Lawrence Livermore National Laboratory

Simulation of High Efficiency Clean Combustion Engines and Detailed Chemical Kinetic Mechanisms Development

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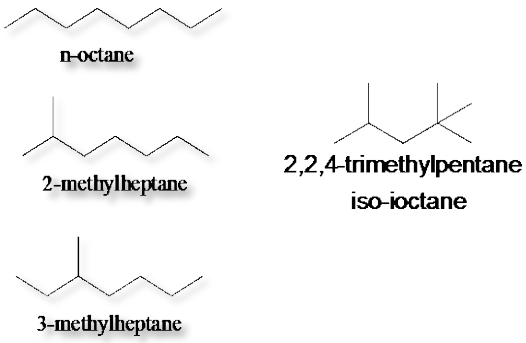
Acknowledgements

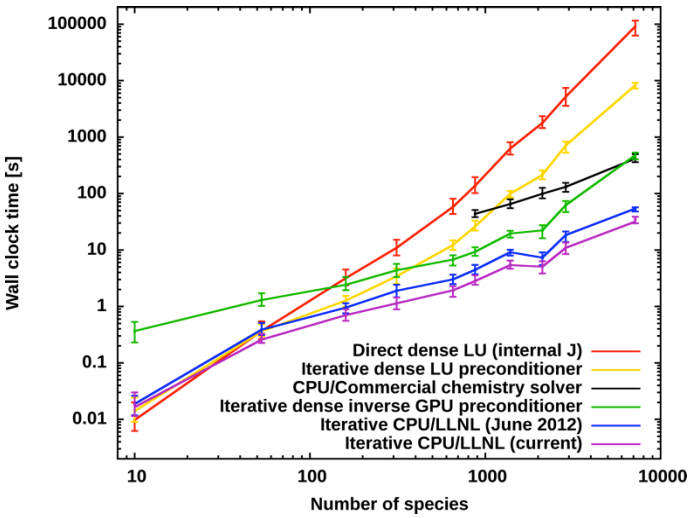
U.S. DOE, Office of Vehicle Technologies Program

Team Leader: Gurpreet Singh

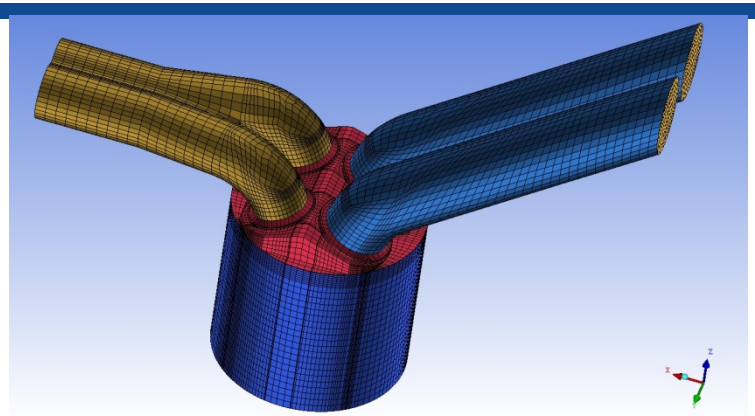
LLNL combustion program encompasses a range of activities in simulations and experiments



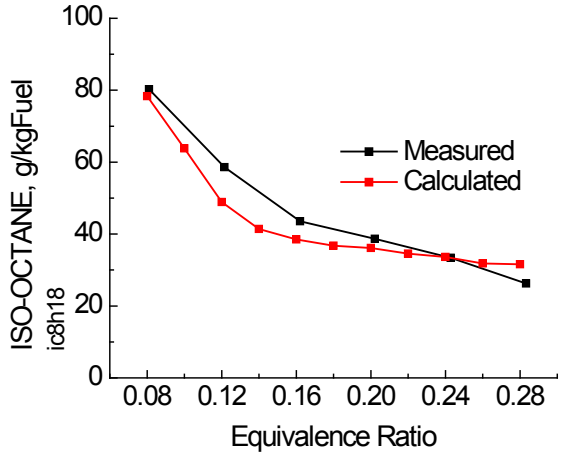
Detailed chemical kinetics mechanism development (Pitz)



Advanced numerics for detailed chemical kinetics (McNenly)



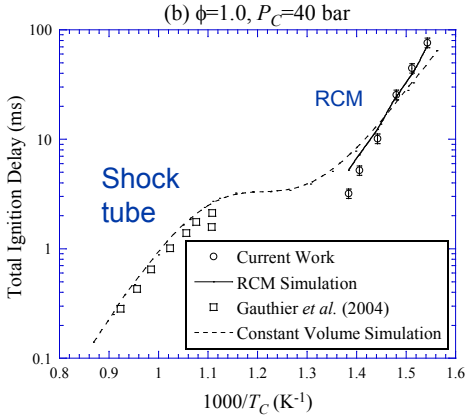
Large scale engine simulation with CFD and detailed chemical kinetics (Flowers)



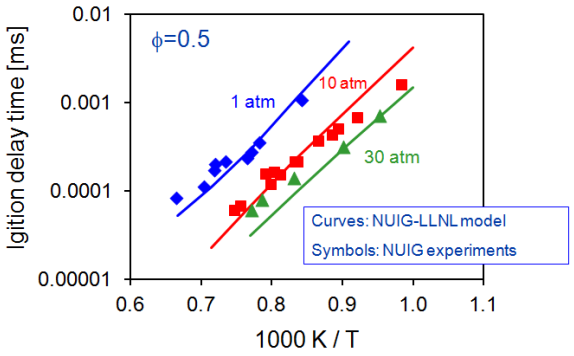
Detailed speciation using GC/MS (Davisson) and C14 analysis (Buchholz)

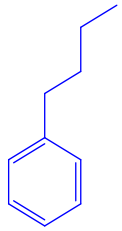
We continue to develop and validate chemical reaction mechanisms for gasoline and Diesel components

- Validated approach and mechanism for gasoline surrogate fuels

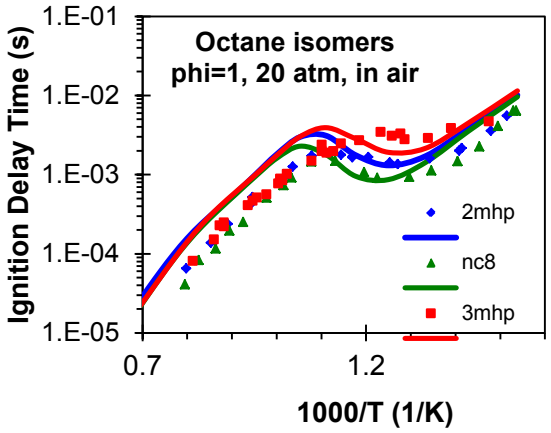


- Development of chemical kinetic model for larger aromatics

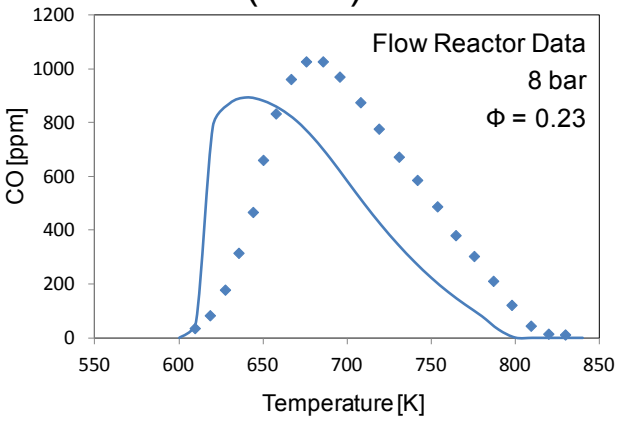




- Determined effect of branching for alkanes on ignition under engine conditions



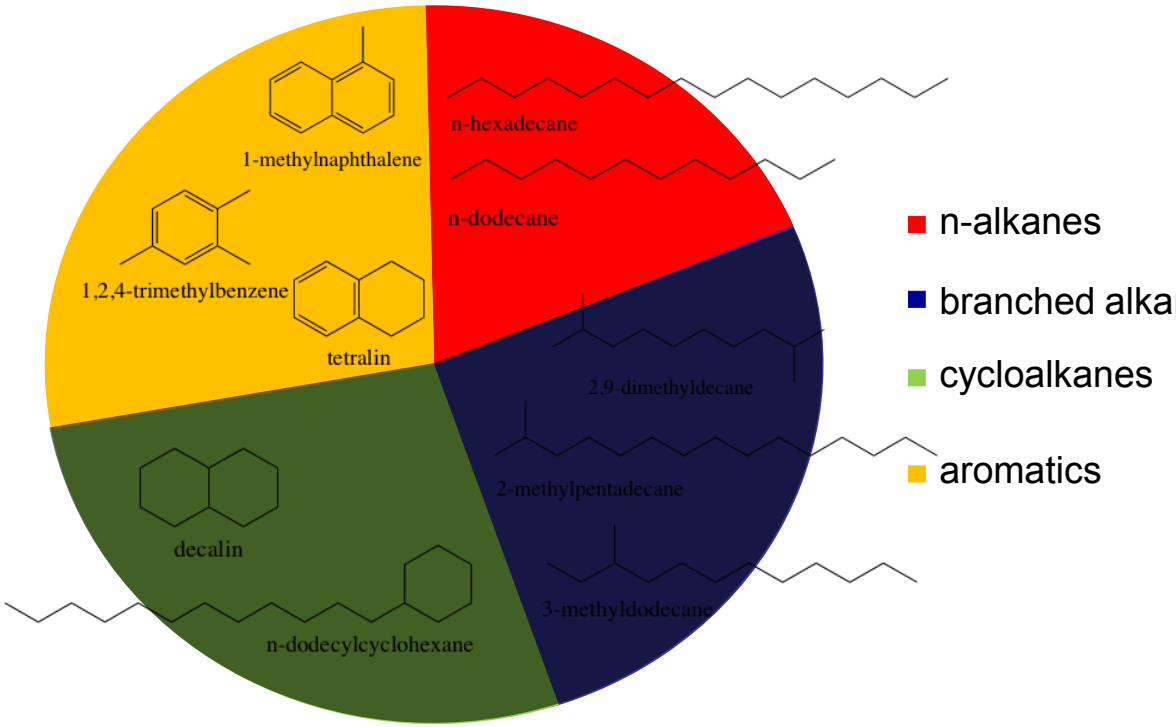
- Developing reduced chemical kinetic model for diesel for engine combustion network (ECN)



(23% m-xylene / 77% n-dodecane)

Surrogates are chemical reaction mechanisms that contain classes of compounds representative of Diesel or Gasoline combustion

Example diesel fuel palette:



Thousands of species
Tens of thousands of reactions

Recent Mechanisms:

- 4-component gas surrogate
- m-xylene/n-dodecane
- n-propylbenzene/n-heptane
- 2-methylalkanes (up to C20)
- 3-methylalkanes (up to C20)

Current Development:

- α-methylnaphthalene
- methylcyclohexane
- di-methylalkanes

Mechanism development is tied closely to validation with a wide range of experiments

- Idealized chemical reactors with/without simplified transport phenomenon

Jet Stirred Reactors

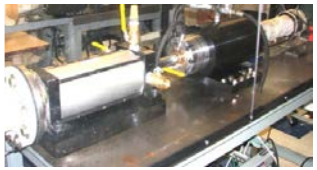
Premixed Laminar Flames

Twin premixed flames

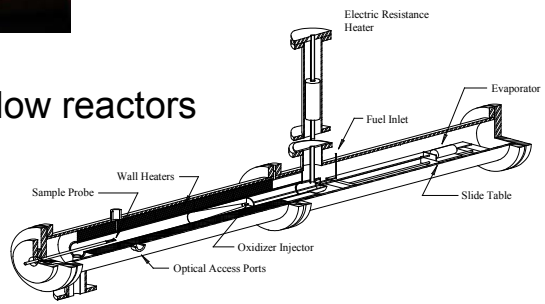
Shock tube

Non Premixed Flames

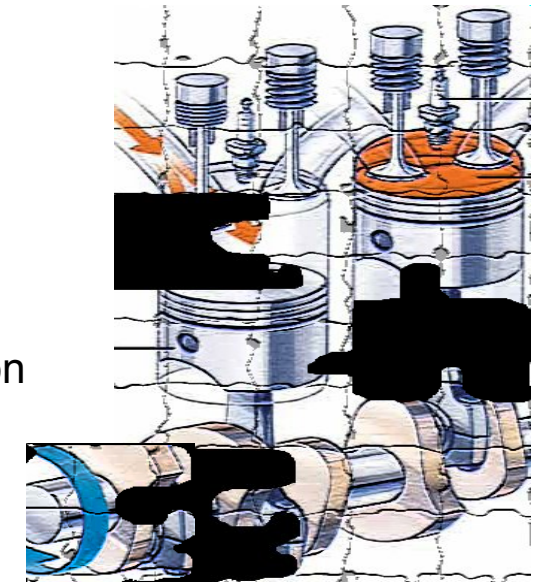
Rapid Compression Machine



High pressure flow reactors



Engine Combustion



Combustion Parameters

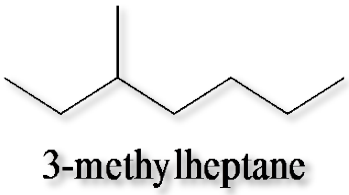
Temperature

Pressure

Mixture fraction (air-fuel ratio)

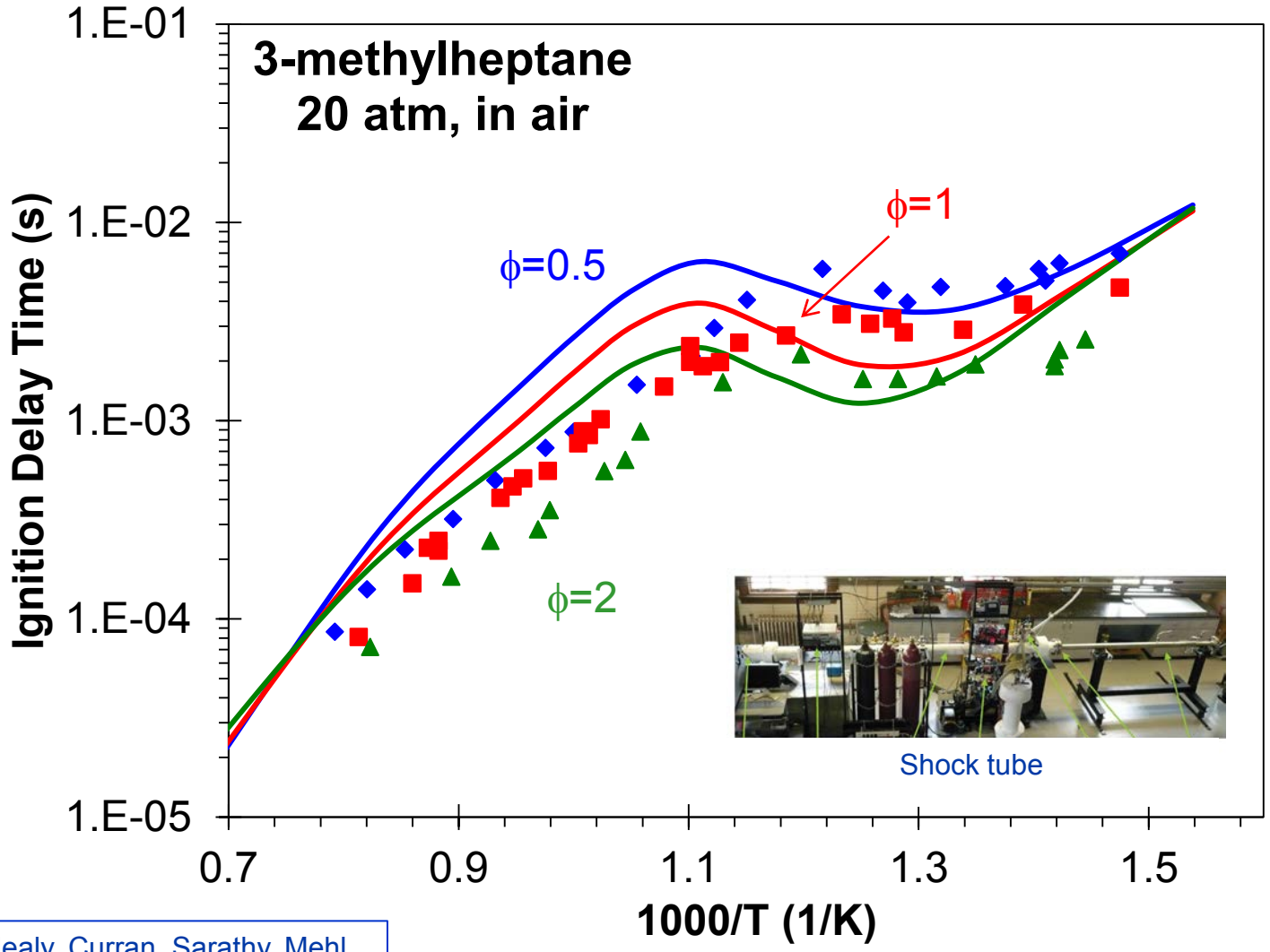
Mixing of fuel and air

Modeling of 3-methylheptane Ignition



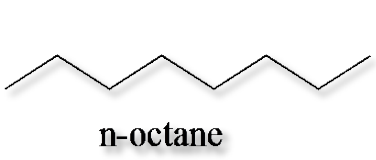
Model is generally within a factor of 1.5-2 of the experimental data.

