Large Eddy Simulation (LES) Applied to LTC/Diesel/Hydrogen Engine Combustion Research

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Overview

Timeline

- Project provides fundamental research that supports advanced engine development projects
- Focused on application of next generation simulation capabilities
- Project scope, directions and continuation evaluated annually

Barriers

- Barriers addressed
  - Development of validated, predictive, multi-scale models with emphasis on:
    - Clean high-efficiency engines using hydrocarbon based fuels (petroleum and non-petroleum) and hydrogen
    - Advanced LTC technologies (i.e., understanding effects of fuel-injection, air-motion, ignition-timing, heat-transfer and engine-geometry on fuel-air mixing, combustion, and emissions over a range of regimes)
  - Advanced simulations of in-cylinder processes will provide insights into:
    - Effects of fuel injection and engine geometry on mixing, combustion, emissions
    - Effects of timing, load, engine speed, heat transfer on mixture preparation
    - Tolerance of combustion to high EGR and mechanisms for controlling ignition timing, etc., …

Budget

- Project funded by DOE/OVT:
  FY08 – $450K
  FY09 – $450K

Partners

- PI's in the Engine Combustion Group at Sandia with emphasis on establishing benchmark simulations of optical engine experiments
- Project lead: Joe Oefelein

High-performance computing (HPC) provides new opportunities for advances in modeling, simulation

- Project objective: Combine three unique capabilities to maximize benefits of HPC for advanced engine combustion research
  - Established theoretical-numerical framework
  - Specialized massively-parallel code
  - Access to "capability-class" computers
- Provides strong link between DOE Office of Science, related HPC systems and Office of Vehicle Technologies
- Awarded INCITE* grant for computer time directly related to this project entitled: "*High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels*"
  - Multiyear CPU allocations for IC-engine related research on the Oak Ridge National Laboratory CRAY XT Platforms
    - 18–million hours in 2008 (32,000 cores)
    - 30–million hours in 2009 (180,000 cores)
    - Hours in 2010 to be determined
  - Requires scaling to *O(100,000)* cores

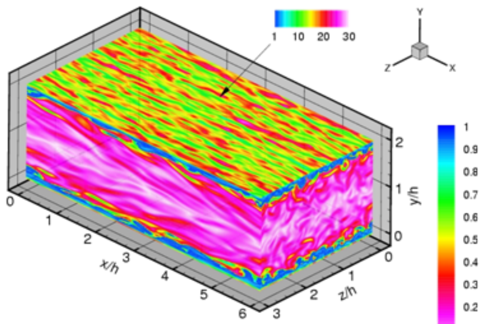
Jaguar is the most powerful computer system for science with world leading performance. The new 1.64-petaflop Cray XT system (Jaguar) has over 180,000 processing cores. Image courtesy of the National Center for Computational Sciences, Oak Ridge National Laboratory.

Office of Science
INCITE
Advancing America's Science and Industrial Competitiveness

****Innovative and Novel Computational Impact on Theory and Experiment***

Theoretical-Numerical Framework (A General Solver Optimized for LES)

- **Theoretical framework**
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray
  - Dynamic SGS modeling (no tuned constants)
- **Numerical framework**
  - All-Mach-number formulation
  - Non-dissipative, conservative
  - Complex geometry
  - Adaptive mesh (ALE)
  - Massively-parallel (MPI)
- **Extensively validated, ported to all major platforms**



