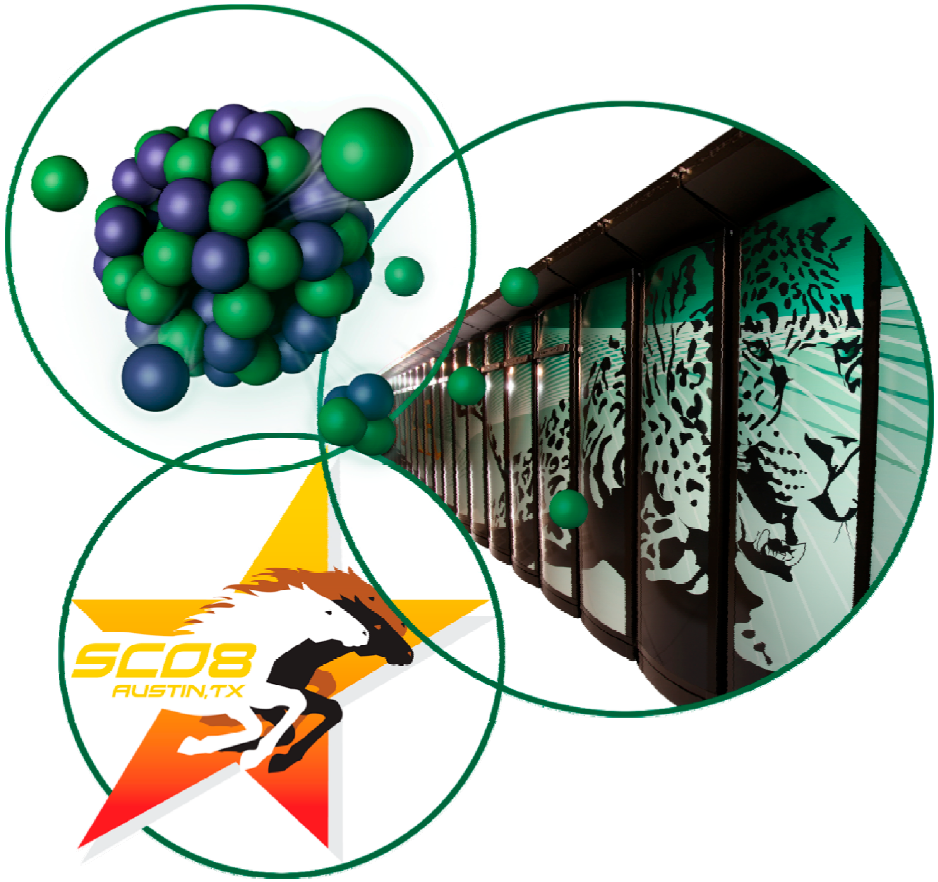
High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels

Application of the Large Eddy Simulation (LES) Technique



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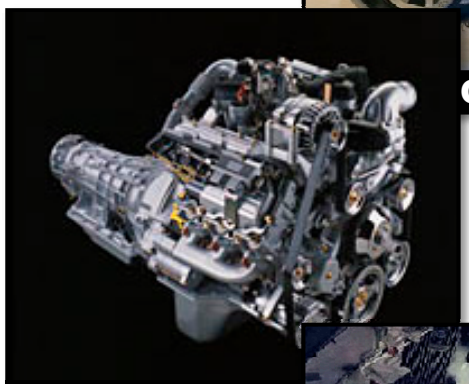
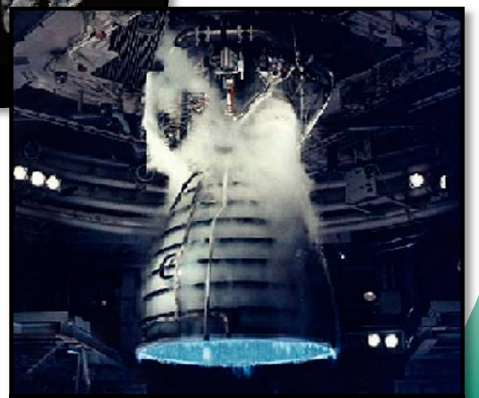
Large Eddy Simulation (LES)

