Lawrence Livermore National Laboratory

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

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Project ID # ACE012

2011 Directions in Engine-Efficiency and Emissions Research (DEER) Conference

Oct 3-6, Detroit, MI

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LLNL-PRES-477791

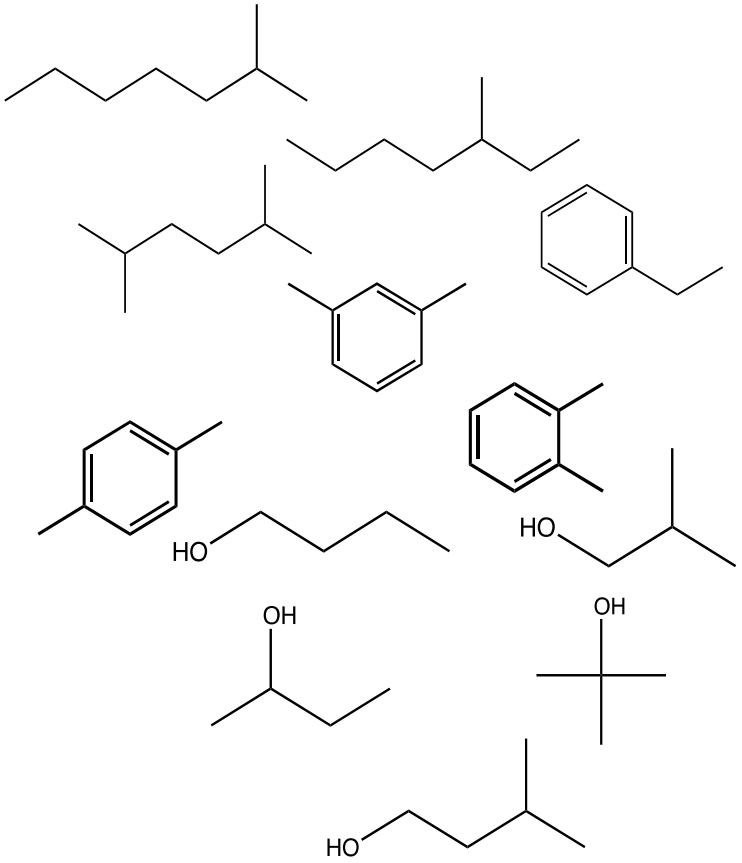
Acknowledgements

Sponsor:

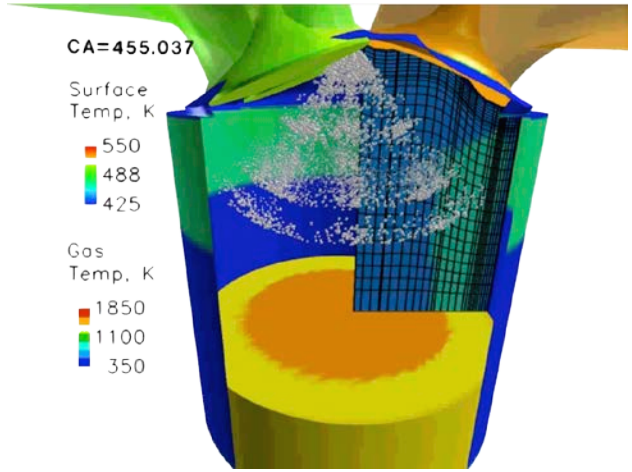
U.S. DOE, Office of Vehicle Technologies

Program Managers: Gurpreet Singh and Kevin Stork

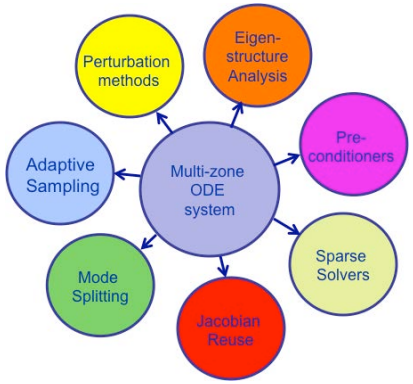
LLNL R&D supports simulation of advanced engine combustion regimes



Detailed chemical kinetics



Coupled CFD+Kinetics for complex fuels

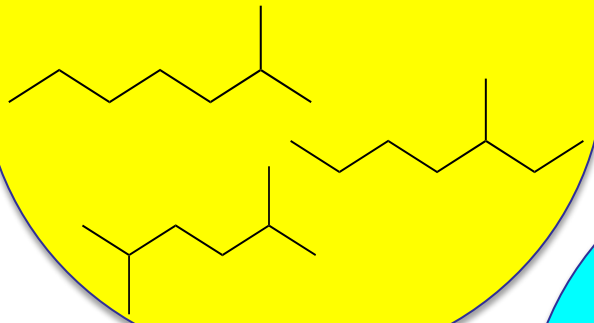


Novel chemical kinetic solvers

Recently Developed Fuel/Surrogate Models

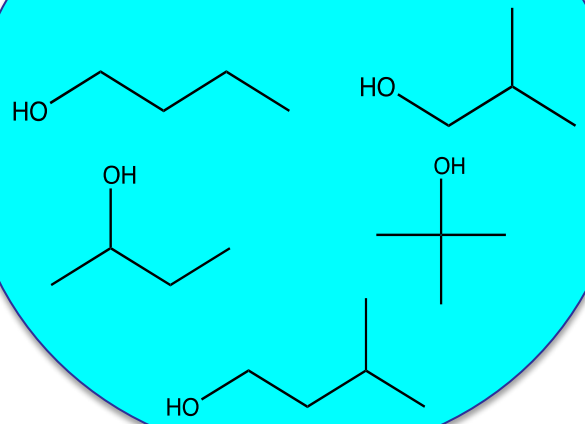
Diesel and Gasoline Surrogates

Branched Alkanes



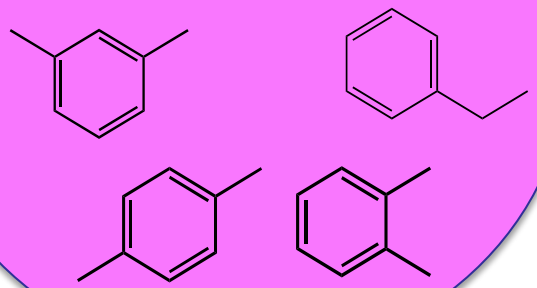
Biofuels / Additives

Alcohols

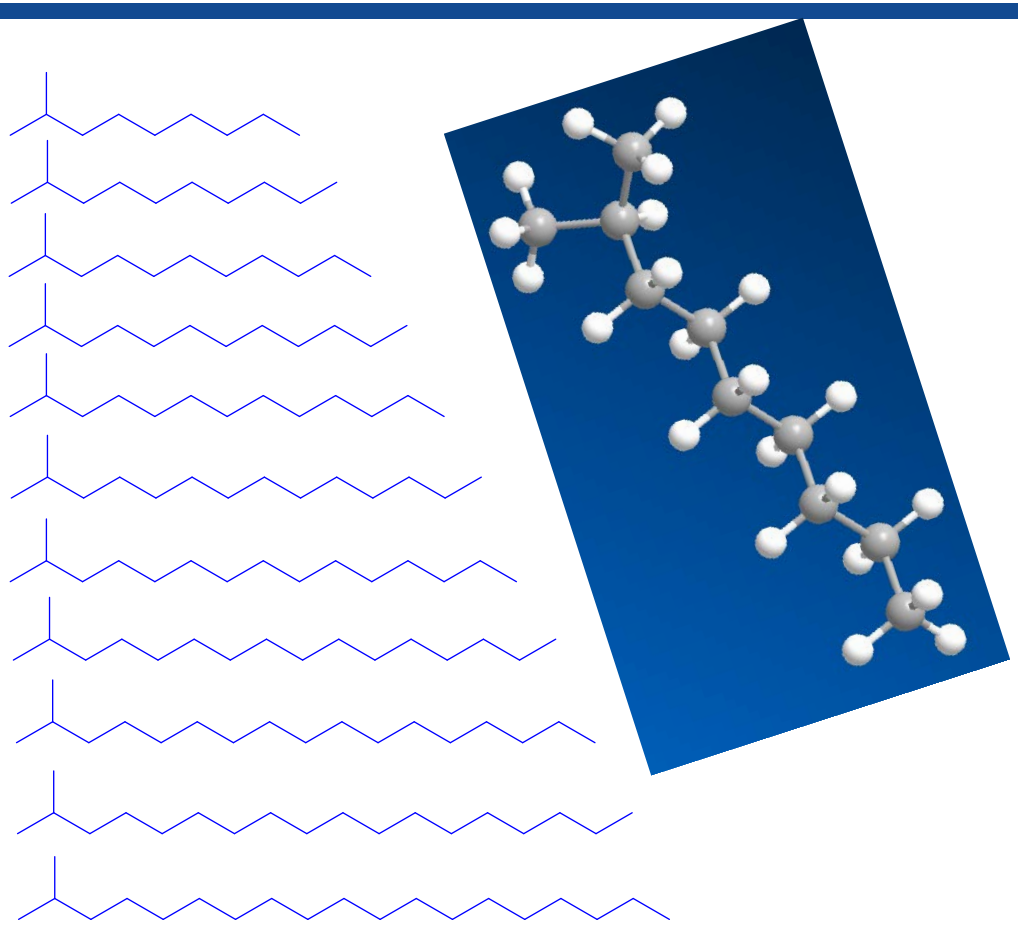


Diesel and Gasoline Surrogates

Aromatics



We have developed Chemical Kinetic Mechanism for n-alkanes and 2-methylakanes up to C_{20}



Includes all n-alkanes upto C_{16} and 2-methylalkanes up to C_{20}, which covers the entire distillation range for gasoline and diesel fuels

Validated against experimental data in shock tubes, flames, and jet stirred reactors.

