Lawrence Livermore National Laboratory

Computationally Efficient Modeling of High-Efficiency Clean Combustion Engines

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This presentation does not contain any proprietary or confidential information

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LLNL-PRES-630352

Overview

Timeline

- Ongoing project with yearly direction from DOE

Budget

- FY11 funding: $740K
- FY12 funding: $740K
- FY13 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

- 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., 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

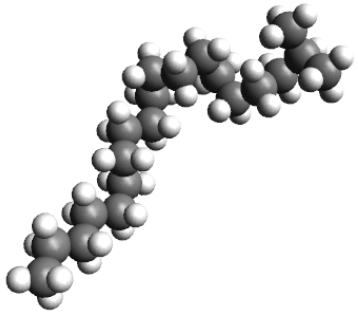
Objective

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



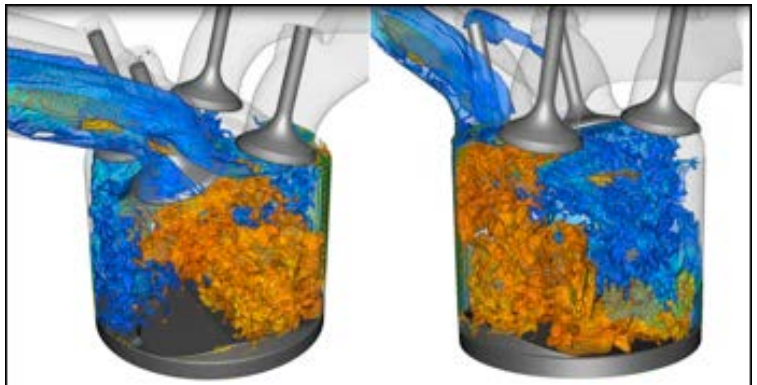
Ex. Biodiesel component

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

7.2K species

53K reaction steps

in highly resolved 3D simulations



Ex. SI/HCCI transition ~10M cells for Bosch in LLNL's hpc4energy incubator

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

n-alkanes

n-hexadecane ($C_{16}H_{34}$)

n-octadecane ($C_{18}H_{38}$)

n-eicosane ($C_{20}H_{42}$)

naphtho-aromatic

tetralin ($C_{10}H_{12}$)

iso-alkane

2,2,4,4,6,8,8-heptamethylnonane ($C_{16}H_{34}$)

aromatics

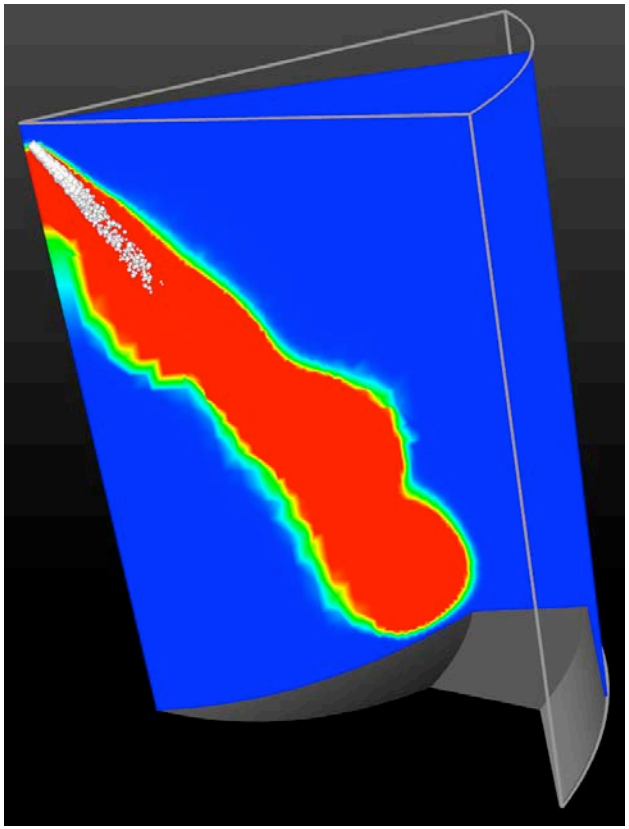
cyclo-alkanes

1,2,4-trimethylbenzene (C_9H_{12})

n-butylcyclohexane ($C_{10}H_{20}$)

1-methylnaphthalene ($C_{11}H_{10}$)

trans-decalin ($C_{10}H_{18}$)



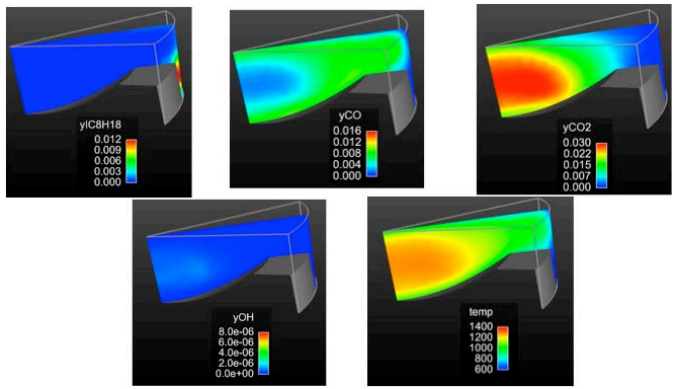
Representative Detailed Chemical Kinetics

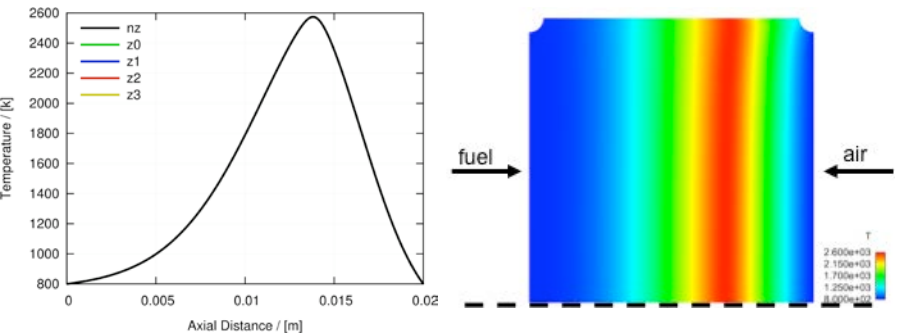
High-Fidelity Fluid Mechanics

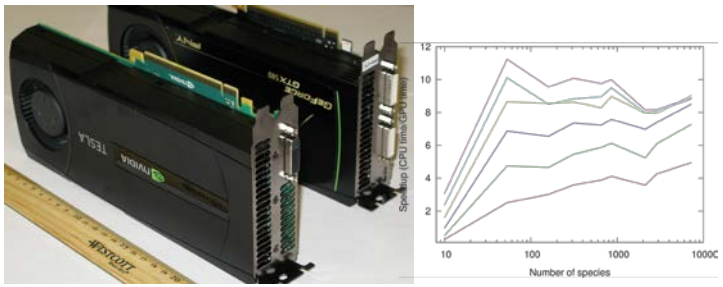
Approach: Develop analysis tools leading to clean, efficient engines in collaboration with industry, academia and national labs