- Turbulent combustion involves interactions over wide ranges of length and timescales
- LES provides mathematical formalism to treat full range of multidimensional scales in a turbulent reacting flow
  - Large energetic-scales are resolved directly
  - Small “subgrid-scales” are modeled
- Used when direct numerical simulations are not feasible
  - Inhomogeneous turbulence characteristics induced by complex geometries
  - High-Reynolds number turbulence-chemistry interactions at high-pressures
  - Device-scale geometries, operating conditions, and run times
- Our focus is on propulsion and power devices (e.g. gas turbines, IC-engines, liquid-rockets)

Gas Turbines



IC-engines



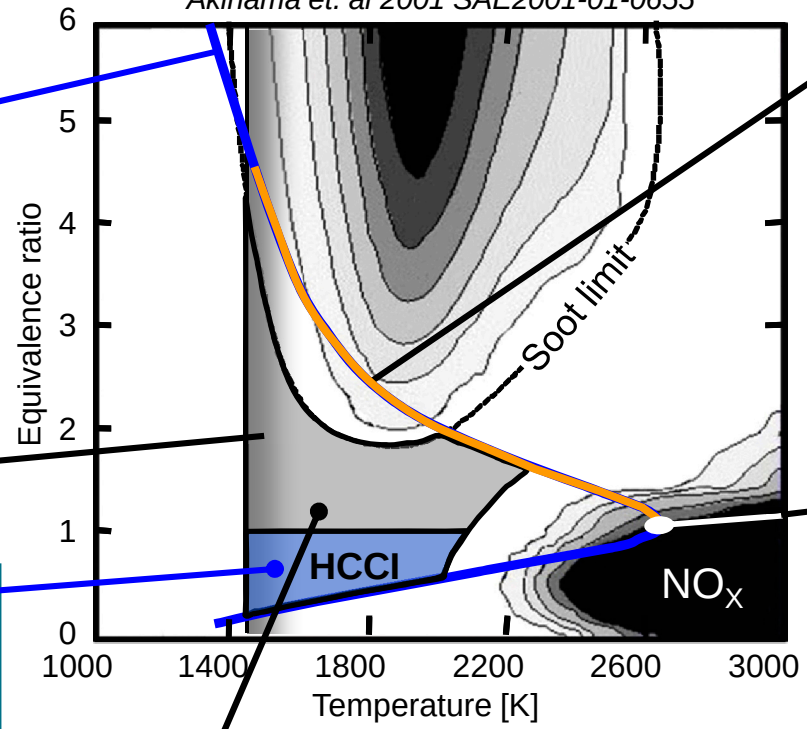
Liquid-rockets

Motivation: Changing World of Fuels and Engines

- **Fuel streams are rapidly evolving**
  - **Heavy hydrocarbons**
    - **Oil sands**
    - **Oil shale**
    - **Coal**
  - **New renewable fuel sources**
    - **Ethanol**
    - **Biodiesel**
    - **Hydrogen**
- **New engine technologies require analysis at actual operating conditions, in actual geometries**
  - **Various direct injection (DI) concepts**
  - **Low-temperature combustion**
- **Mixed modes of turbulent combustion, complex mixture preparation strategies**
- **Advanced scientific understanding is necessary to develop next-generation predictive models**

Example: If optimized, homogeneous charged compression ignition (HCCI) engines can deliver both high efficiency and low emissions

Akihama et. al 2001 SAE2001-01-0655

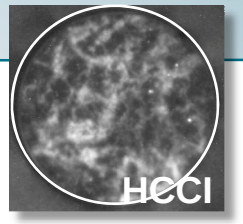


Adiabatic flame temperature in air

CO to CO_2 conversion diminishes

HCCI

- A form of LTC that is mostly premixed
- Lean or dilute with EGR

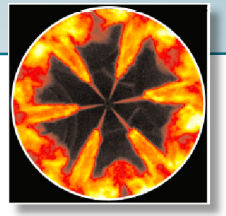


Low Temperature Combustion (LTC)