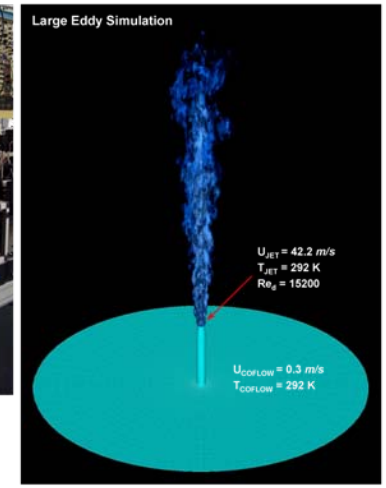
High-Re Wall-Bounded Flows

DLR-A Flame: Re_d = 15,200

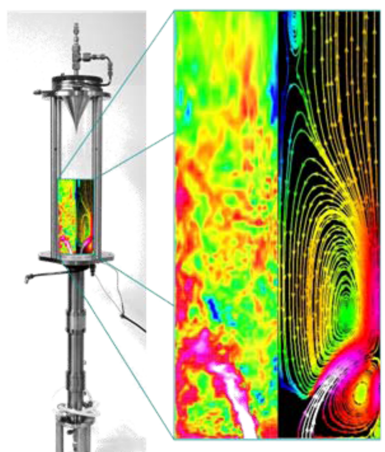
Fuel: 22.1% CH_4, 33.2% H_2, 44.7% N_2

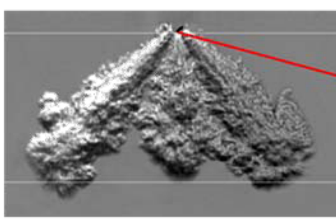
Coflow: 99.2% Air, 0.8% H_2O

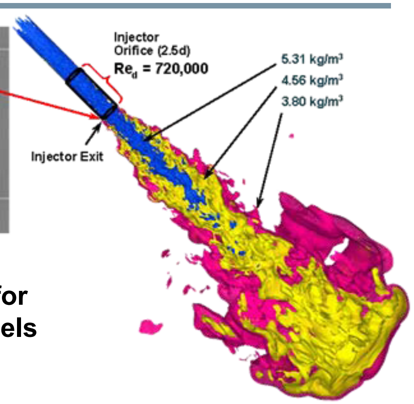
Detailed Chemistry and Transport: 12-Step Mechanism (J.-Y. Chen, UC Berkeley)



Nonpremixed Flames


Premixed Flames





High-Pressure Injection, Mixing, and Combustion for Arbitrary Hydrocarbon Fuels

Complex Geometries (Optical Engines) …

Oefelein, J. C. (2006). Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, 42: 2-37.

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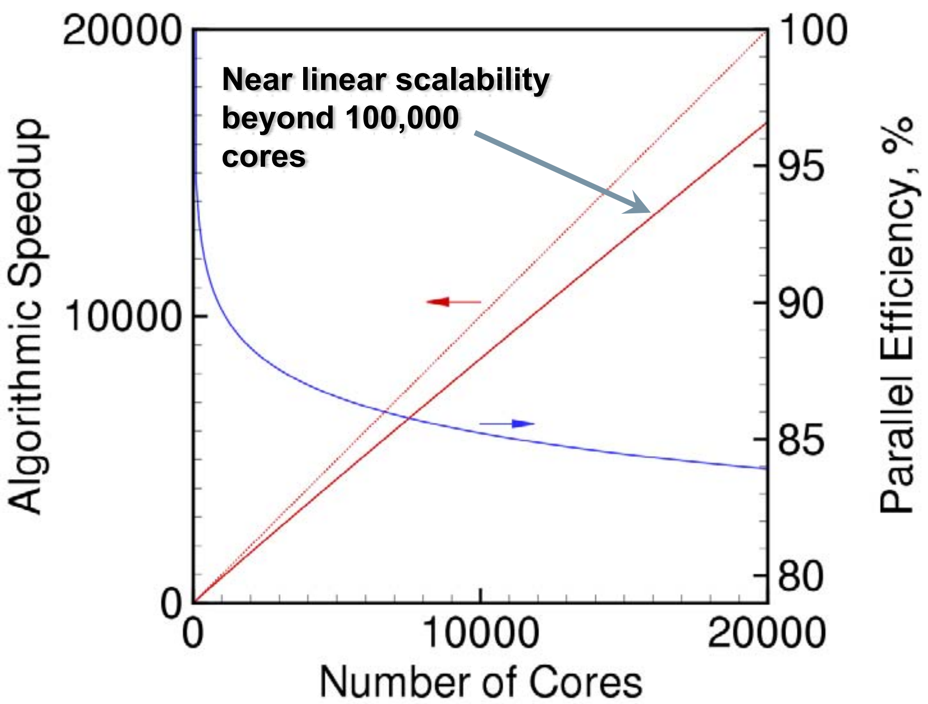