Model slightly faster than shock tube data in the NTC region



W. Wang, Li, Oehlschlaeger, Healy, Curran, Sarathy, Mehl, Pitz, Westbrook, Proc. Combust. Inst. (2012).

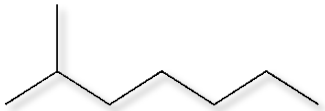
Modeling the effect of branching on ignition



n-octane

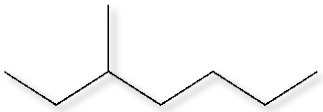
RON

-19.0



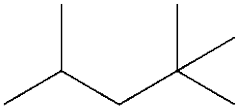
2-methylheptane

21.7



3-methylheptane

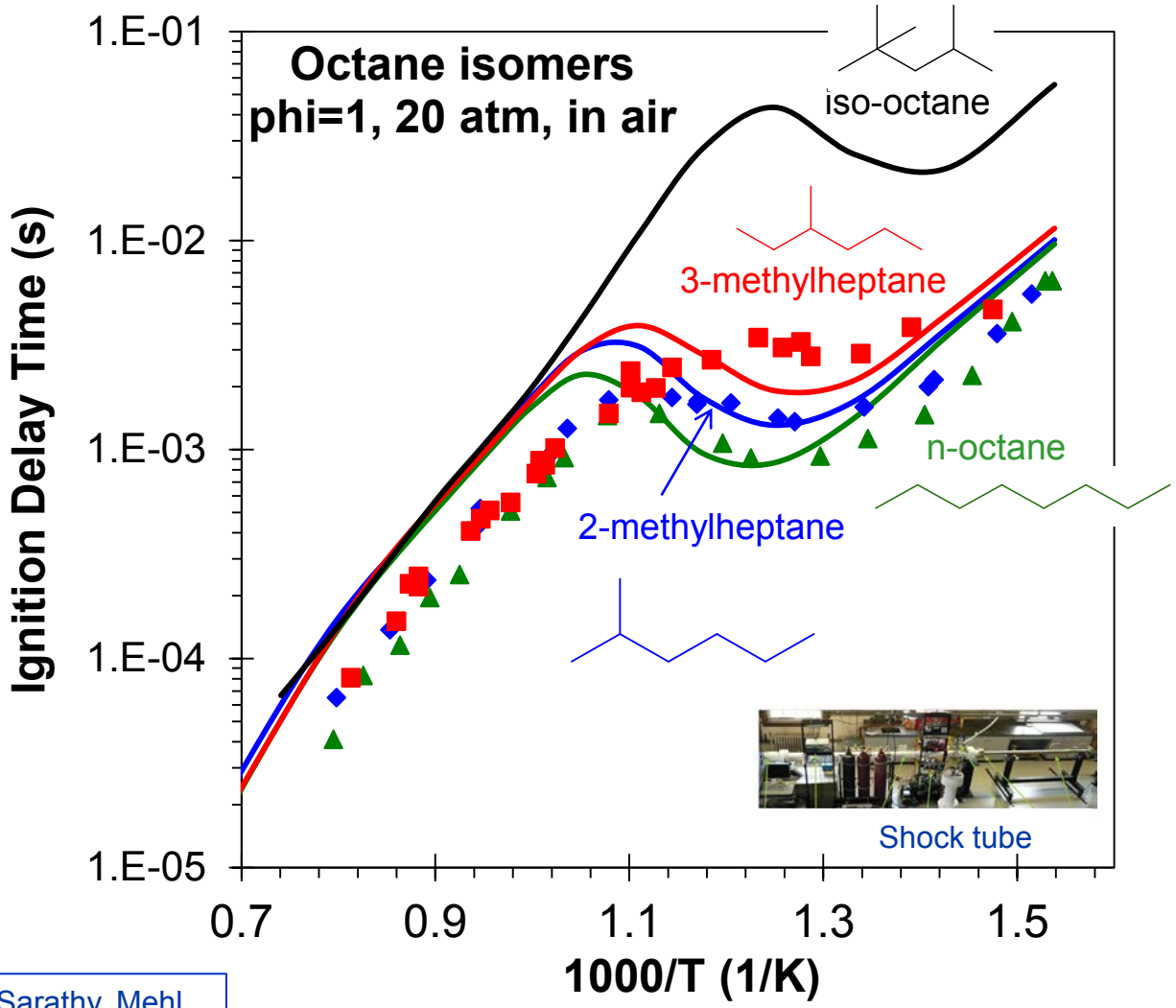
36.8



2,2,4-trimethylpentane

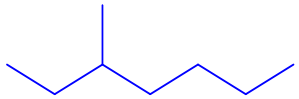
iso-ioctane

100



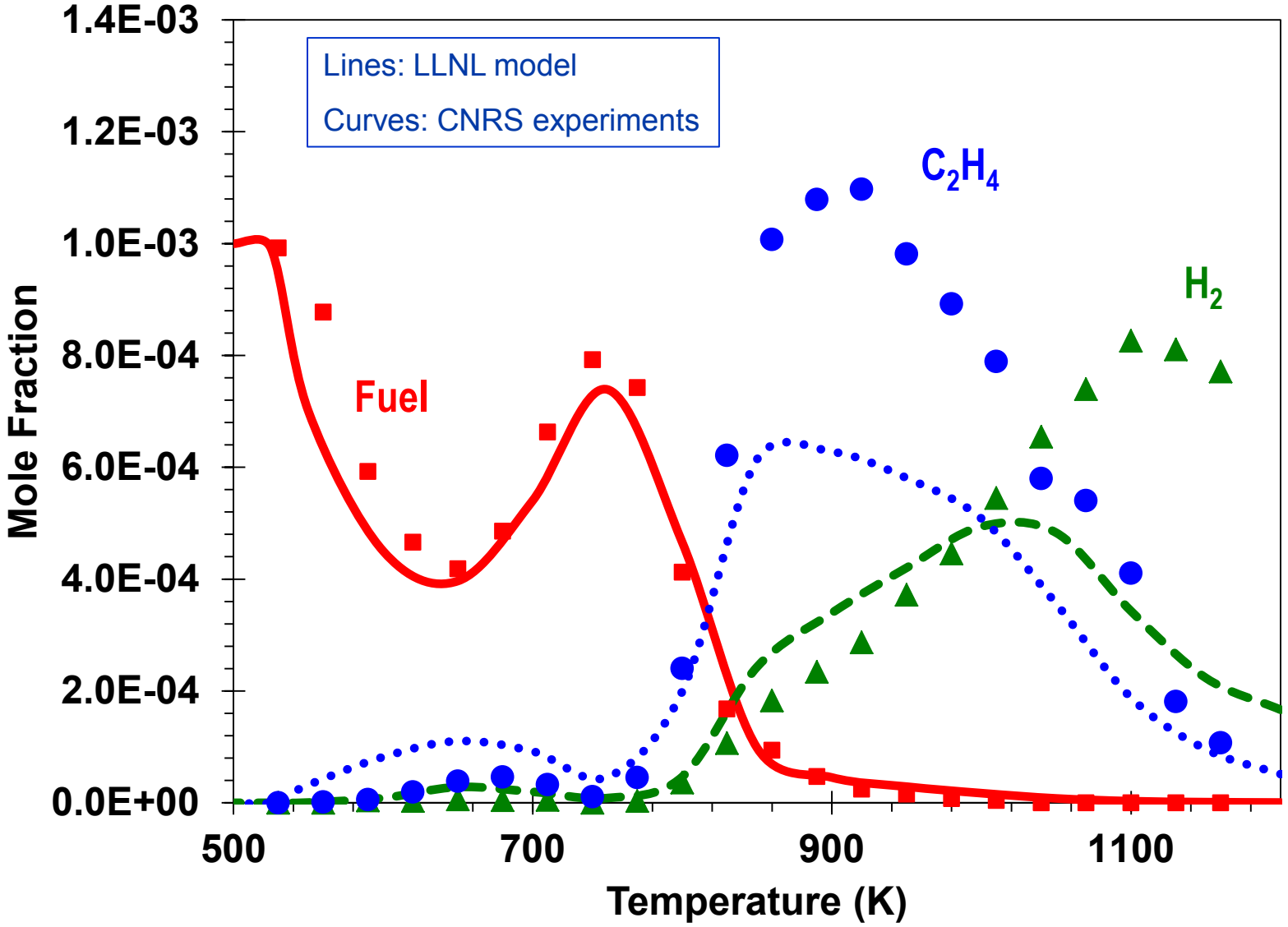
W. Wang, Li, Oehlschlaeger, Healy, Curran, Sarathy, Mehl, Pitz, Westbrook, Proc. Combust. Inst. (2012).

JSR 3-Methylheptane Results



Dagaut et al. CNRS (2010)

Experiments performed at CNRS, Orleans (F. Karzenty, C. Togbe G. Dayma, P. Dagaut)



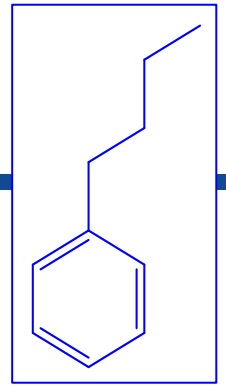
10 atm

$\phi = 1$

$\tau = 0.7$ sec

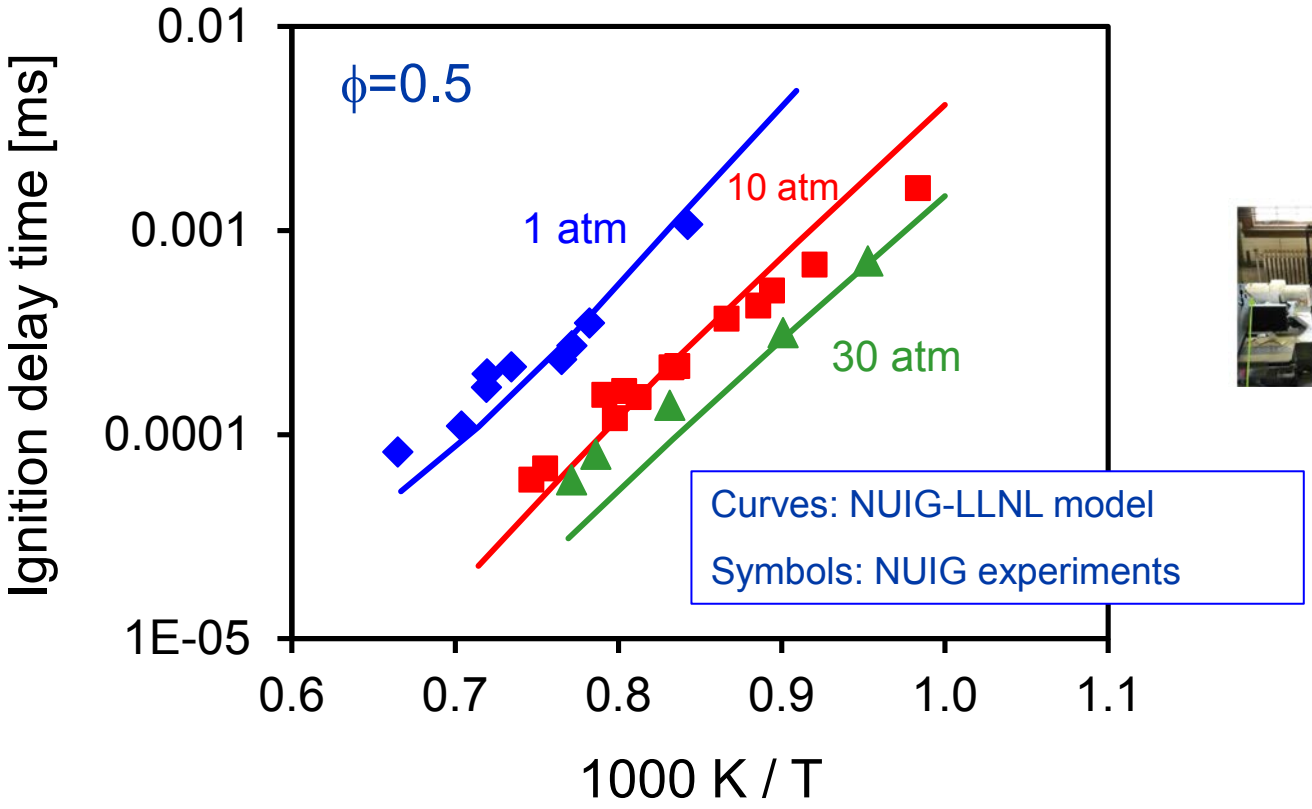
Good prediction of low T and high T reactivity

Larger aromatics: Shock tube ignition of n-butyl benzene at high pressure



n-butylbenzene

Shock tube



Experiments: Tobin,Yasunaga and Curran, NUIG, Ireland (Combust. Flame 2011)

Mechanisms are available on LLNL website and by email

http://www-pls.llnl.gov/?url=science_and_technology-chemistry-combustion

- Ethanol
- Dimethyl Ether
- CH4, C2H4, C2H6, C3H8, and nC4H10
- CH4, C2H4, C2H6, C3H6, C3H8, and NOx
- C8-C16 n-Alkanes
- Cyclohexane
- Methylcyclohexane
- Methyl Butanoate and Methyl Formate
- Methyl Decanoate
- Methyl Decenoates
- Biodiesel Surrogates
- Dimethyl Carbonate
- Heptane, Detailed Mechanism
- Heptane, Reduced Mechanism
- iso-Octane
- 2-Methyl Alkanes
- Primary Reference Fuels: iso-Octane / n-Heptane Mixtures
- 2,2,4,4,6,8,8-Heptamethylnonane
- Organophosphorus Compounds under Incineration Conditions
- Organophosphorus Compounds in Propane

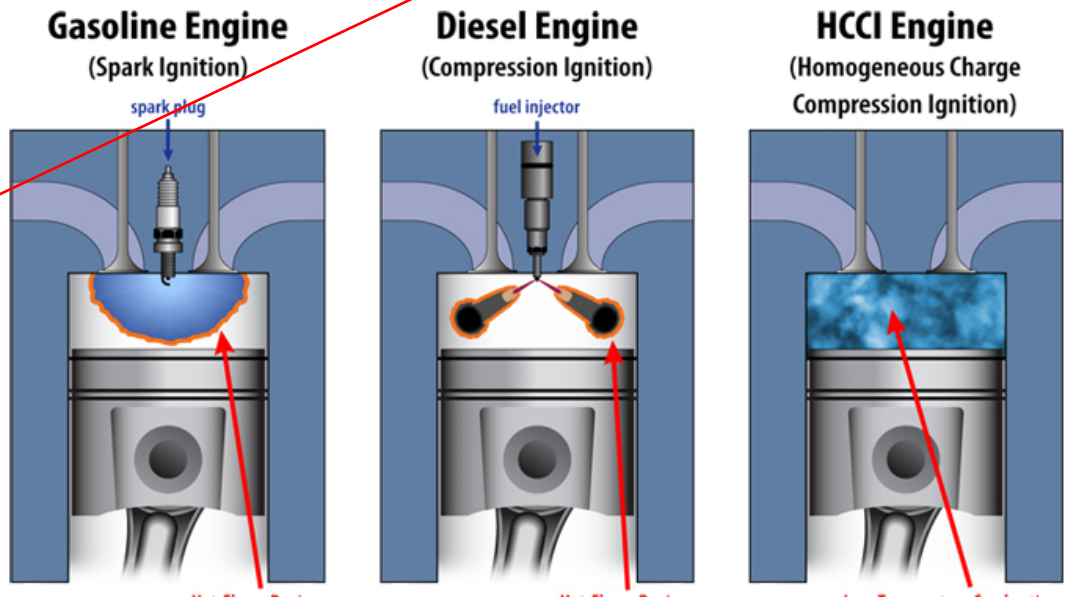
Combustion Chemistry

Go Directly to Mechanisms...