- Diesel-like efficiency
- Low NOx, soot, hydrocarbon emissions
- Challenges: Operation limited to low loads. Controlling combustion difficult
- Detailed analysis of in-cylinder processes is required

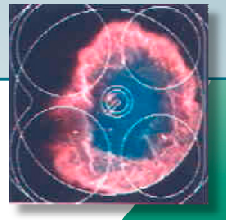
Diesel Combustion

- Controlled timing and HRR
- High efficiency (relative to SI)
- High NOx and soot



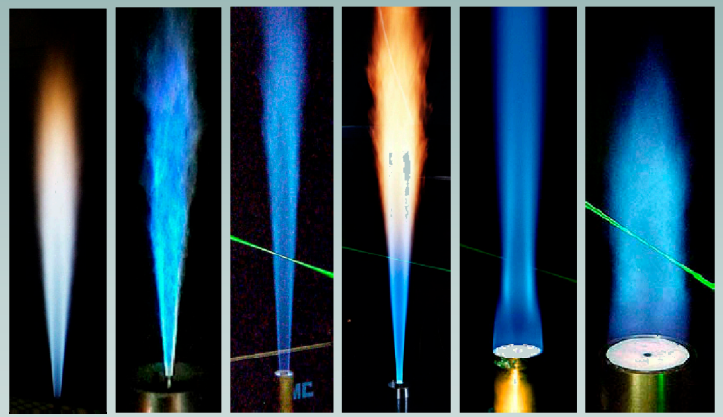
Spark-Ignition Combustion

- Controlled timing and HRR
- Low NOx, hydrocarbon emissions
- Low efficiency (relative to diesel)



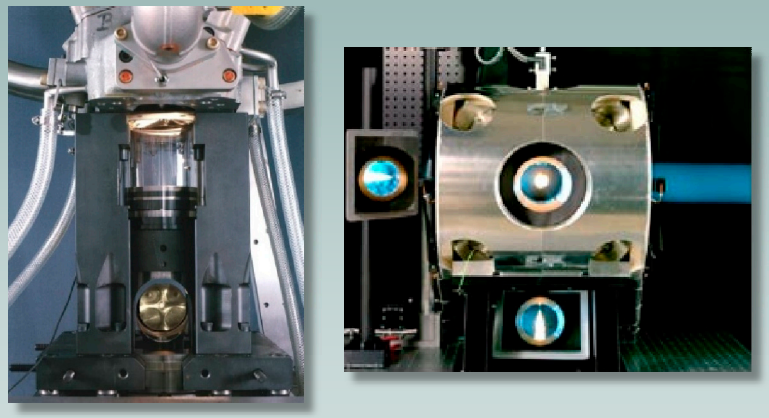
Two core projects under Reacting Flow Research and Advanced Engine Combustion programs

LES of Turbulence-Chemistry Interactions in Reacting Flows
DOE Office of Basic Energy Sciences

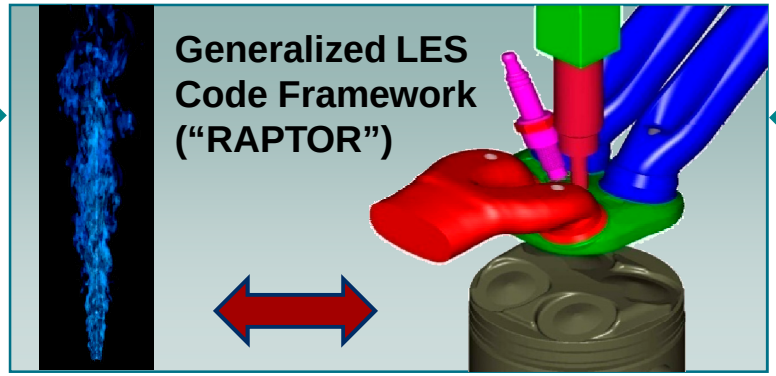


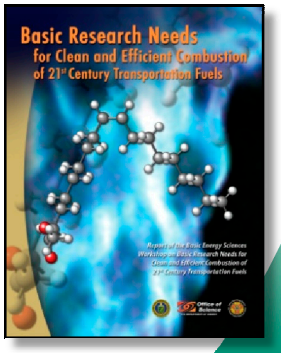
TNF Workshop
www.ca.sandia.gov/TNF

LES of High-Pressure, Low-Temperature Engine Combustion Processes
DOE Office of Vehicle Technologies