- Strong (fine-grain) scaling attributes exhibited on the ORNL NCCS CRAY XT4 (Jaguar)
- Weak (coarse-grain) scaling on 150,000 cores being benchmarked as part of DOE "Joule Code Metric"

One of the first "capability-class" codes that handles relevant physics & geometry for ICE applications

Approach

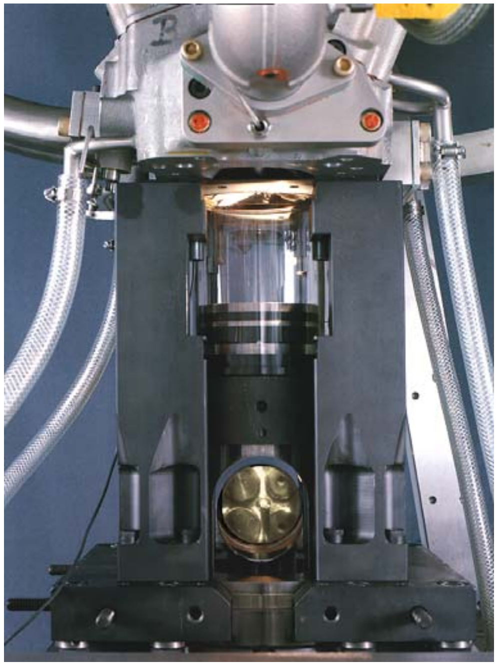
- Combine state-of-the-art LES with existing expertise in optical engine experiments
  - High-fidelity simulations that identically match geometry, etc.
  - Computational benchmarks that complement experimental data
- Adhere to strict algorithmic, model implementation and grid resolution requirements
  - Non-dissipative spatial stencils, no explicit artificial dissipation
  - High-quality hex-grids, minimal stretching and cell deformation
  - Detailed high-level models for SGS closure
- Enhance investment in experiments by providing additional source of detailed quantitative information
  - Move beyond current simulation approaches and constraints
  - Provide fundamental insights not available anywhere else
  - Establish foundation for advanced model development

Milestones

- Develop improved high-pressure multiphase models for time-accurate treatment of direct-injection processes
  - Initial emphasis on high-pressure hydrogen injectors, model validation using data from Petersen and Ghandhi (U. Wisconsin)
  - Direct applicability to liquid hydrocarbon injectors (collaboration with Musculus, Pickett (www.ca.sandia.gov/ECN))
- Perform high-fidelity simulations of optical H_2-ICE (Kaiser *et al*.)
  - Validation through comparison of measured, modeled results
    - Chemiluminescence Imaging and Particle Image Velocimetry (PIV)
    - Planar Laser Induced Fluorescence (PLIF)
  - Detailed analysis of in-cylinder direct-injection mixing and combustion processes (3D dynamics)
- Systematically extend to HCCI engine experiments (Dec *et al*.)
  - Detailed studies of low temperature combustion processes
  - Treatment of complex hydrocarbon processes