- 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
- Make accurate and efficient models accessible to industry
- Democratize simulation: bring chemical kinetics-fluid mechanics computational tools to the desktop PC

Milestones: We have developed and validated detailed engine modeling tools







- Validated new multi-zone scheme, quantified accuracy and fidelity for zone stratgies (July 2012)
- Implemented advanced solvers with Converge multi-zone, orders of magnitude reduction in simulation time (Sept 2012)
- Validated Multi-dimensional simulations of isooctane PCCI using Converge multi-zone with detailed chemistry (Nov 2012)
- Demonstrated CFD/multi-zone applied to GDI SI and PCCI operation (Dec 2012)
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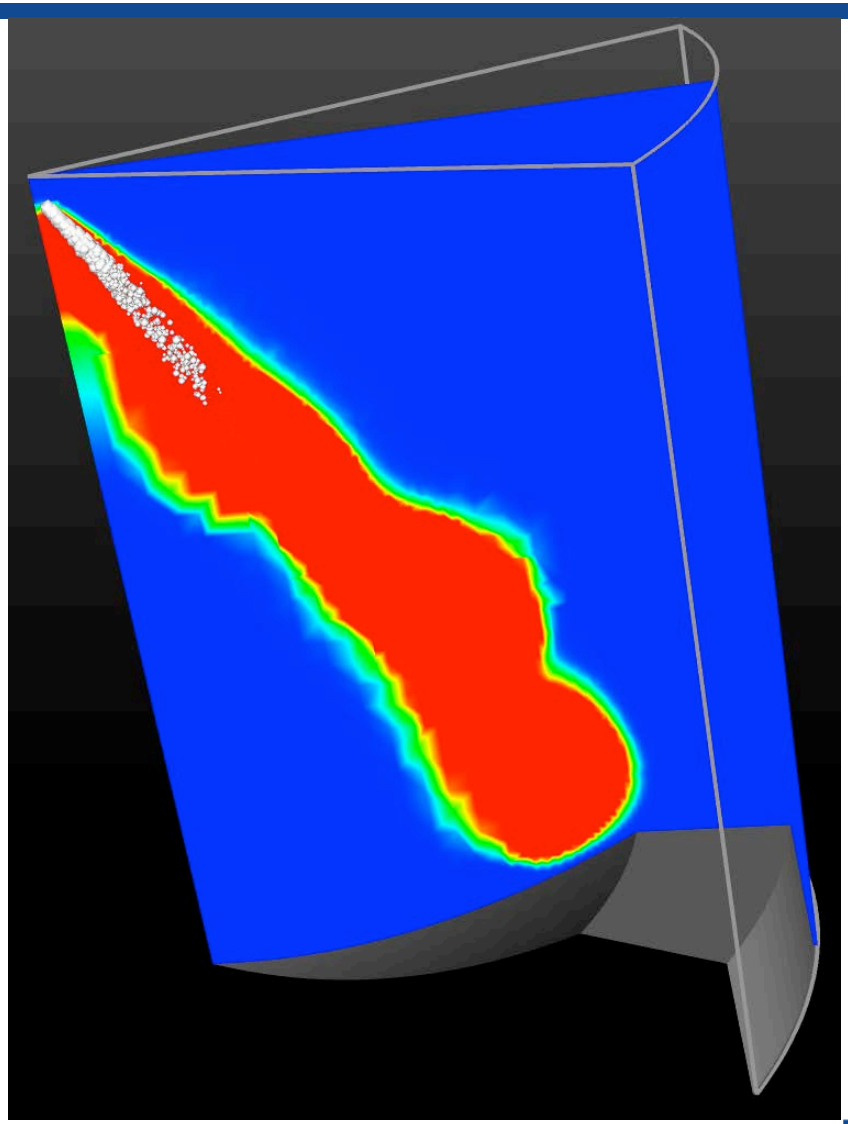
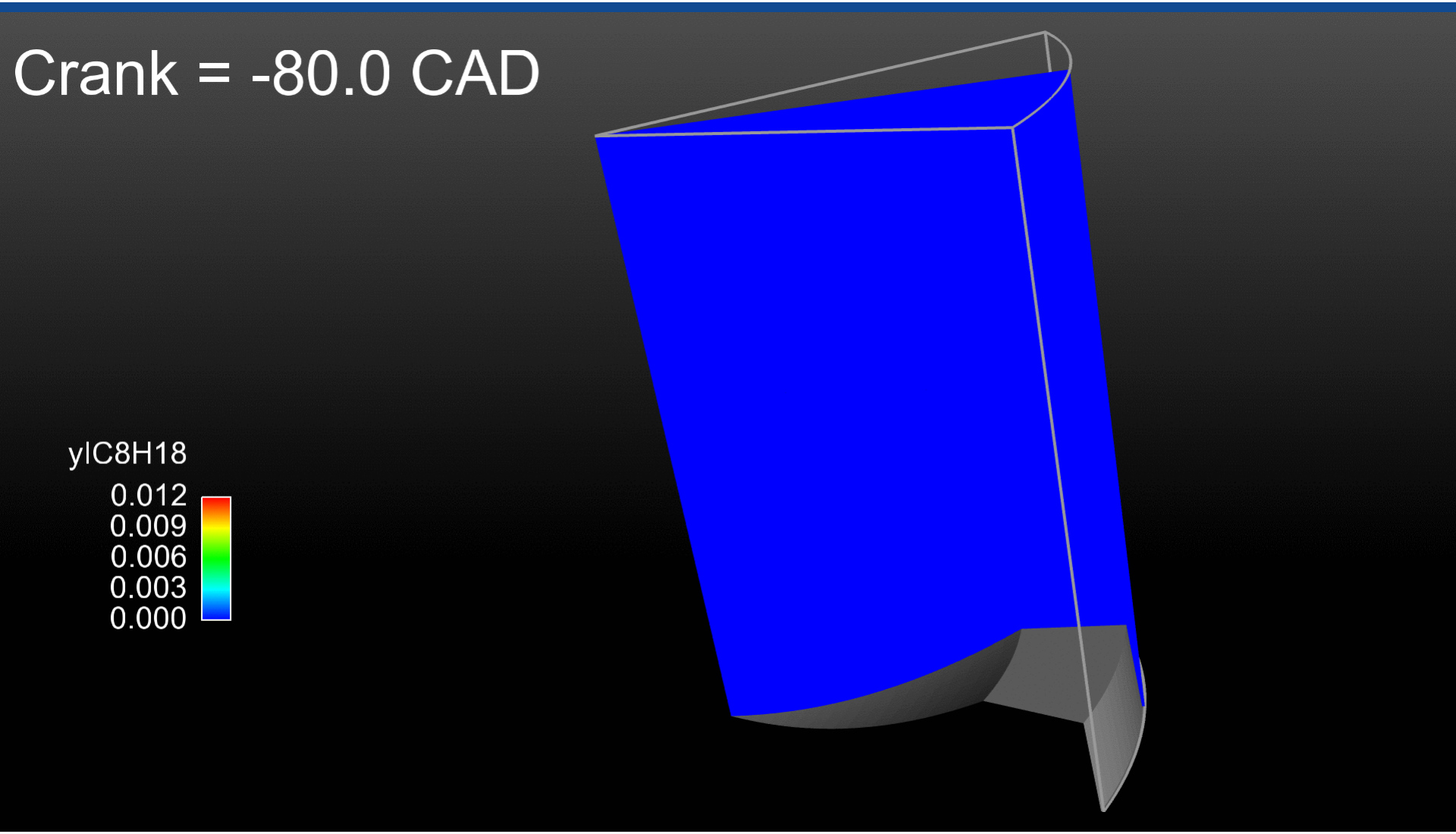
- New license agreement for advanced CPU/GPU solvers with Convergent Sciences (April 2013)