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



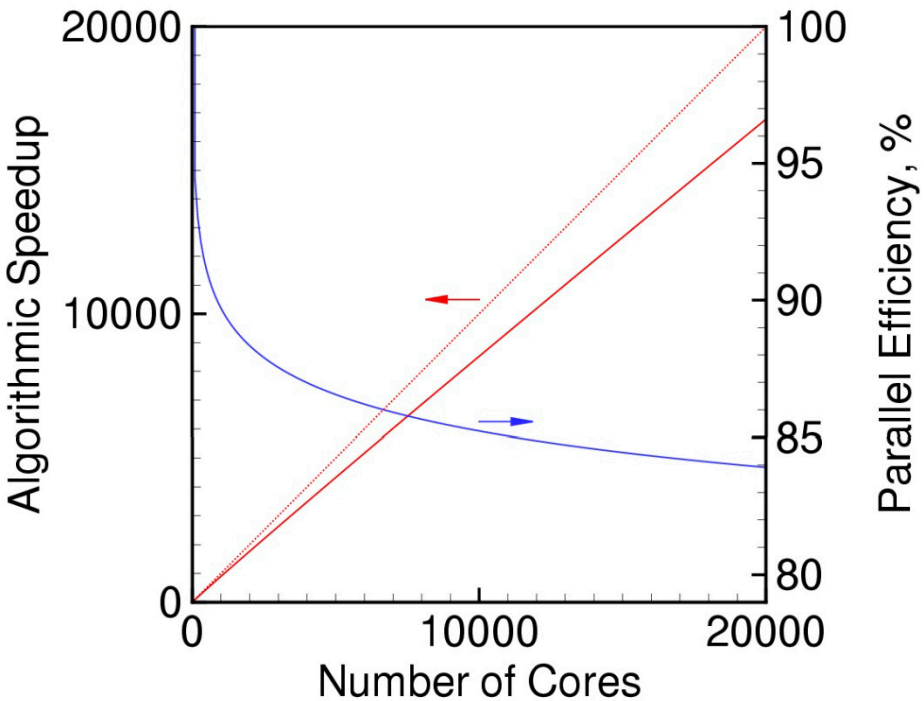


Basic Research — **Applied Research**

Bridges Gap Between Science and Applications

Theoretical-Numerical Framework "RAPTOR" (a general solver optimized for LES)