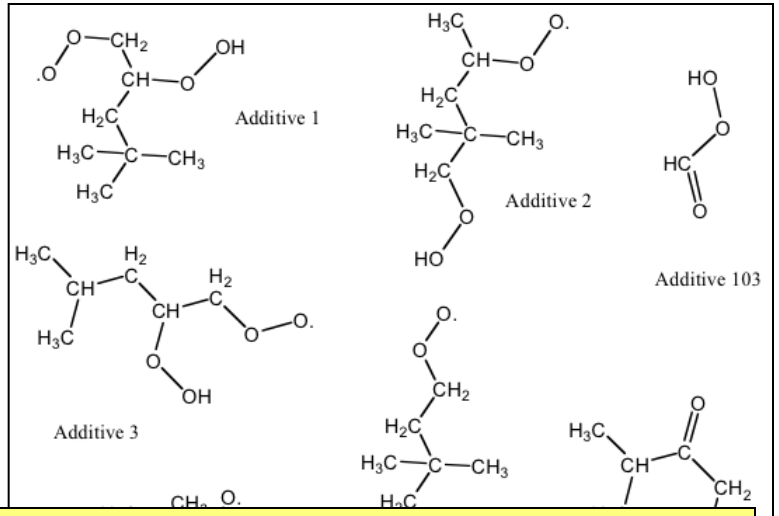
The central feature of the Combustion Chemistry project at LLNL is our development, vali
and application of detailed chemical kinetic reaction mechanisms for the combustion of
hydrocarbon and other types of chemical fuels. For the past 30 years, our group has bu
hydrocarbon mechanisms for fuels from hydrogen and methane through much larger fue
including heptanes and octanes. Other classes of fuels for which models have been dev
include flame suppressants such as halons and organophosphates, and air pollutants su
soot and oxides of nitrogen and sulfur.

Reaction mechanisms have been tested and validated extensively through comparisons bet
computed results and measured data from laboratory experiments (e.g., shock tubes, laminar
flames, rapid compression machines, flow reactors, stirred reactors) and from practical systems
(e.g., diesel engines, spark-ignition engines, homogeneous charge, compression ignition (HCCI)
engines). We have used these kinetic models to examine a wide range of combustion systems.

2-Methyl Alkanes



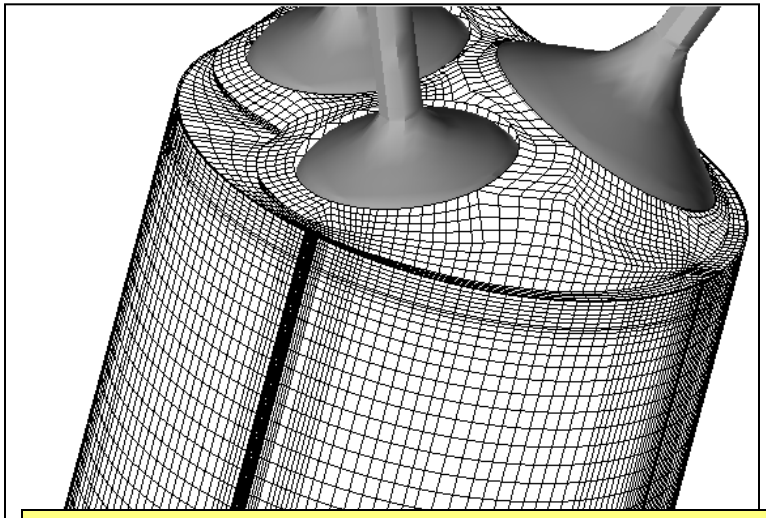
Challenge: new HECC modes require computationally expensive models fully coupling detailed kinetics with CFD



Detailed Chemistry

Mechanisms for large fuel molecules contain +7000 species (*e.g.* LLNL 2-methyl and 3-methyl-alkane mechanisms)

+



3D Fluid dynamics

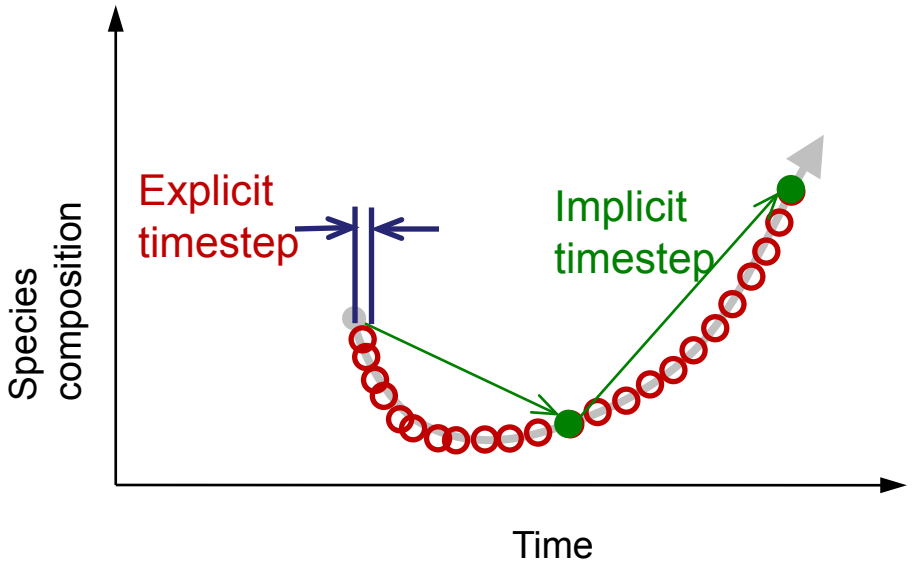
1M – 10 M fluid cells for well-resolved engineering mixing and turbulence model (Enaux *et al.*)

= 300,000 Pflop/s (chem-only), roughly a decade on current 12-core workstations = Not available for design

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 High Efficiency Clean Combustion 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

For combustion chemistry, implicit solvers allow for much larger time steps to resolve ignition



During ignition:
Δt (explicit) = 10^{-12} to 10^{-15} seconds
Δt (implicit) = 10^{-6} to 10^{-8} seconds

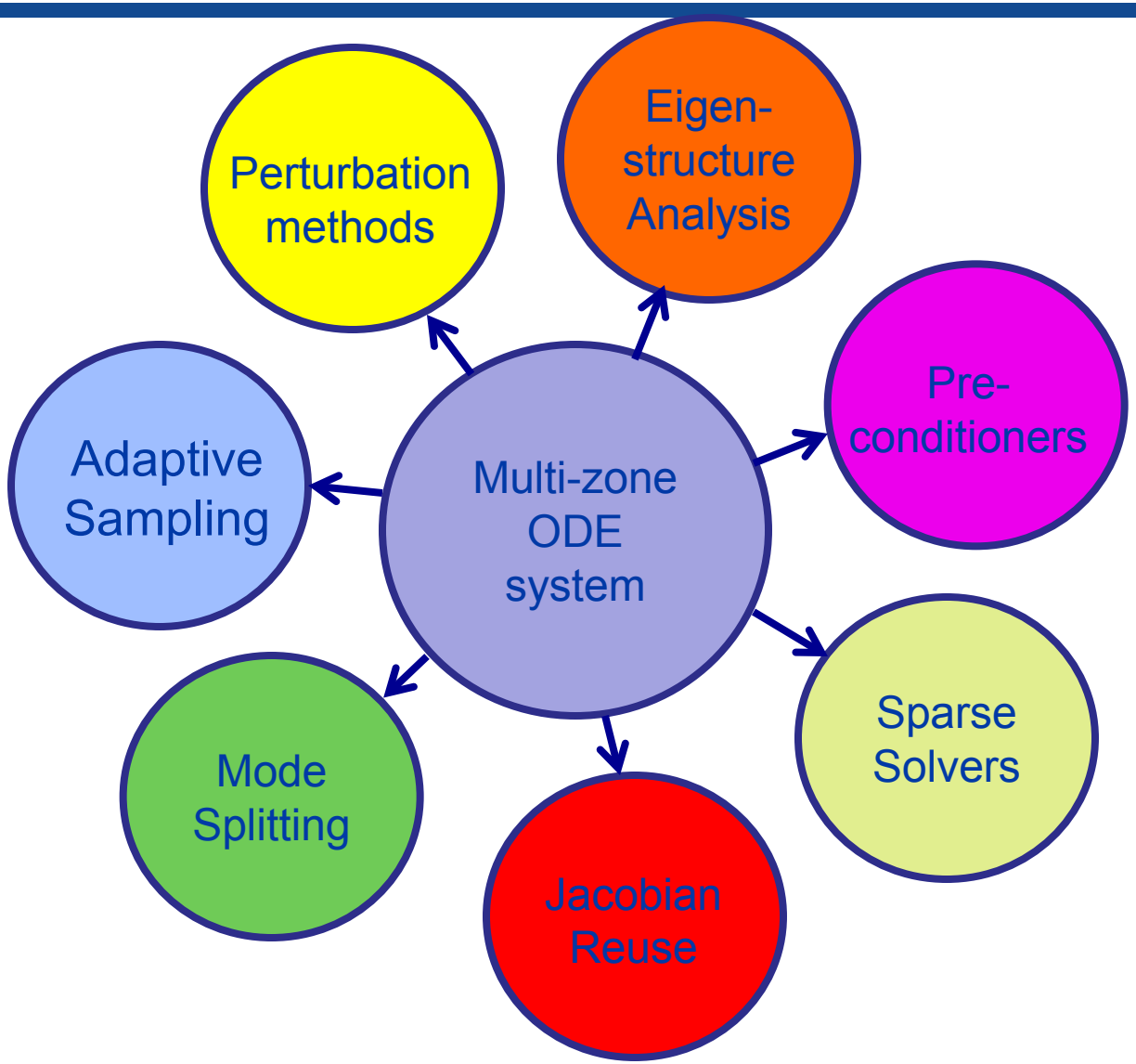
Explicit: directly solve differential equations (easy but many steps)

$$\frac{\partial x_1}{\partial t} = f_1(t, x_1, \ldots, x_N)$$
$$\frac{\partial x_2}{\partial t} = f_2(t, x_1, \ldots, x_N)$$
$$\vdots$$
$$\frac{\partial x_N}{\partial t} = f_N(t, x_1, \ldots, x_N).$$

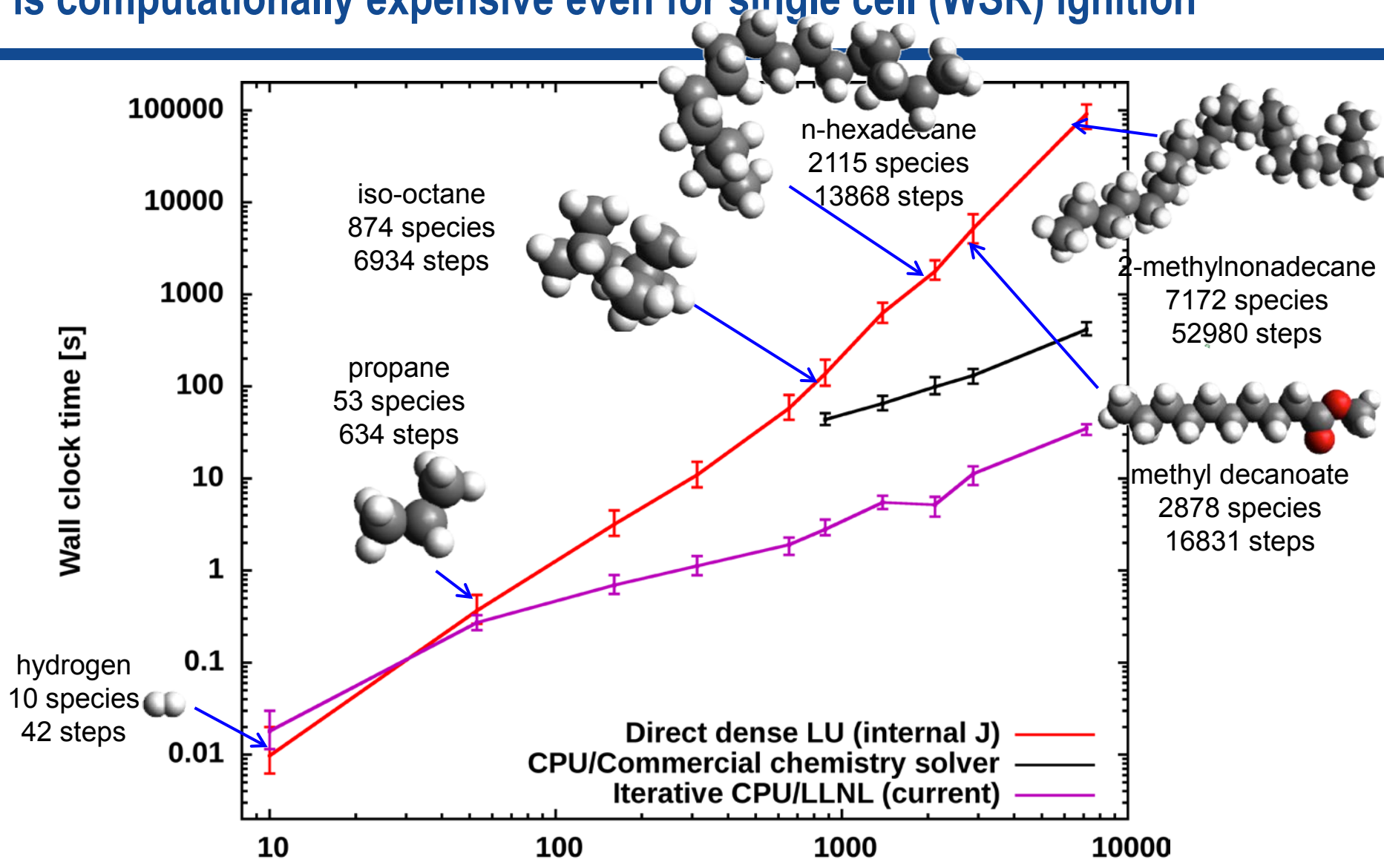
Implicit: Invert a matrix (hard but fewer steps)