FY2013 Accomplishment – Validating Converge multi-zone for Early-Direct Injection PCCI

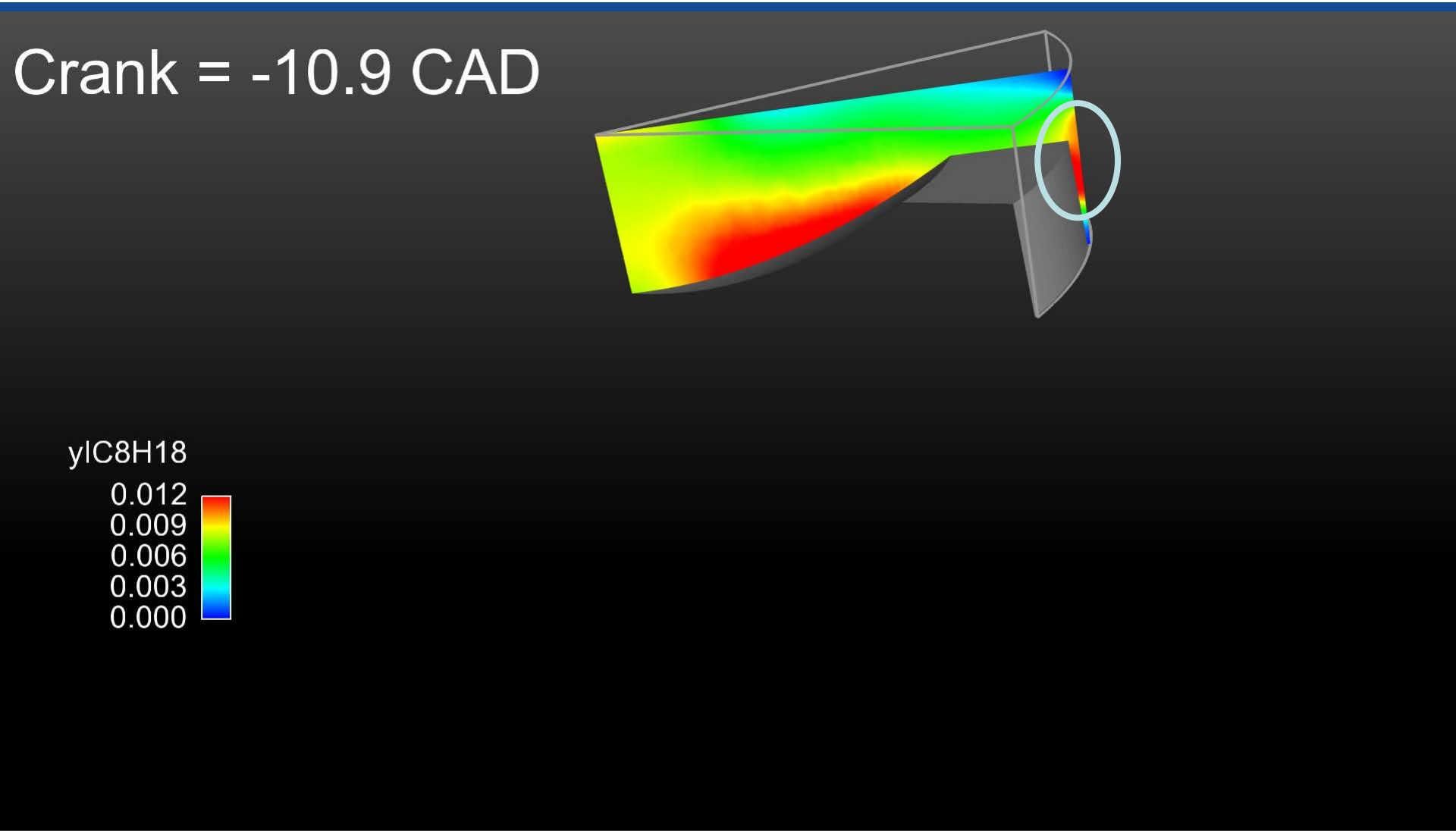
- Sandia (Dec) isooctane data
- Converge spray models (RT/KH)
- LLNL multi-zone and AP solver
- 874 species ic8h18 mechanism
- Closed cycle
- 45 degree sector
- 200K cells (at BDC)
- Low load (phi=0.12 overall)



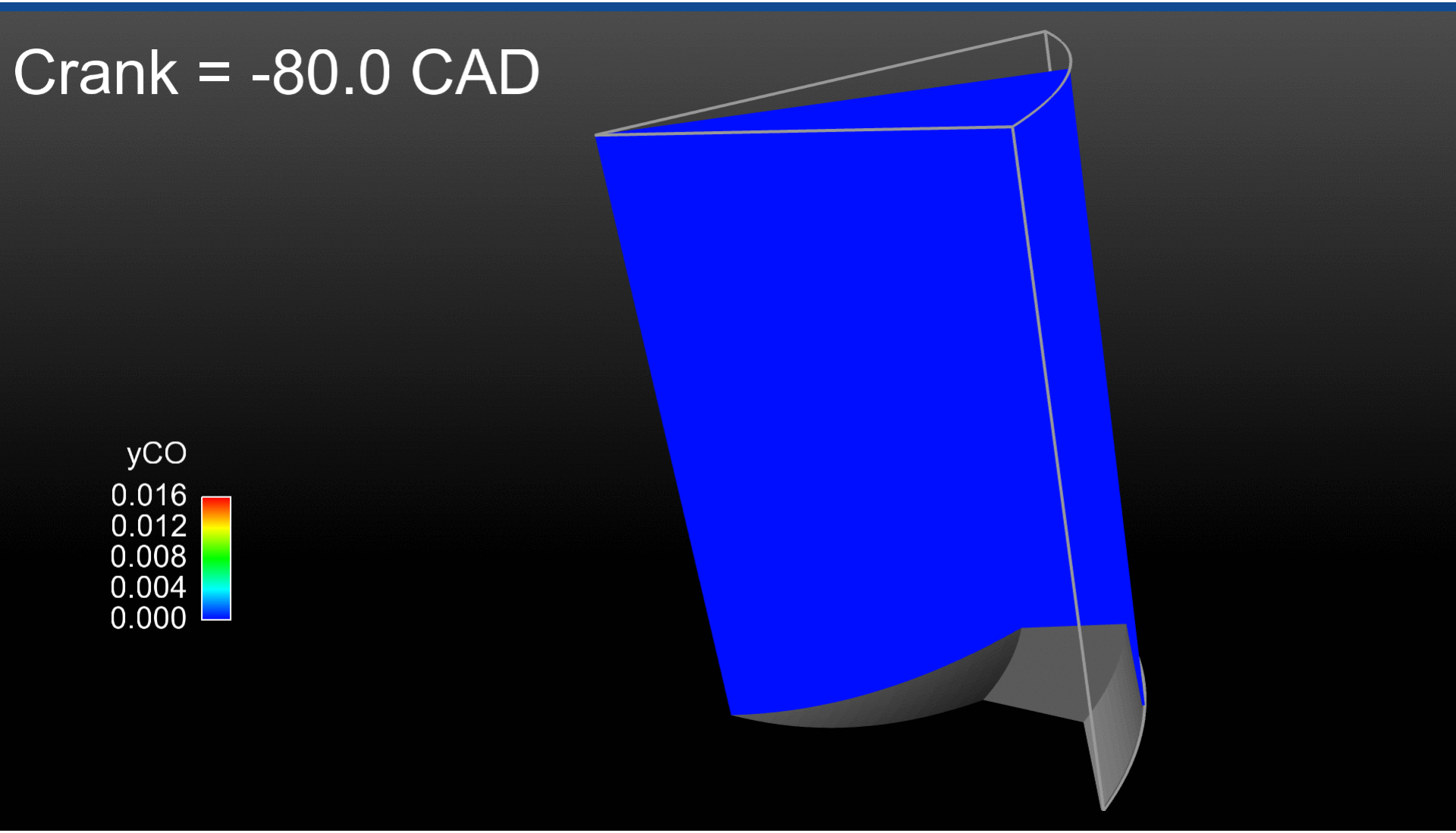
Fuel concentration is highest near bowl with some fuel entering the ring crevice



