate of heat release

CO2, CO and OH

Fuel, C7H16, and NO

Converge multi-zone provides the same accuracy while reducing the simulation time by a factor of 10
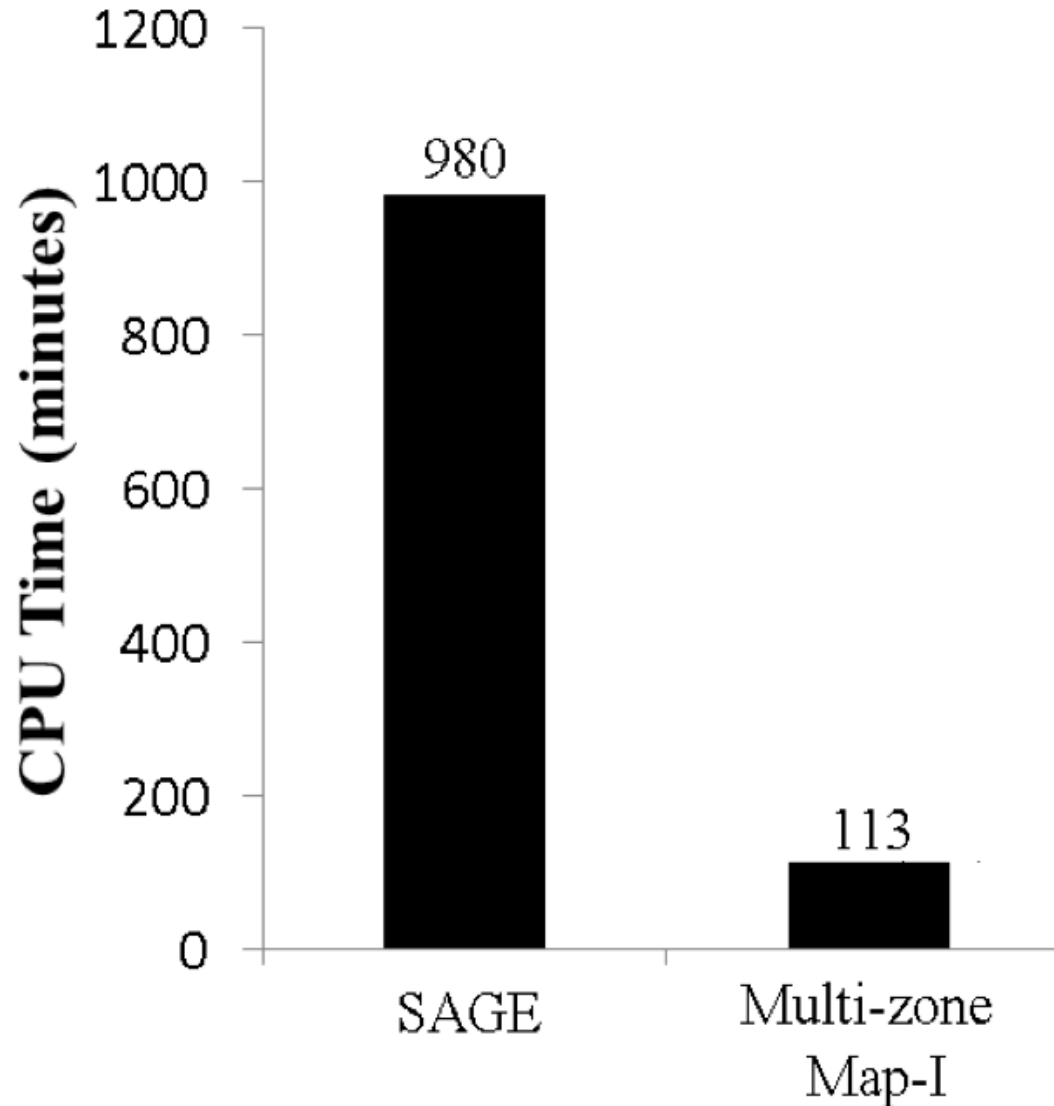
