Sustainable TRANSPORTATION

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

DOE Perspective - the Need for High Performance Computing in Engine Simulation

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Advanced Combustion Engine R&D
Vehicle Technologies Office

Presented at the ANL Workshop for High-Performance Computing Enabled Engine Simulations
November 12-13, 2014

Outline

- Federal Role
- DOE Vehicle Technologies Office (VTO) goals
- DOE/VTO Advanced Combustion Engine R&D Program
- Need for HPC in engine modeling
- CFD and HPC roadmap from VTO
- Role of national labs in advancing computational research
- How CFD and high-fidelity experiments have advanced engine technology through DOE funded research
- Summary

The Federal Role

- Facilitate development of precompetitive technical knowledge base through investments in fundamental and applied R&D
- Undertake High-Risk Mid- to Long-Term Research
- Utilize Unique National Lab Expertise and Facilities
- Help Create a National Consensus
- Enable public-private partnerships to integrate R&D into industrially useful design tools

Oil Dependency is Dominated by On-Road Vehicles

- Transportation is responsible for 2/3 of U.S. petroleum usage
- On-Road vehicles responsible for ~80% of transportation petroleum usage
- About 1/3 of U.S. GHG emissions from transportation

More than 240 million vehicles on the road

- Economic security, energy security, and environmental stewardship
- Changing energy landscape
  - Natural gas
  - Electrification
  - Fuel Economy Standards

The Cost of Oil is Not Just Monetary

Vehicle Technologies Office - Goals

Reducing oil imports by 1/2 by 2020

Decreasing Petroleum Dependency and Reducing Greenhouse Gas Emissions

Efficiency — *Combustion Efficiency, Vehicle Lightweighting, Electric Drive*

Fuel Substitution — *Biofuels, Natural gas, Electricity*

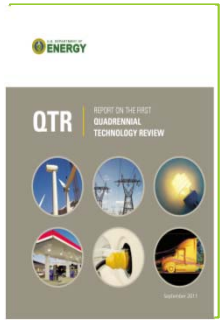
Clean Cities

Deployment — *Clean Cities, Competitions, Education*

Opportunity for Increased ICE Efficiency

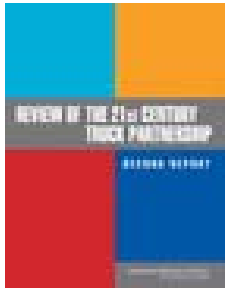
Increasing the efficiency of internal combustion engines (ICEs) is one of the most promising and cost-effective approaches to improving the fuel economy of the U.S. vehicle fleet in the near- to mid-term.

"The performance, low cost, and fuel flexibility of ICEs makes it likely that they will continue to dominate the vehicle fleet for at least the next several decades. ICE improvements can also be applied to both hybrid electric vehicles (HEVs) and vehicles that use alternative hydrocarbon fuels." DOE QTR 2011[1]



DOE 2011

"The DOE-funded research in advanced engine combustion … addresses important aspects for achieving an integration of advanced combustion processes that should be important enablers for achieving the 55 percent BTE goal as well as providing ongoing improvements." - NRC Report 2012[2]

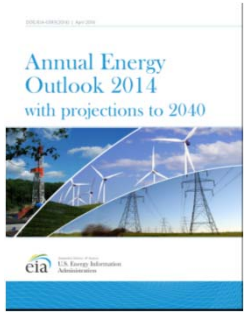


NRC 2012

"…better understanding of the combustion process and emissions production can help to overcome a major barrier to more advanced ICEs, this work is important to the country. …" NRC Report 2013[3]

NRC 2013

EIA *AEO 2014*[3] reference case scenario - even by 2040, ***over 99% of vehicles sold will have ICEs***.



DOE 2014

[1] Quadrennial Technology Review, DOE 2011
[2] *Review of the 21st Century Truck Partnership: 2nd Report,* NRC 2012
[3] *Review of the Research Program of the U.S. DRIVE Partnership: 4th Report,* NRC 2013
[4] *Annual Energy Outlook 2014*, April 2014.

Advanced Combustion Engine R&D

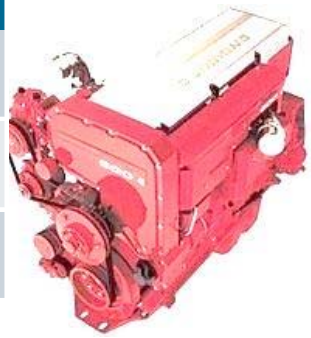
Strategic Goal: Reduce petroleum dependence by removing critical technical barriers to mass commercialization of high-efficiency, emissions-compliant internal combustion engine (ICE) powertrains in passenger and commercial vehicles

Primary Directions

- Improve ICE efficiency through advanced combustion strategies
- Develop aftertreatment technologies
- Explore waste energy recovery with mechanical and advanced thermoelectric devices

Performance Targets*

	Light-Duty		Heavy-Duty	
	2015	2020	2015	2020
Engine brake thermal efficiency	--	--	50%	55%
Fuel economy improvement	25 – 40%	35 – 50%	20%	30%
NOx & PM emissions	Tier 2, Bin 2	Tier 3/LEV III	EPA Standards	EPA Standards



*compared to 2009 model year baseline

Overall ACE R&D Approach

Fundamental R&D

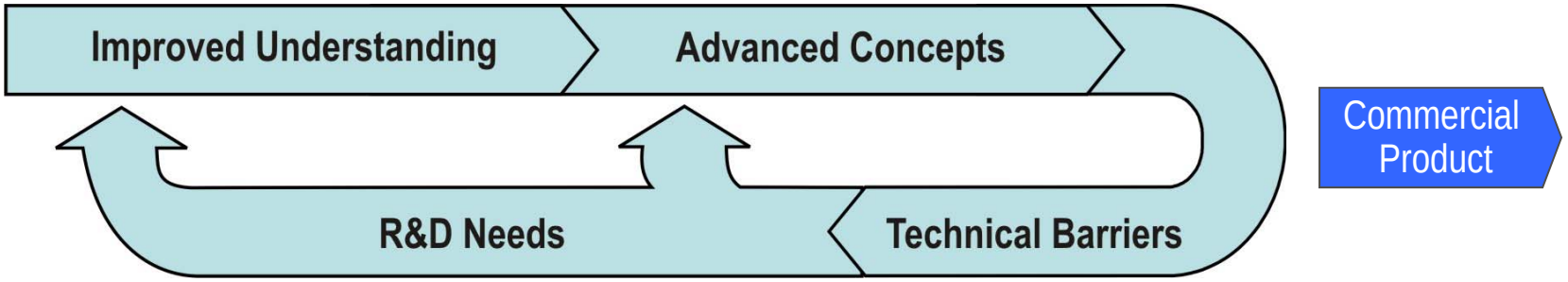
- SNL – Advanced Combustion Strategies (LTC, lean-burn gasoline, advanced Diesel)
- LLNL – Chemical kinetics models (Combustion, fuels and emissions)
- LANL – CFD modeling of combustion
- ANL – X-ray fuel spray characterization, modeling and simulation
- PNNL – Catalyst Characterization (NOx and PM Control)
- Universities – Complementary research

Fundamental to Applied Bridging R&D

- ORNL – Experiments and simulation of engines and emission control systems (bench-scale to fully integrated systems)
- ANL – fuel injector design, engine experiments and simulation