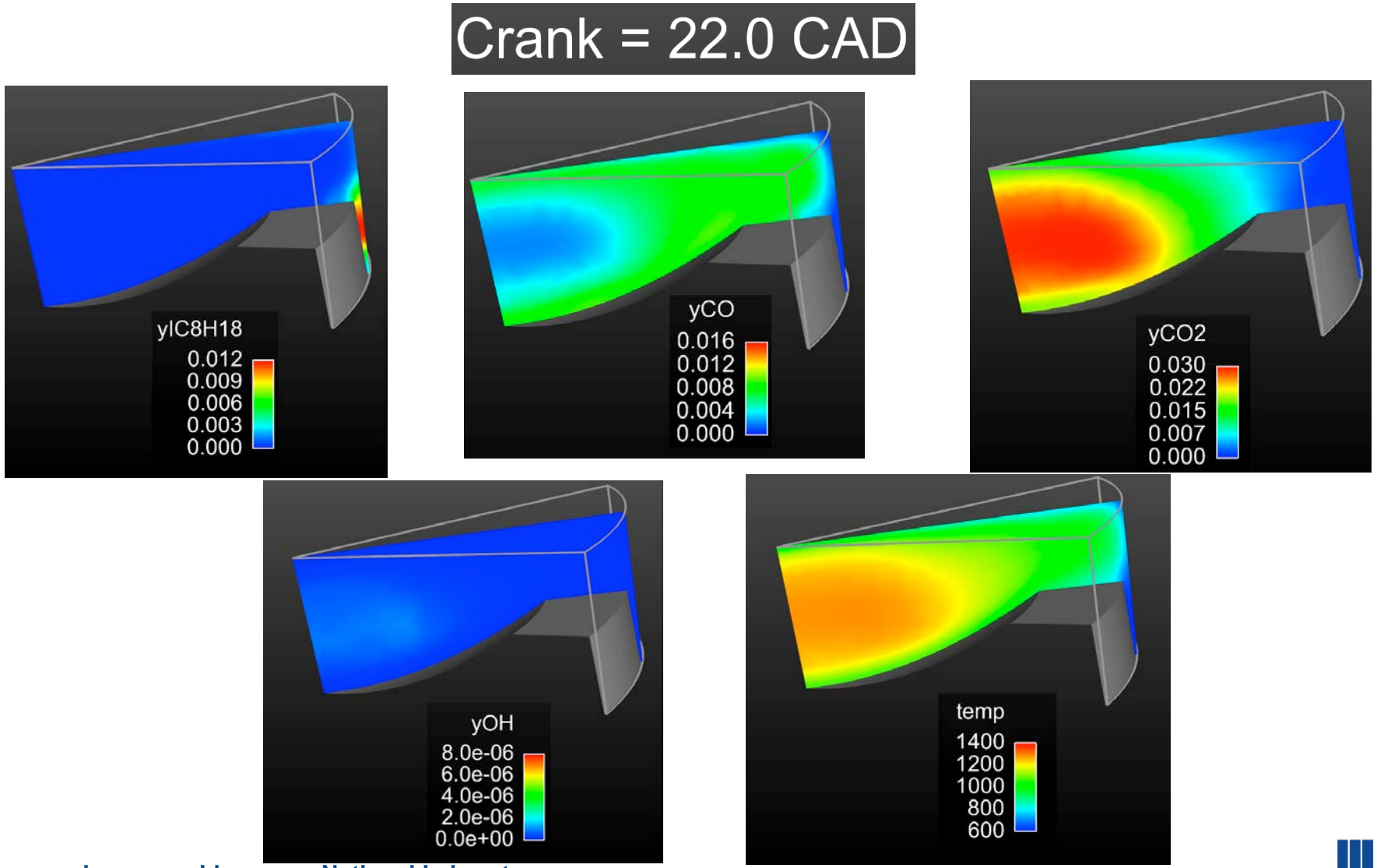
Fuel distribution in cylinder just before significant conversion occurs



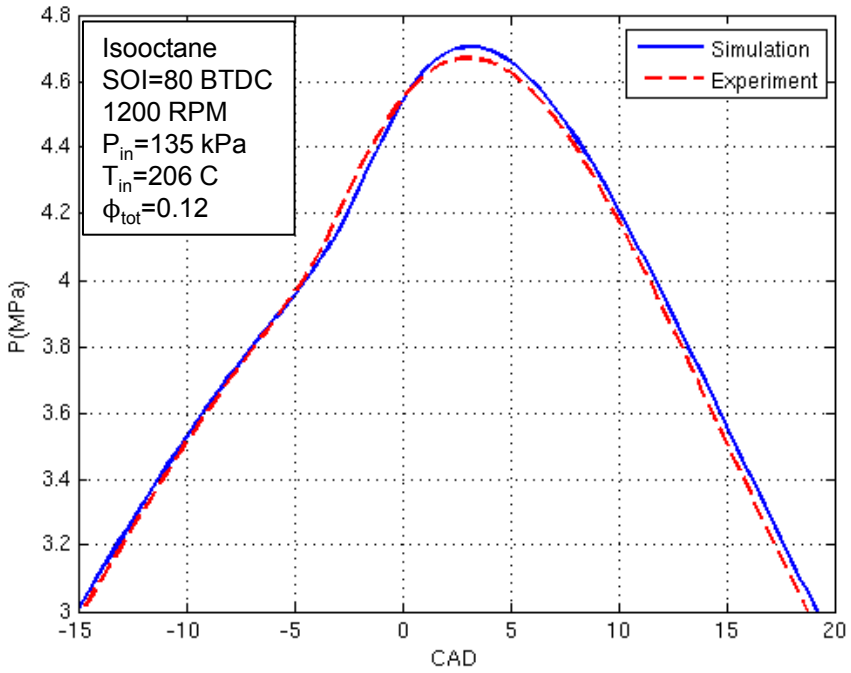
CO is not fully converted away from the central core of the combustion chamber