We have developed a standalone multi-zone kinetics engine model for use in engine cycle simulation codes
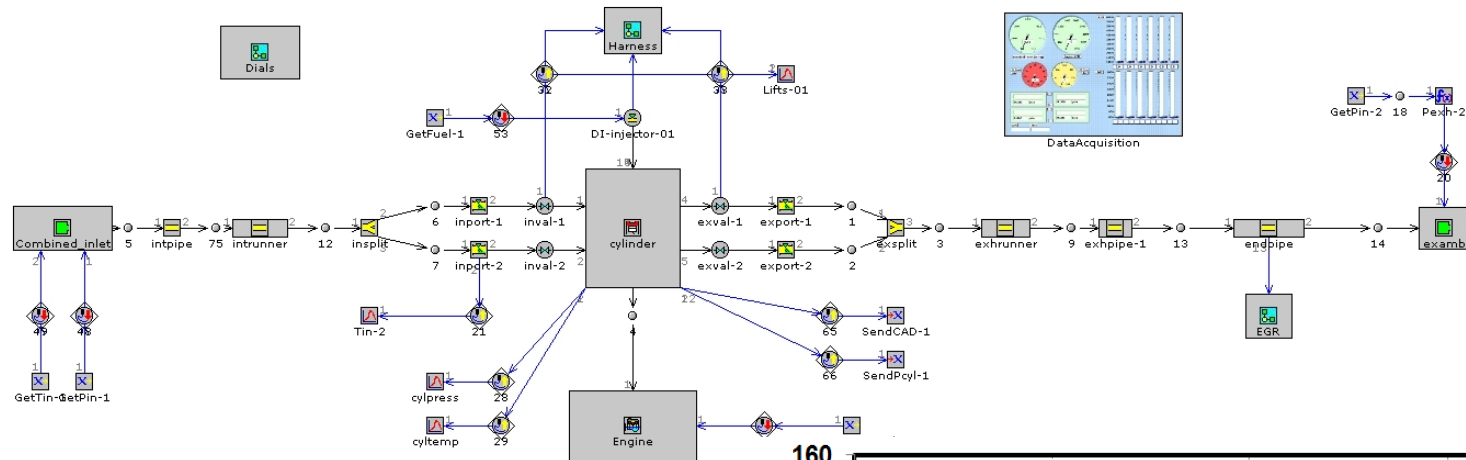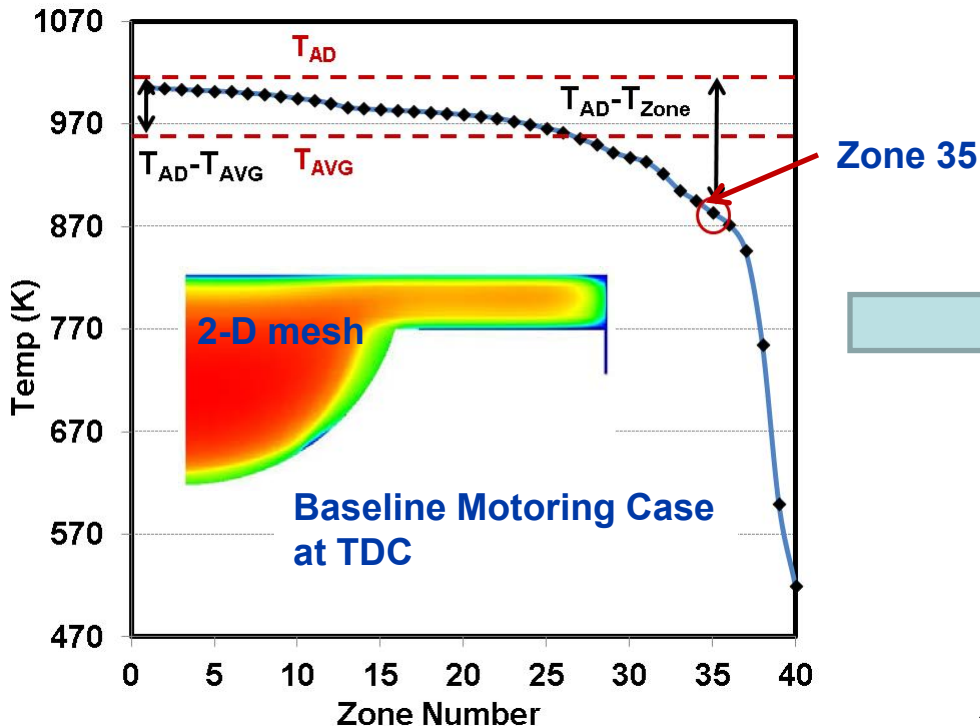