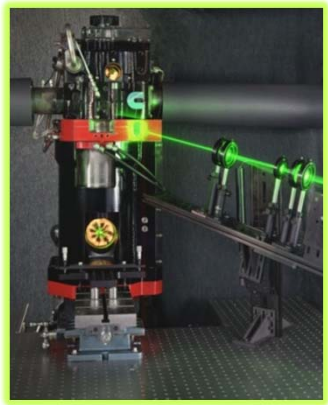
Competitively Awarded Cost-shared Industry R&D

- Automotive and engine companies,– engine systems
- Suppliers – enabling technologies (sensors, ignition, VCR, WHR)

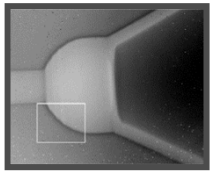


Research Tools Bridge Fundamentals to Application

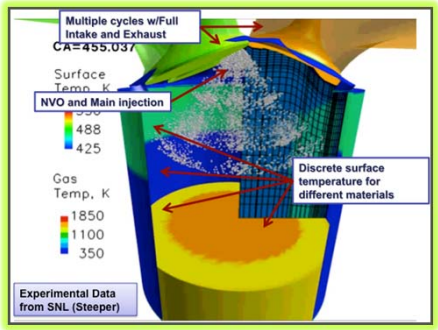
- Close coupled modeling and experiments
  - Advanced diagnostics including optical, laser, x-ray, and neutron based techniques
  - Multi-dimensional computational models and combustion simulators
  - Fuel kinetics
  - Multi- and single-cylinder engines



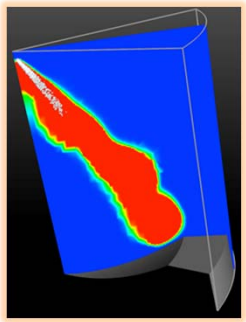
Optical Engine



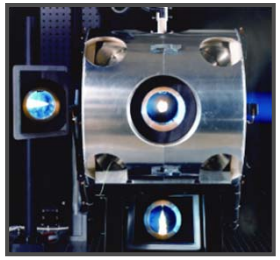
Nozzle Sac X-Ray Image



Engine Simulation



Chemical kinetic solver interfaced to CFD code



LTC Simulator

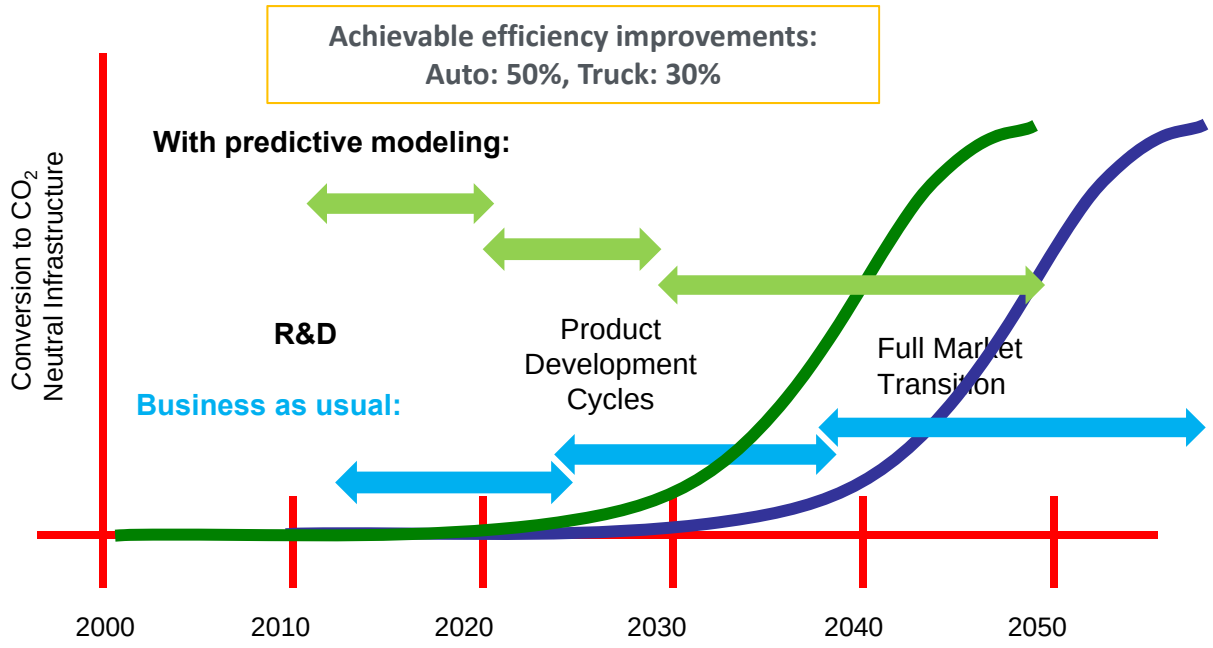
HCCI & Lean-burn Gasoline

- Close collaboration between industry, national labs and universities
- Cross-cuts light- and heavy-duty engine R&D

Leading to engine modeling tools widely used in industry

What is the impact *if* new engine simulation tools are developed?

- Design, testing, and calibration portions of the product development cycle can all be shortened and cheaper
  - Calibration savings alone could reduce the product development cycle time and cost by 25-50% (industry dependent)
- Expand design space to broad range of design concepts
- Reach for the theoretical limits of thermodynamic efficiency
  - Potential for saving 4 M barrel of petroleum per day



Product Development Must Be Accelerated To Meet Energy Goals

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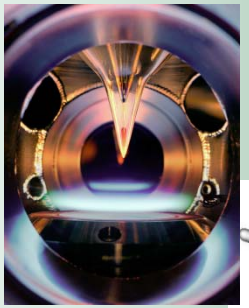
Science-Based Engine Design - An early example

Basic Science

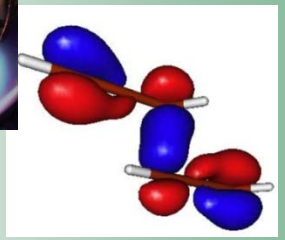
BES

Sustained support in 2 areas

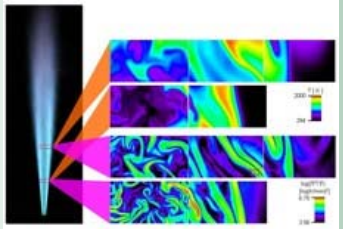
Development of predictive chemistry in model flames



Computational kinetics and experiments



Advance laser diagnostics applied to model flames

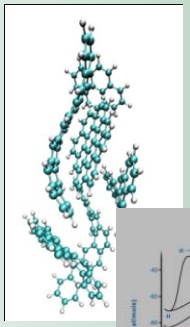


Laser-based chemical imaging

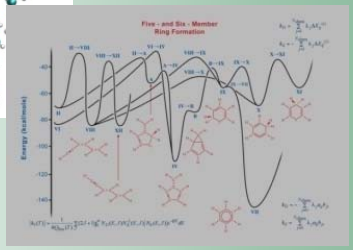
Applied R&D

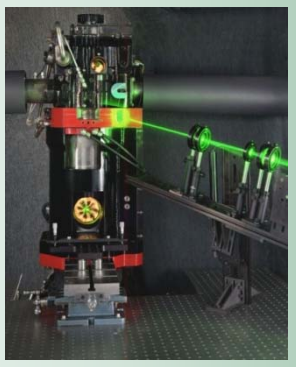
BES → EERE

Applications of chemistry and diagnostics to engines



Predictive chemical models under realistic conditions



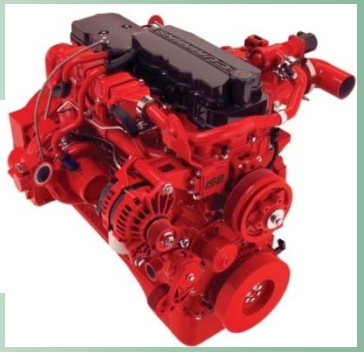


Laser diagnostics of diesel fuel sprays in engine cylinders

Manufacturing/ Commercialization

Cummins and Dodge

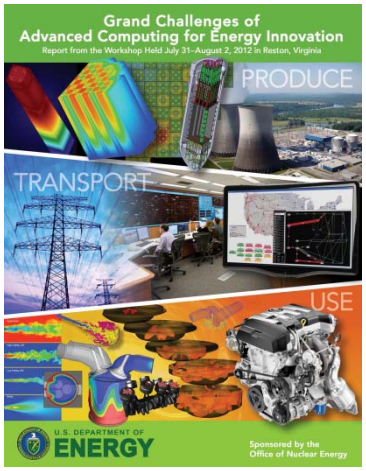
Cummins used simulation tools and improved understanding of diesel fuel sprays to design a new diesel engine with reduced development time and cost and improved fuel efficiency.