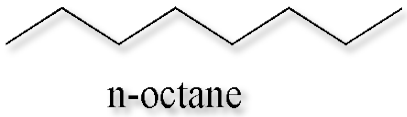
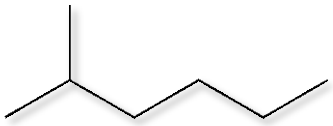
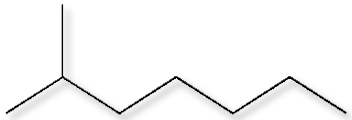
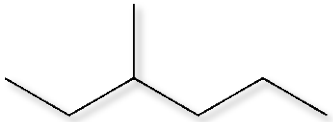
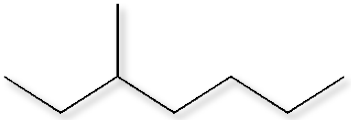
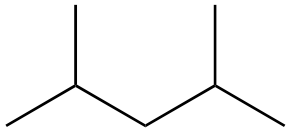
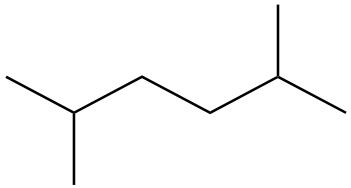
Complete Mechanism

7,200 species

31,400 reactions

S.M. Sarathy, C.K. Westbrook, M. Mehl, W.J. Pitz, et al., Combustion and Flame, 2011

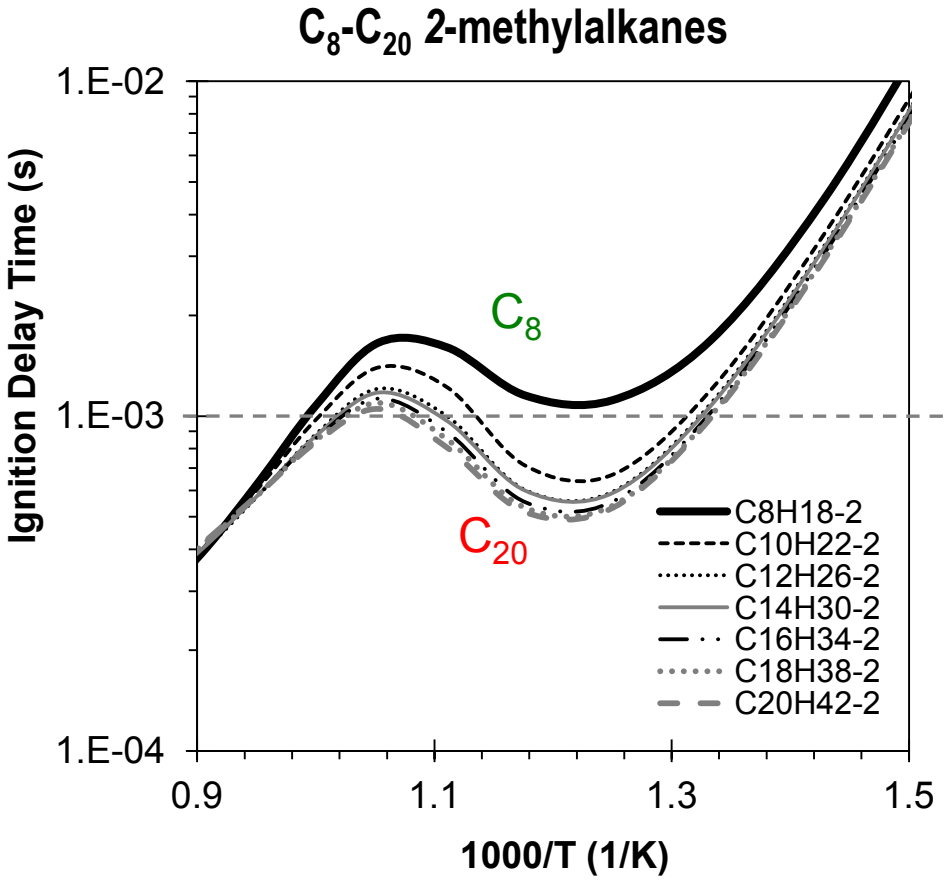
Branching reduces propensity for ignition

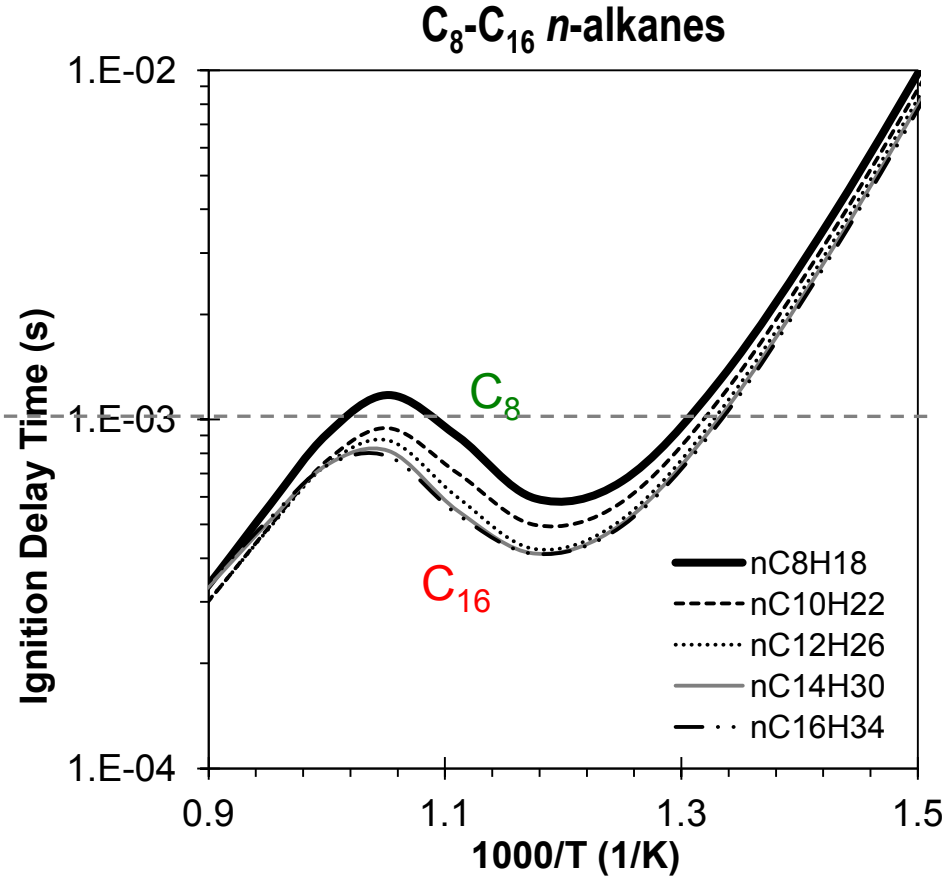
C_7H_{16}	Research Octane Number[1]	Derived Cetane Number[2]	C_8H_{18}	Research Octane Number[1]	Derived Cetane Number[2]
 n-heptane	0	53.8	 n-octane	-19.0	57.6
 2-methylhexane	42.4	43.5	 2-methylheptane	21.7	52.6
 3-methylhexane	52.0	?	 3-methylheptane	36.8	?
 2,4-dimethylpentane	83.1	?	 2,5-dimethylhexane	55.5	?

1. C. Morley Comb. Sci. Tech. 55, 15 (1987)
2. Ratcliff et al. NREL (2010)

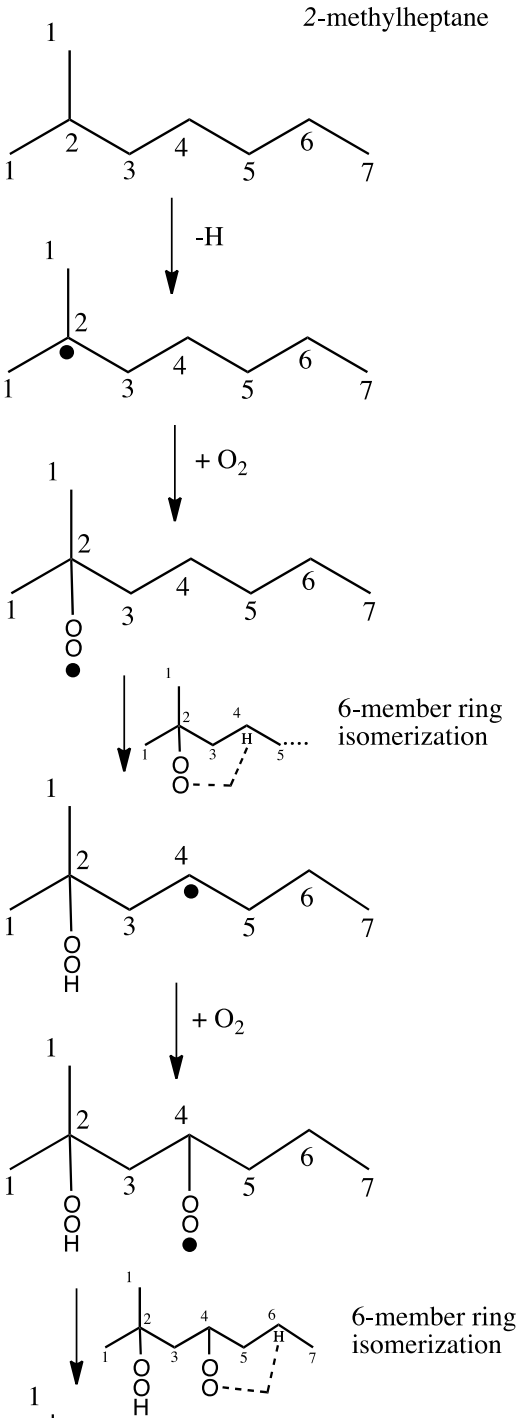
Reactivity increases with chain length; *2*-methylalkanes are less reactive than *n*-alkanes of the same chain length.

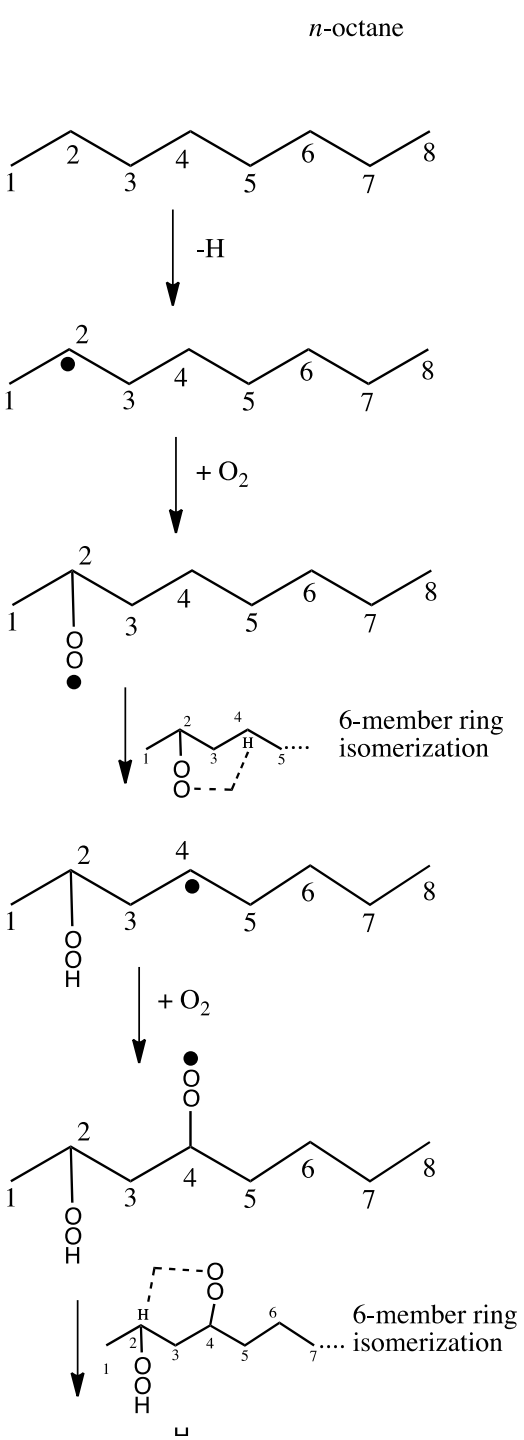
ϕ = 3, 20 atm (Diesel Ignition Conditions)





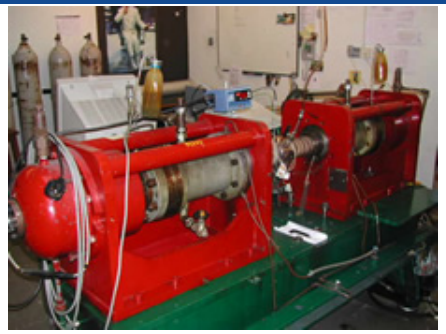
Low Temperature (700 K) Chain Branching Reaction Pathways