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

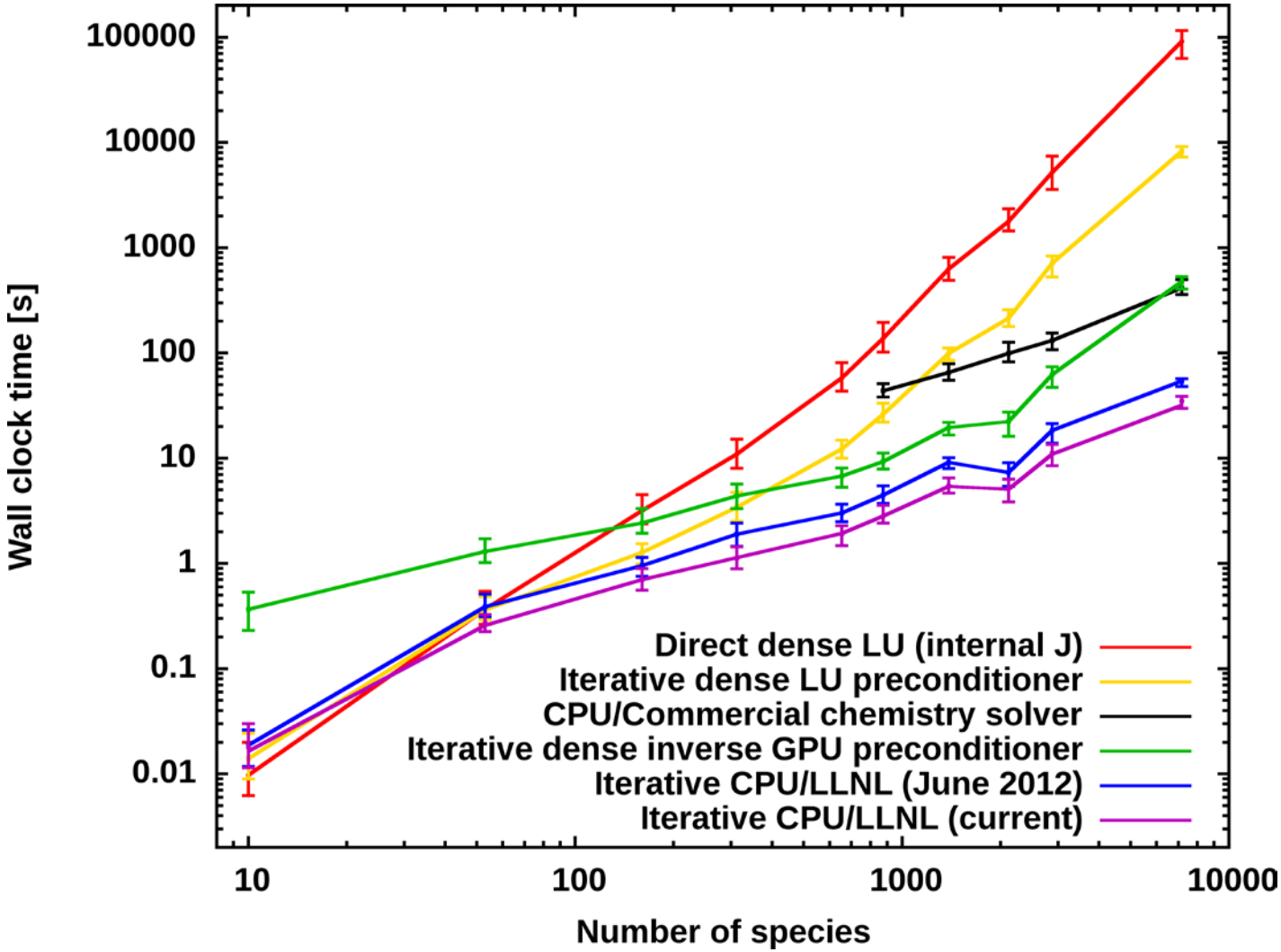
Opportunities for 1000x speedup in computational chemistry cost through applied mathematics



Using the default stiff-ODE integrator options for large mechanisms is computationally expensive even for single cell (WSR) ignition



We have developed solvers that reduce chemistry simulation time by orders of magnitude



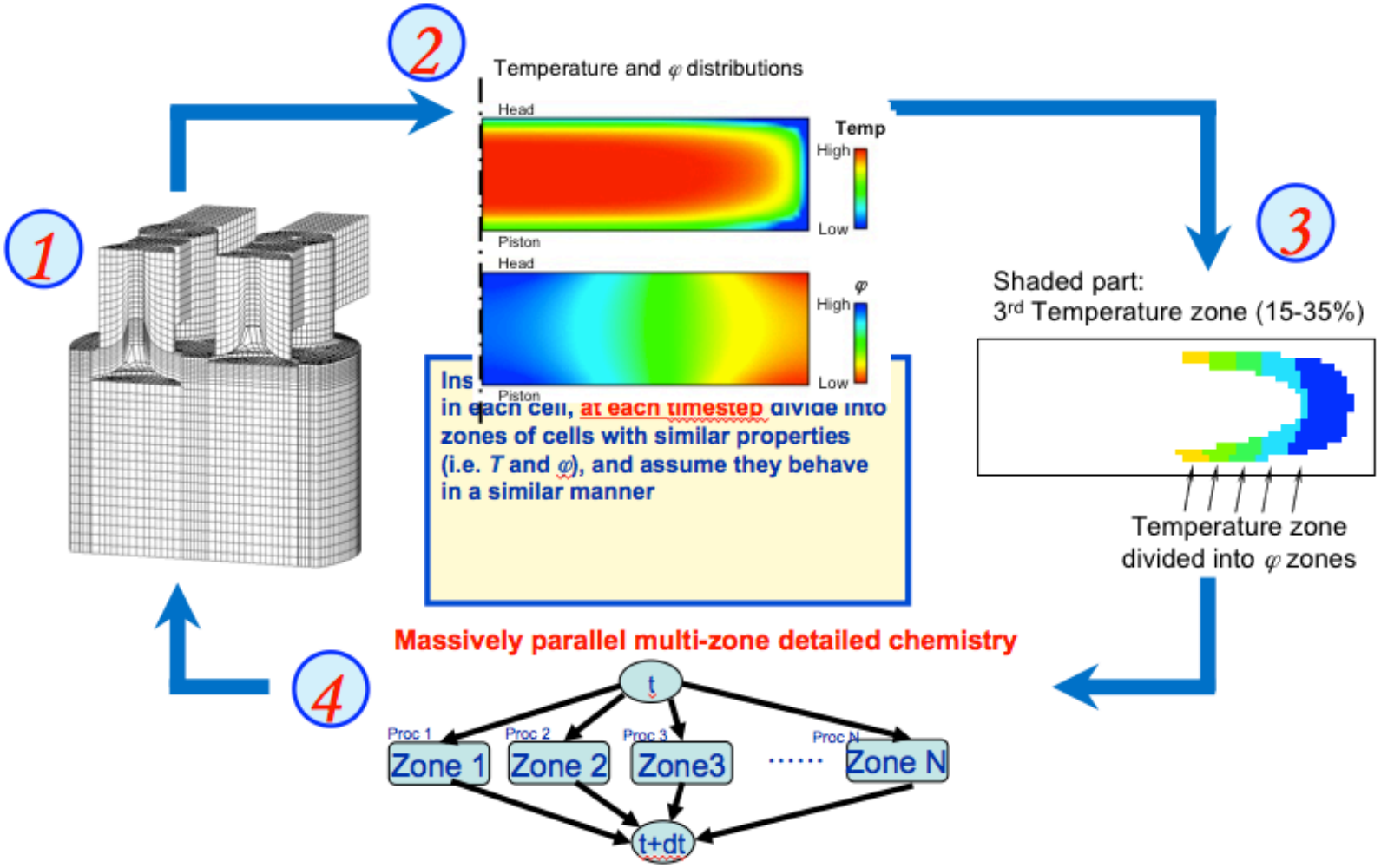
Standard method (>1 day)

Commercial solver (7 min)

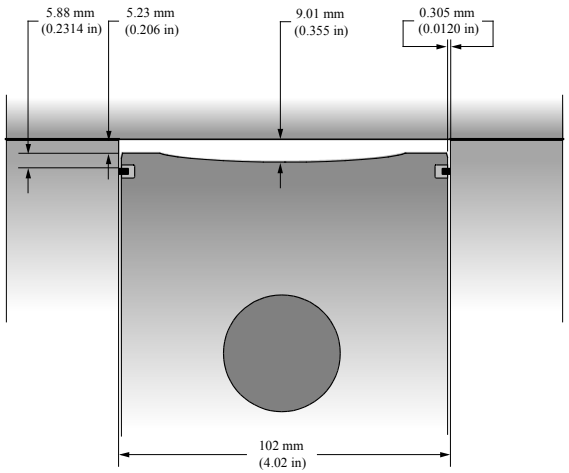
LLNL Adaptively Preconditioned Solver (30 sec)

The LLNL CFD/multi-zone solves flow in XYZ space and chemistry in temperature-chemistry space

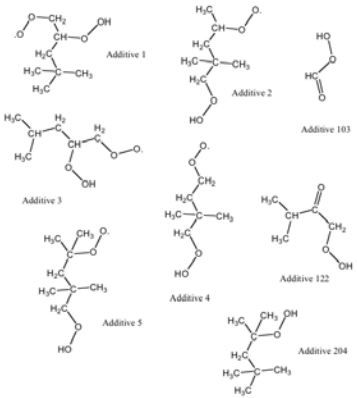
Chemistry can be solved with 100s of reactors, independent of the CFD resolution



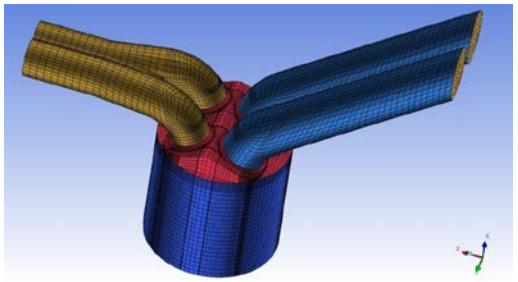
The Combustion Simulation Group combines detailed kinetics, CFD, and solvers for engine simulation



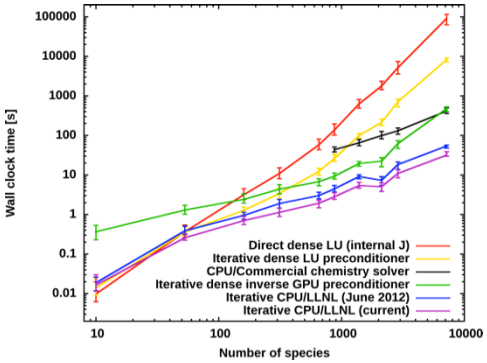
Experiments by partners
(e.g. Sandia, Oak Ridge)



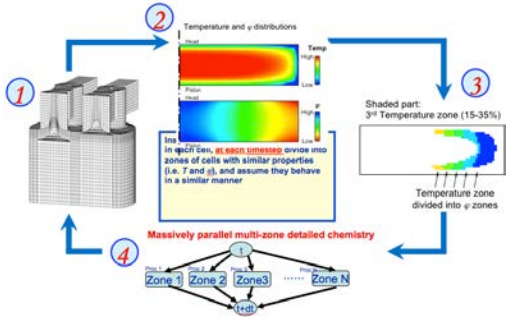
Kinetics from LLNL (Pitz)
and others



Engine CFD (Converge,
OpenFOAM)

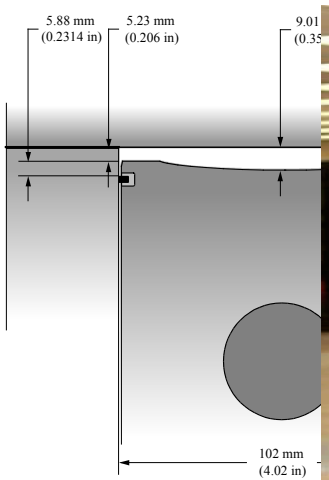


Kinetics Solvers from
LLNL (McNenly)

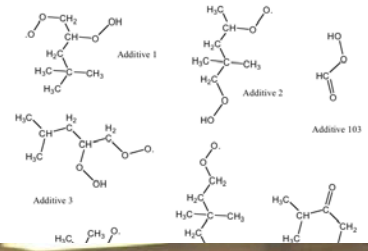


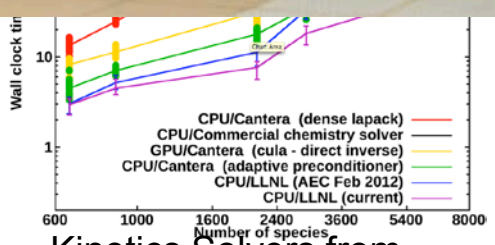
Multizone from LLNL
(Flowers)

This work is further enabled by LLNL large-scale computing resources (multiple TFLOPs available to us)

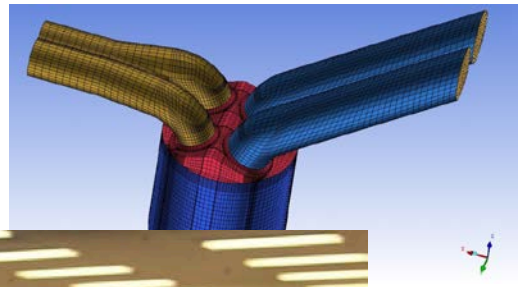


Experiments by partners
(e.g. Sandia, Oak Ridge)

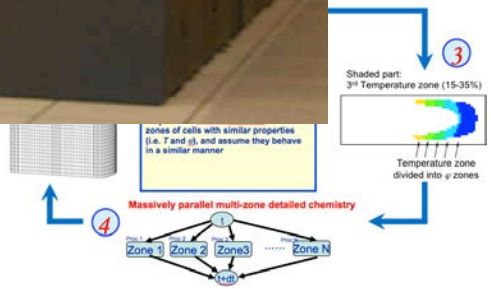




Kinetics Solvers from
LLNL (McNenly)



nverge,



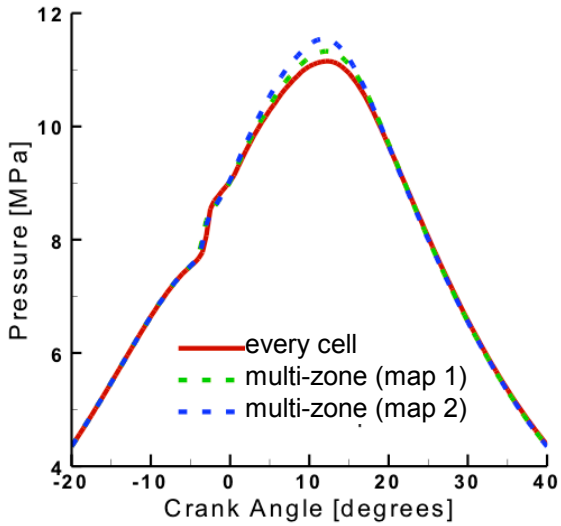
Multizone from LLNL
(Flowers)