- Multi-zone integrated into GT-Power

- Resolves cycle-to-cycle feedback for NVO HCCI

For block-preconditioned solver, 10 zone model is 10-15 sec/cycle with 252 species mechanism

Accurate HCCI cycle simulations are possible by a single up-front motored CFD simulation
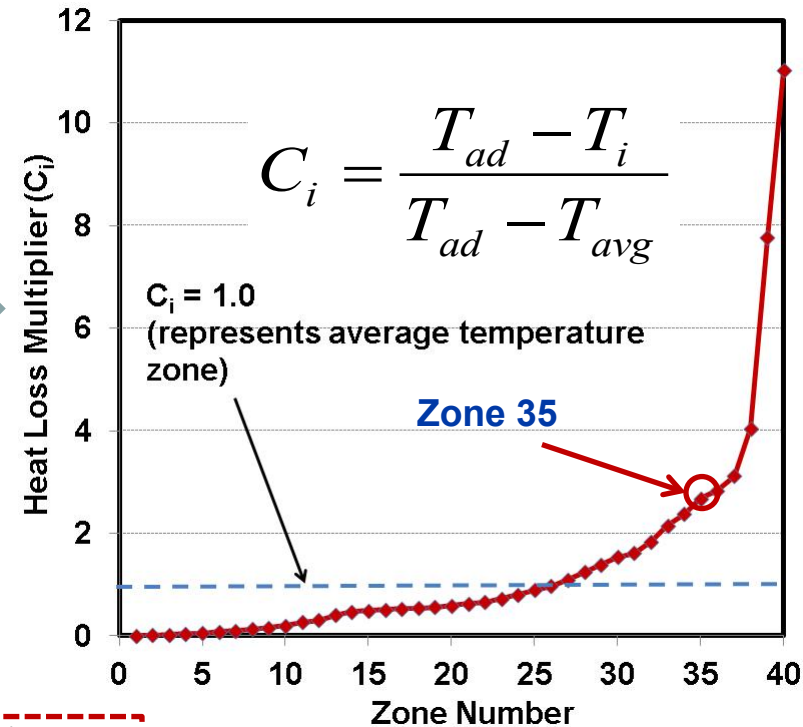
CFD Temp. Distribution at TDC

T_{AD}

$T_{AD}-T_{Zone}$

Zone 35

$T_{AD}-T_{AVG}$ T_{AVG}

2-D mesh

Baseline Motoring Case at TDC

Zone heat loss multipliers

$$C_i = \frac{T_{ad} - T_i}{T_{ad} - T_{avg}}$$

$C_i = 1.0$
(represents average temperature zone)

Zone 35

Heat Loss from zone 'i'

$$\dot{q}_i = C_i \frac{m_i}{m_{tot}} \dot{q}_{overall}$$

From Modified Woschni based on T_{avg}

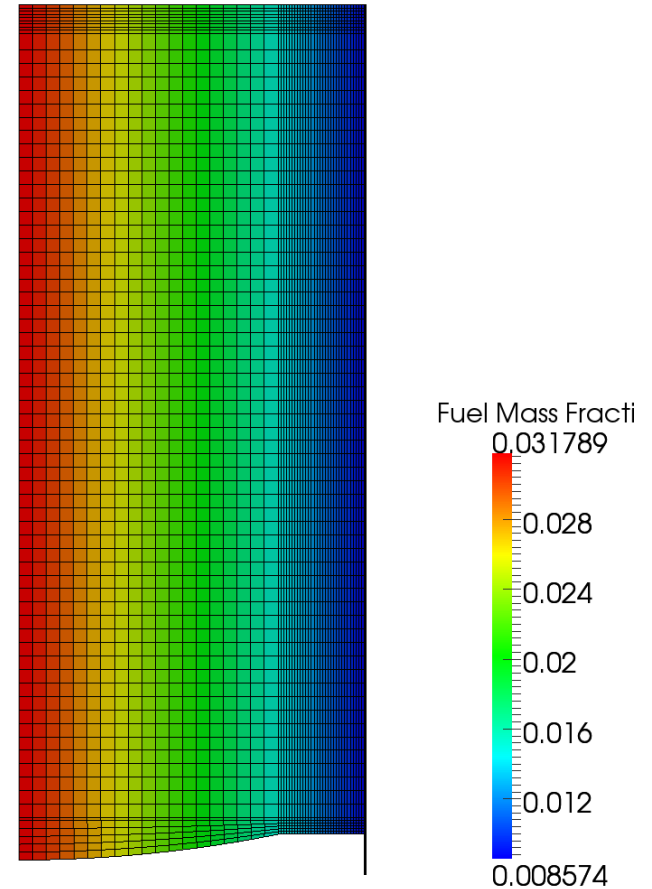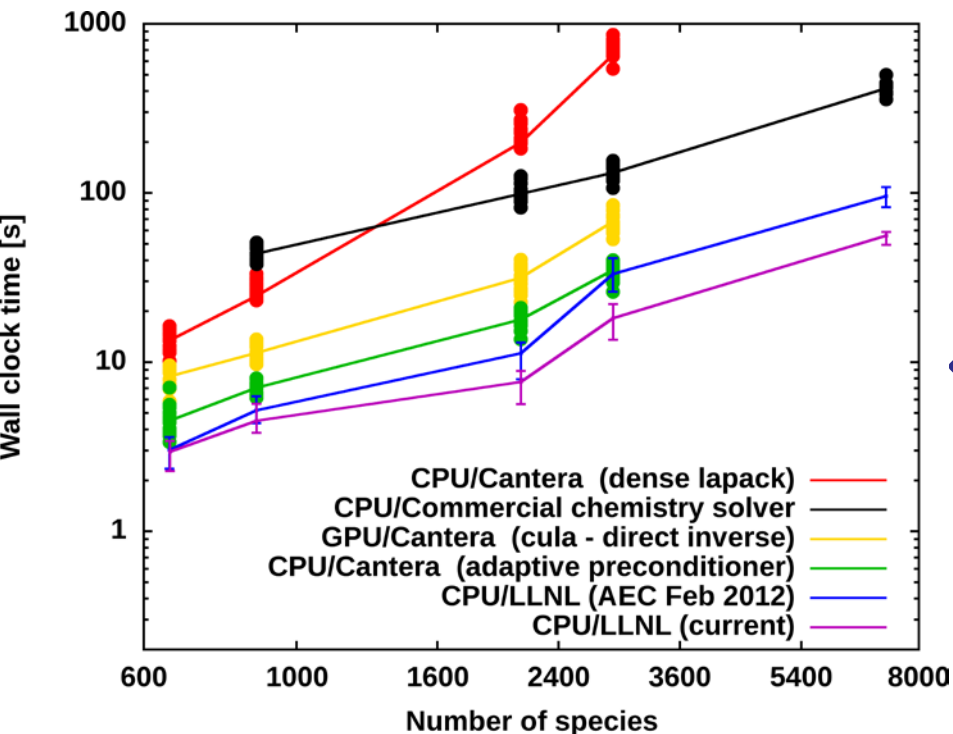**Procedure done ONCE (only at TDC) to determine C_i's.**