ISB 6.7 liter Cummins diesel engine first marketed in the 2007 Dodge Ram pickup truck; more than 350,000 sold

The Need for HPC in Engine Modeling

"**Combustion engines consume energy and generate pollution**. … "High Performance Computing (HPC) has become a predictive, proactive tool that is fully integrated into the product development process... There is …desire for greater simulation accuracy to reduce risks and allow more analysis of the available design space…; need for multi-physics coupled models as well as better post-processing and data management tools…; need for continued software development for HPC architectures …"



Workshop on the Grand Challenges of Advanced Computing for Energy Innovation, July 31 to August 2, 2012

[http://ams.labworks.org/challenges_workshop/materials]

Advanced Computing *(as defined in the report)*

- Modeling and simulation
  - Improved dimensionality, resolution and fidelity
- Data Analytics
  - Extracting knowledge out of large data
- Enabled by **High Performance Computing**
  - Hardware, Middleware, Applications Software
  - Capabilities potentially deployable a full range of systems (laptops and up)

Office of Science (SC)-Advanced Scientific Computing Research (ASCR) - Support for ACTT

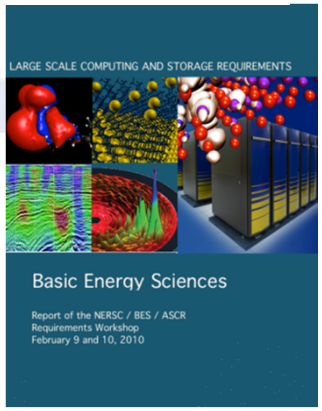
- Leverage facilities expertise
  - Petascale energy applications
  - Facilities design and operations
  - Acquisitions expertise
- Requirements validation
- Connectivity to Energy Sciences Network (Esnet)
- Computer Science & Applied Math
  - Scientific Discovery through Advanced Computing (SciDAC) for Energy
  - CoDesign for Energy
- Resource Allocation

Oak Ridge Leadership Computing Facility

Argonne Leadership Computing Facility

SciDAC
Scientific Discovery through Advanced Computing

ESnet
Energy Sciences Network



National Energy Research Scientific Computing Center

Defining DOE/VTO Role in CFD Modeling

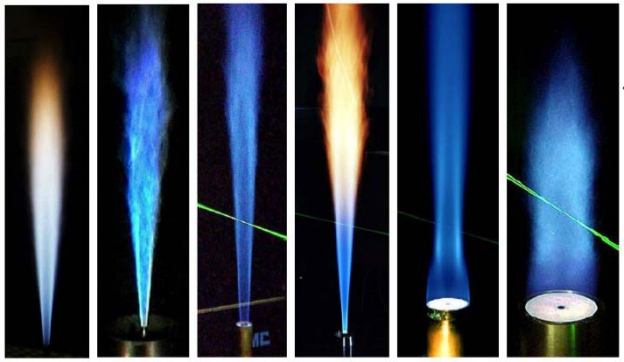
- Long-Term Vision: Engine development cycle can be significantly shortened with improved CFD modeling and simulation capabilities.
- Workshop Objectives: Understand the needs of OEM's so a roadmap can be developed which defines DOE/VTO role and defines roles for participants (i.e., industry, universities, national laboratories).
- General DOE Role: Facilitator and coordinator of the various CFD community members for **pre-competitive** development and implementation activities.
  - Support science-based model development and refinement (DOE/SC/BES ➡ DOE/EERE/VTO);
  - Coordinate and support collaborative efforts amongst community members, e.g., ECN (DOE/EERE/VTO);
  - Improve industry access to CFD and HPC resources (DOE/EERE/VTO);
  - Continue advancement of High Performance Computing (HPC) resources at the national labs (DOE/SC/ASCR);
  - Support HPC software development, including formal Uncertainty Quantification (UQ) (DOE/SC/ASCR).
- Follow on actions: Final Workshop report; Technology Roadmap, potential solicitations.

Workshop on Defining DOE/VTO Role in Supporting Development of Advanced Engineering CFD Codes, August 18, 2014 .

DOE role … provide science-base that addresses technical barriers

Basic ← Unified Code Framework (RAPTOR) → Applied

DOE Basic Energy Sciences Program



TNF Workshop
www.ca.sandia.gov/TNF

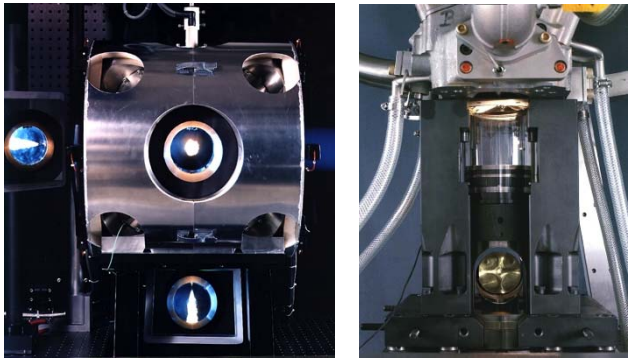
Detailed jet flame data for model development but low Reynolds number and simple fuels

Re ≈ *O(10,000)*

Device relevant measurements but limited due to complex geometry, flow, and fuels

Re > *O(100,000)*

DOE Vehicle Technologies Program



Engine Combustion Network
www.ca.sandia.gov/ECN

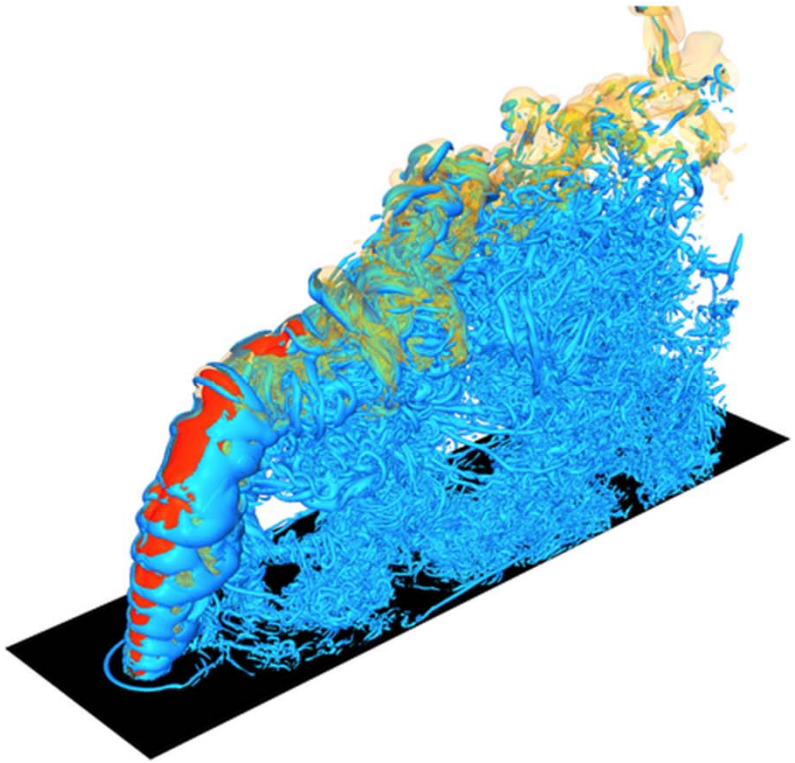
Goal … use "high-fidelity" LES and "first-principles" models to develop the science base needed to formulate affordable engineering CFD models