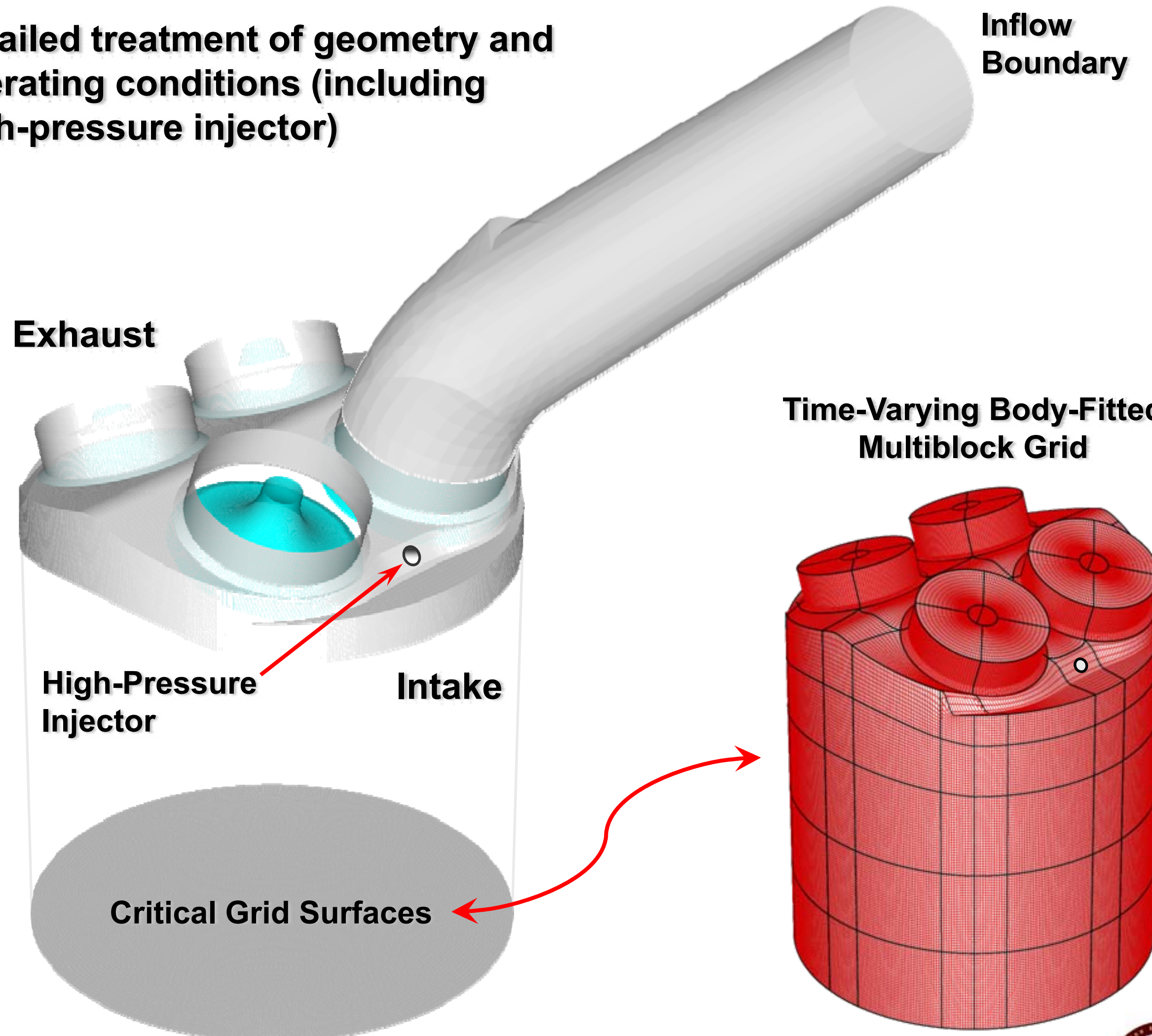
Technical accomplishments achieved in all three areas as follows

CRF Optically Accessible Hydrogen-Fueled IC-Engine



Engine Specifications	
Compression Ratio	9 – 12
Bore	92 *mm*
Stroke	85 *mm*
Peak Turbulence Intensity	2.85 *m/s*
Integral Length Scale	2 *mm*
Thermal Layer Thickness	6.3 *μm*
Kolmogorov Length Scale	5.6 *μm*
Reaction Zone Thickness	3.9 *μm*
Turbulent Reynolds Number	2550

Detailed treatment of geometry and operating conditions (including high-pressure injector)