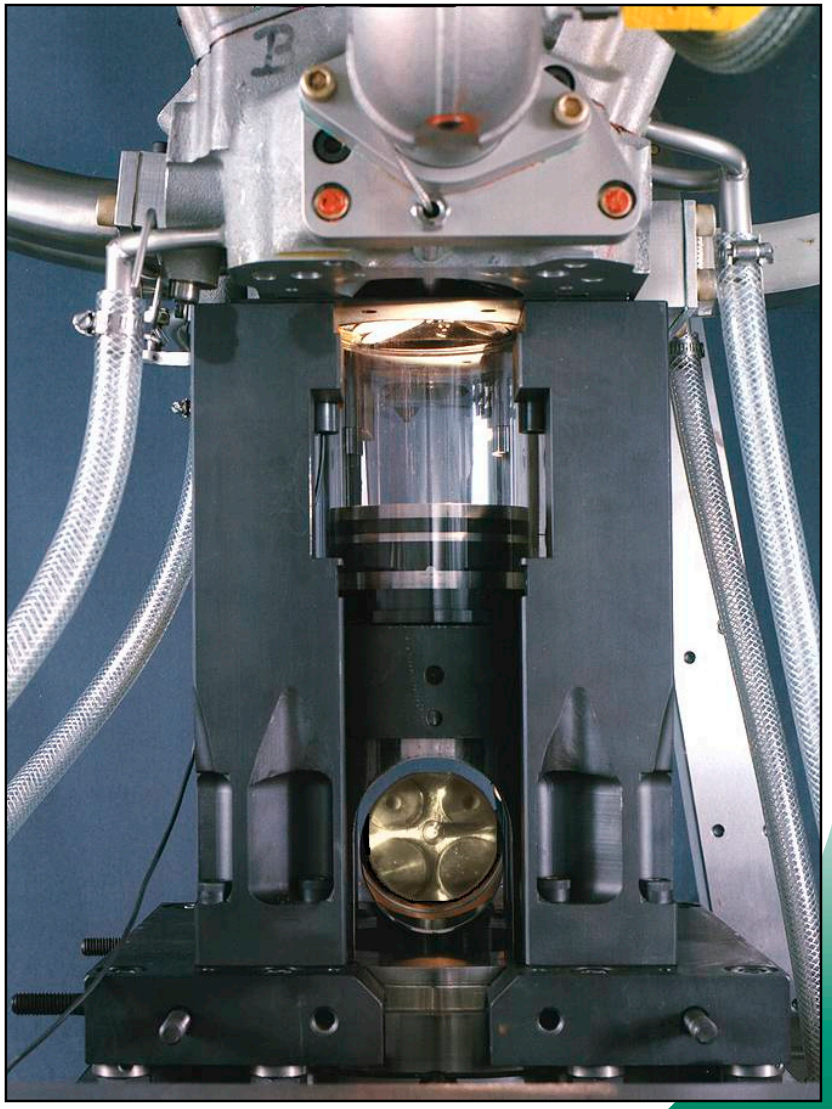
- **Theoretical framework**
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray
  - Dynamic SGS modeling (no tuned constants)
- **Numerical framework**
  - Dual-time, all-Mach-number
  - Generalized preconditioning
  - Non-dissipative, conservative
  - Complex geometry
  - Adaptive mesh (ALE)
  - Massively-parallel (MPI)
- **Validated for variety of flows**
- **Ported to all major platforms**



Strong scaling attributes of the RAPTOR software exhibited on the ORNL NCCS CRAY XT4 (Jaguar)

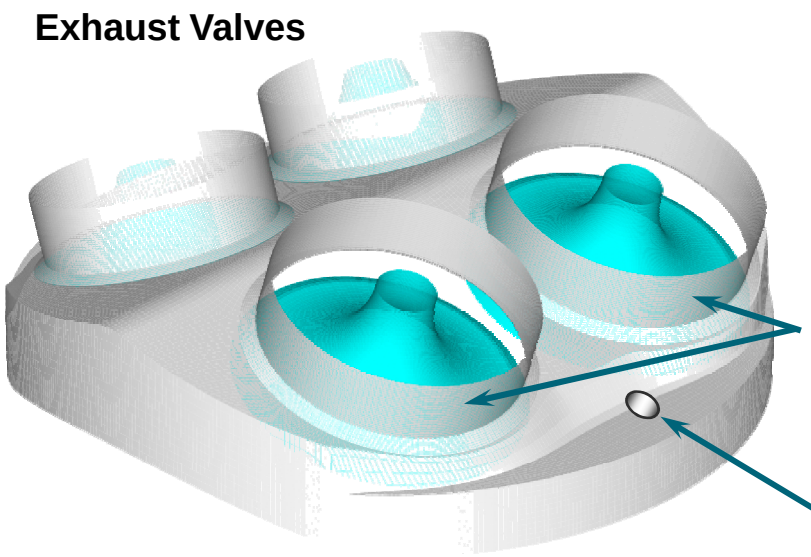
Current Focus: Apply RAPTOR to Sandia Optically Accessible Hydrogen-Fueled IC-Engine (INCITE 08)