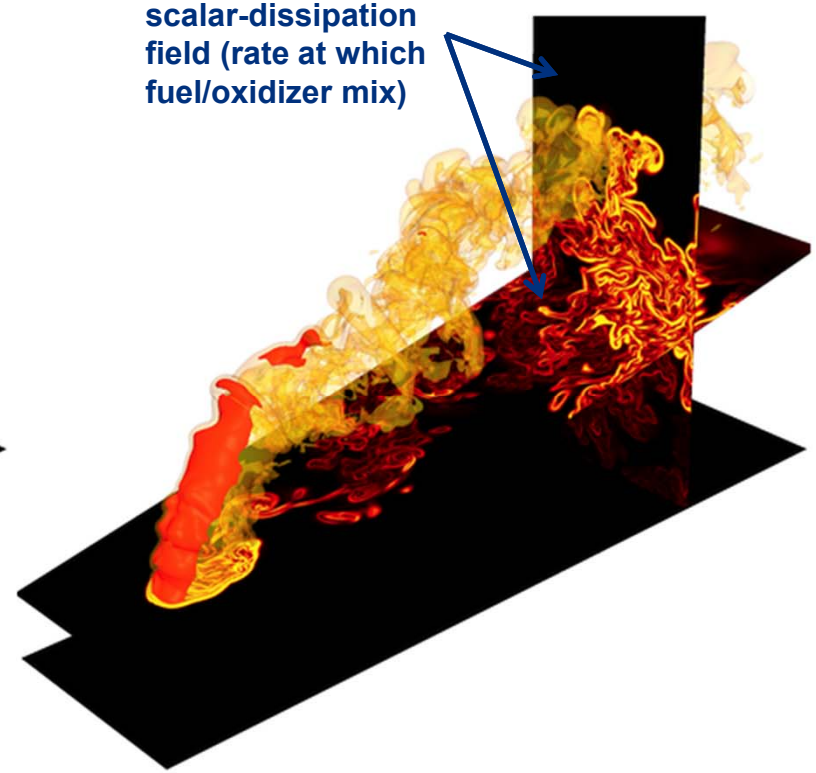
- Complement key experiments, provide quantitative information not otherwise available
- Match detailed engine geometry and operating conditions (i.e., high Re)
- Retain full governing physics
- Validate using available experimental data, then extract:
  - fundamental data and insights not available from experiments alone
  - data needed to formulate affordable models
- Use high-performance computing as enabler (both local and DOE platforms)

“High-fidelity” LES & “first-principles” models have specific definitions

Liquid n-Decane-air jet-in-cross-flow:

- **Re = 100,000 (jet), 620,000 (cross-flow)**
- **P = 40 *bar* (supercritical)**





- **Mixture fraction isosurface (high)**
- **Mixture fraction isosurface (low)**
- **Vorticity (reveals structure)**

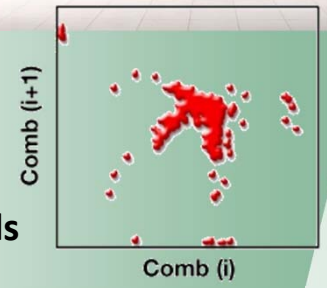
- **“High-fidelity” LES resolves scalar dissipation (cut-planes) with structurally/physically correct dynamics**
- **“First-principles” models involve no tuned constants and lim Δ→0 = DNS**

High Performance Computing Could Accelerate Engine Design and Optimization

Basic Science

DOE Office of Science

Fundamental expertise in combustion instability mechanisms and leadership in high performance computing including the world's fastest supercomputer



TITAN Use Awards

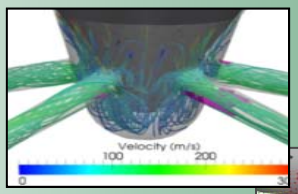
- ALCC 32.5M hrs
- OLCF 17M hrs

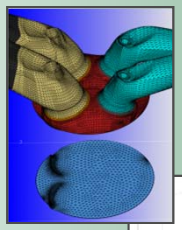
Applied R&D

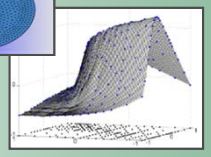
DOE/EERE/VTO

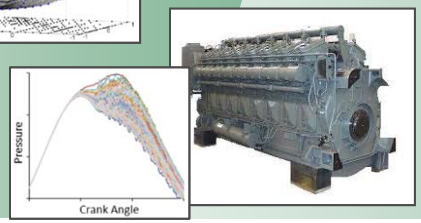
Accelerating high pressure fuel injector design optimization and providing new insights into combustion instability phenomena

Injector image *(source GM)*









OAK RIDGE National Laboratory

Manufacturing/ Commercialization

GM/Ford/GE

Research in close collaboration with automobile and engine manufacturers will directly impact the development of the next generation of high efficiency engines