SAME C_i's are used for all RPM, intake conditions and loads.

We are incorporating advanced solvers into our Parallel CFD multi-zone model and benchmarking performance

New solvers (adaptive preconditioner) have been successfully implemented and tested in multi-dimensional parallel CFD

Geometry: 2D sector mesh (trapped volume)

Duration: -155 to 5 CAD

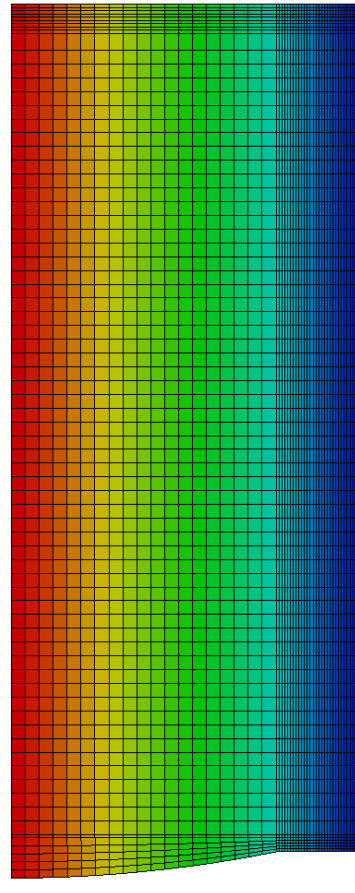Mesh Size: 0.4K-8K cells

Mechanism: 258 species iso-octane
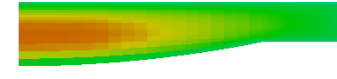
Chem Zones: 25-400

Processors: 12

Benchmark:

D. Flowers, S. Aceves, and A. Bajajimopoulos,
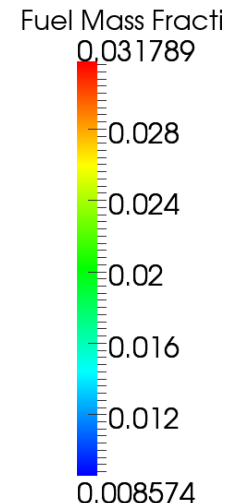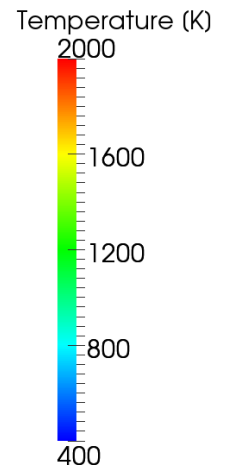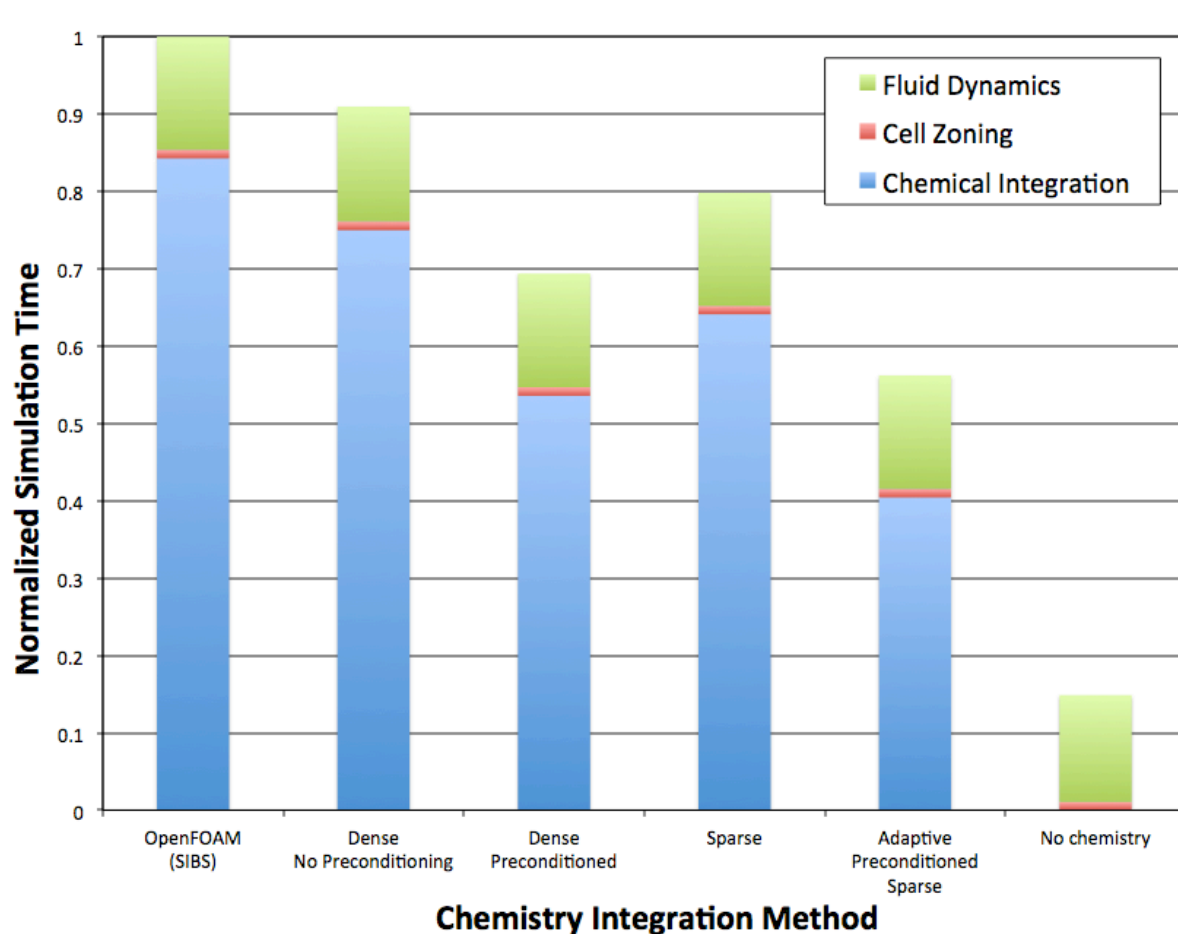
SAE-2006-01-1363
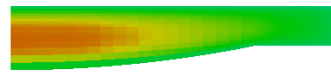

CA = 4 deg BTDC

CA = 25 deg BTDC

CA = 75 deg BTDC

Fuel Mass Fracti
0.031789
0.028
0.024
0.02
0.016
0.012
0.008574

Temperature (K)
2000
1600
1200
800
400

The adaptive preconditioner used in fully coupled CFD-Multizone is shown to provide speedup - even with "only" 250 species
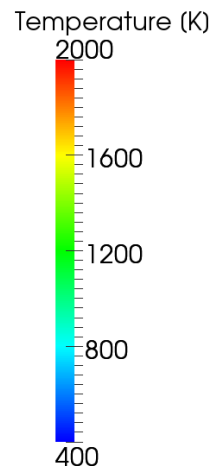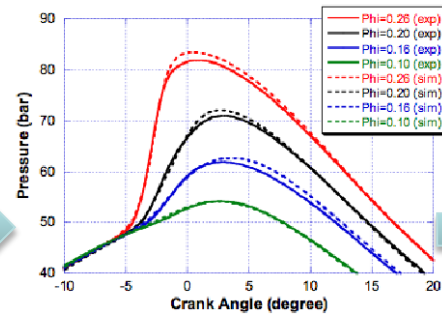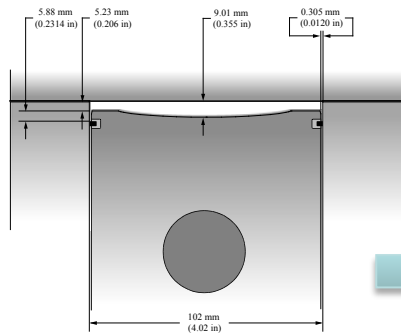