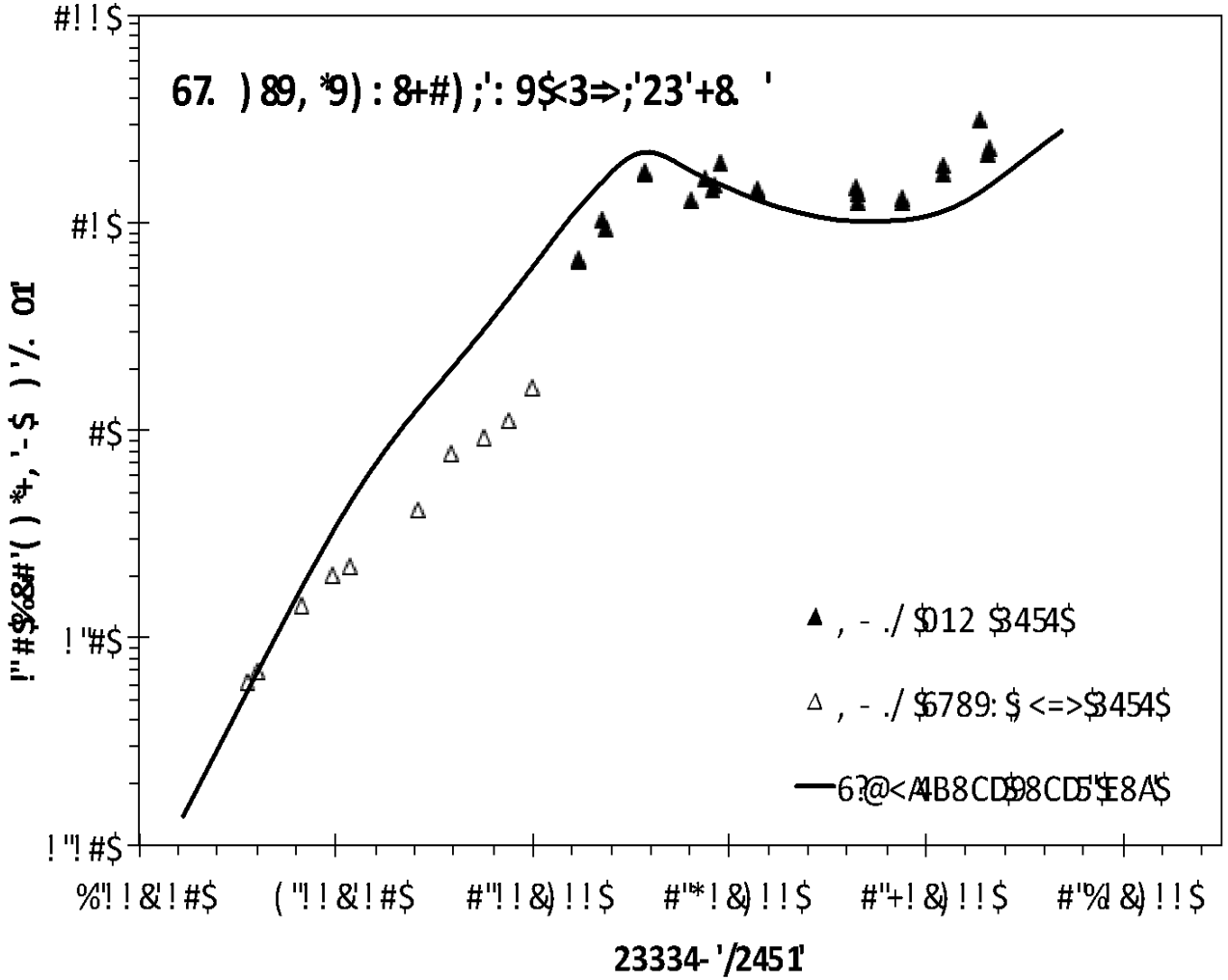


Experimental validation is underway with a number of collaborators

- Rapid Compression Machine Ignition
  - NUI Galway, Ireland
- Counterflow Diffusion Flames
  - University of Toronto
  - UC San Diego
- Shock Tube Ignition Delay
  - RPI, New York
- Jet Stirred Reactor
  - CNRS Orleans, France



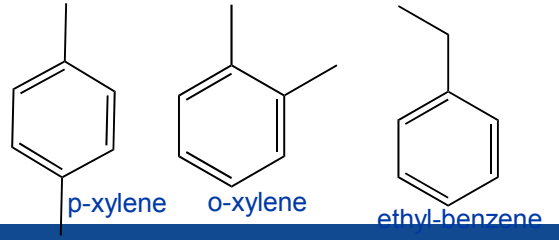
Shock Tube and RCM 2-methylheptane experiments show good agreement with our mechanism



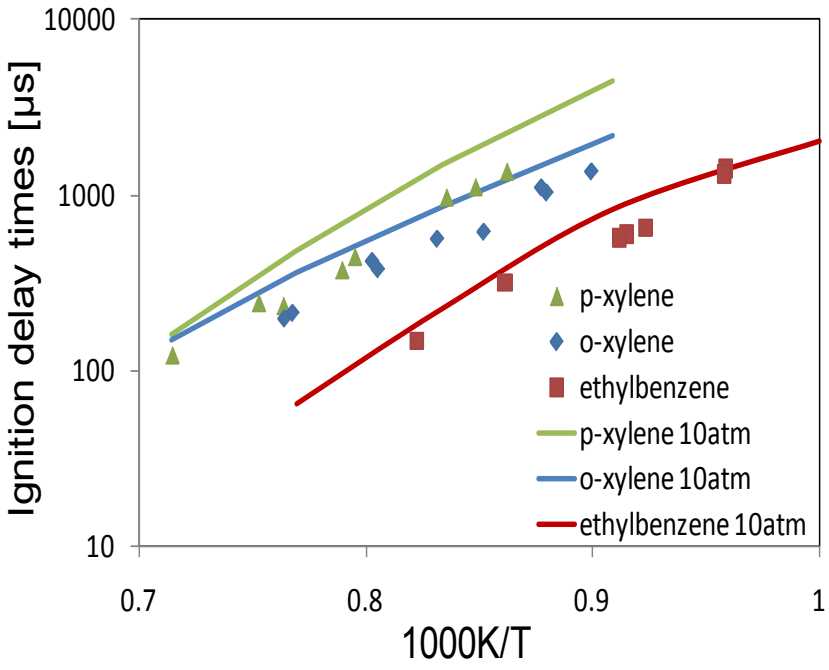
NUIG RCM

Overall reasonable prediction of low reactivity for an *a priori* kinetic model

We are also developing and validating mechanisms for complex C_8 Aromatics

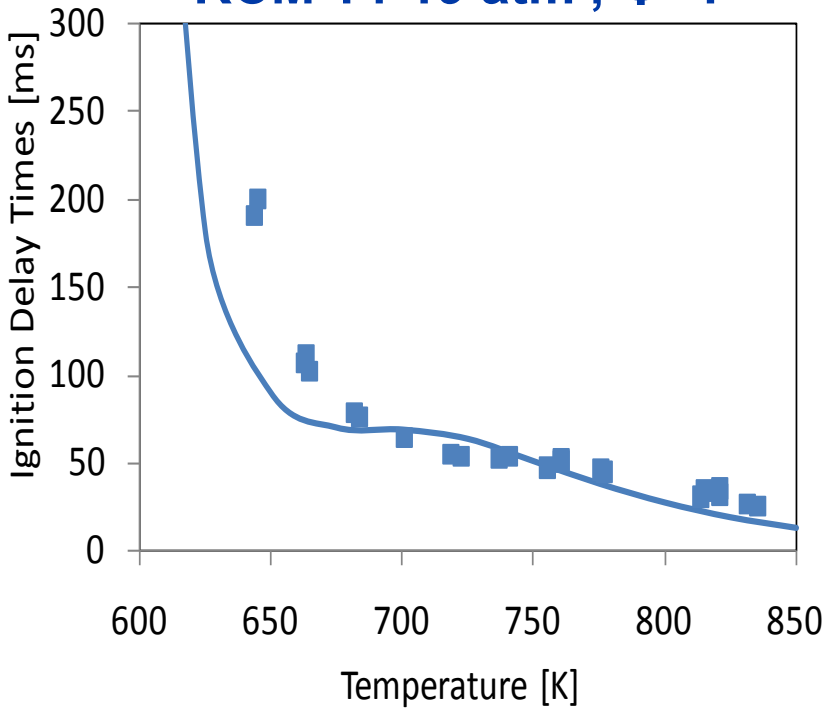


ST 10 atm , Φ=1



RCM comparisons: Lines are calculations, data are from H.-P.S. Shen, M.A. Oehlschlaeger, Combustion and Flame 2009, 156, 1053–1062

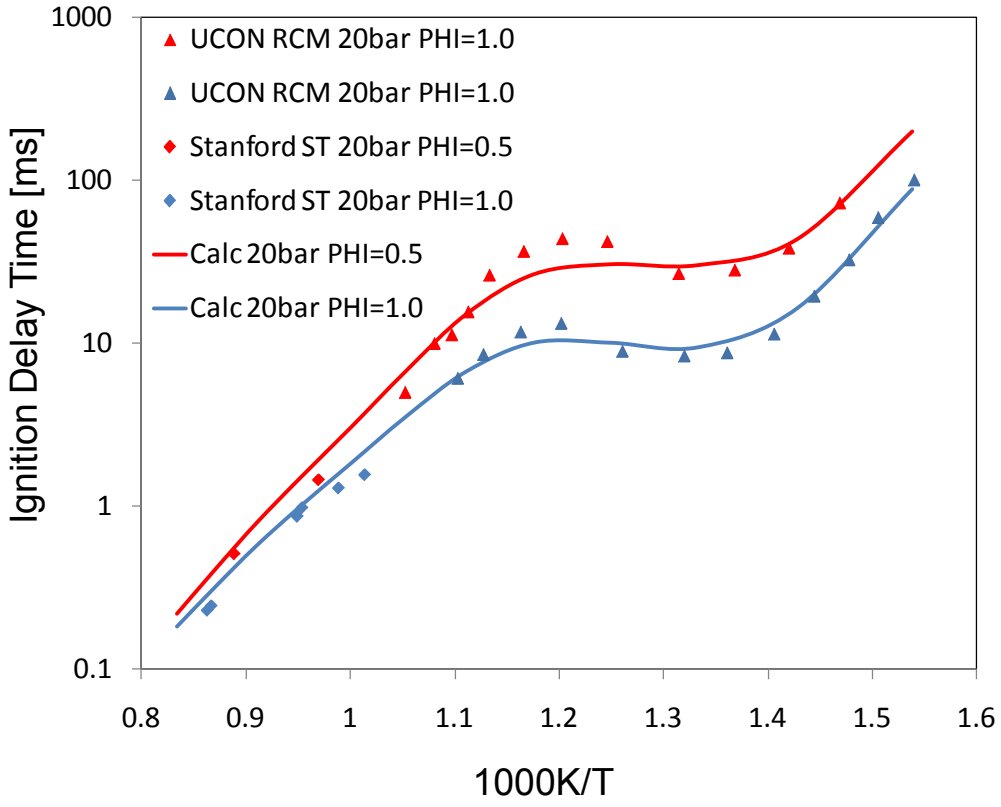
o-Xylene, RCM 14-19 atm , Φ=1



A. Roubaud, O. Lemaire, R. Minetti, and L.R. Sochet, Comb. Flame 2000, 123, 561–571

The model correctly reproduces the relative reactivity in terms of ignition of different C8 aromatics