GM RESEARCH & DEVELOPMENT

Ford

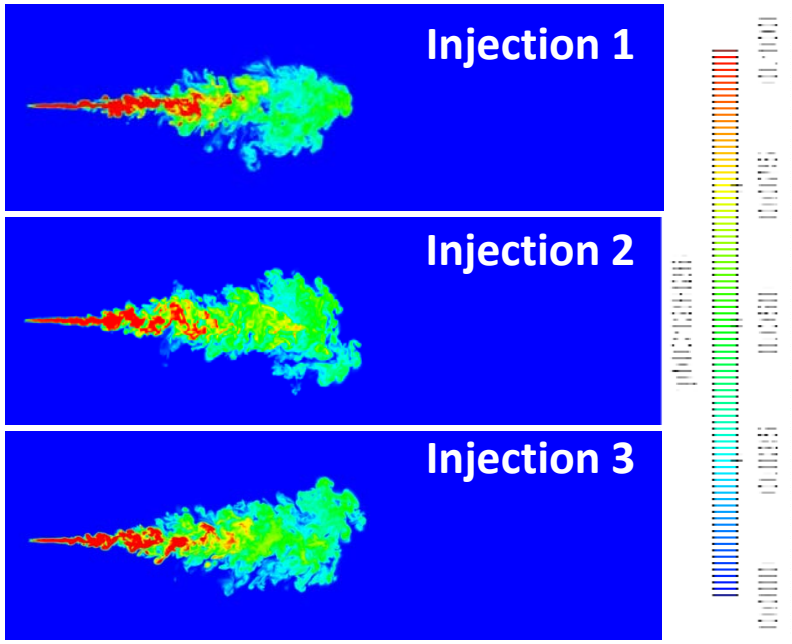
GE Global Research

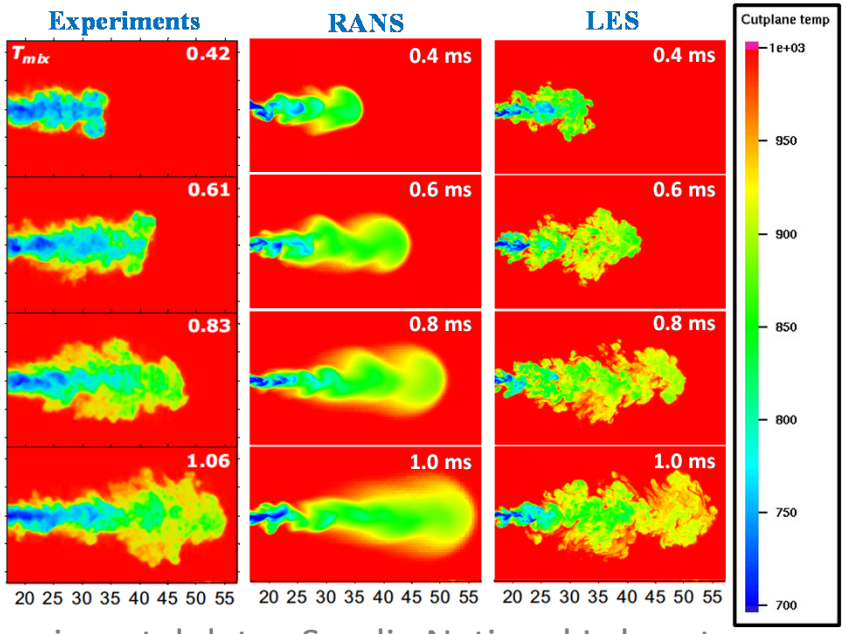
Making use of unique world class resources to address real-world challenges

Cyclic Variability with Large Eddy Simulations

Project Impact

- High-fidelity Large Eddy Simulations (LES) can capture flow structures which lower fidelity (RANS) approaches cannot predict
- LES can predict cycle-to-cycle variations during each injection event. Further research to predict engine misfire!





Experimental data : Sandia National Laboratory

Computational Details

- High-temporal and spatial resolutions results in less sub-grid scale modeling with the LES
- Each cycle: 1 month on 256 cores; need at least 8-10 cycles
- Simulations performed at Fusion cluster at Argonne together with **Cummins Engine Company** and **Convergent Science Inc.**

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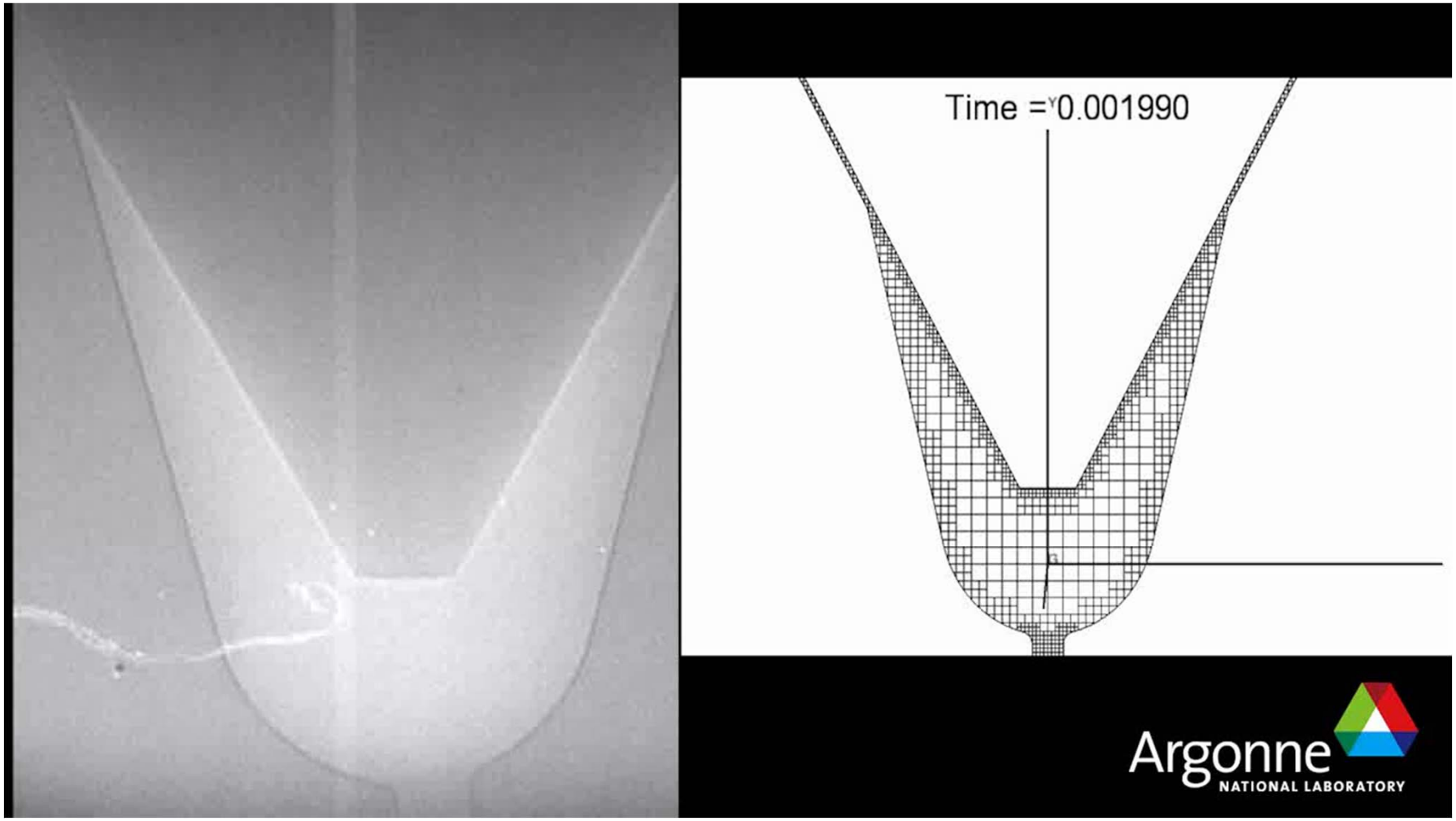
X-ray Imaging of Injector Needle Wobble