Typical in-cylinder turbulence scales at start of combustion	
Compression Ratio	9.1
Bore	92 *mm*
Stroke	85 *mm*
Cylinder Volume at BDC	634.81 cm^3
Cylinder Volume at TDC	69.759 cm^3
Peak Turbulence Intensity	2.85 *m/s*
Integral Length Scale	2 *mm*
Thermal Layer Thickness	6.3 *μm*
Reaction Zone Thickness	3.9 *μm*
Kolmogorov Length Scale	5.6 *μm*

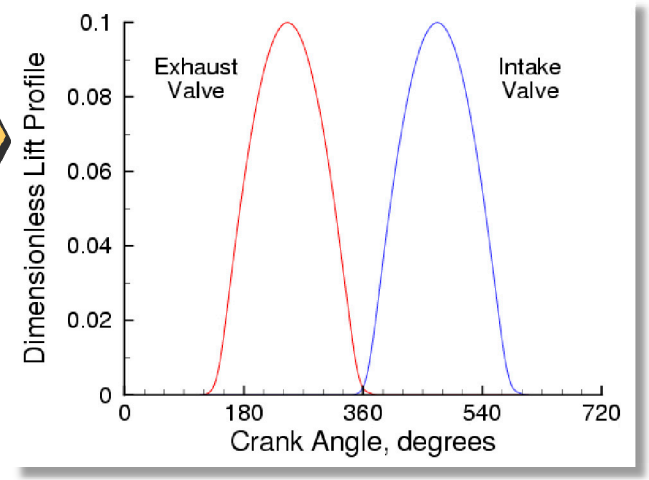


- **Identically match geometry, boundary, and operating conditions**
- **Identify key phenomena, provide detailed information not available from experiments alone**
- **Establish scientific foundation for advanced model development**

Goal: Detailed treatment of geometry, operating conditions (including high-pressure injector)

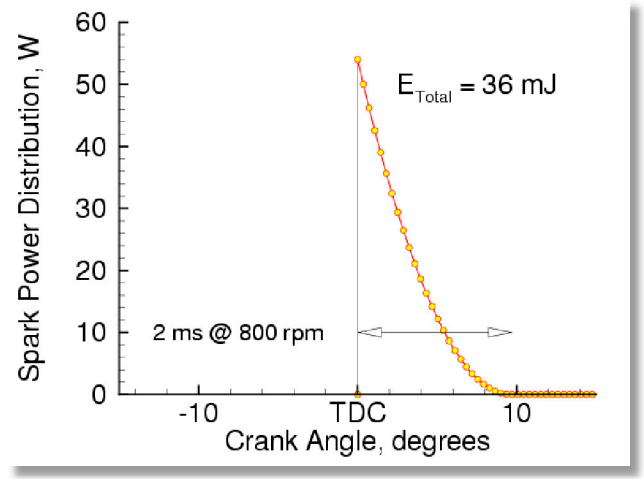


Valve lift profiles measured directly from camshaft

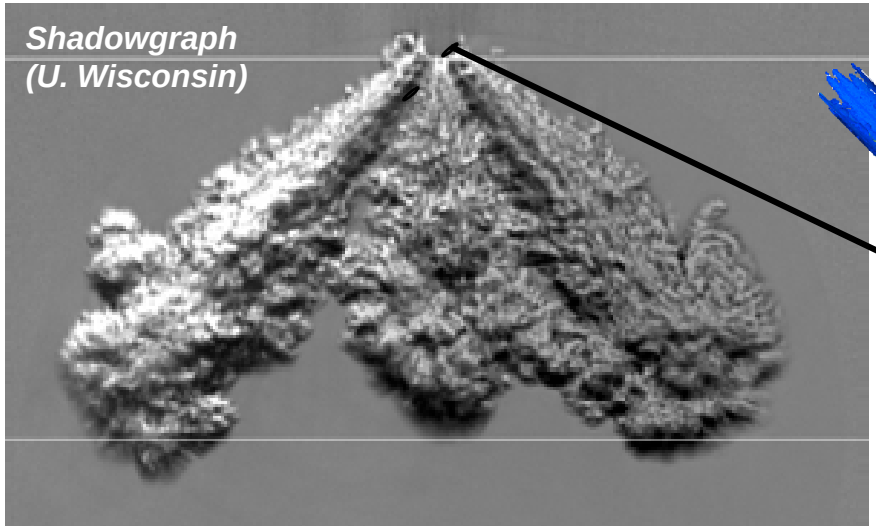


Detailed view of critical grid surfaces

Spark ignition simulated by distributing total integrated energy over defined spark volume (1 mm^3) and adding as source to total energy equation