CA = 4 deg BTDC

CA = 25 deg BTDC

CA = 75 deg BTDC

Temperature (K)

LLNL sensitivity and uncertainty analysis tools are being applied to improving kinetic rates at elevated pressure using engine data
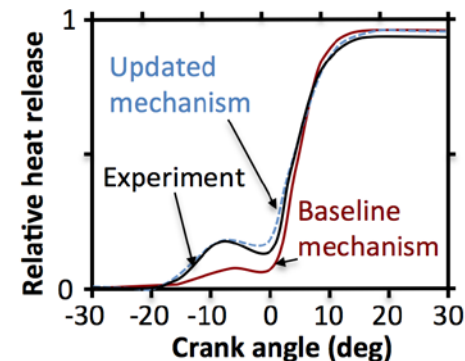

Engine experiments varying P_{in}, T_{in}, fuel flow, EGR, RPM, etc.

Large-scale Multi-zone simulations of engine operation

Objective function: Quantifying experiment and simulation agreement
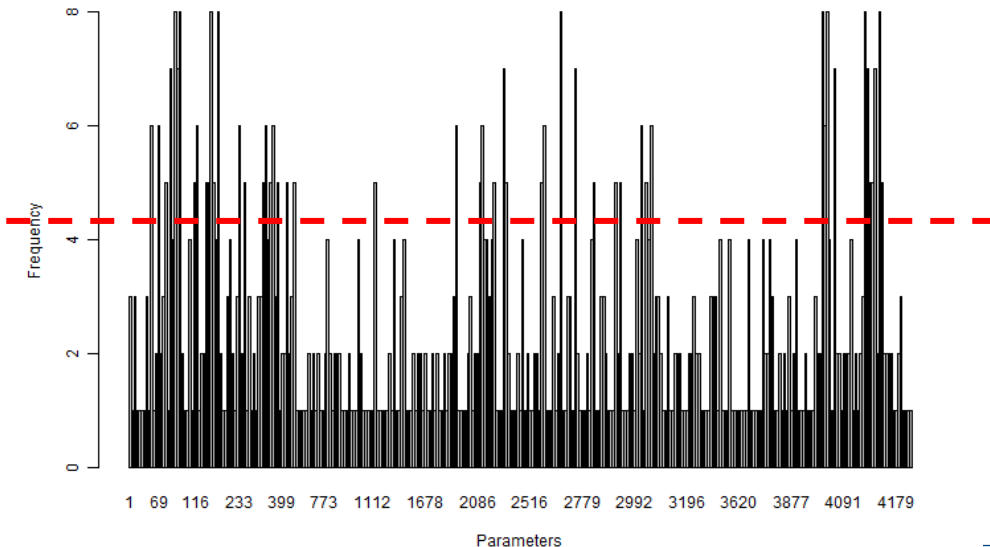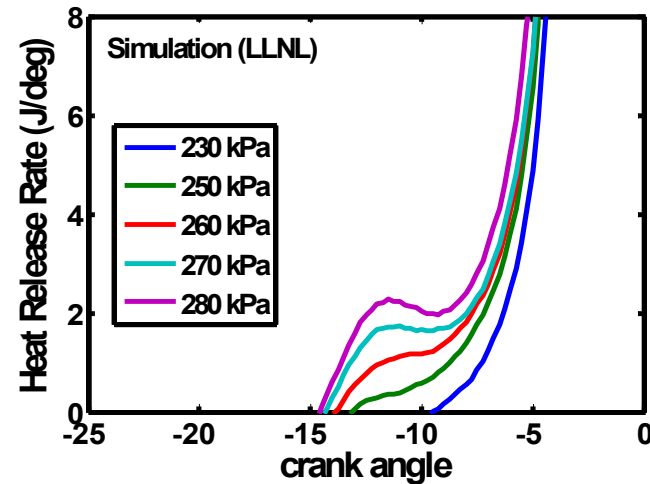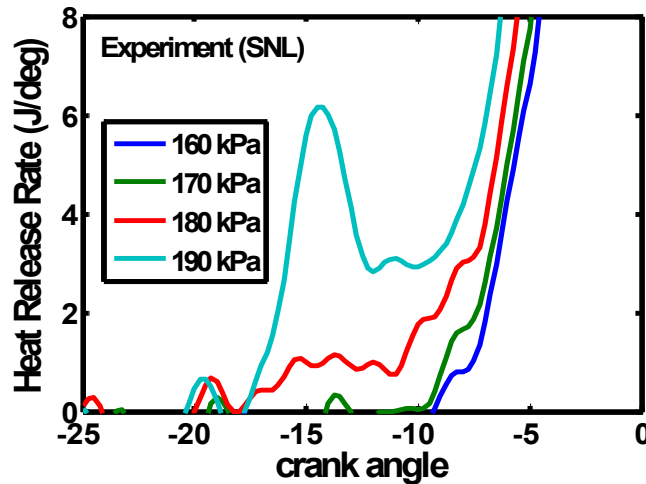
Refined chemical kinetic mechanism