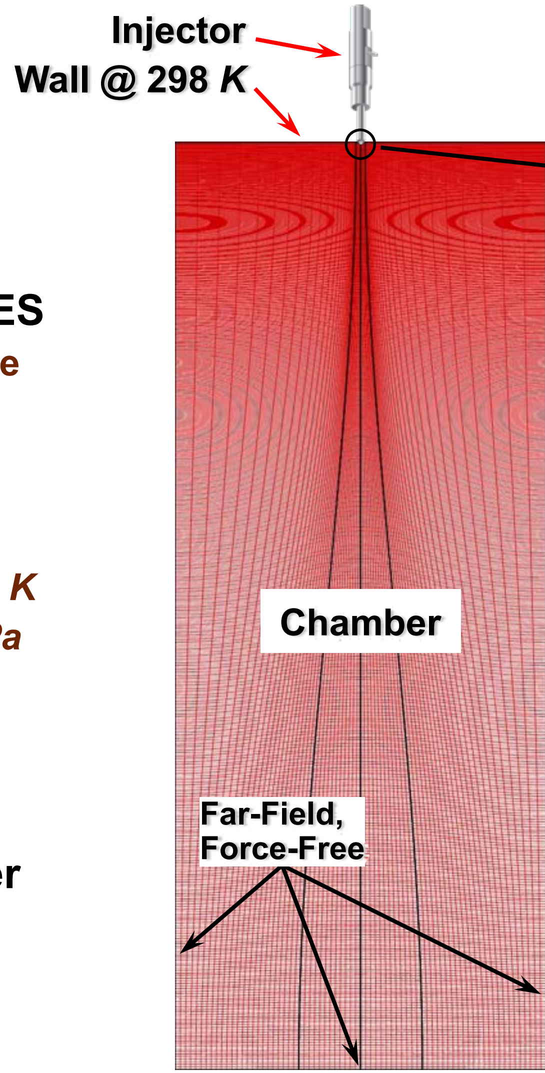
High-fidelity models for treatment of transient high-pressure injection processes

- **Available Data:**
  - Schlieren visualizations and corresponding penetration data
    - H_2 injected into quiescent chamber of N_2 or CO_2
    - Injection pressures of 52 and 104 bar
    - Chamber densities of 1.15 to 12.8 kg/m^3
  - Parametric study using 3, 7, 9, 13 hole injectors, 36 cases total
- **Objectives:**
  - Systematic validation: Investigate issues related to initial transients and requirements for in-cylinder calculations
  - Establish appropriate resolution criteria and time-dependent boundary conditions

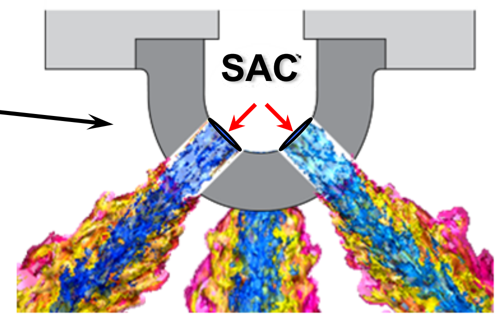
1. B. R. Petersen and J. B. Ghandhi (2006). Transient high-pressure hydrogen jet measurements. *SAE Transactions, Volume 115* (Paper 2006-01-0652, SAE World Congress, April 3-6, Detroit, Michigan)
2. B. R. Petersen (2006). Transient high-pressure hydrogen jet measurements. *Masters of Science in Mechanical Engineering*, University of Wisconsin-Madison

Computational Domain and Boundary Conditions (3-Hole Injector)

- **Cross-section of 3D grid**
  - Injector mounted at head-end
  - Outer shaft diameter: 7.5 *mm*
  - Chamber size 750L x 300D *mm*
- **Resolution for wall-resolved LES**
  - 1-million cells per injector orifice
  - 3.5-million cells in chamber
  - Optimal stretching
- **Initial conditions**
  - Injector: H_2 at 10.4 *MPa* and 298 *K*
  - Chamber: N_2 at 101, 336, 722 *kPa* and 298 *K*
- **Detailed thermodynamics and transport**
- **50,000 – 100,000 CPU hours per case on CRAY XT platforms**