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

- Converge is widely used in industry for engine simulation

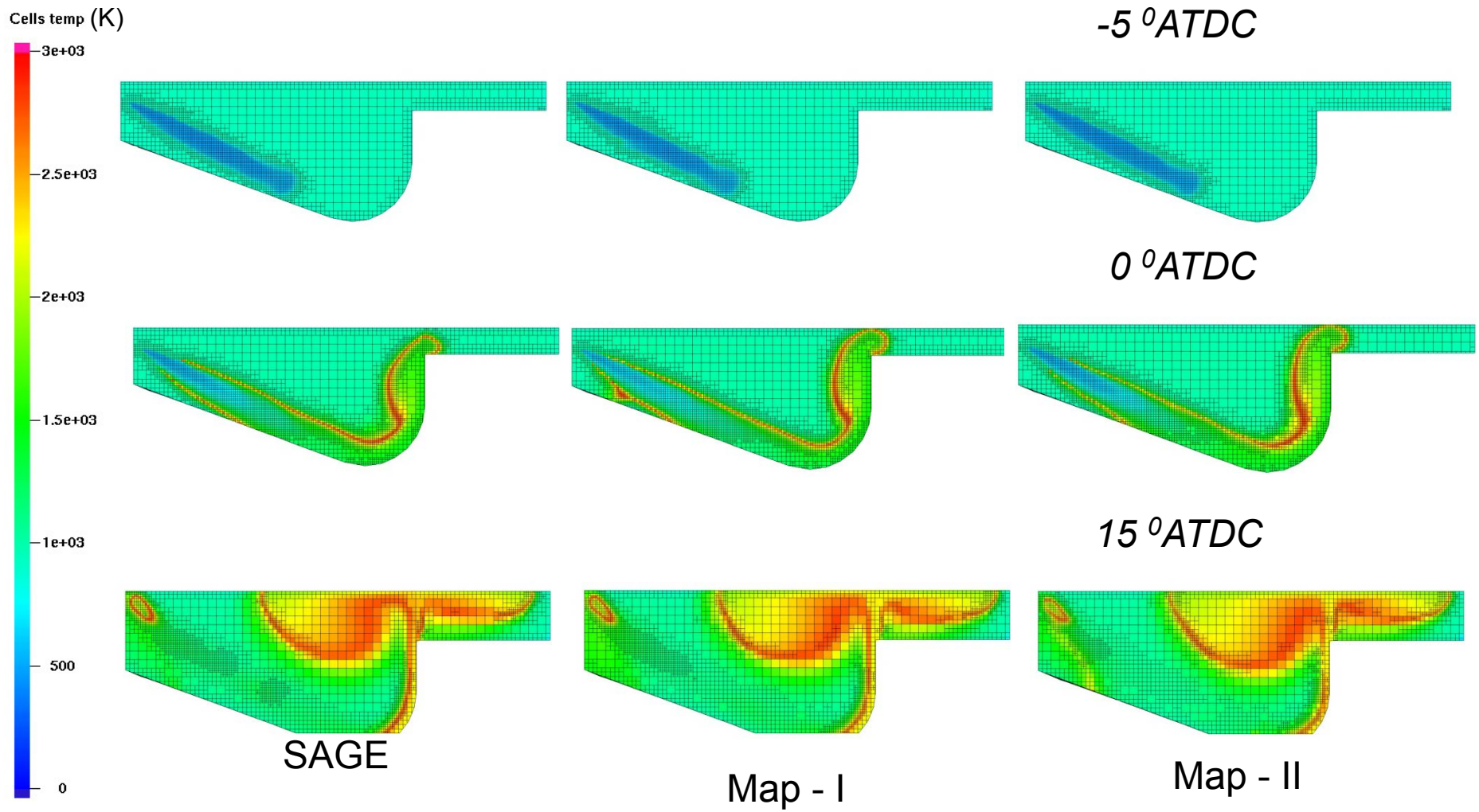
SCOTE Direct Injection Test Case

Bore x stroke (mm)	137.2 x 165.1
Compression ratio	16:1
Engine speed (rev/min)	1600
Start of injection (°ATDC)	-9
Temperature at IVC (K)	355
Pressure at IVC (bar)	2
EGR (% by mass)	0%

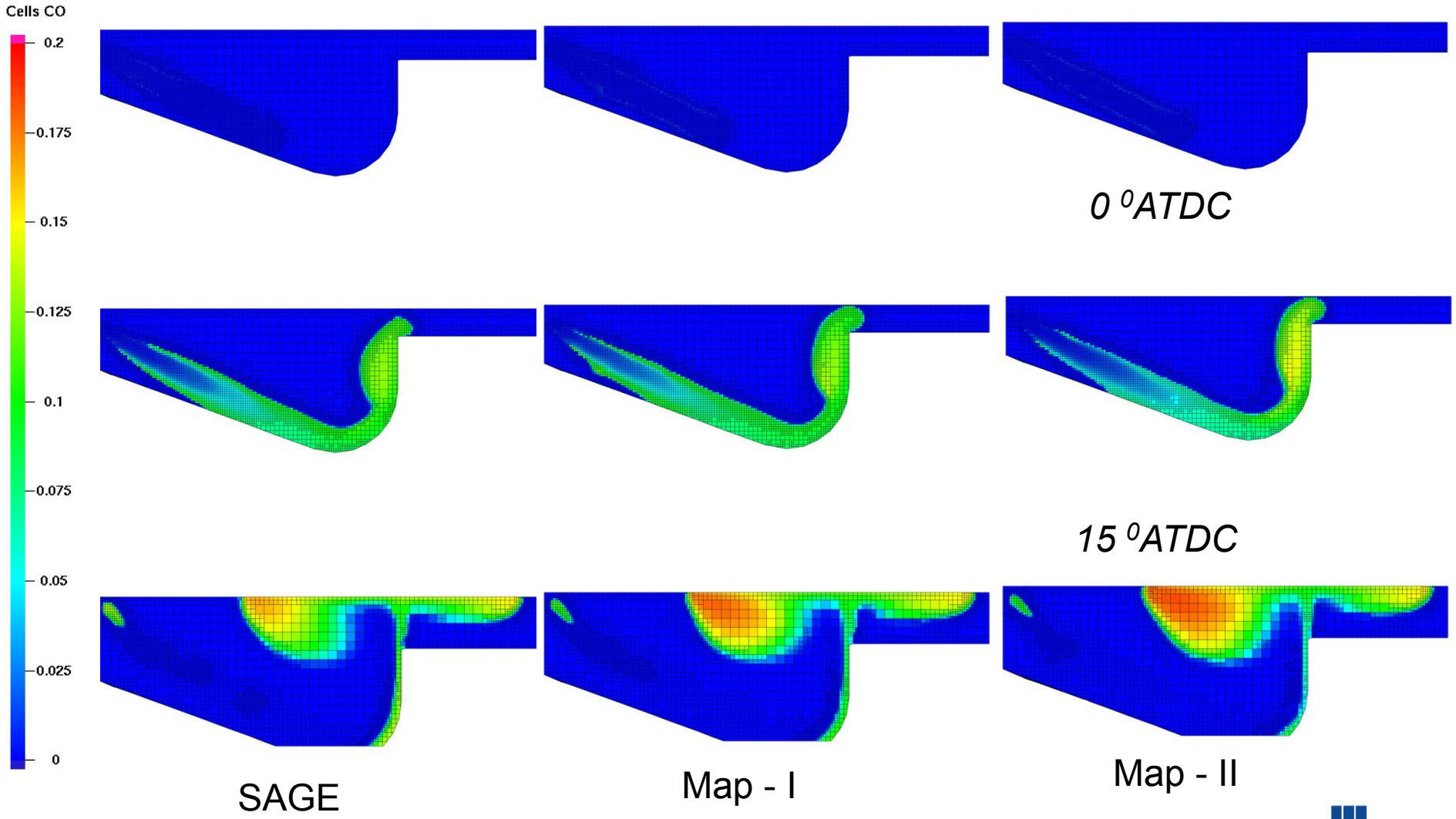


In-cylinder pressure predicted by CONVERGE for every-cell and multi-zone model

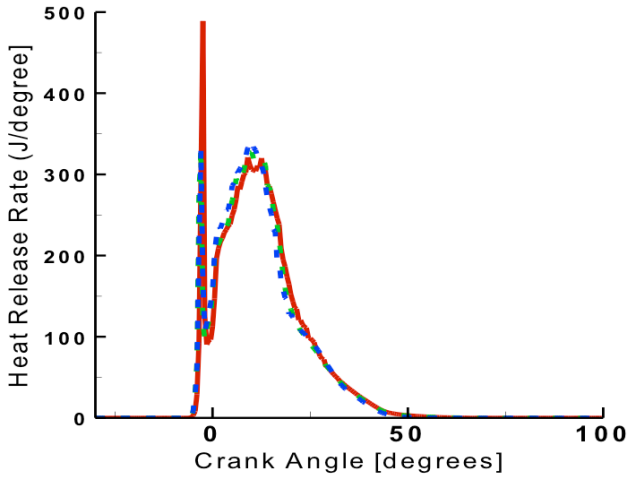
Multi-zone model in CONVERGE shows very good agreement between spatial and temporal temperature evolution



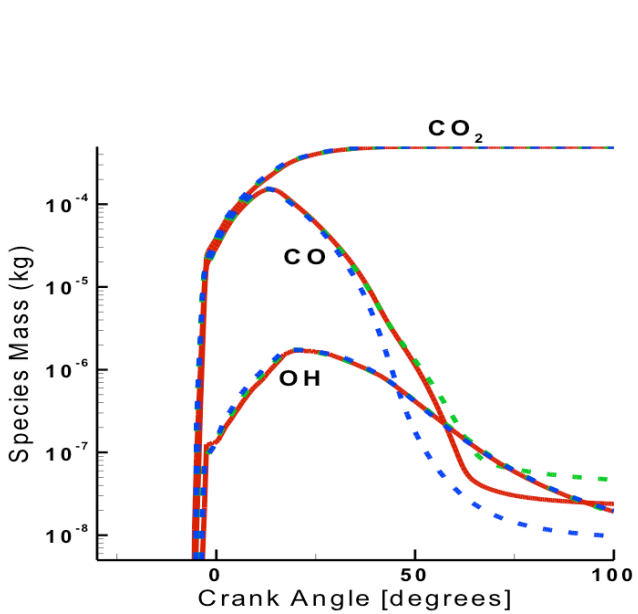
Similarly, CONVERGE predicted carbon monoxide evolution compares well between multi-zone and every-cell



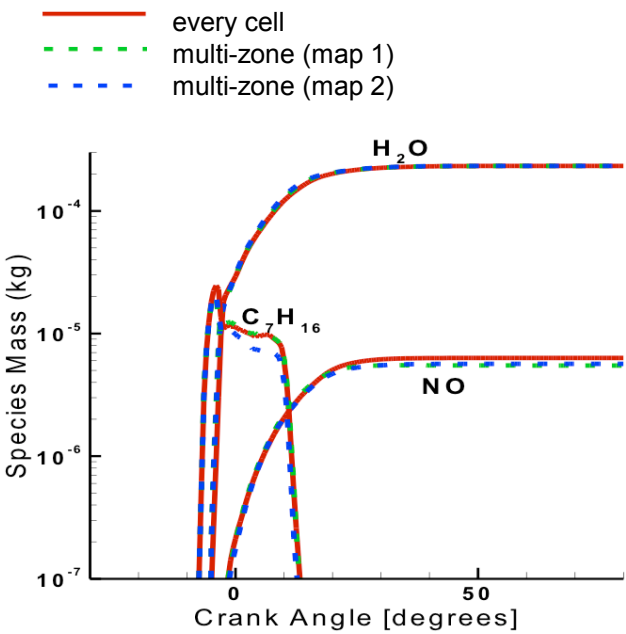
Predictions are very consistent between CONVERGE every-cell and multi-zone simulations