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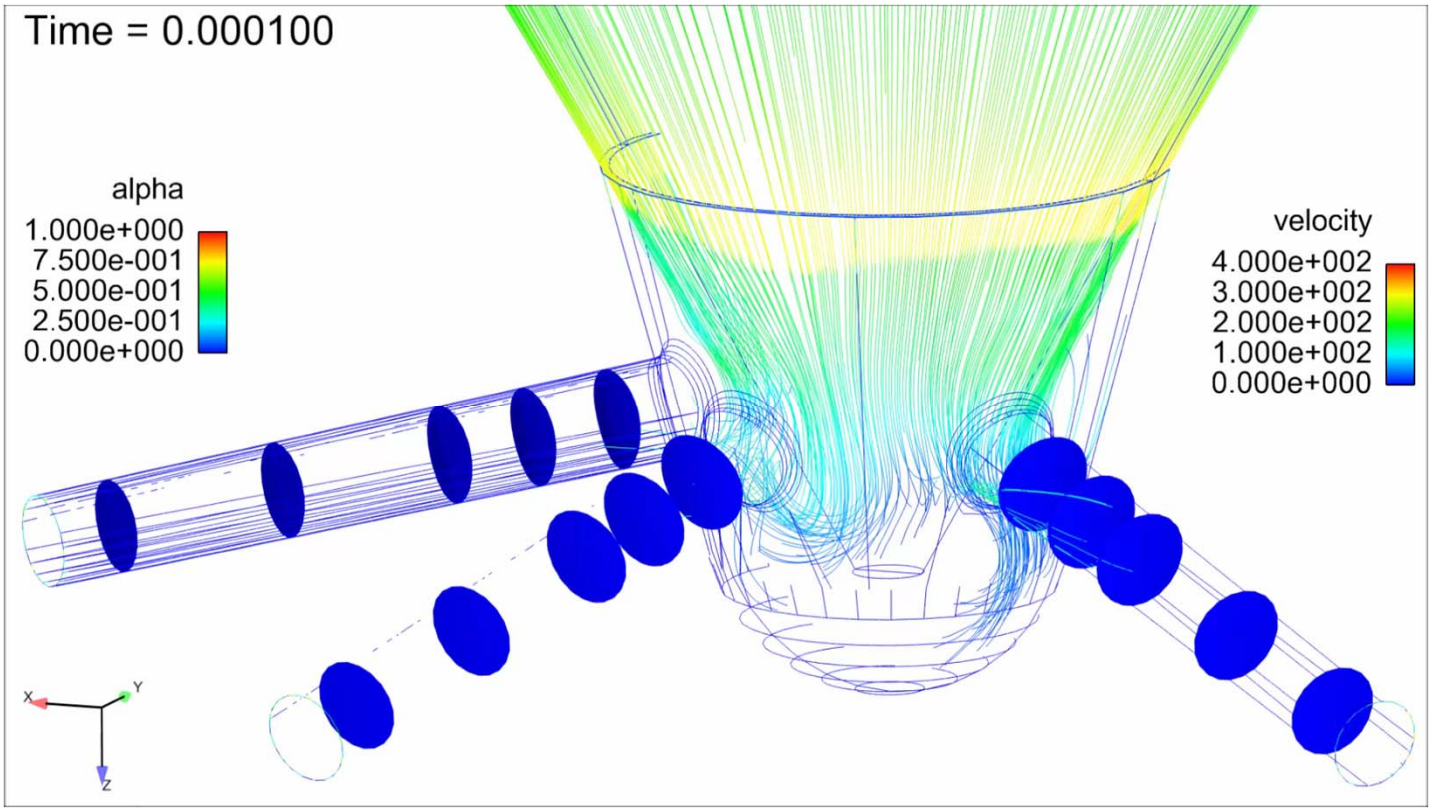
Multi-hole Nozzle Two-phase Flow Simulations

Project Impact

- **Plume-to-plume variations** in Multi-hole nozzles can now be captured
- Influence of **needle transients on fuel spray development** can now be predicted!

Computational Details

- High-temporal and spatial resolutions resulting in **grid-convergent solutions**
- Each Simulation: 1 month on 64 cores; Need 20+ simulations



Production GM multi-hole diesel injector simulation at Argonne

Argonne NATIONAL LABORATORY
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Engine Combustion Network (ECN) – DOE/VTO-funded web-based collaboration to better CFD tools

Experiment

Sandia
Argonne
IFPEN
CMT
CAT
GM
Delphi
Bosch
TU/e
Ist. Motori
Mich. Tech.
Meiji
Infineum
Chalmers
KAIST
Aachen
Melbourne

CFD codes used

CONVERGE
Star CD
Open FOAM
KIVA
ANSYS Fluent & CFX
FORTE
RAPTOR
other research codes…

CFD approaches

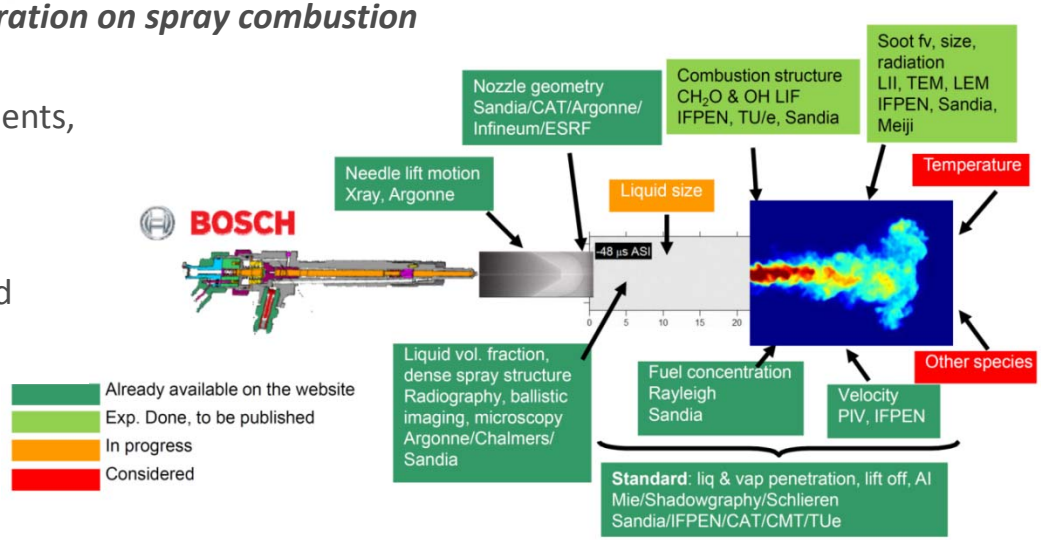
RANS
LES
High-fidelity LES
Eulerian-Eulerian
Eulerian-Lagrangian
Dense fluid
many spray and combustion variants…

Modeling submissions

Sandia
Argonne
IFPEN
CMT
PoliMi
UMass
UNSW
Penn St.
TU/e
UW-Madison
Purdue
ETH-Zurich
Aalto
Aachen
DTU
Cambridge
Georgia Tech
Chalmers
GM

ECN collaboration on spray combustion

- Spray A diesel experiment:
  - over 40 different measurements, more than 10 institutions
  - ~15 years of research performed in ~3 years
- Focused effort using advanced modeling at these conditions (over 16 teams)
  - High-fidelity models used to improve engineering modeling tools



ECN organization

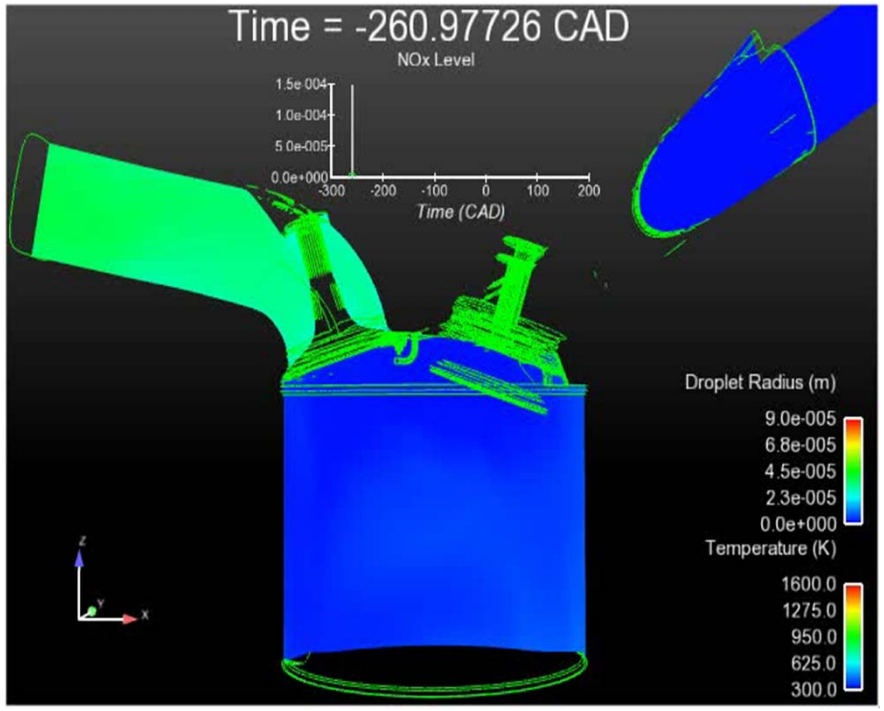
- Monthly web meetings
- Workshop organizers gather experimental and modeling data, perform analysis, understand differences, provide expert review
- Very tight coordination because of target conditions