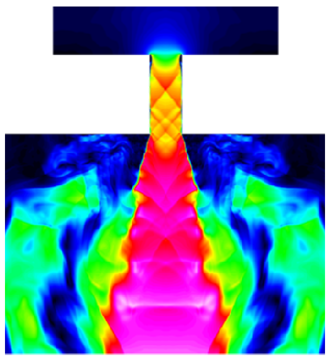


Injector Tip



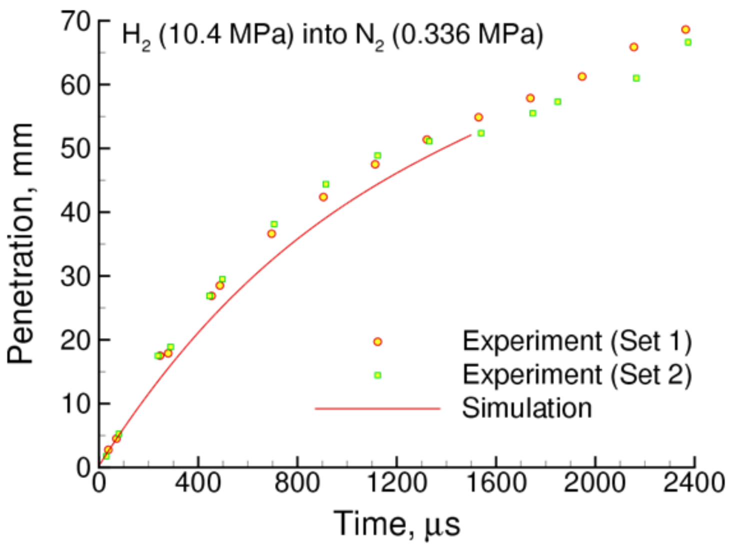
Inflow to orifices approximated using ramp function with superimposed fluctuations

Idealized SAC

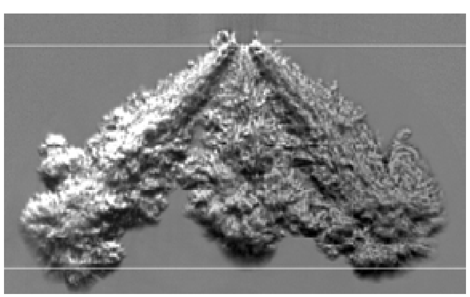


Mean profiles at orifice inlets determined using idealized SAC configuration

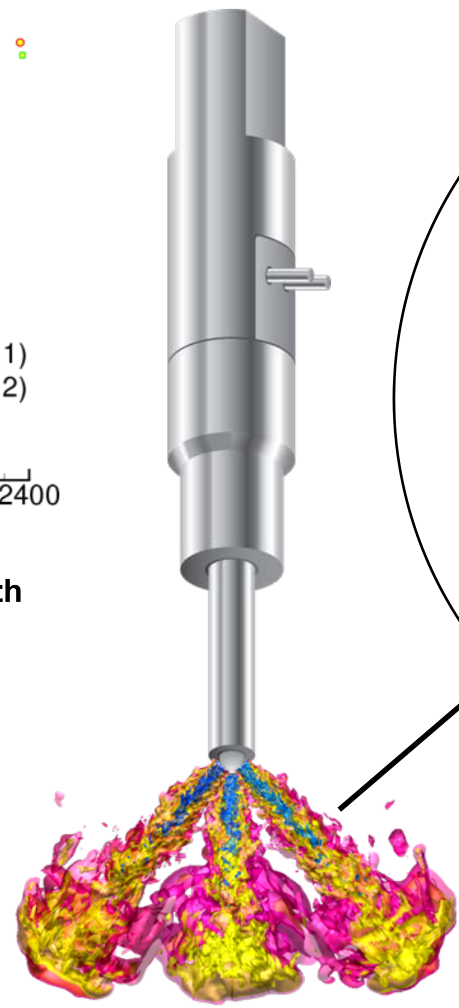
Good agreement with penetration data and shadowgraphs, detailed treatment of turbulence