Rate of heat release

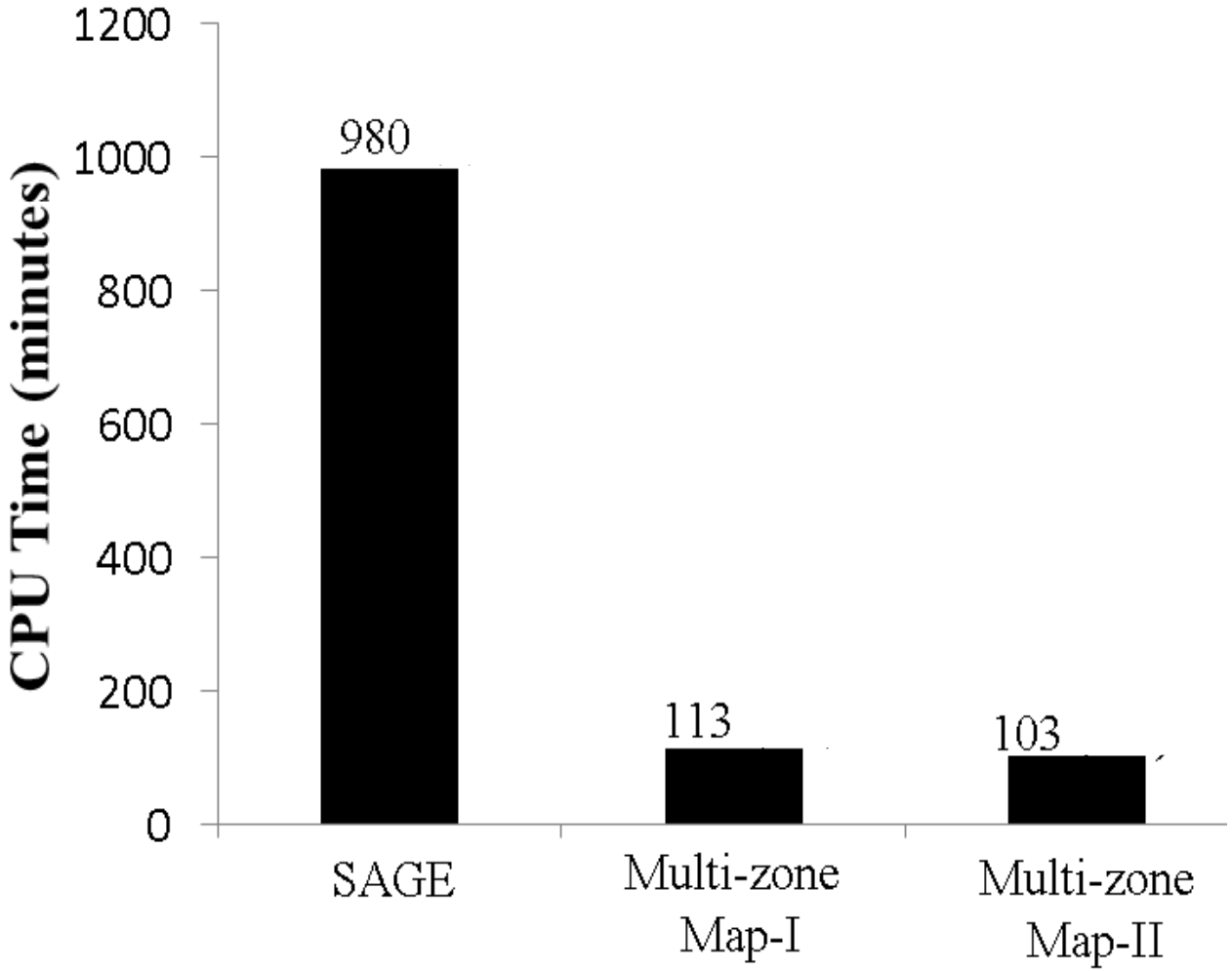


CO2, CO and OH



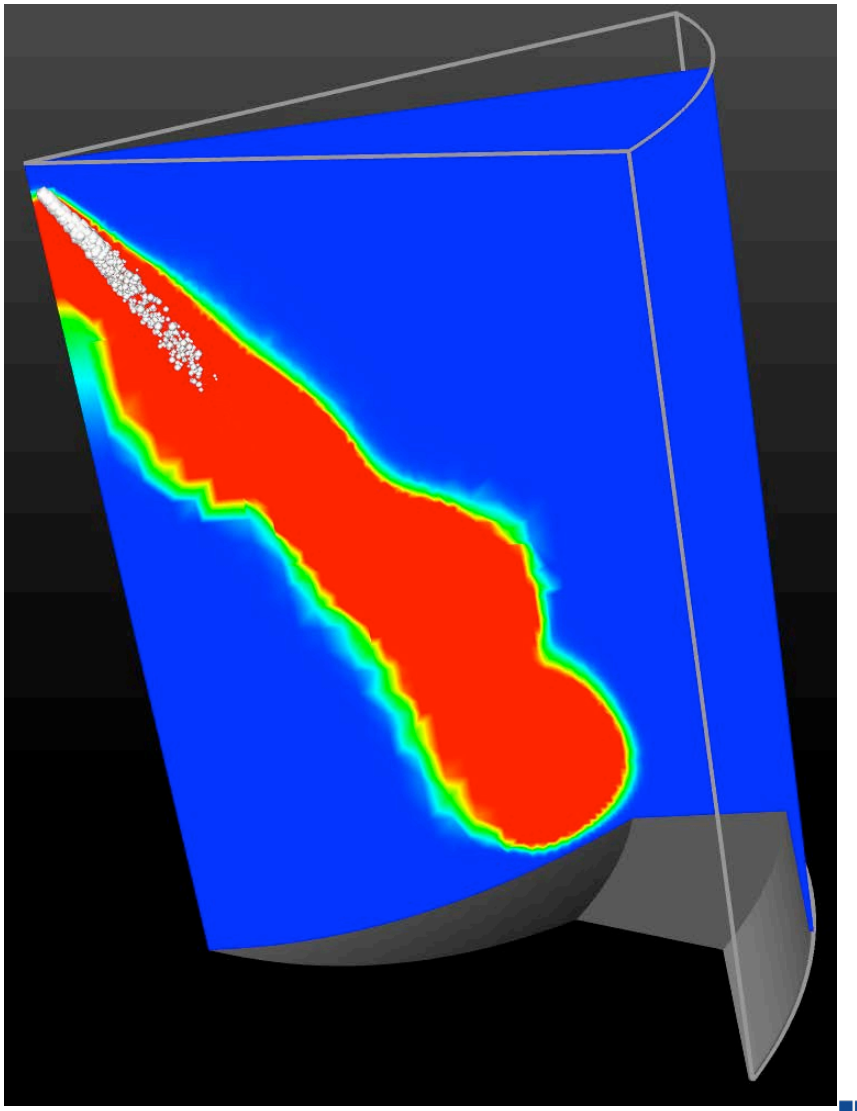
Fuel, C7H16, and NO

Converge multi-zone provides the same accuracy while reducing the simulation time by a factor of 10

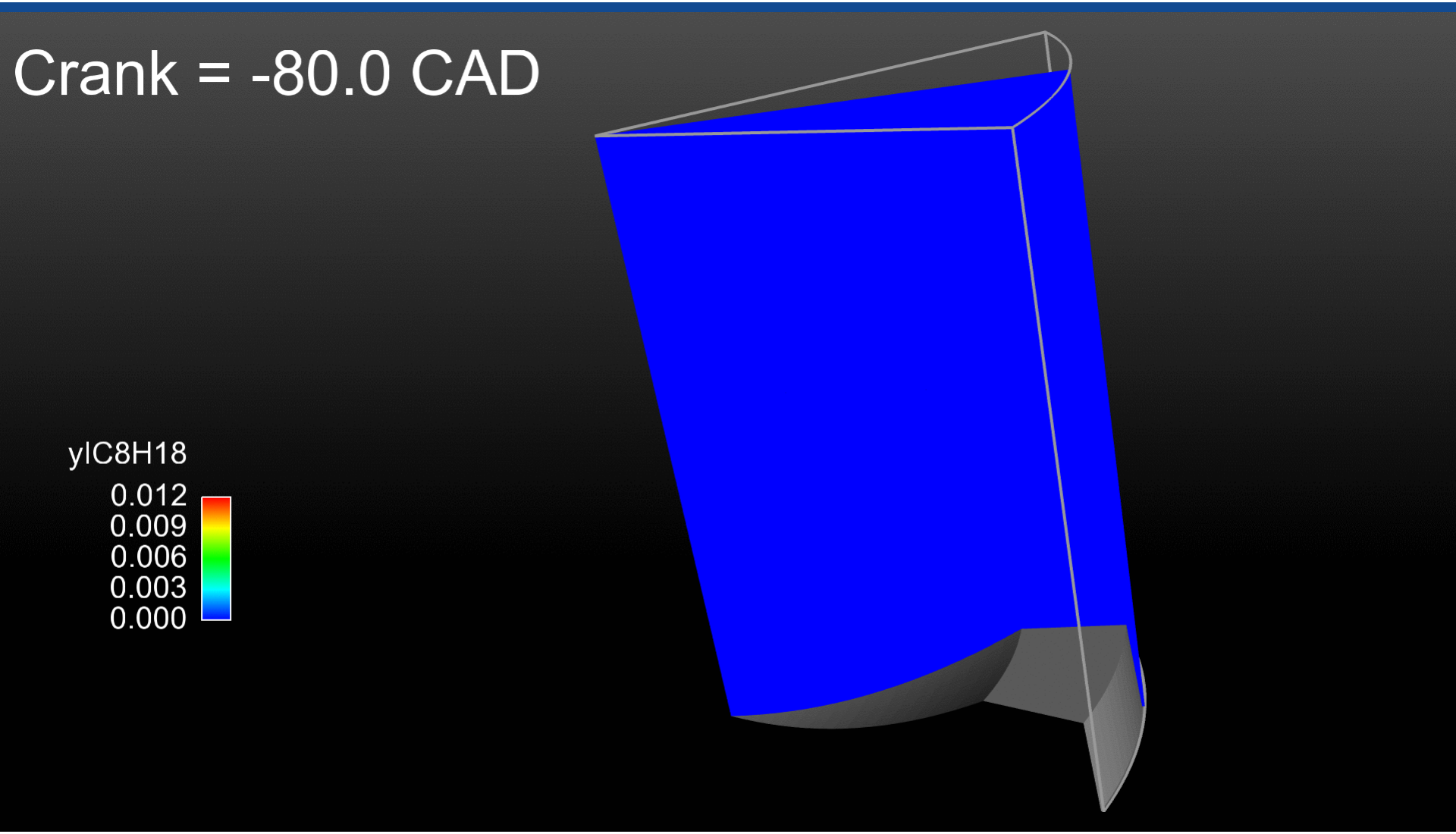


We are doing a systematic study of using the Converge multi-zone for investigating Early-DI PCCI

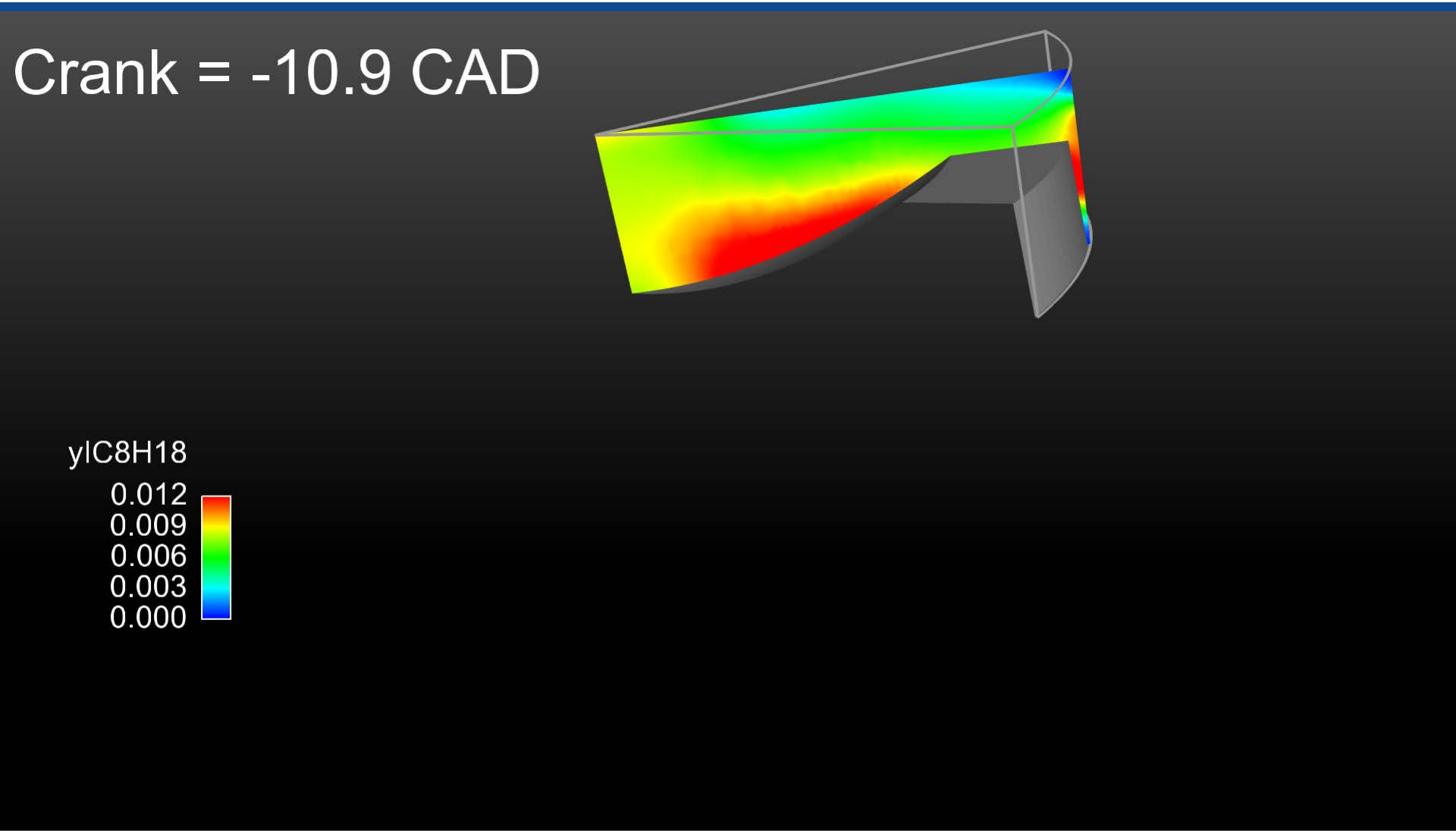
- Sandia (Dec) isooctane data
- Converge spray models (RT/KH)
- LLNL multi-zone and AP solver
- 874 species ic8h18 mechanism
- Closed cycle
- 45 degree sector
- 200K cells (at BDC)
- Low load (phi=0.12 overall)



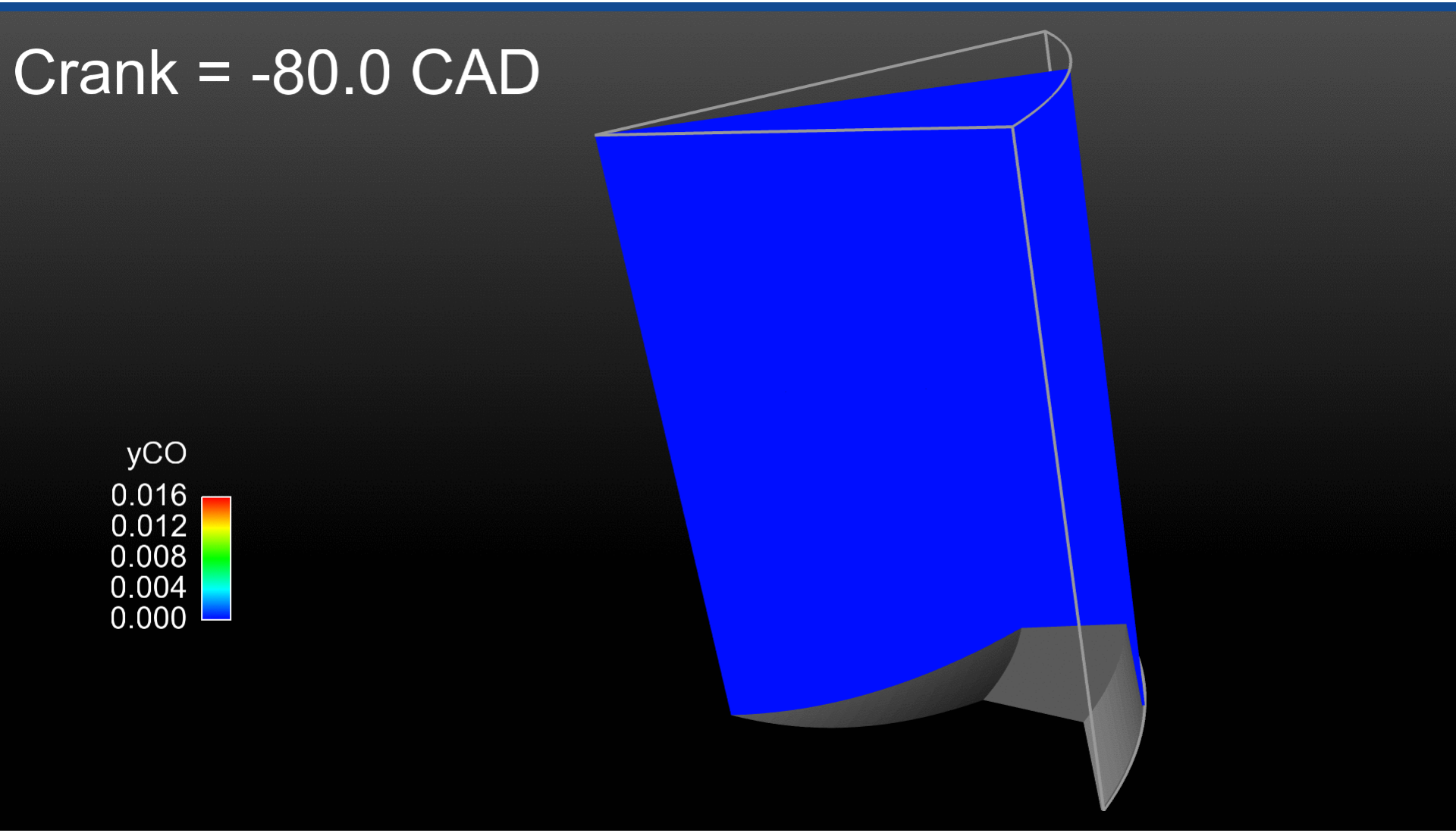
Fuel concentration is highest near bowl with some fuel entering the ring crevice