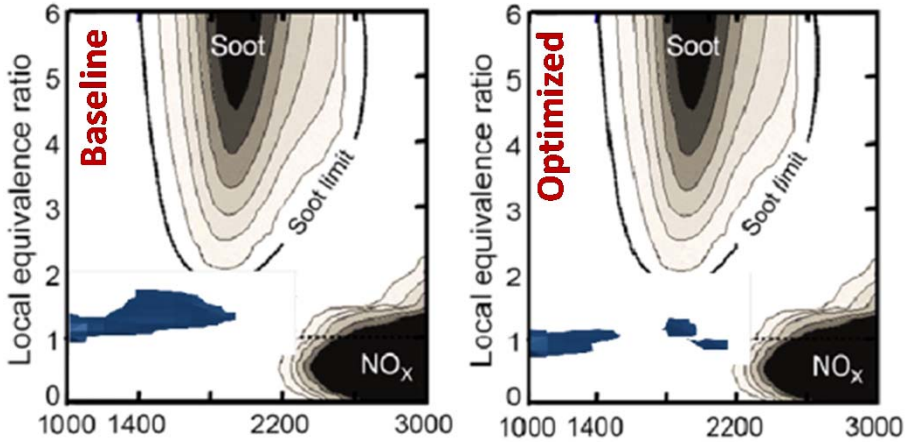
Most of industry use ECN data to test their CFD practices

Fuel Economy Optimization with High-Fidelity Simulations

Project Impact

- Specific fuel consumption was **optimized using genetic algorithm** based tools and **CONVERGE** CFD code for **Chrysler LLC**.
- Predicted optimized speed-load conditions corroborated very well with experimental measurements on a Chrysler Dual-fuel combustion engine at Argonne
- The **optimized conditions also showed considerably lower emissions** compared to the baseline





Computational Needs

- 400 engine simulations performed to achieve optimized fuel economy and emissions
- Each simulation generation takes about a week on 24 cores

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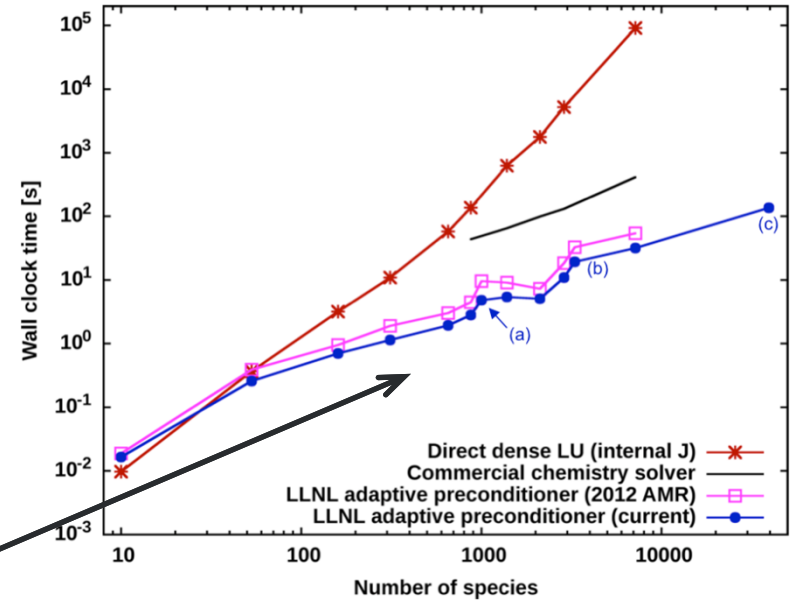
The Advanced Combustion Numerics project enables accurate chemistry models to be used in engine CFD simulations (LLNL)

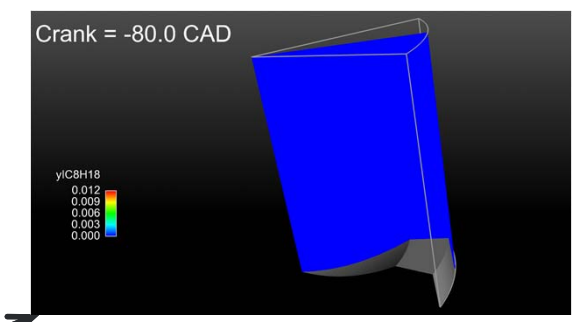
Motivation:

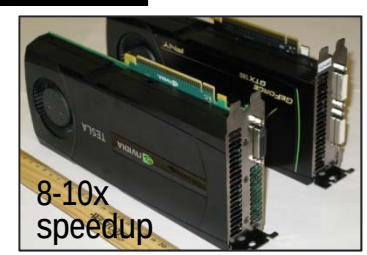
- Accurate fuel chemistry is needed in CFD models to capture the ignition, performance and emission properties of kinetically controlled advanced combustion modes (e.g., HCCI, PCCI and RCCI)
- The most accurate chemical kinetic mechanisms for transportation fuels contain 1,000s of species - previously thought impractical for engine CFD

Accomplishments:

- New chemistry solver using adaptive preconditioner technique speeds up detailed kinetic calculations orders of magnitude over traditional methods
- The new solver has interfaces to common CFD codes
- The new solver has been licensed to Convergent Science Inc. whose ConvergeCFD code is used by many of the automotive and diesel engine MOU partners
- The new solver has been ported to the general purpose graphical processing unit (GPU)







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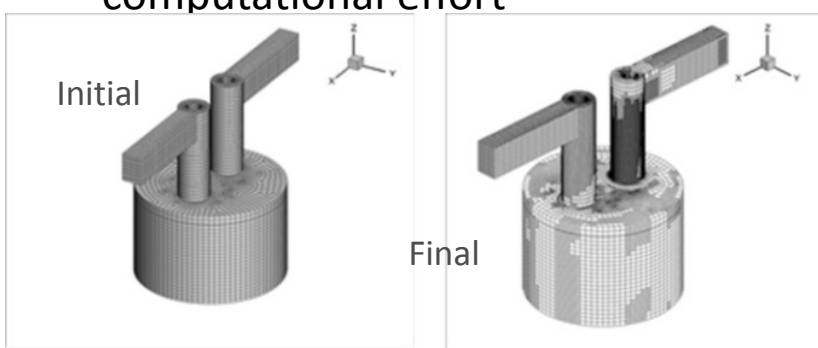
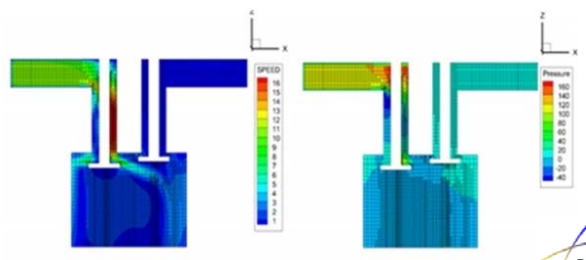
LANL's KIVA-hpFE: Toward Predictive Engine Modeling