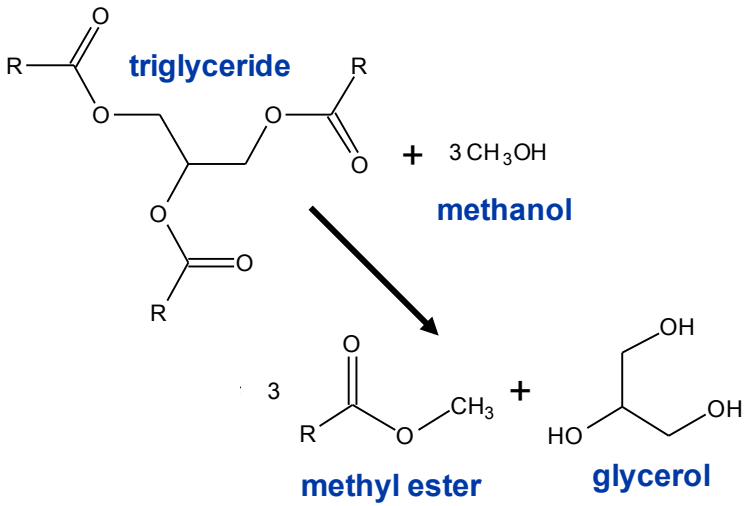
We have built a gasoline surrogate that is predictive of RCM ignition delay data

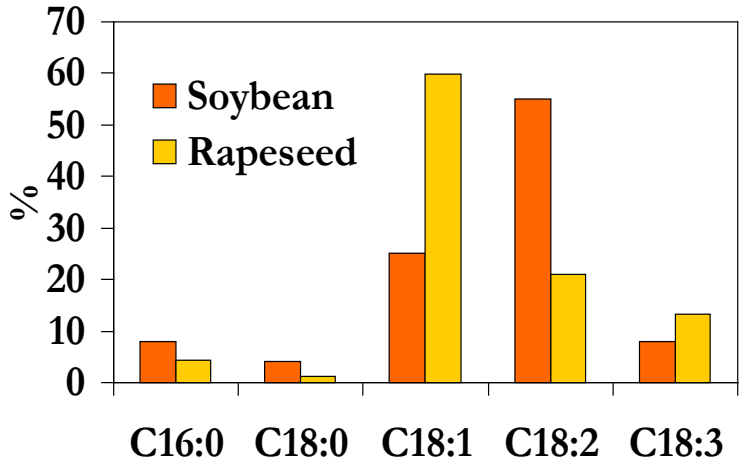


The research gasoline used at Sandia in previous and current HCCI experiments was tested in the UCON Rapid Compression Machine.

The experimental ignition times are compared with simulations obtained using the gasoline surrogate proposed by LLNL

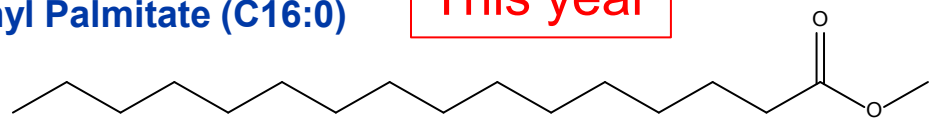
We have complete mechanisms for the 5 principle components of soybean and rapeseed biodiesels



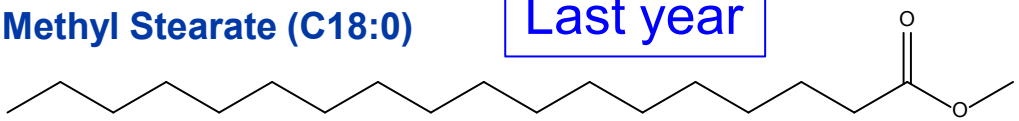


Fatty acid methyl esters (FAMEs):

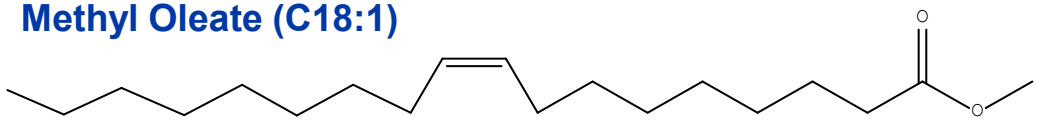
Methyl Palmitate (C16:0) This year



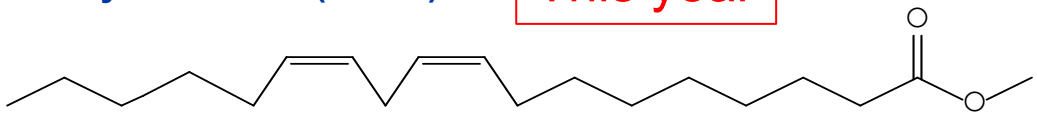
Methyl Stearate (C18:0) Last year



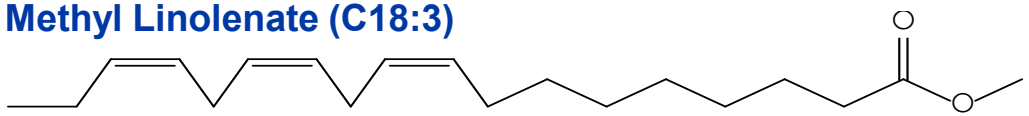
Methyl Oleate (C18:1)



Methyl Linoleate (C18:2) This year

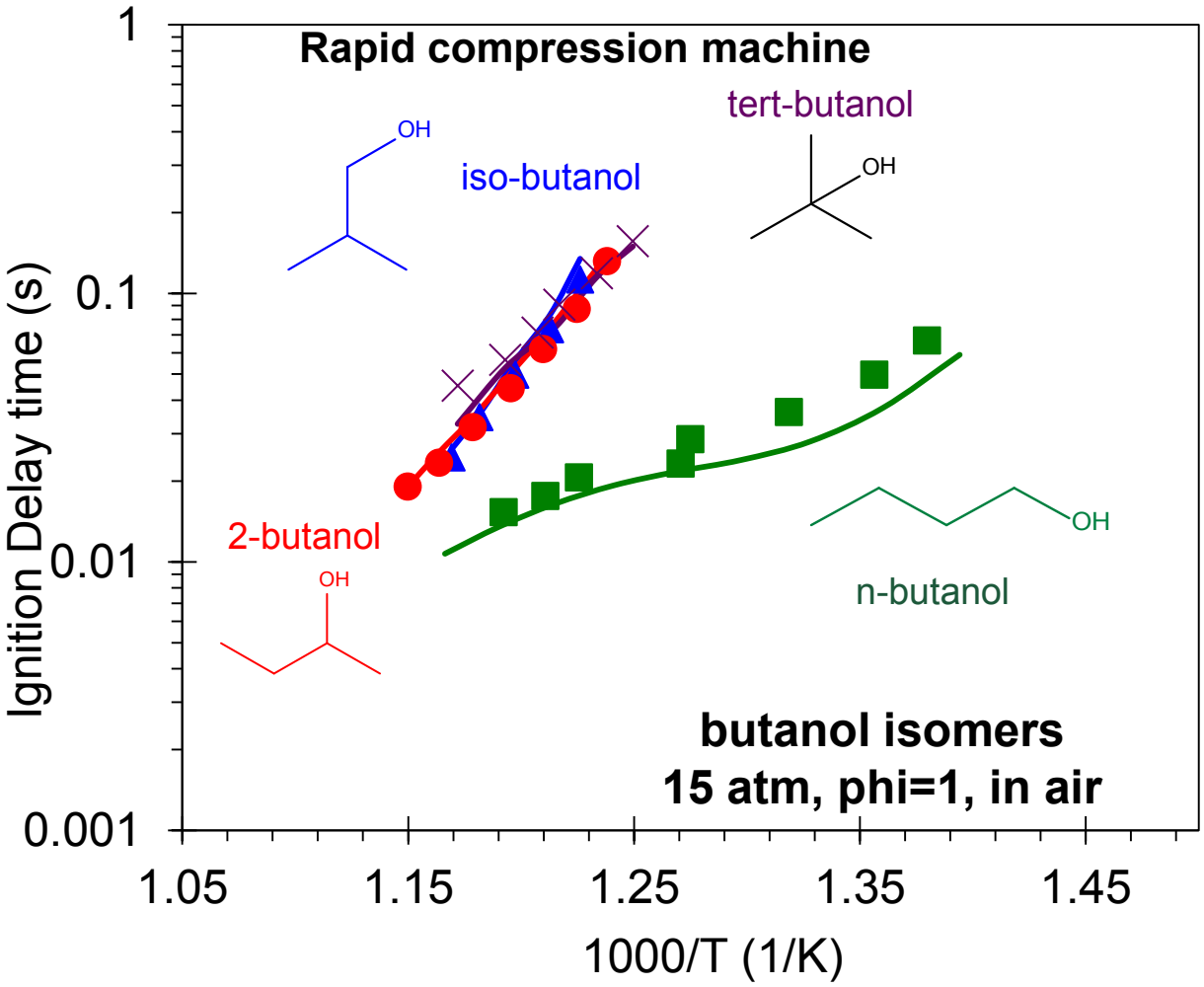


Methyl Linolenate (C18:3)

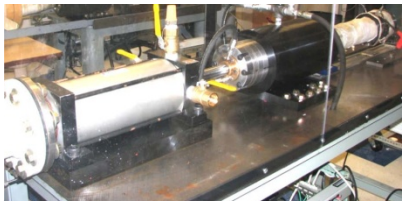


Model with all 5 components now published and available: Westbrook, Naik, Herbinet, Pitz, Mehl, Sarathy and Curran, "Detailed chemical kinetic reaction mechanisms for soy and rapeseed biodiesel fuels," Combustion and Flame, 2011.

Supporting interest in Bio-butanol as an alternative fuel, we have developed and validated mechanisms for several butanol isomers



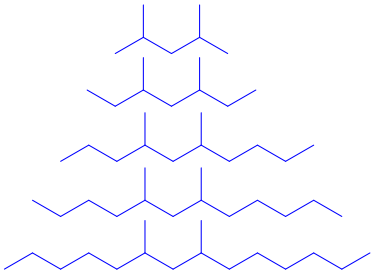
Symbols:
experimental data
Sung et al.,
AIAA paper, 2011



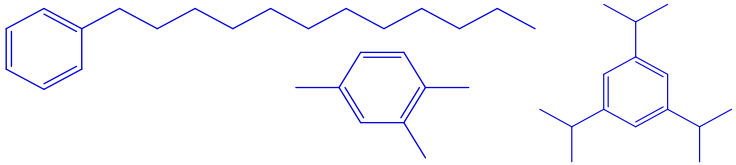
Rapid compression machine
University of Connecticut

Simulations including RCM volume traces better predict experimental ignition delay times.