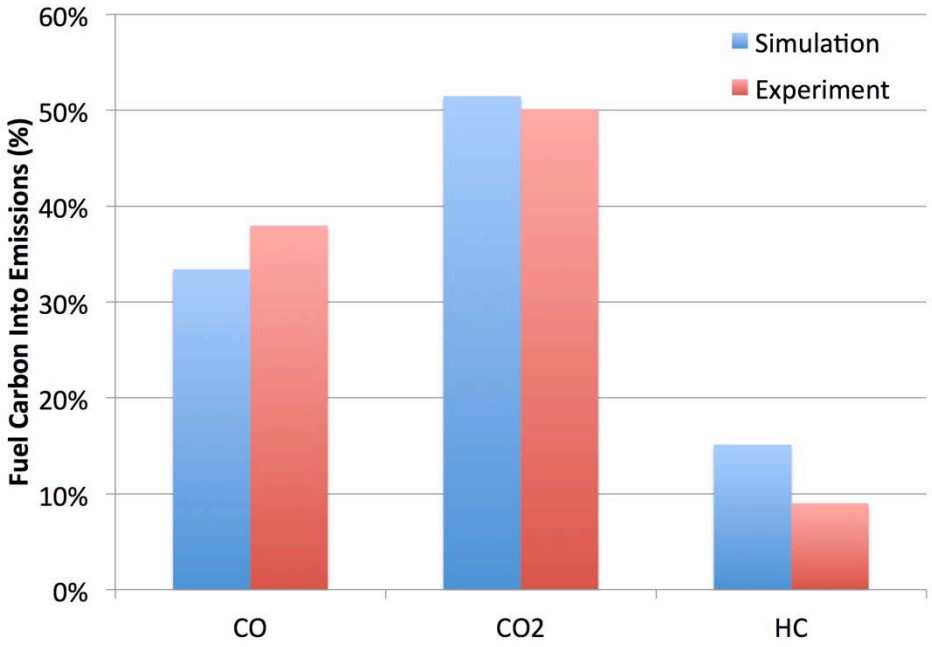


Full conversion of fuel occurs in the center of the combustion chamber, partial reaction in squish region



Very good agreement on in-cylinder pressure and emissions without tuning modeling parameters





- Mesh refinement and multi-zone parameter refinement studied to achieve “grid” convergence

FY2013 Accomplishment - 25x reduction in chemistry time for multi-zone with latest LLNL solver in Converge Multi-zone

HCCI Engine Simulation

Cummins B-series geometry

Homogeneous iso-octane/air mixture

Equivalence ratio ~0.2

Multi-zone T-Φ bins:

ΔT = 10 K

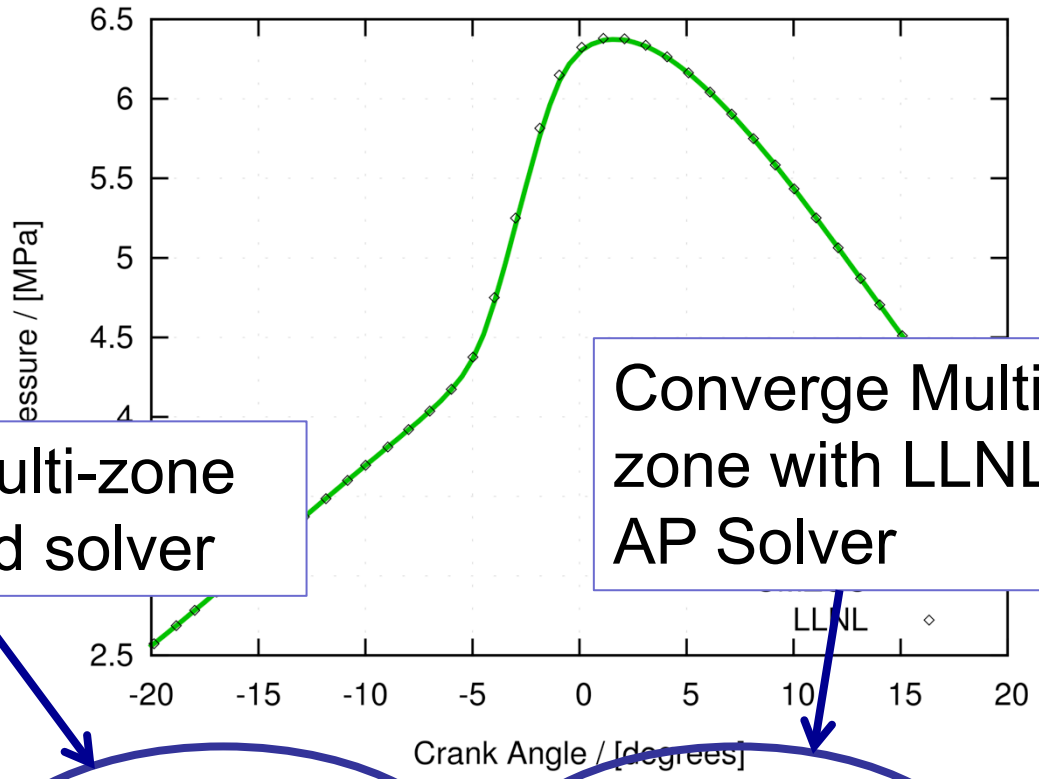
ΔΦ = 0.1

~250,000 cells at BDC

Max num. zones = 122

857 species LLNL iso-octane mechanism

24 processor MPI run



Converge Multi-zone with standard solver

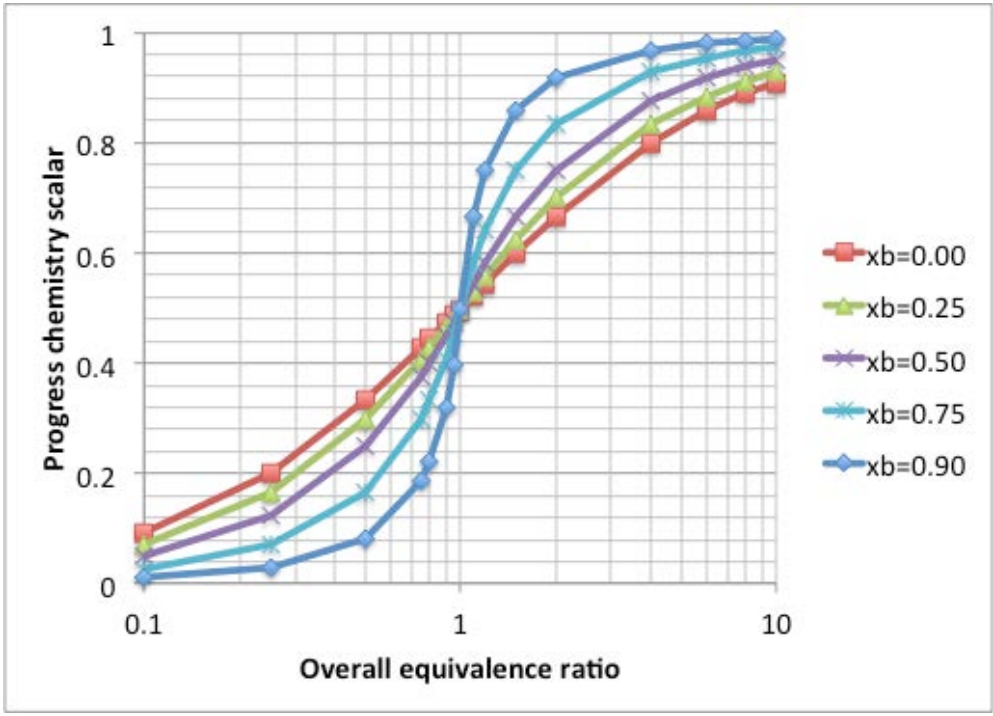
Converge Multi-zone with LLNL AP Solver

Total Simulation Time (wall clock):	CMZ = 15.66 hrs	CMZ-LLNL = 10.2 hrs
Chemistry Time* (avg. per proc.):	CMZ = 5.26 hrs	CMZ-LLNL = 0.2 hrs

*includes zoning time

FY2013 Accomplishment: New zoning approach developed and zone discretization strategies validated

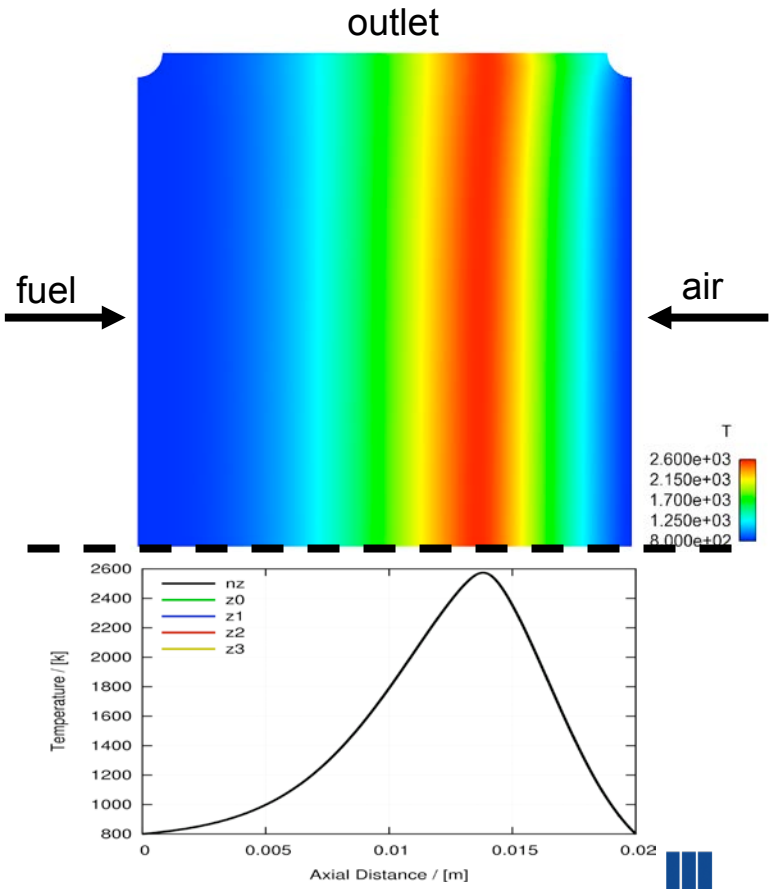
- Fast solver utilization
  - Adaptive Preconditioner
  - CPU/GPU hybrid
- Zoning strategies
  - New discretization parameters
  - N-dimensional zoning
- Alternative remap
- Error metrics and error control



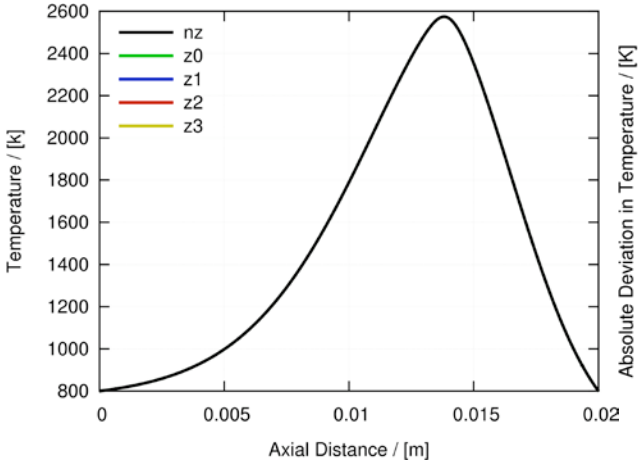
Non-premixed reactor designed to investigate accuracy and efficiency of multi-zone compared to every-cell kinetic chemistry

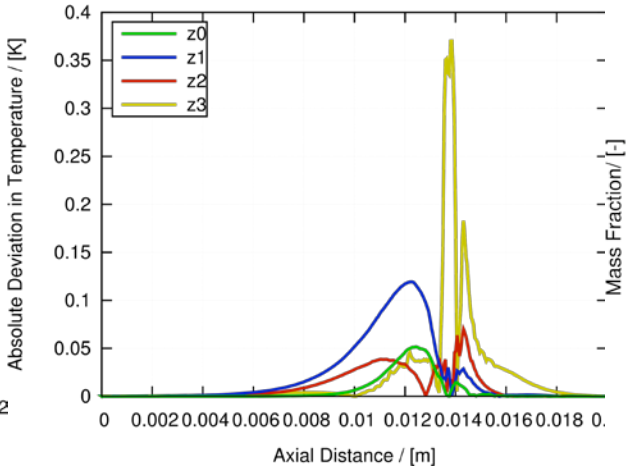
- Multi-zone Test Case:
  - 2-D domain (2 cm x 2 cm)
  - H_2 fuel / Air oxidizer
  - Atmospheric Pressure
  - 800 K inlet temperature
  - Laminar
  - Steady state solution
  - ~64,000 cells
  - LLNL Hydrogen Mechanism (10 species / 21 reactions)
  - Future work with large hydrocarbon mechanisms

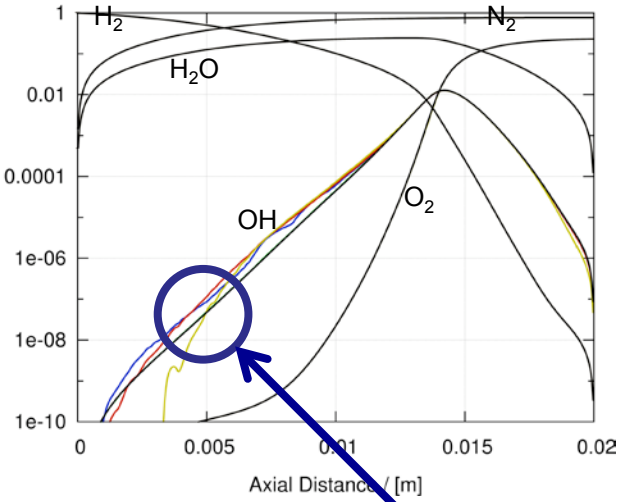
Counter flow laminar flame include diffusion and high stratification of fuel and air