New *hp*-adaptive **Finite Element Method (FEM) for turbulent reactive flow modeling** increases **KIVA's accuracy, robustness**, and range of applicability

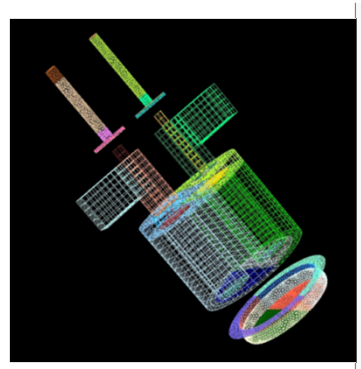
- grid enrichment (h), polynomial order enrichment (p); ***FEM*** *error measure drives* resolution (numerical error is very near zero
- excellent spatial accuracy with minimal computational effort

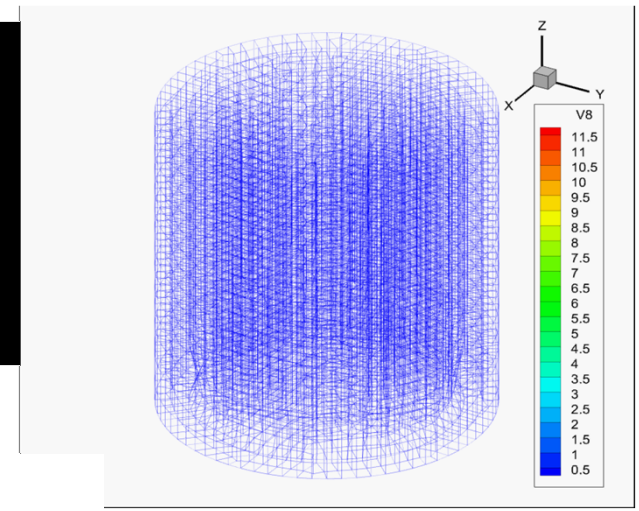


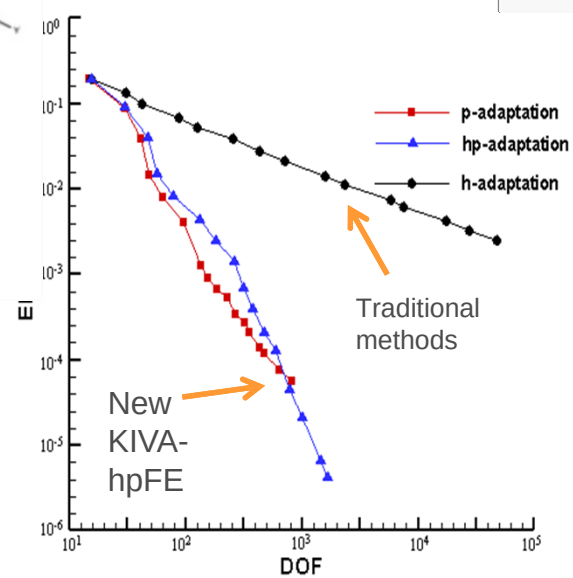
Initial and final grids at given crank angle



- **Superior actuated parts movement**
  - **New local-ALE is robust (no tangle) & accurate**
  - 2nd order spatial convergence having ~zero error







- **KIVA-hpFE** is accurate for all flow regimes with k-ω RANS, LES turbulence and thermal analysis

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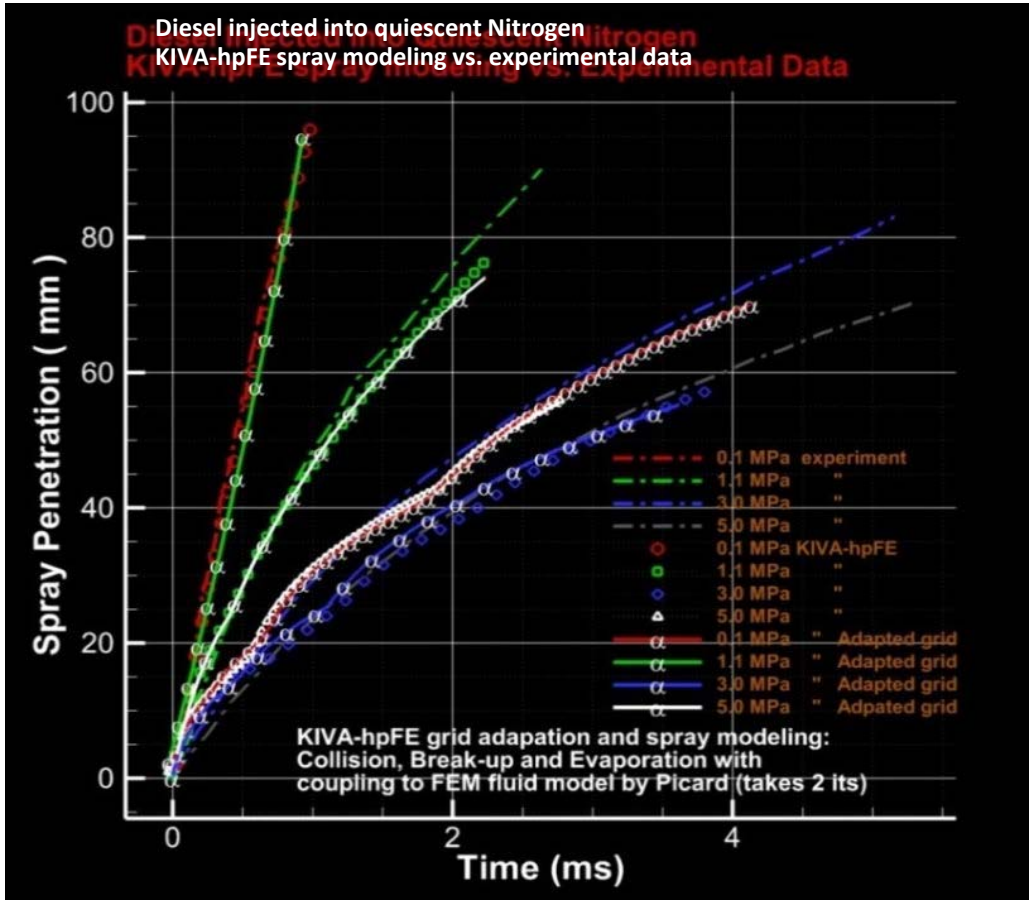
Other KIVA Enhancements

- **Spray Modeling**
  - Is now: Spatially convergent and temporally accurate
  - Uses precise values of momentum
  - Precise coupling - fluid and droplet



- **Fast CAD to CFD grid generation**
  - Overlaying parts for easy/ automatic grid generation
- **Plasma Kernel Spark Model**
  - Spark wattage f(t) (from ignition specification)
  - Kernel heat loss as f(t) - function of time
  - Now nearly exact calculation of LHV from Chemistry
- **Improved parallel performance vs. conventional methods**
  - Theoretical up to 40 to 60x speedup

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Summary

- EERE VTO Advanced Combustion Engine R&D, in collaboration with industry, academia and the national labs, contributes to increases in engine efficiency and vehicle fuel economy.
- DOE maintains large user facilities and employs a core of engineers, computer scientists and applied mathematicians who can help industry take full advantage of supercomputing capabilities.
- CFD and high-fidelity experiments have improved engine efficiency and reduced development time - new roadmap aims to further support industry needs.
- There are opportunities to utilize DOE's Advanced Computing capabilities for predictive simulation of ICEs.

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