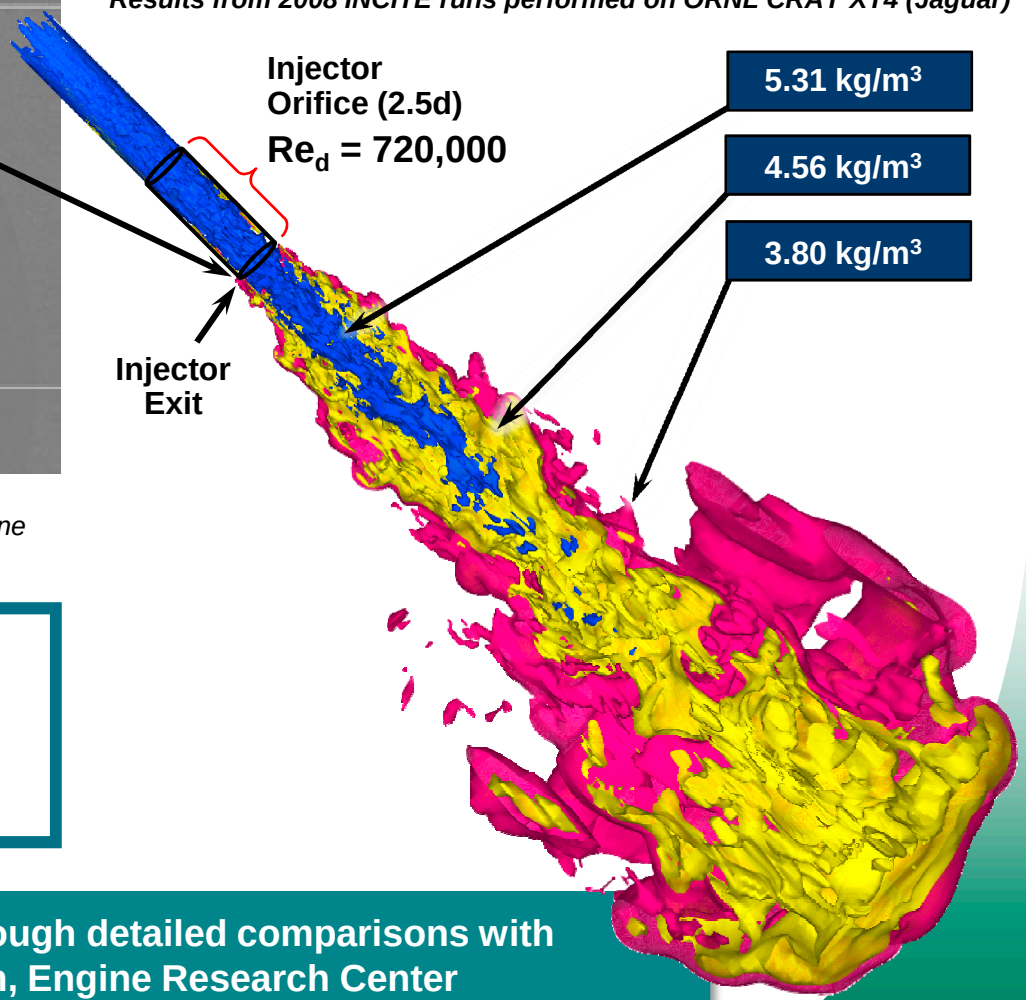
Accuracy of in-cylinder calculations hinges on detailed treatment of high-Reynolds number, high-pressure injection processes



T.G. Drozda and J.C. Oefelein (2008). Large eddy simulation of direct-injection processes for high-pressure, low-temperature engine applications. SAE World Congress, Paper 2008-01-0939