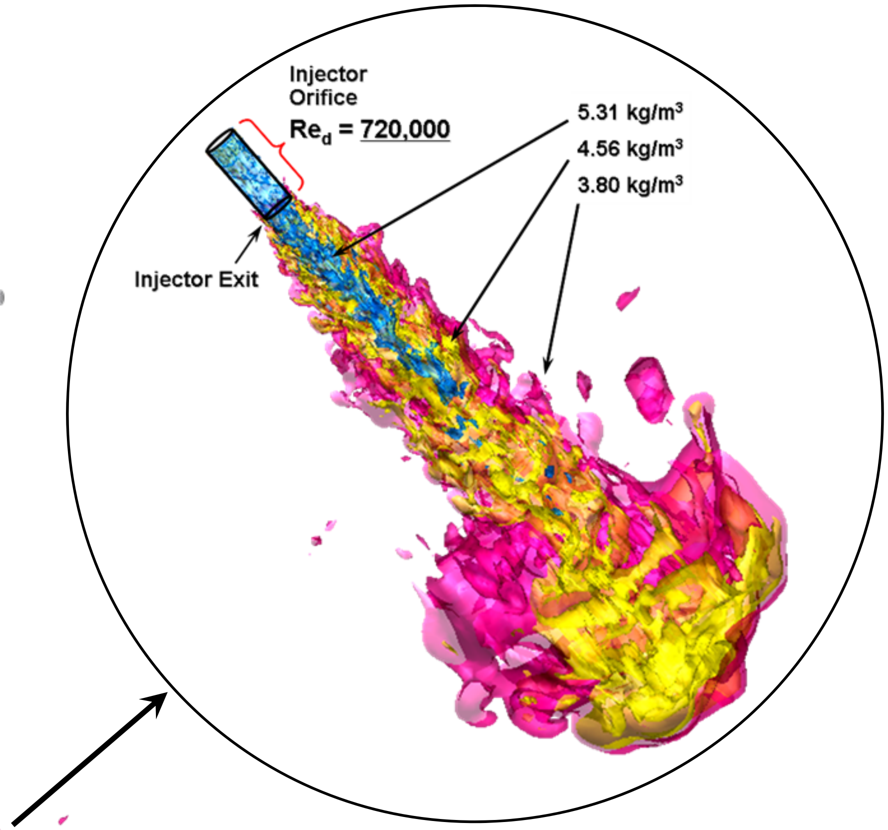
Representative comparison of LES with penetration measurements



Shadowgraph (U. Wisconsin)

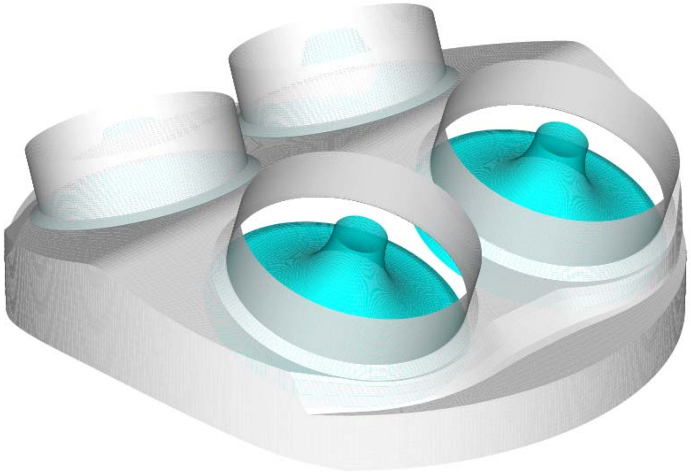


Large Eddy Simulation

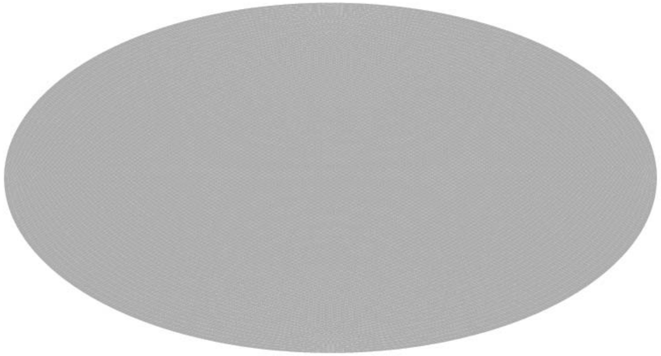


Iso-Contours of Density ($H_2 - N_2$)	
Orifice Diameter	0.8 *mm*
Injection Pressure	10.4 *MPa*
Injection Temperature	298 *K*
Chamber Pressure	0.336 *MPa*
Chamber Temperature	298 *K*