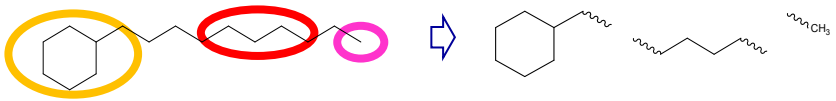
We continue to build and validate kinetic mechanisms for both conventional and alternative fuels



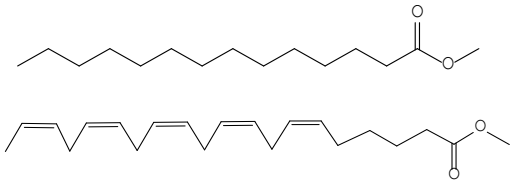
Dimethyl-alkanes



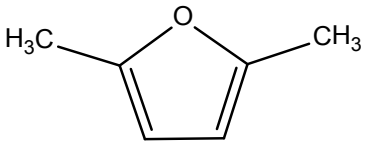
Larger alkyl aromatics

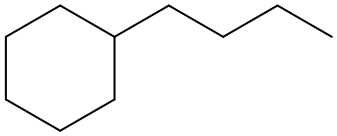


Functional Group methodology

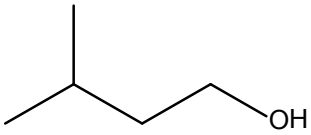


Algal derived biofuels





Biomass derived fuel



Iso-pentanol validation

Mechanisms are available on LLNL website and by email

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

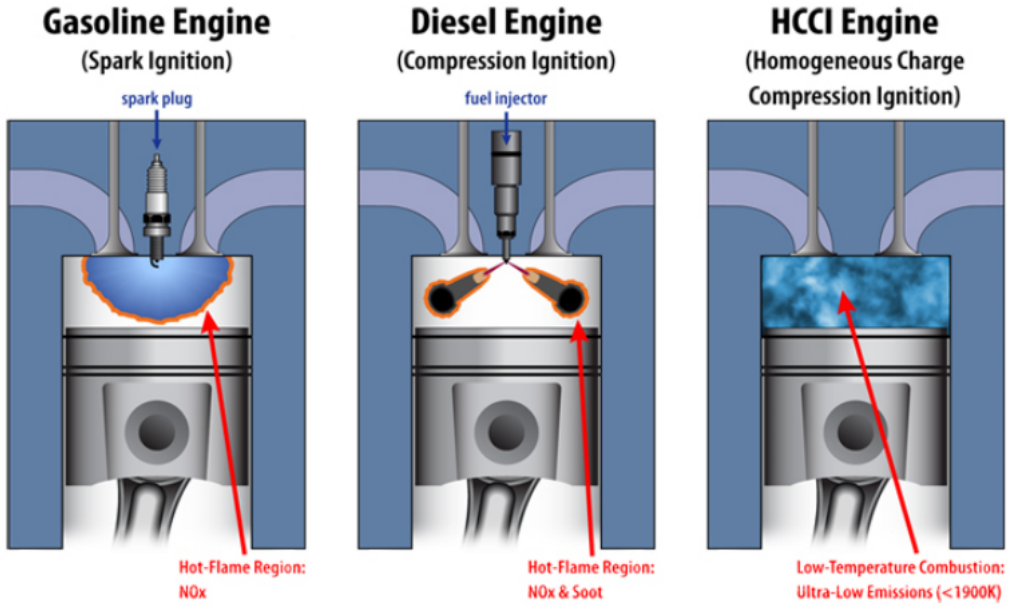
- Ethanol
- Dimethyl Ether
- CH4, C2H4, C2H6, C3H8, and nC4H10
- CH4, C2H4, C2H6, C3H6, C3H8, and NOx
- C8-C16 n-Alkanes
- Cyclohexane
- Methylcyclohexane
- Methyl Butanoate and Methyl Formate
- Methyl Decanoate
- Methyl Decenoates
- Biodiesel Surrogates
- Dimethyl Carbonate
- Heptane, Detailed Mechanism
- Heptane, Reduced Mechanism
- iso-Octane
- 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 Flames
- Organophosphorus

Combustion Chemistry

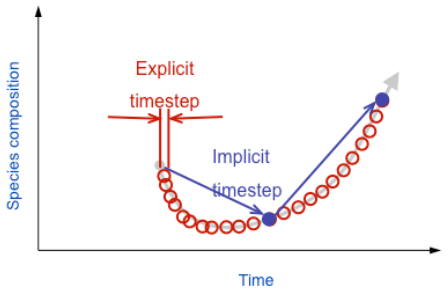
Go Directly to Mechanisms...

The central feature of the Combustion Chemistry project at LLNL is our development, validation, 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 built hydrocarbon mechanisms for fuels from hydrogen and methane through much larger fuels including heptanes and octanes. Other classes of fuels for which models have been developed include flame suppressants such as halons and organophosphates, and air pollutants such as soot and oxides of nitrogen and sulfur.

Reaction mechanisms have been tested and validated extensively through comparisons between 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.



Large chemical kinetic mechanisms can be difficult to solve numerically, we develop methods to enable detailed kinetics in engine simulations



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

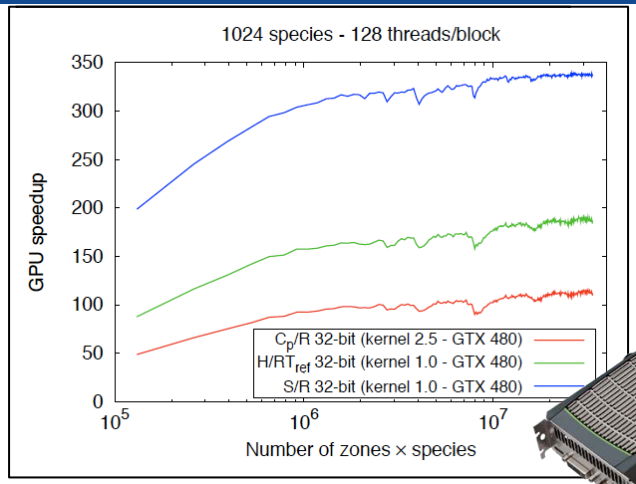
Explicit Update
(lower cpu/step)

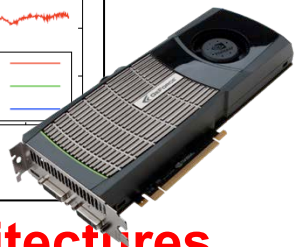
$$\frac{\partial x_1}{\partial t} = f_1(t, x_1, \ldots, x_N)$$
$$\frac{\partial x_2}{\partial t} = f_2(t, x_1, \ldots, x_N)$$
$$\vdots$$
$$\frac{\partial x_N}{\partial t} = f_N(t, x_1, \ldots, x_N).$$

Implicit Update
(more trajectory data)

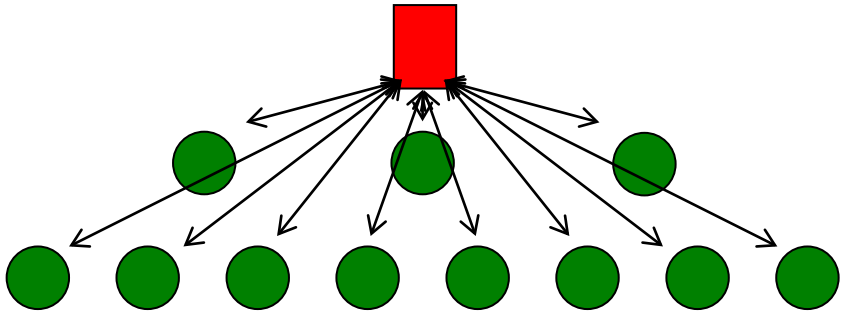
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial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

Improved Numerics

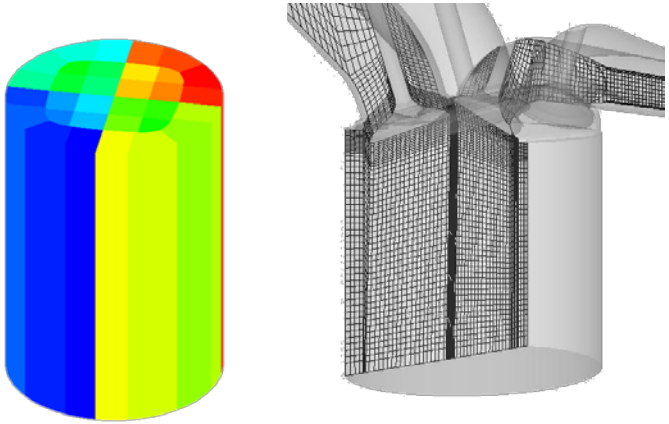




New Computing Architectures

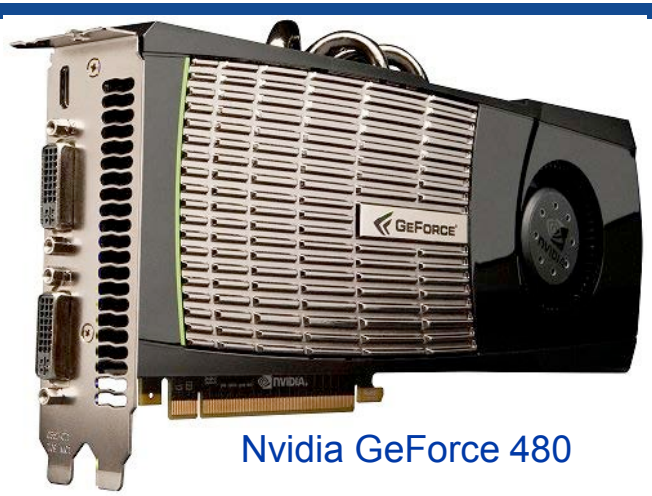


CFD+multi-zone development

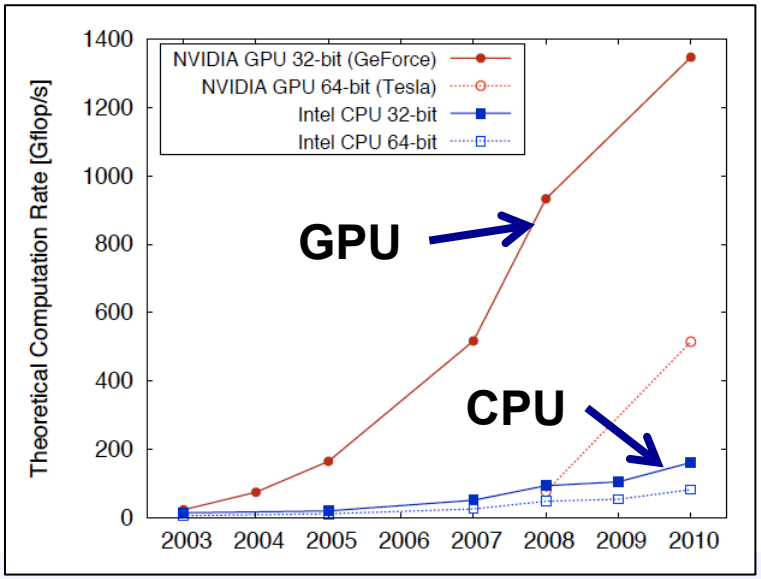


Parallel CFD and MZ-chemistry

Graphical Processing Units (GPUs) can bring supercomputing to the desktop workstation