1000s of simulations use sensitivity to update chemical kinetic rate parameters

We are investigating disparities in predicted low temperature heat release at elevated pressures

- 85000 simulations (500,000 CPU hrs) systematically adjust all 4800 kinetic rate parameters
- Screening identified a set of 47 rate parameters that most strongly affect LTHR

Collaboration: We have ongoing interactions Industry, National Labs, and Universities

- **Convergent Science Inc**; Multi-zone model development
- **Advanced Engine Combustion (AEC)** working group (Industry, National labs, Univ. of Wisc.); biannual presentations
- **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
- **Los Alamos National Laboratory**; Kiva4 development
- **Other Universities**: UC Berkeley, University of Wisconsin, University of Michigan, Lund Institute, Chalmers University, Tianjin University
- **Ford**; gaseous direct injection
- **Delphi**; direct injection
- **Bosch**; High Performance Computing of HCCI/SI transition
- **GM**; Diesel engine
- **Volvo**; multi-zone cycle simulation

Collaboration with Bosch using LLNL supercomputing resources to simulate SI to HCCI transition
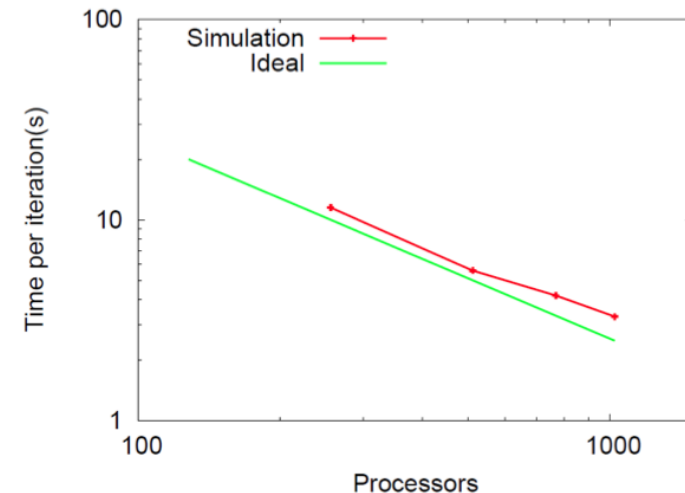
- LLNL hpc4energy incubator has dedicated 12 Million CPU hours for these simulations
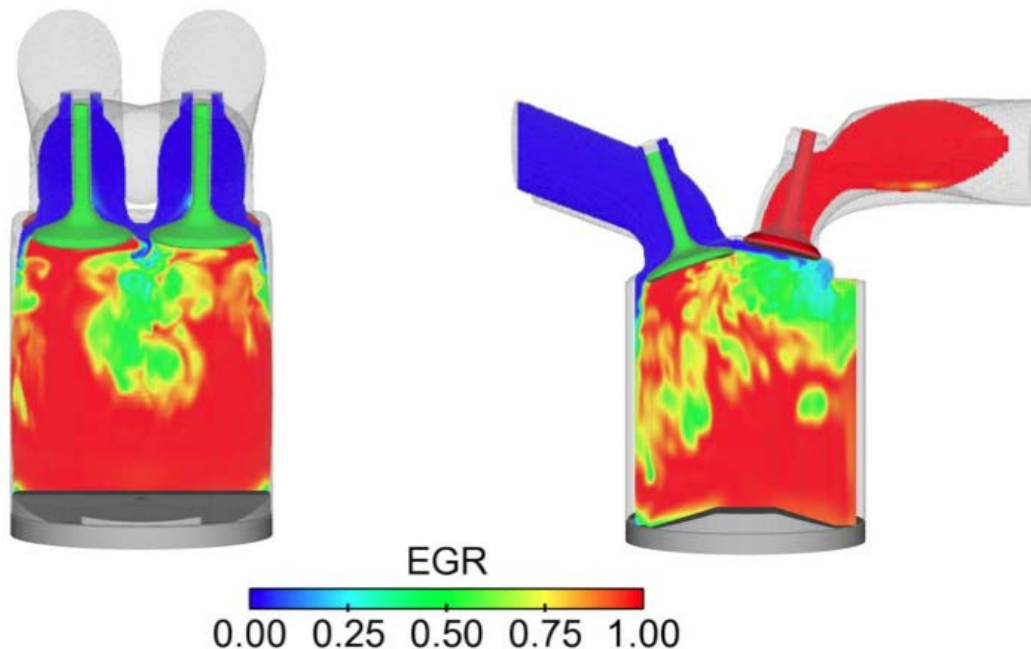
EGR