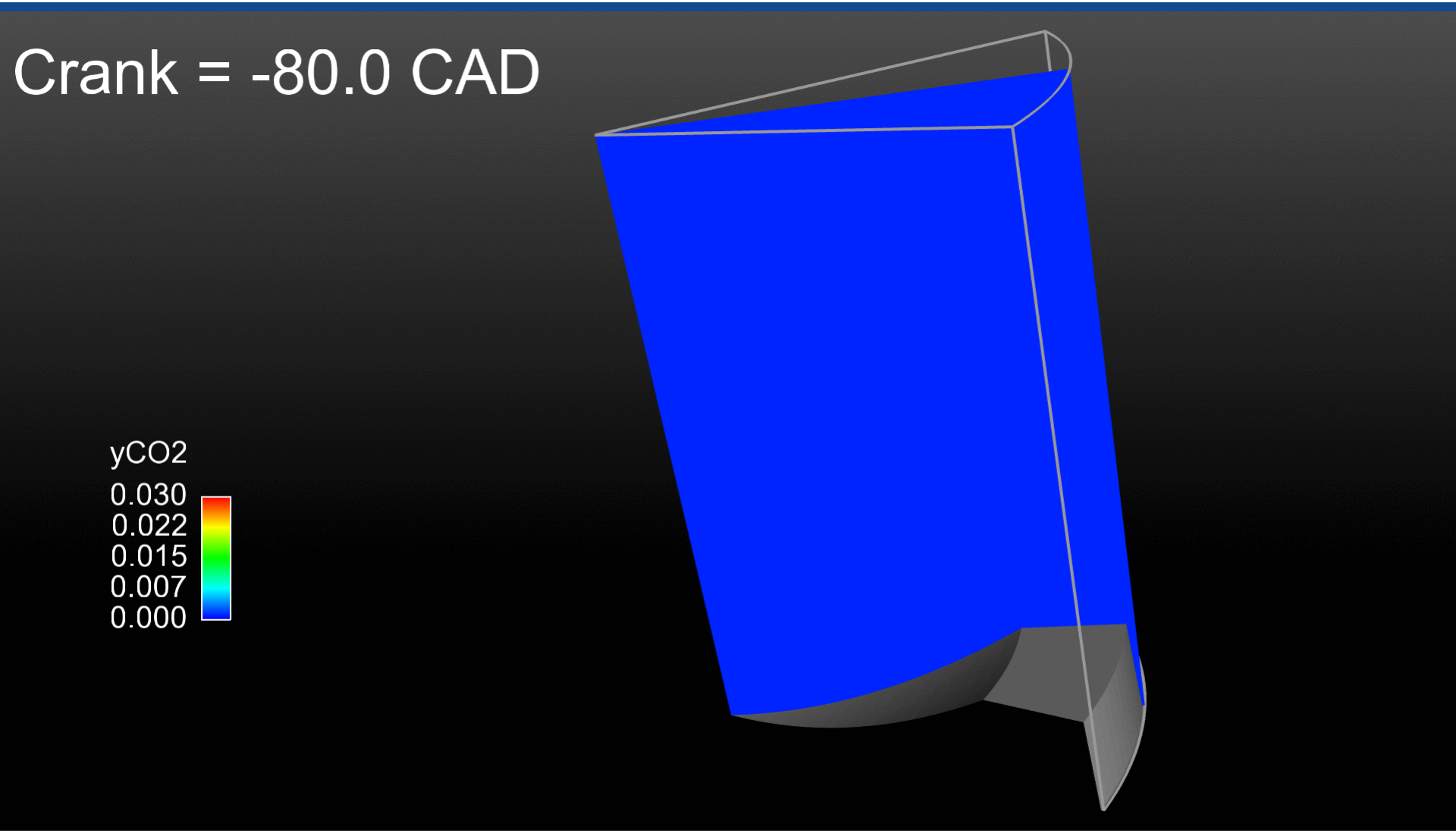
Fuel distribution in cylinder just before significant conversion occurs



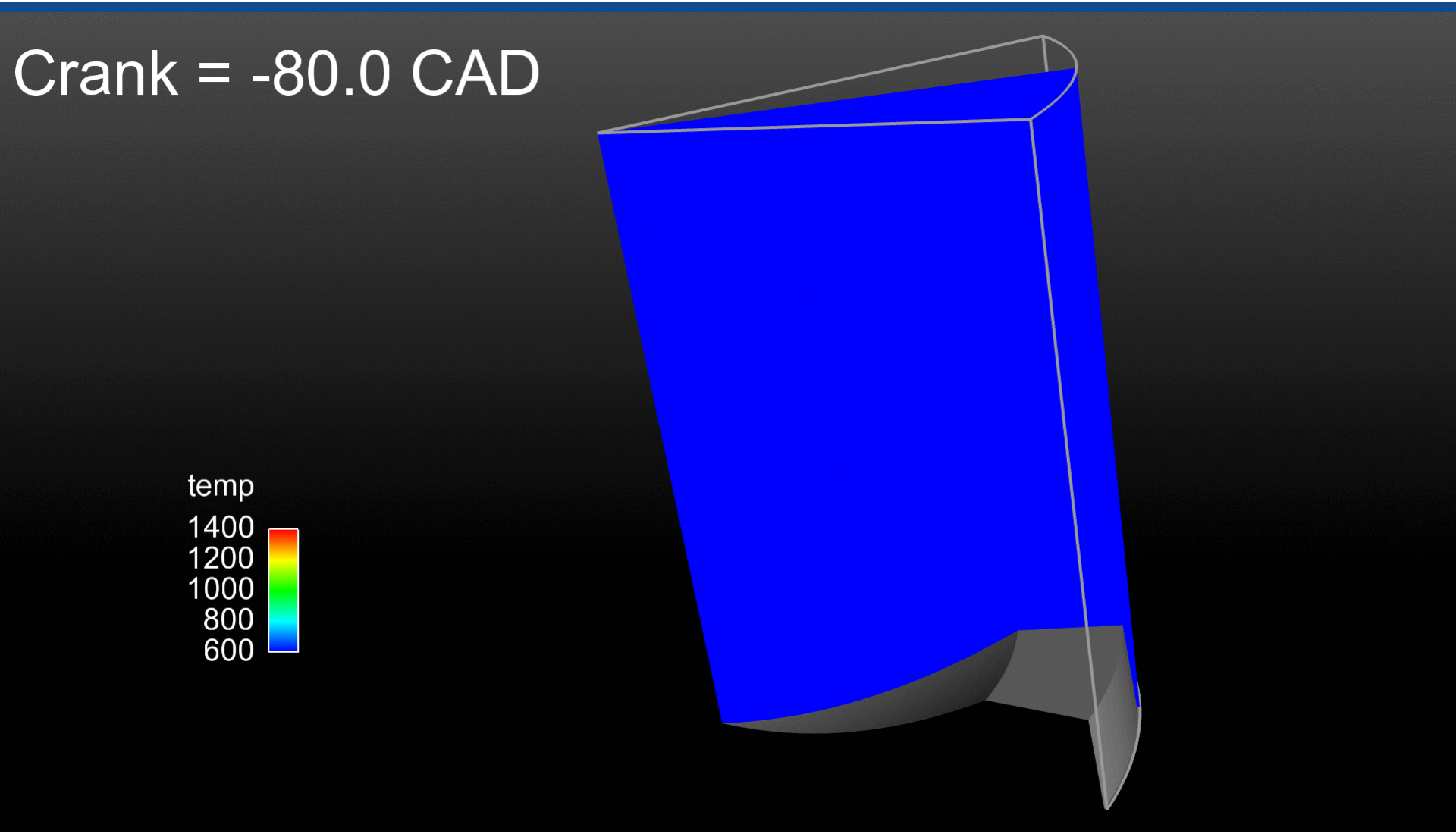
CO is not fully converted away from the central core of the combustion chamber



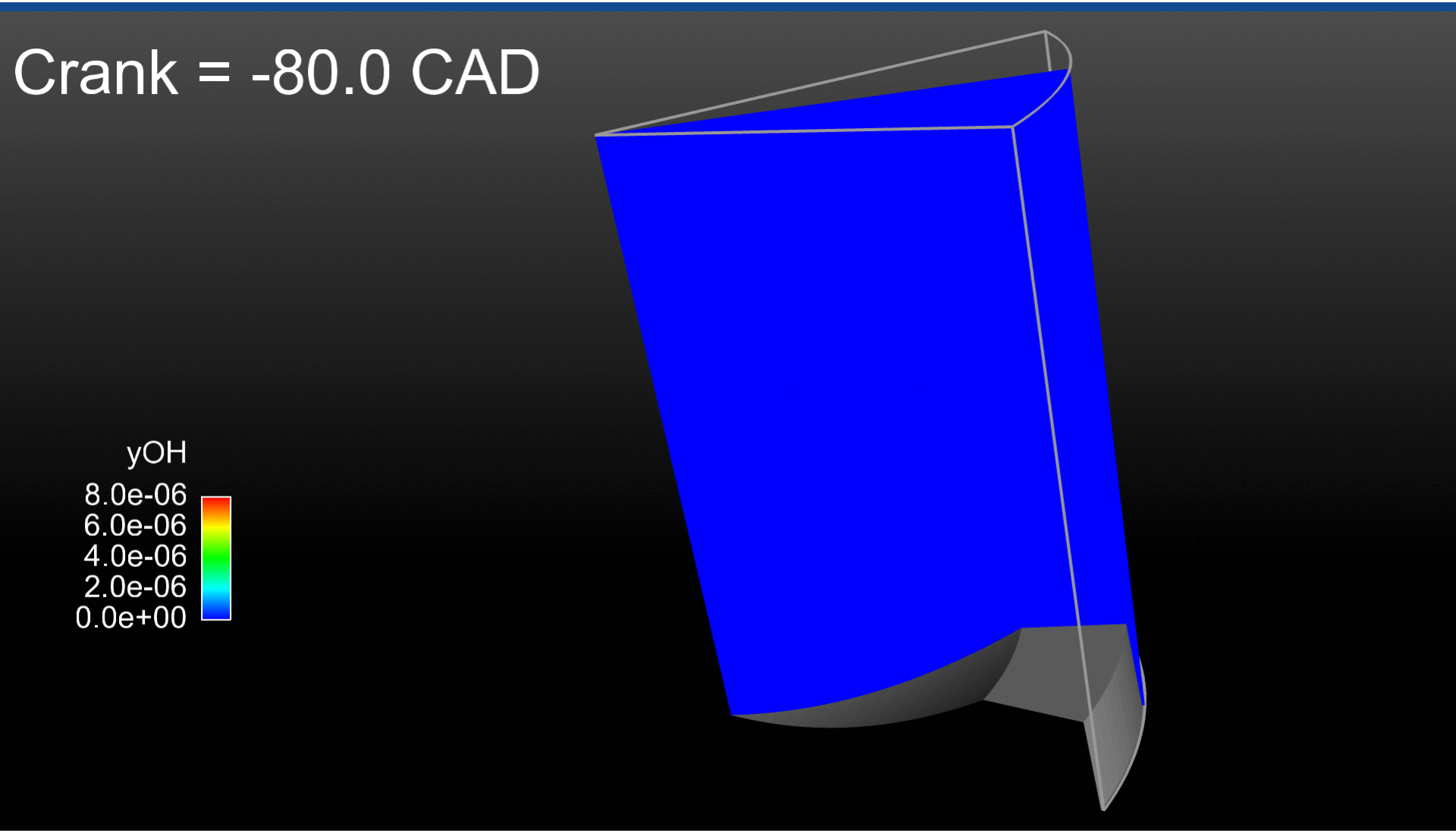
CO2 shows regions of more complete combustion



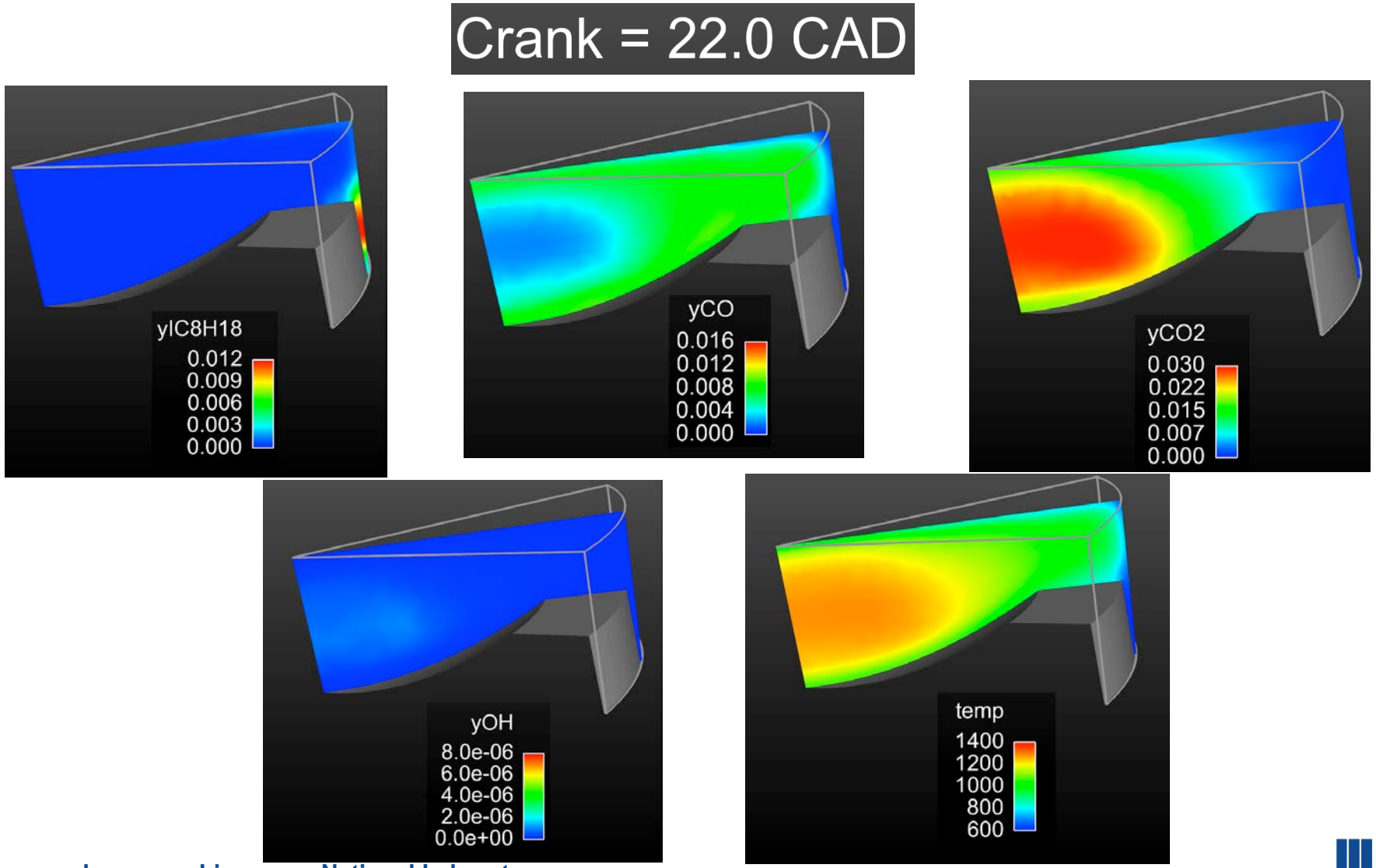
Temperatures exceed 1400K in the complete combustion region



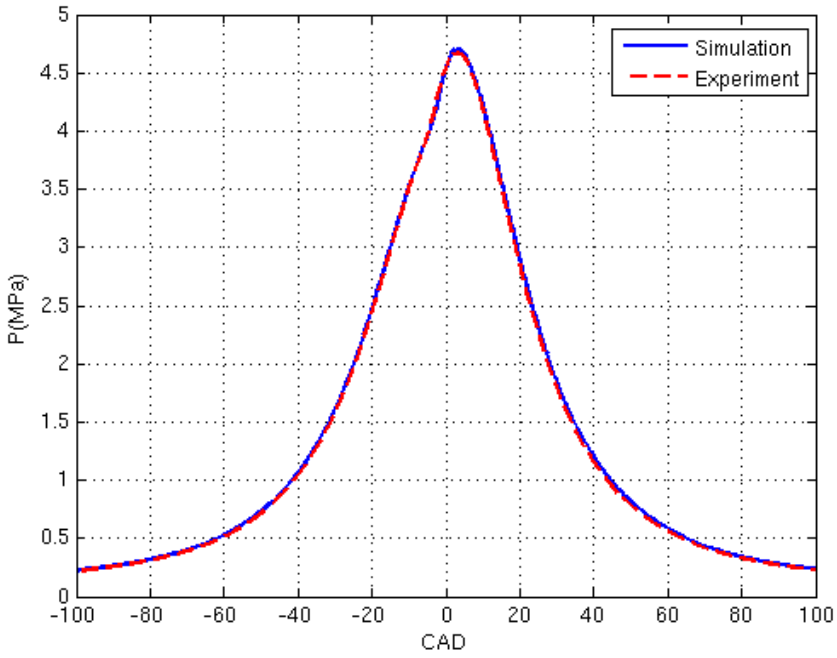
OH production hindered by low local temperatures