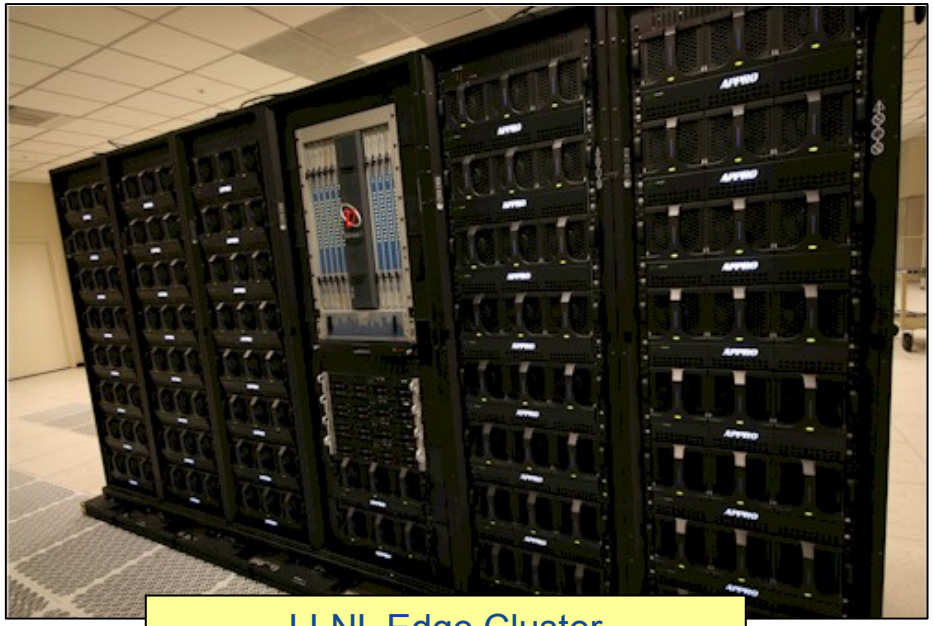
Nvidia GeForce 480

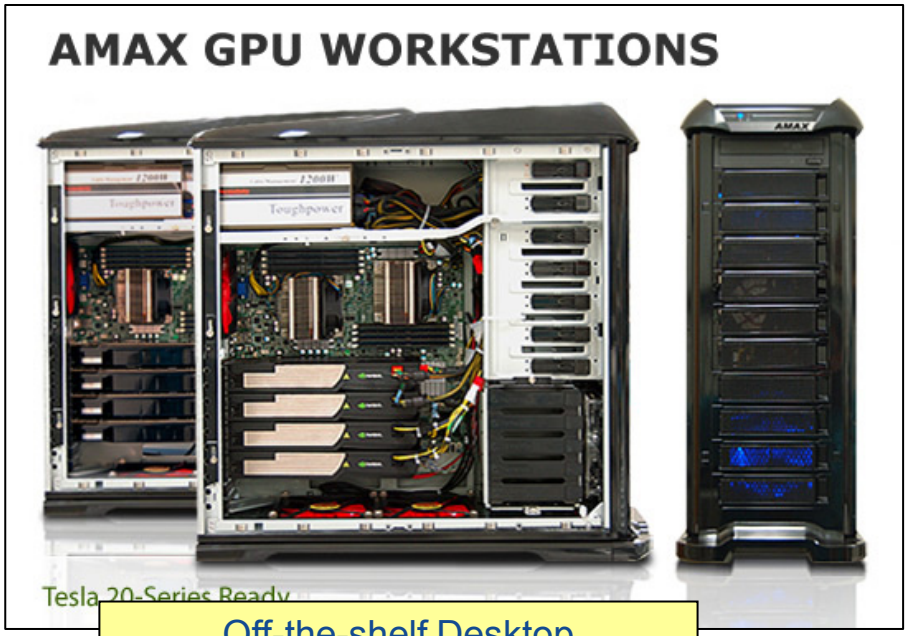


Data from NVIDIA's, "CUDA C Programming Guide Version 3.1," 2010.

- ½ Teraflop for $500
- 480 parallel processors
- Codes must be redesigned to take advantage of architecture
- Massively parallel computing on the desktop
- Fortran/C++ Compilers designed for GPUs now available

LLNL is a center for research on using GPU architectures for large-scale scientific simulations

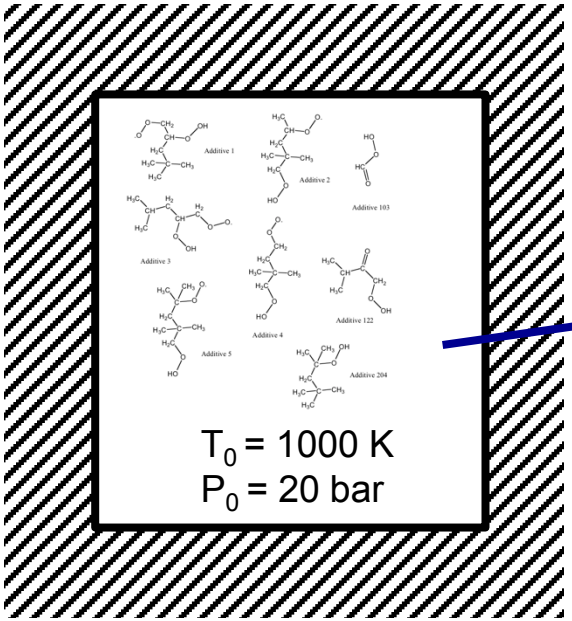


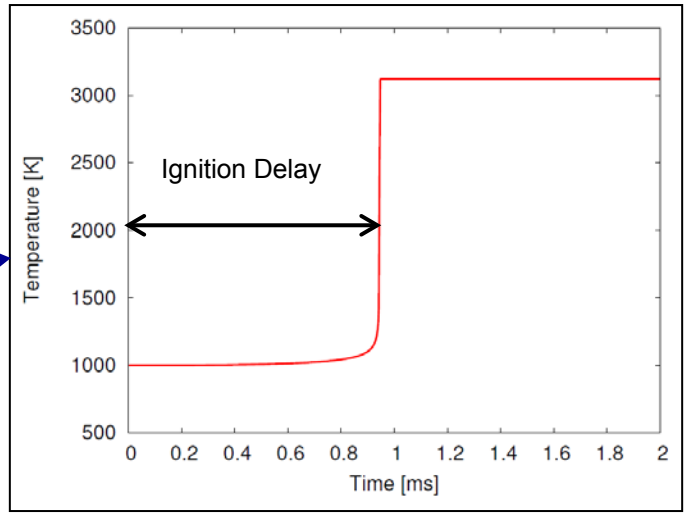


LLNL Edge Cluster		
GPUs:	412	
Type:	Tesla M2050	
Cores:	185,000	GPU
	2,500	CPU
Tflop/s:	212 (64-bit)	
Price:	4 - 5 M$	

Off-the-shelf Desktop		
GPUs:	1	
Type:	Tesla C2050	
Cores:	448	GPU
	8	CPU
Tflop/s:	0.5 (64-bit)	
Price:	5.7 K$	