This model allows us to quantify prediction quality of zoning and remapping strategies, and computational efficiency





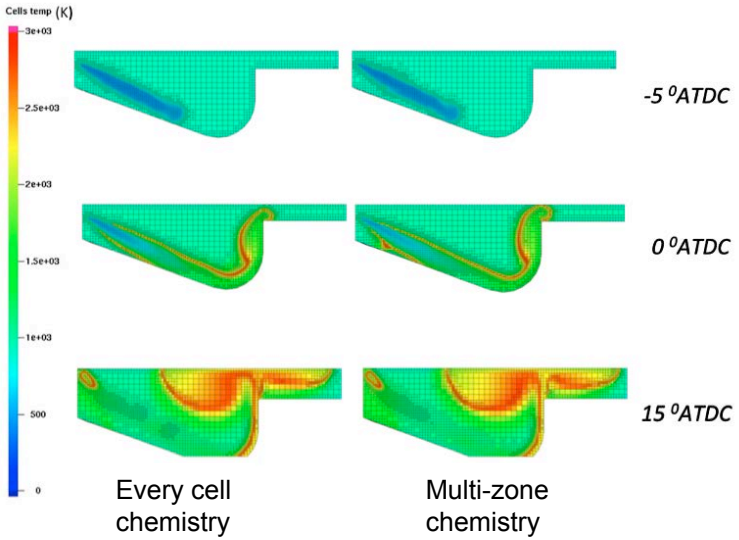


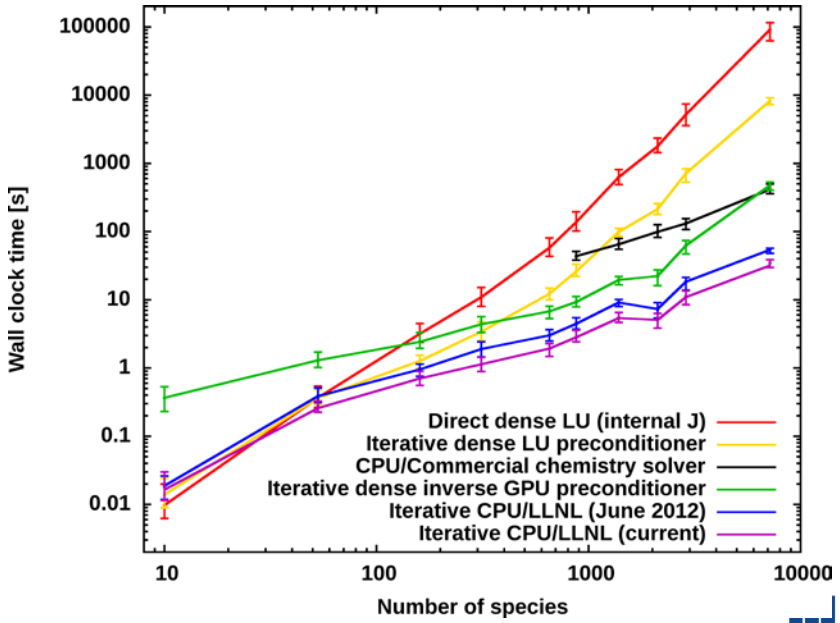
Remap affects minor species

Label	ΔT	Δf	# of Zones	Chemistry Speedup	Overall Speedup
nz	Every Cell Chemistry		63680	1	1
z0	1	0.002	3773	13.2	9.6
z1	5	0.005	749	54.6	19.3
z2	10	0.01	372	91.8	22.6
z3	20	0.02	186	132.9	23.5

FY2013 Accomplishment: New license agreement with Convergent Science for CPU and GPU based chemistry solvers

- Non-exclusive amendment to multi-zone license agreement from 2010
- 4 year extension (through 2017)
- Includes multi-zone, latest adaptively preconditioned solvers and GPU based solvers





LLNL collaborating with Cummins, Converge, IU to develop the GPU chemistry solver

- IU Big Red II Supercomputer
- Hybrid CPU/GPU machine
  - CPU compute nodes
    - Two AMD 16 core CPU
  - GPU compute nodes
    - One AMD 16 core CPU
    - One K20 2496 core GPU
  - 1020 total nodes
  - 1.006 petaflops
- To be commissioned spring 2013

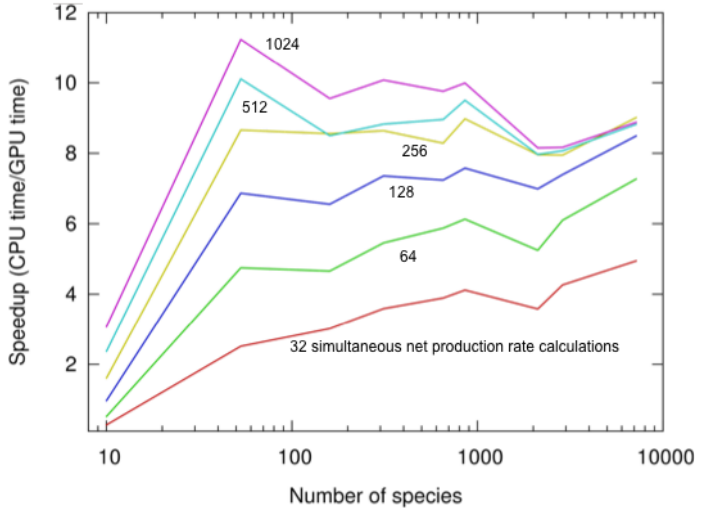
CONVERGENT SCIENCE

INDIANA UNIVERSITY

FY2013 Accomplishment: Potential 10x reduction in chemistry time for multidimensional CFD with GPU-assisted advanced solver

LLNL-Converge GPU chemistry solver developed on LLNL Edge Cluster

LLNL Edge Cluster	
GPUs	412 Tesla M2050
Cores	185,000 GPU, 2,500 CPU
Tflop/s	212 (64-bit)



GPU solver most effective in multi-reactor (e.g. CFD) simulations

Readily applicable for simulation on ~$5000 GPU-equipped engineering workstation

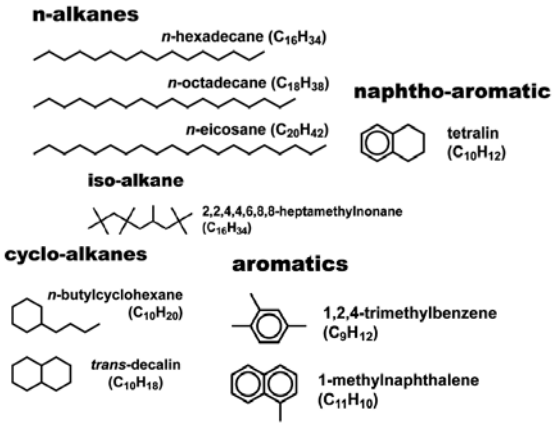
Collaboration – We have ongoing interactions with industry, national laboratories, and universities

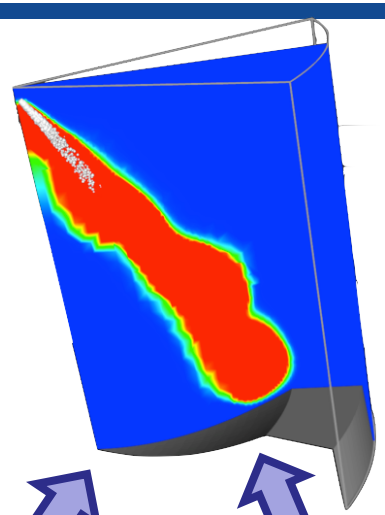
- **Cummins**; CPU/GPU solvers for Converge CFD to run biodiesel engine simulations on new Indiana Univ. GPU supercomputer.
- **Ford**; gaseous direct injection, chemistry solver/mechanism assistance
- **Volvo**; multi-zone cycle simulation, OpenFOAM model development
- **Bosch**; High Performance Computing 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 14C 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 – There are many ways to work with us

- Chemistry solver support for MOU partners
- 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.