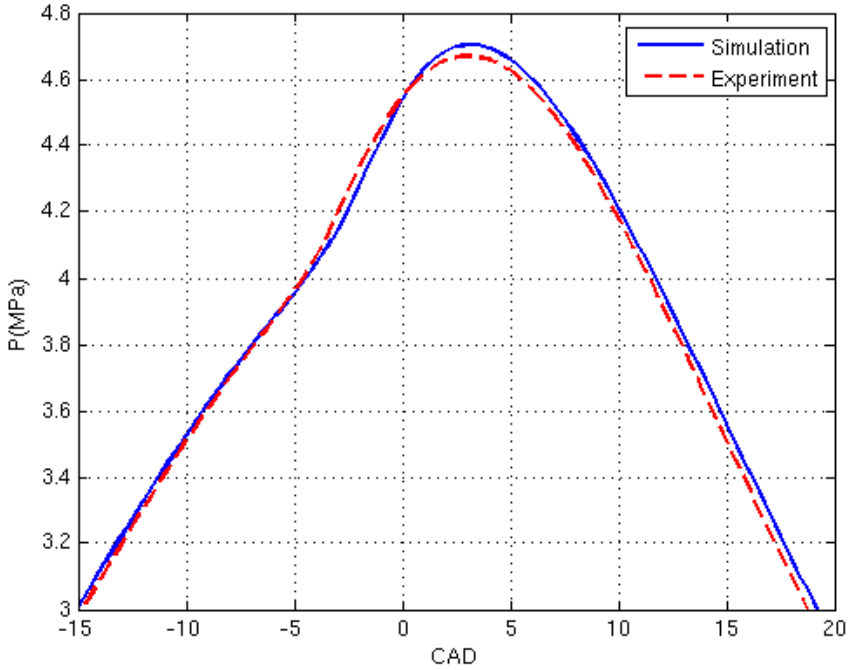


Full conversion of fuel occurs in the center of the combustion chamber, partial reaction in “squish” region



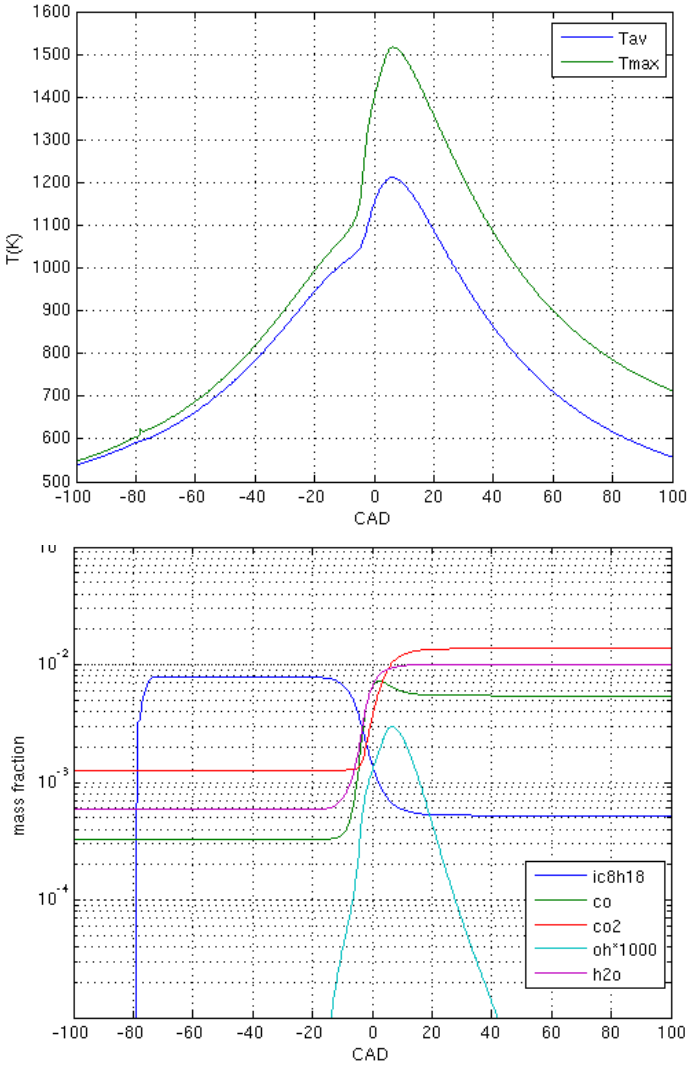
Very good agreement on in-cylinder pressure without tuning modeling parameters

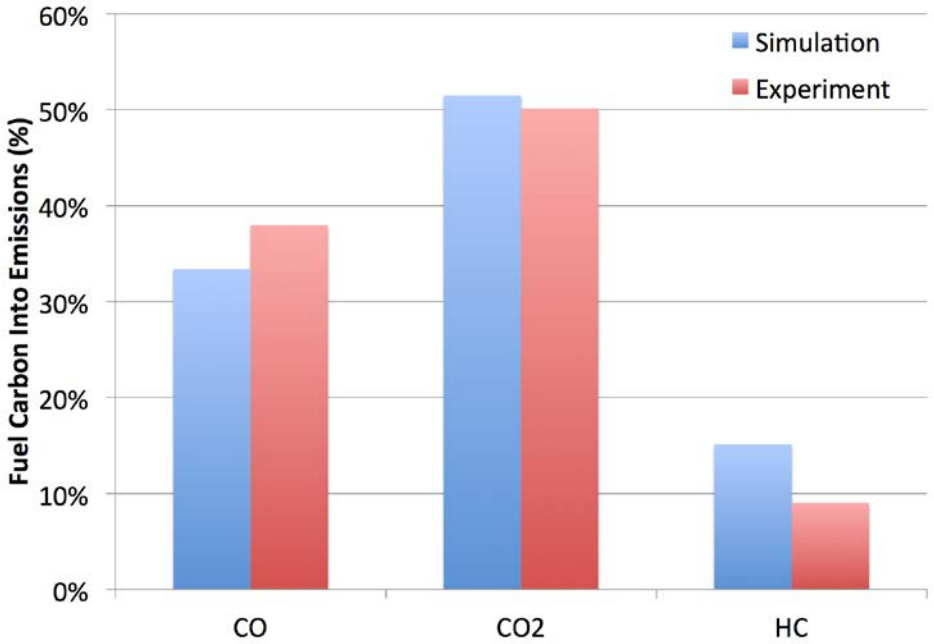




- Mesh refinement and multi-zone parameter refinement studied to achieve “grid” independence

Converge multi-zone predicted emissions compare very well with experiment





Adaptive preconditioned solver dramatically reduces chemistry time for 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

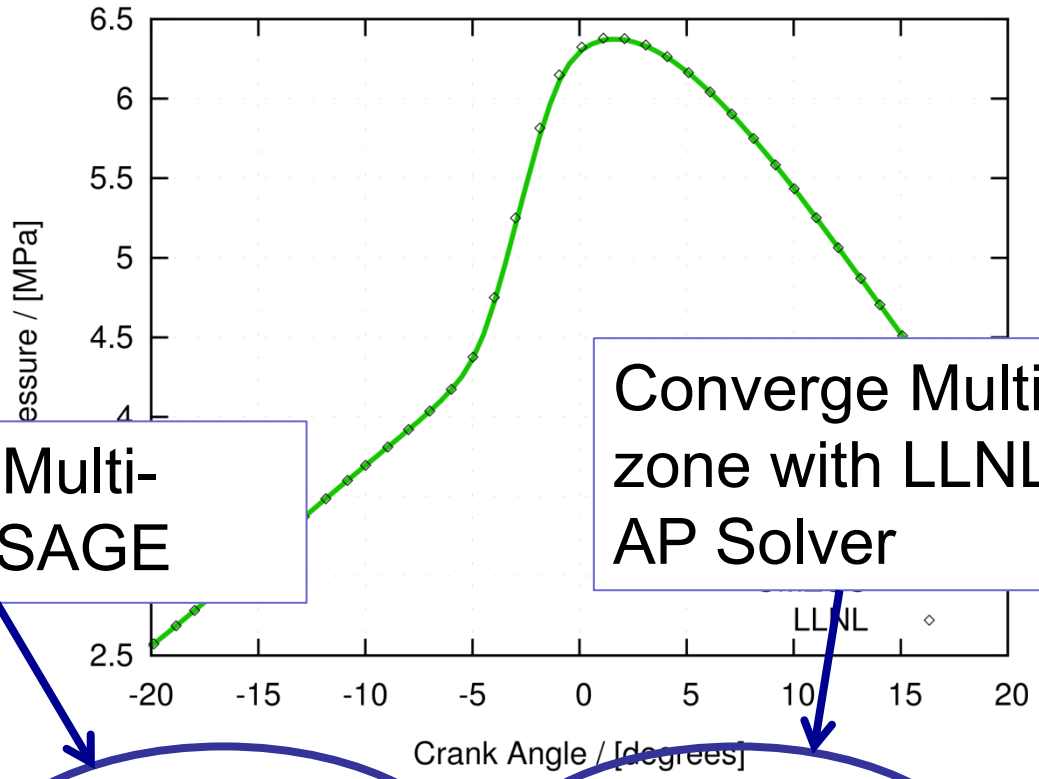
ΔΦ = 0.1

~250,000 cells at BDC

Max num. zones = 122

857 species LLNL iso-octane mechanism

24 processor MPI run



Converge Multi-zone with SAGE

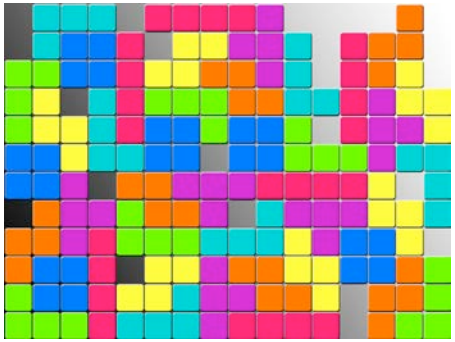
Converge Multi-zone with LLNL AP Solver

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

*includes zoning time

We use OpenFOAM as our platform for model development

open source



Modular

OpenFOAM

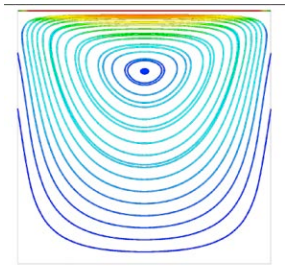
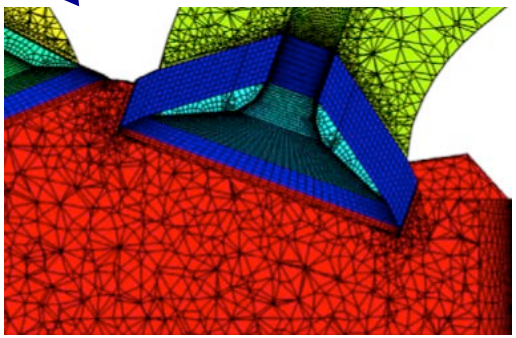


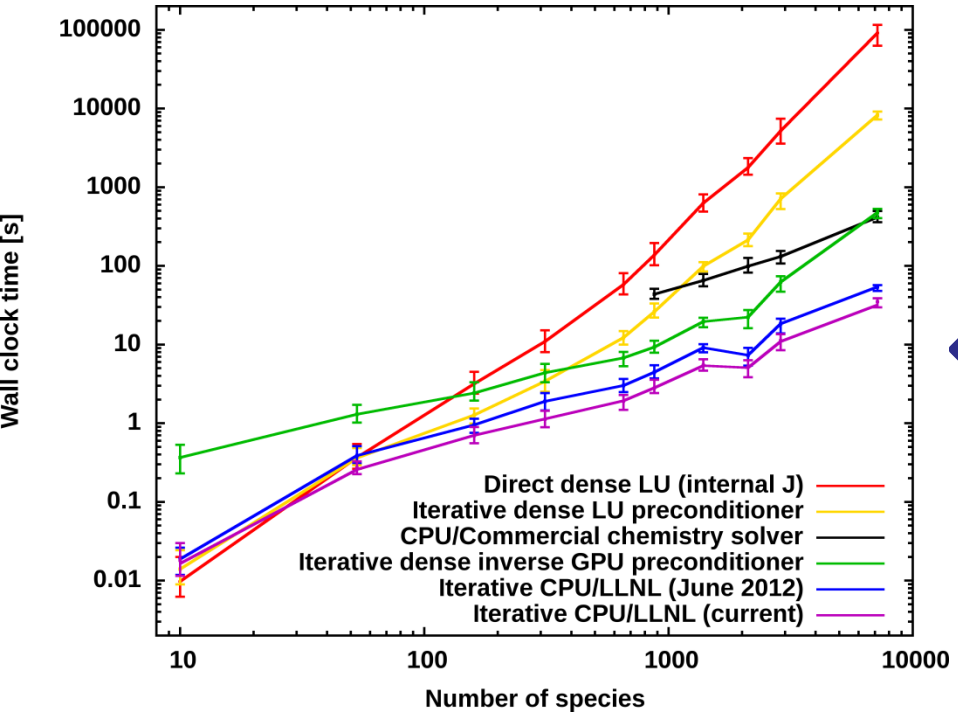
Figure 2.9: Streamlines in the *cavity* case.

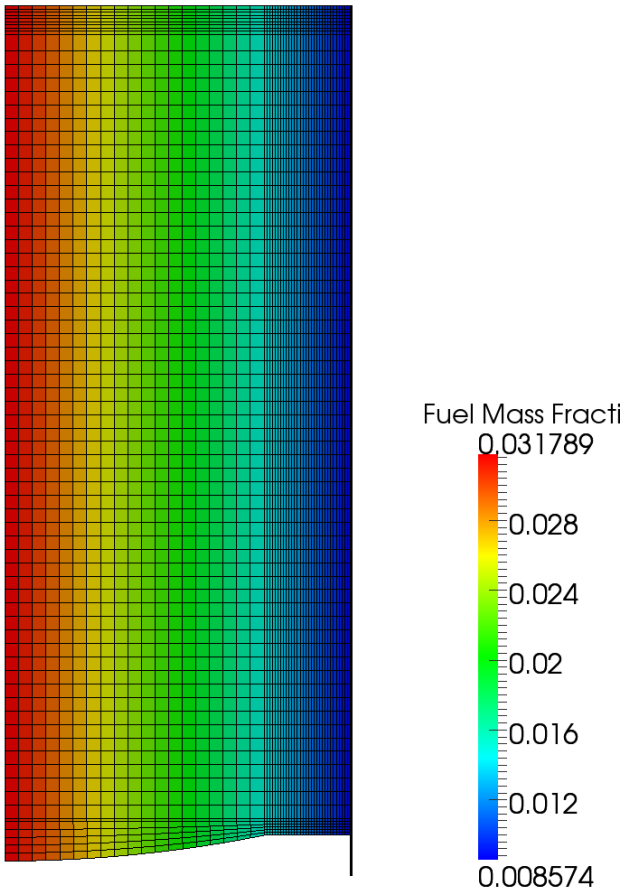
General CFD



Engines

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





Ongoing and Future Work

New chemical kinetic mechanisms

- Large alkyl aromatics
- larger n-alkanes (above C16)(important to get end of distillation curve)
- Improved gasoline and Diesel surrogates

Improved detailed chemical kinetics solvers

- Larger average timesteps per species
- Adaptive preconditioning scheme for GPU
- Extended error control schemes

CFD/Kinetics simulation tools

- Integrator based remap
- Reactor initialization estimator
- Convergence and validation with HPC