Constant volume ignition delay is the basis for numerical chemistry development

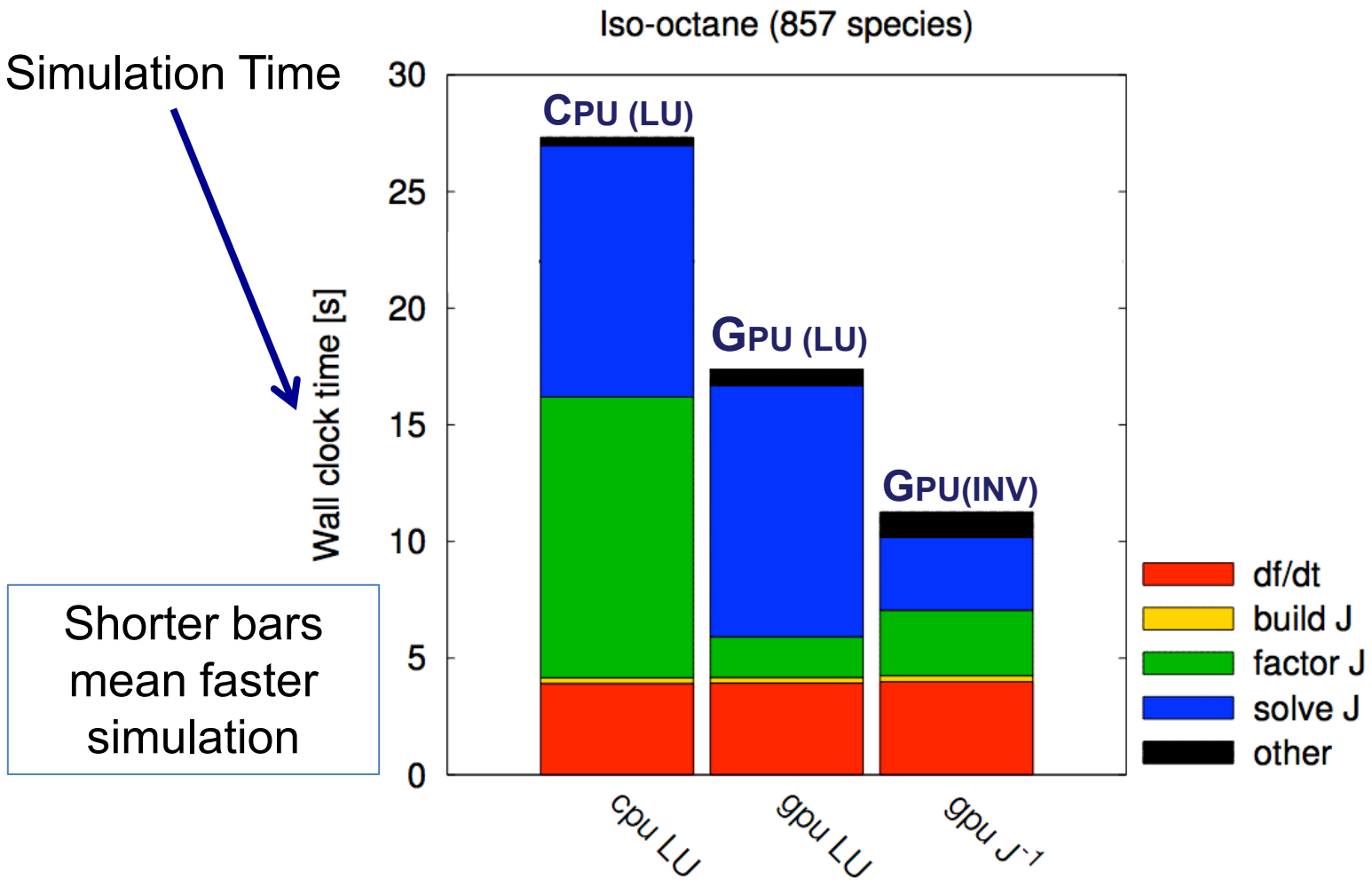




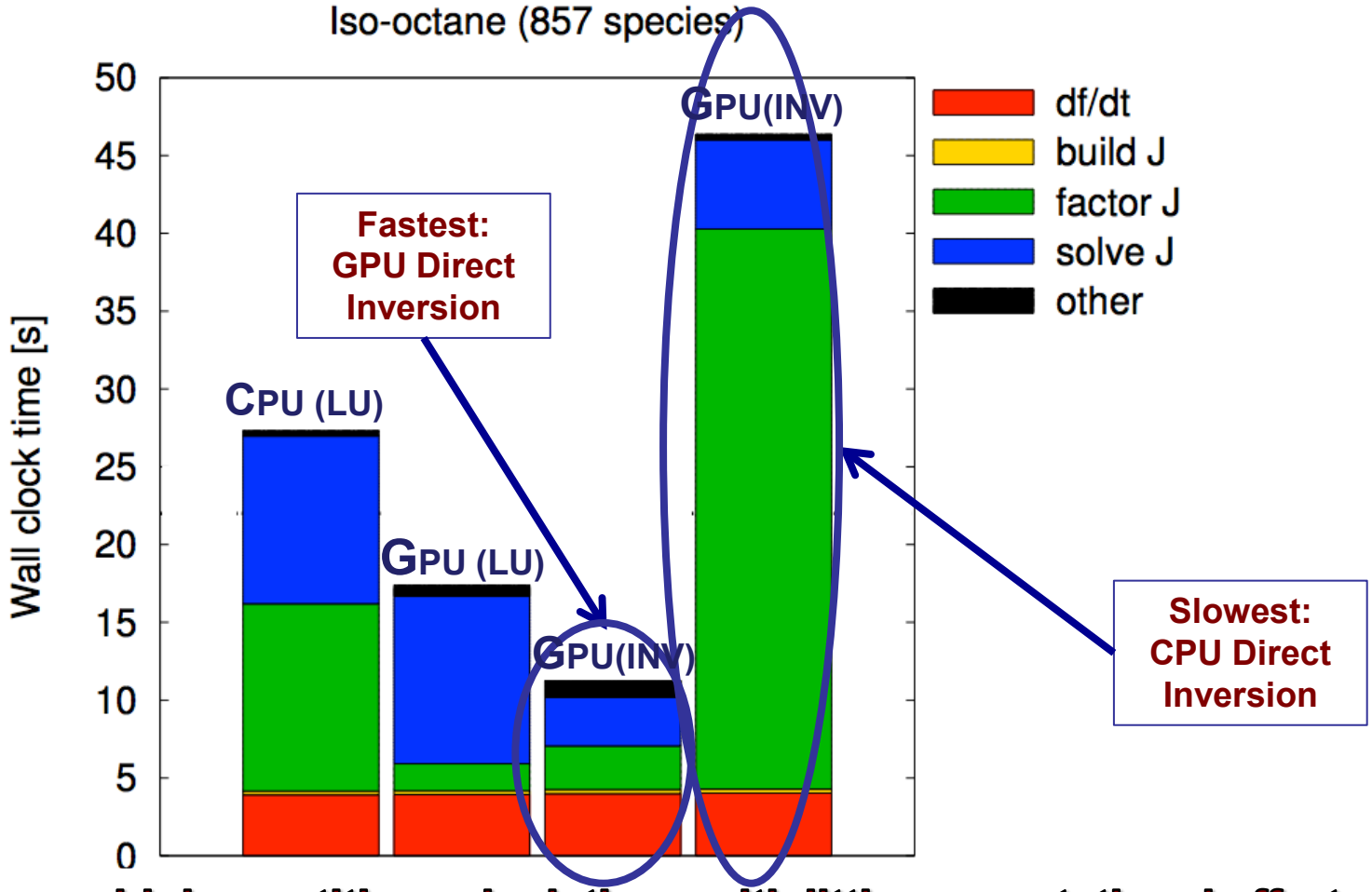
Constant Volume Reactor **Temperature Time History**

The Constant Volume Reactor is the basic unit for chemistry in multidimensional CFD codes

We are doing ignition delay calculations with large mechanisms to determine best practices for GPUs



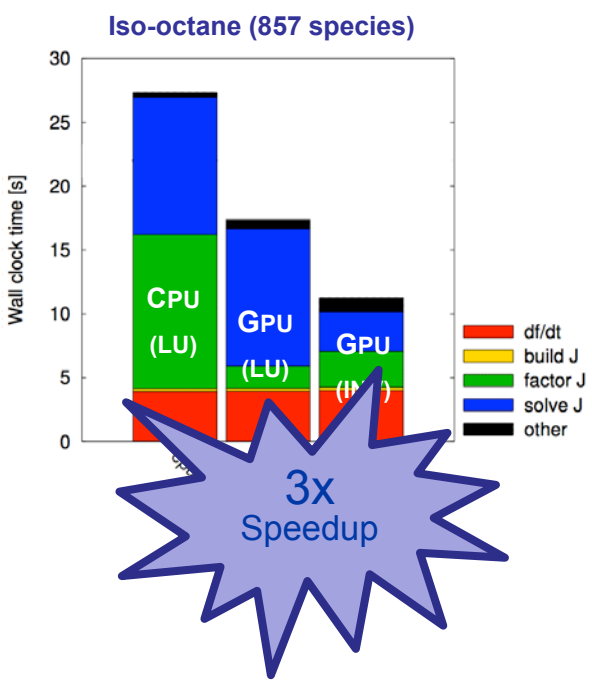
Direct matrix inversion is the most effective solver strategy on the GPU, but performs poorly on the CPU

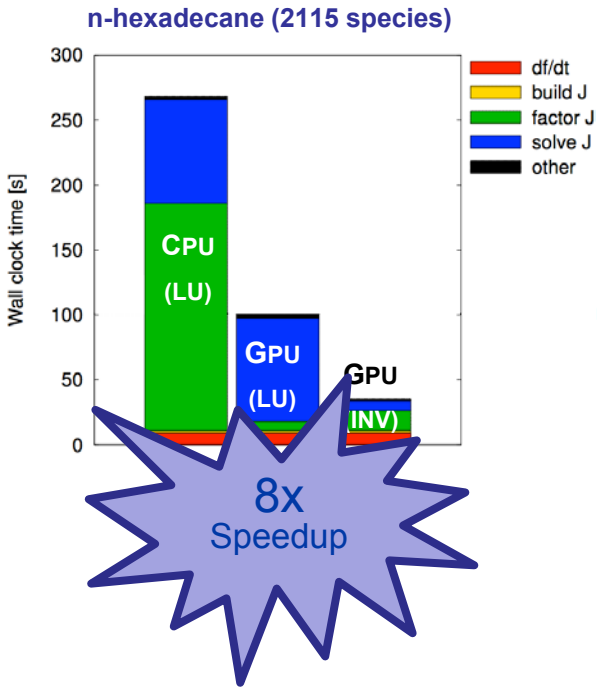


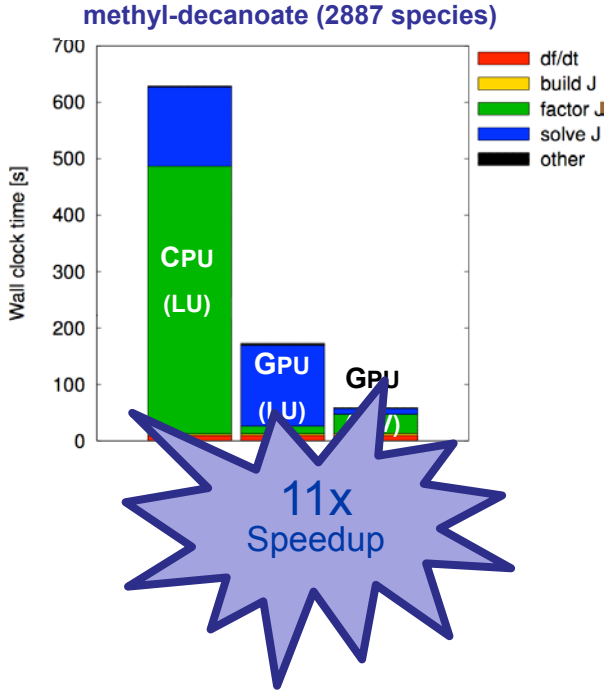
GPUs can do many high repetitive calculations with little computational effort

CPUs get bogged down by these kinds of calculations

We have achieved up to 11x speedup with GPU for ignition delay with large mechanisms

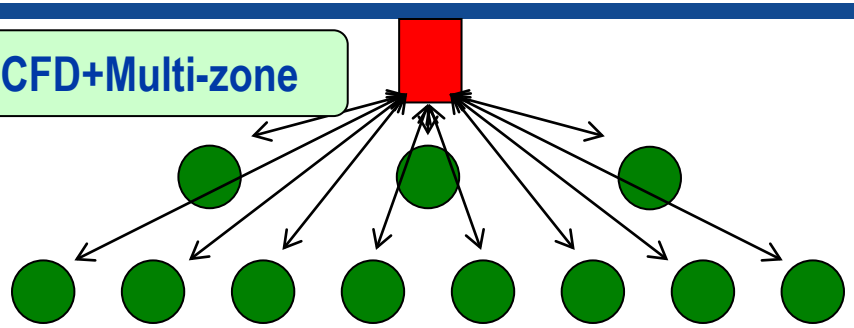




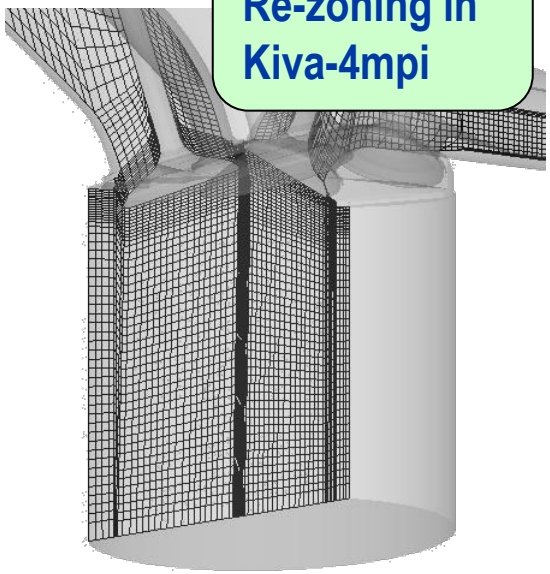


We have done extensive submodel development and testing to enable large-scale parallel CFD for engine simulation