Large Eddy Simulation

Results from 2008 INCITE runs performed on ORNL CRAY XT4 (Jaguar)



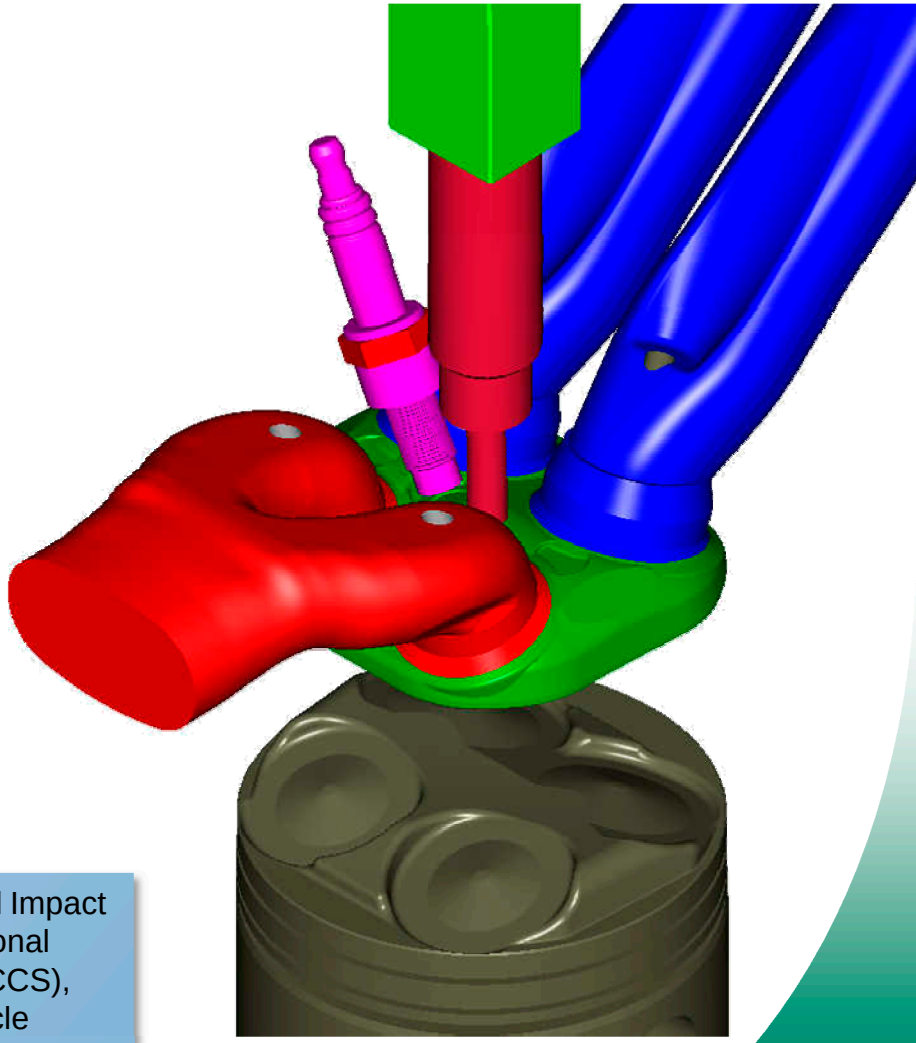
Iso-Contours of Density (H_2 – N_2):

- $d_{orifice}$ = 0.8 *mm*
- $p_{injector}$ = 10.4 *MPa*, $T_{injector}$ = 298 *K*
- $p_{chamber}$ = 0.34 *MPa*, $T_{chamber}$ = 298 *K*

Scalar-mixing model for LES validated through detailed comparisons with experiments at the University of Wisconsin, Engine Research Center

Full engine calculations in geometry shown to the right are currently in progress

Multi-scale simulations of turbulent combustion will provide the foundational science required to develop a validated, predictive combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications. This will enable transportation technology breakthroughs, assuring American competitiveness, U.S. energy security, and minimizing harmful environmental emissions



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