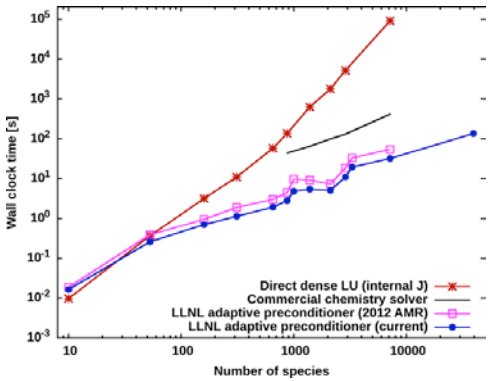
Future work: Predictive 3D simulation of Diesel combustion with full (>10,000 species) detailed chemistry



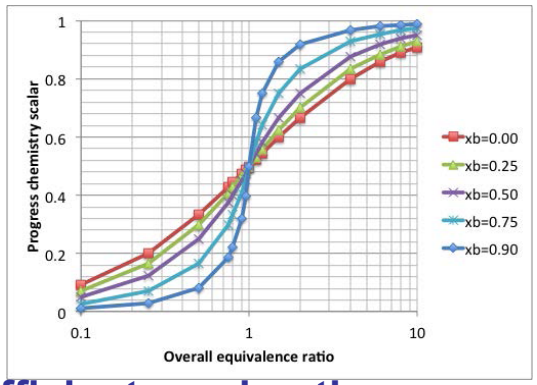


High fidelity Diesel engine simulations

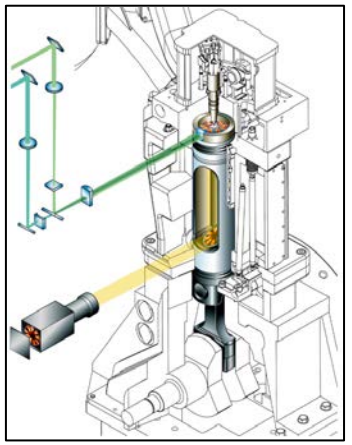
9-species Diesel mechanism
>10,000 species (Pitz, LLNL)



Accelerated kinetic solver tools (McNenly, LLNL)



Efficient combustion models (Flowers, LLNL)

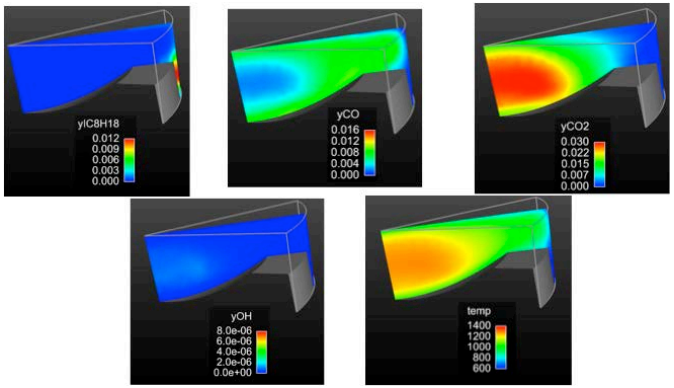


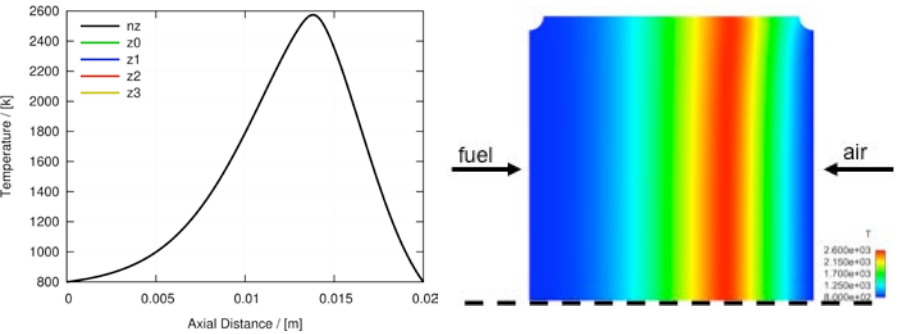
High quality experiments (Mueller, SNL)

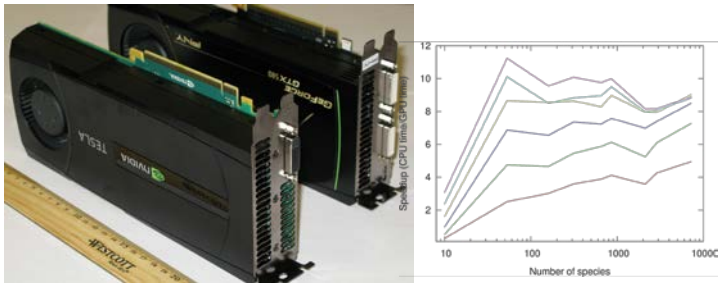
Future work: Improve physical accuracy and computational efficiency of engine combustion modeling tools

- ***Improved parallel CFD with chemistry***
  - Multi-zone improvements: Jacobian or other improved remap; error–bound driven zoning strategy.
  - Improve computational performance for operator-split, every-cell chemistry in CFD: quasi-steady-state, partial equilibrium, perturbative methods, fully-coupled chemistry/advection/diffusion.
  - Improve computational performance for species advection/diffusion calculations.
- ***Engine simulation with LLNL parallel CFD with chemistry***
  - Fuel effects in HCCI/PCCI engines (Pitz/Mehl full and reduced mechanism for RD387, Certification Fuel, Ethanol based on J. Dec Experiments)
  - Diesel predictive engine model with detailed chemistry, spray, soot (Pitz/Mehl mechanism, C. Mueller Experiments)
- ***Mechanism rate optimization with multiple engine operating points***
  - Sensitivity analysis of multi-zone models and CFD codes for HCCI
  - Compare CFD codes with phenomenological multi-zone
  - Uncertainty quantification simulations applied for HCCI experiment design
  - Improve large kinetics mechanism using large-scale uncertainty quantification tools
- **Continue technology transfer and licensing activities**

Summary: We are providing industry and researchers with accurate and efficient engine combustion modeling tools







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