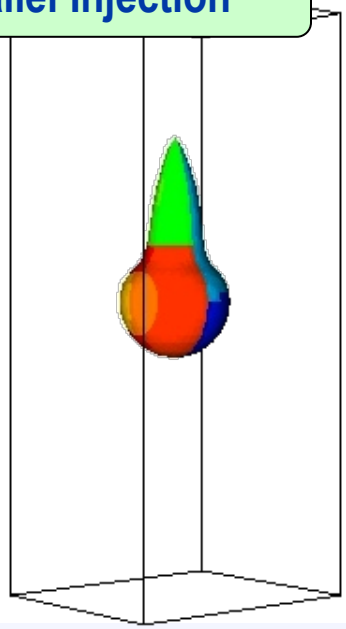
Parallel CFD+Multi-zone



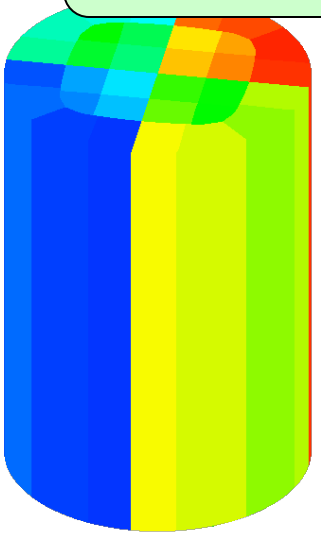
Robust Grid Re-zoning in Kiva-4mpi



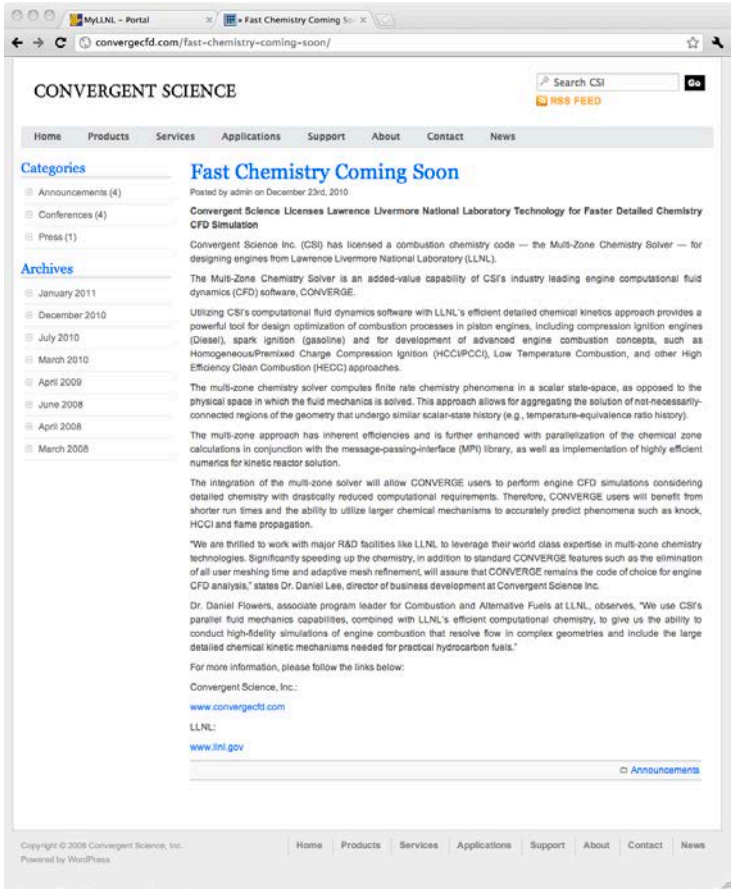
Parallel Injection



Mesh Partitioning Strategies



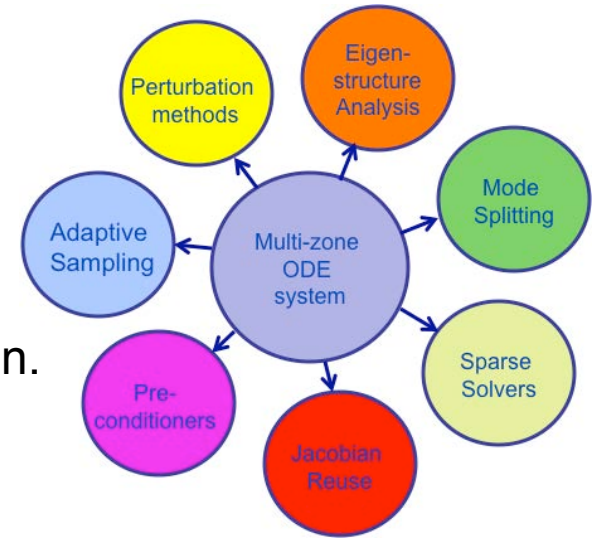
We completed a 5 year licensing agreement for the LLNL Multi-zone Model with Convergent Science Inc. (CSI)



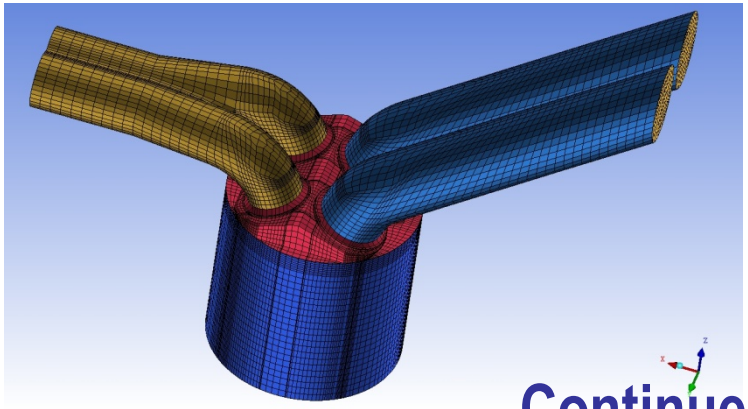
- CONVERGE from CSI is high performance parallel CFD solver widely used in US industry
- LLNL has CONVERGE-MZ licenses for complex 3D problems on our large-scale parallel computers
- LLNL is working with CSI to implement and test the CONVERGE multi-zone model

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

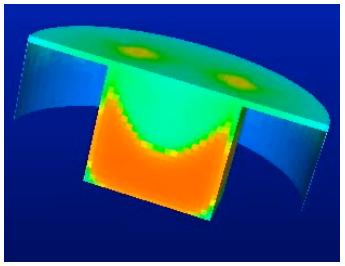
- ***Improved computational chemistry solvers***
  - Sparse solvers (CPU & GPU)
  - More efficient data structures
  - Hybrid solver solutions
  - Solver parallelization compatibility
  - Reaction sort with submatrix direct inversion.
  - New integration error control logic
  - Increase GPU shared memory reuse
  - GPU particle motion/collision algorithms
- ***Improved parallel CFD with chemistry***
  - Multi-criteria multi-zone
  - Spray parcel models
  - Spray initialization



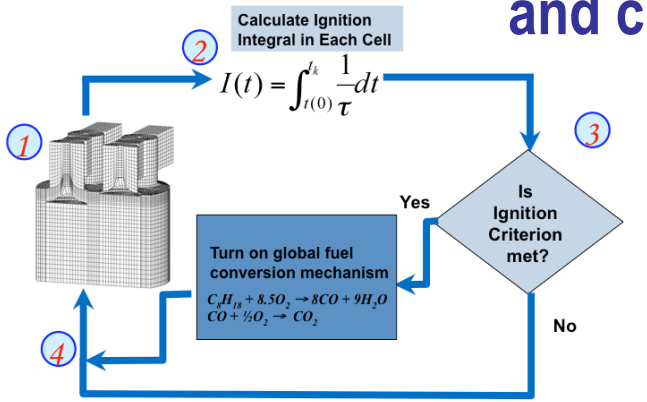
Future work: extend applicability and computational efficiency of analysis tools

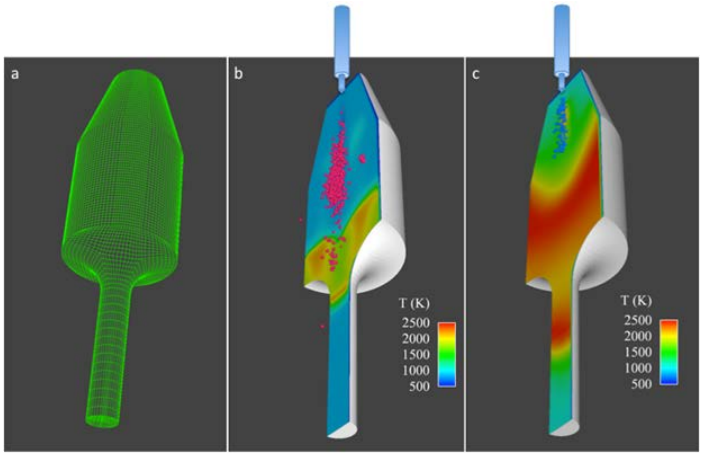


Enable 3-D fluid mechanics and detailed kinetics in today's desktop PCs



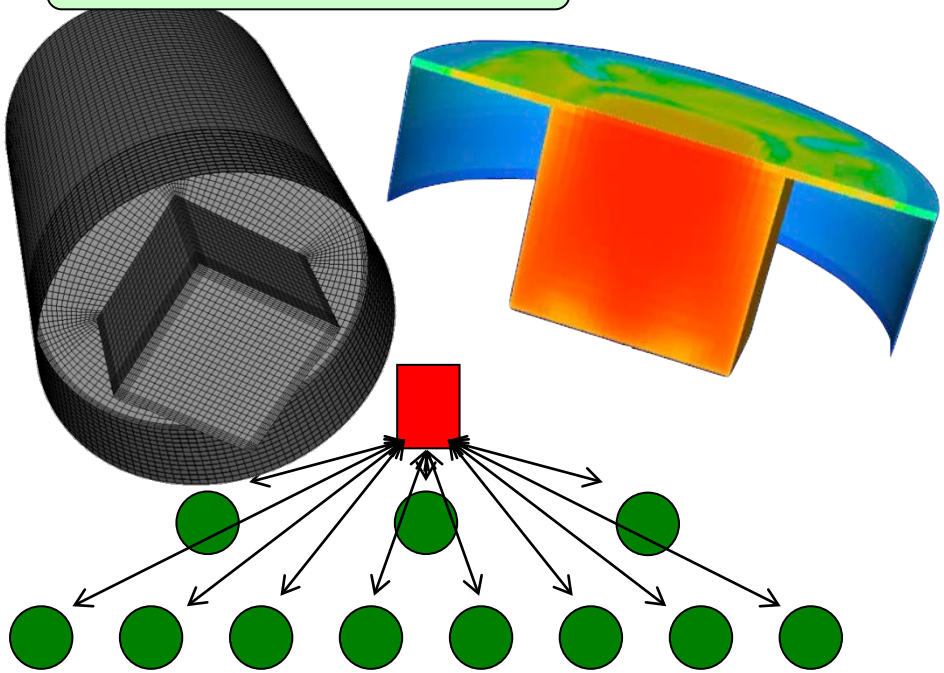
Continue to validate and develop parallel CFD, multi-zone, and ANN for highest fidelity in fluids and chemistry



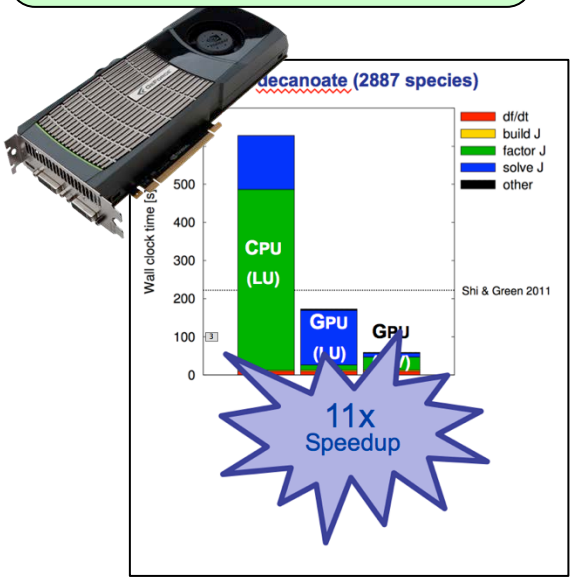


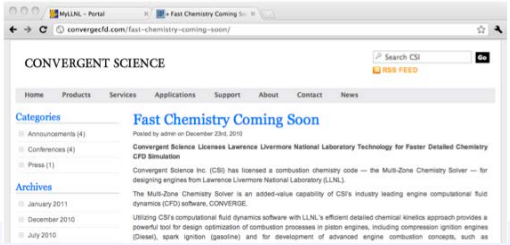
Summary: we are enhancing our analysis capabilities and improving computational performance

Parallel CFD+Multi-zone



Accelerated Combustion Chemistry Simulation





Model Commercialization