0.00 0.25 0.50 0.75 1.00

Simulations use ~32M computational cells

Engine simulation code scales well to 1000s of processors

Future Work: We will explore strategies for improving efficiency of engine CFD and chemistry simulations

- **Tech transfer of models to Industry/MOU partners**
  - We are actively developing means to release models to partners
  - We will build on CONVERGE license agreement
- **Improved parallel CFD with chemistry**
  - Overcome bottleneck due to reinitialization of each kinetic zone at each time step
    - Operator splitting: species transport, energy, chemistry are discretely and sequentially calculated over a time step
    - Final integrator state of chemical kinetic reactor from one time step will not be the same as the initial state for the next time step due to transport (convection, diffusion, zoning)
    - Recalculating the initial state is computationally expensive

    - *We will develop a method to adequately estimate the initial state (e.g. Jacobian) of the integrator based on prior step states and transport information*

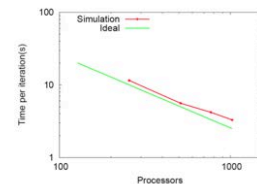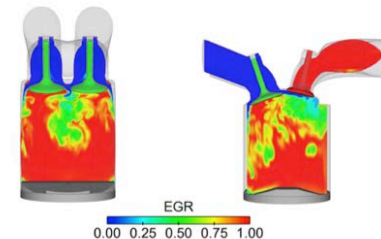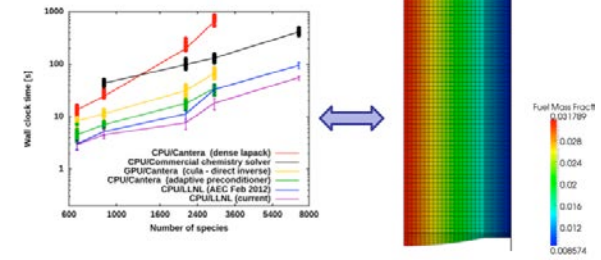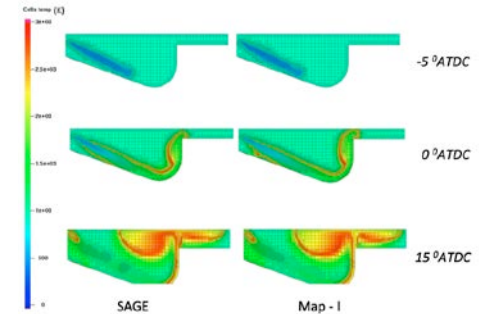**Lawrence Livermore National Laboratory**

Future work: extend applicability and computational efficiency of analysis tools

- ***Improved parallel CFD with chemistry***
  - Incorporate latest solvers in LLNL CFD packages and CONVERGE
  - ODE guided zone-to-cell remap for CFD multi-zone
  - Multi-criteria multi-zone for multi-component fuels
- ***Engine simulation with LLNL parallel CFD with chemistry***
  - Simulating high quality engine experiments from Sandia (PCCI, RCCI, CIDI) using latest high resolution CFD and multi-zone with large detailed mechanisms (~1000 species)
    - Successfully conducted closed-cycle simulations with 10M cells, 1000 species
- ***Mechanism rate optimization with multiple engine operating points***
  - Evaluate sensitivity of LTHR at high pressure for a wide range of engine operating conditions, optimize rate parameters
  - Develop general framework for mechanism optimization from engine data

Summary: We continue R&D activities that enable high fidelity simulation of advanced high-efficiency engines

- Collaboration with licensee Convergent Sciences Inc. on engine combustion simulation

- Multi-zone model for cycle simulation (in GT-Power)

- Improved kinetic solvers integrated into parallel CFD

- Optimization method for improving kinetic mechanisms with engine experimental data

- Large-scale computing of SI-to-HCCI transition

- Detailed simulation of Sandia engine experiments
  - Dec, Steeper, Sjoberg, Mueller engine

Simulations use ~32M computational cells

Engine simulation code scales well to 1000s of processors