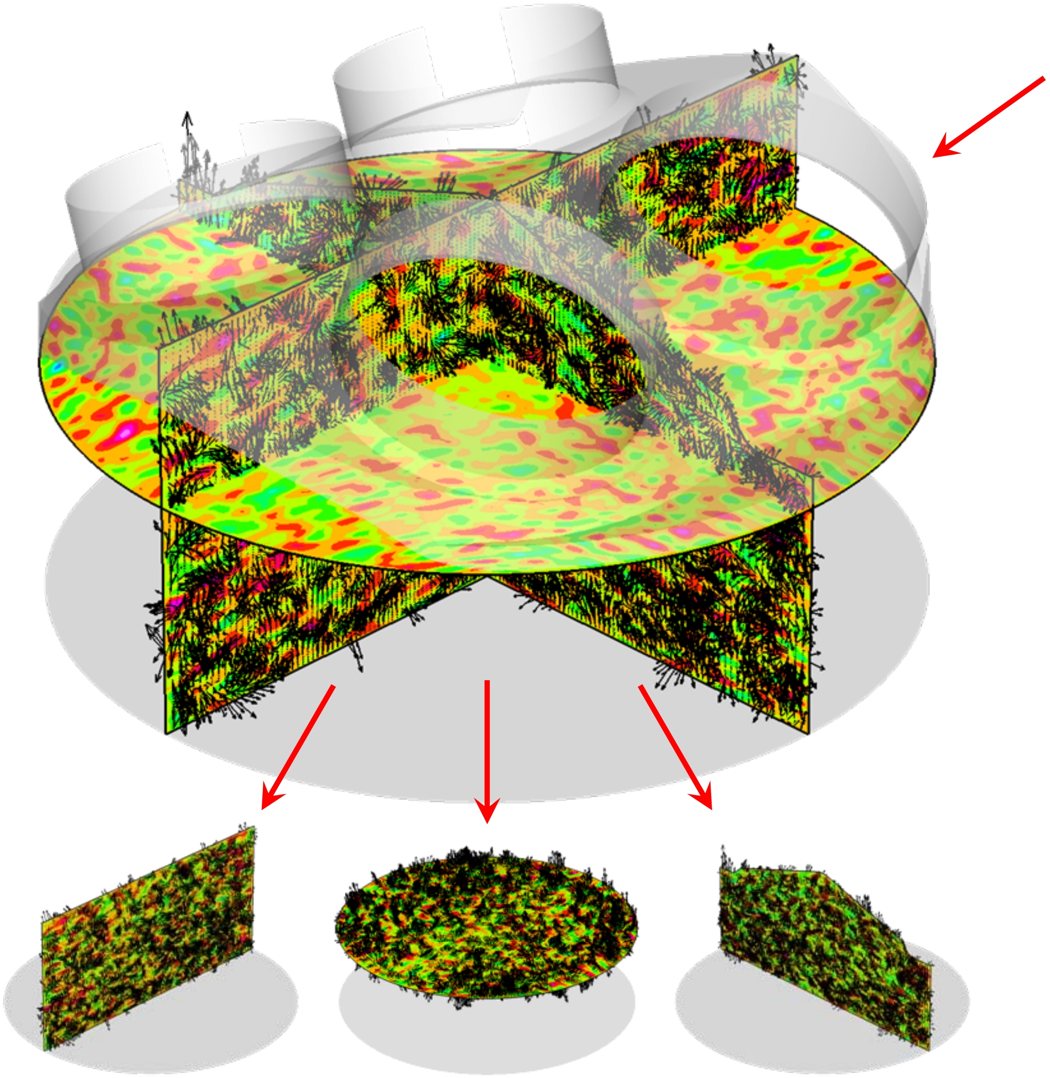
Analysis of In-Cylinder Flow Dynamics



Animation



Comparisons with PIV Data



Instantaneous velocity field from LES showing out of plane components (-60 CAD BTDC)

- Goals:
  - Validation using available data
  - Study 3D dynamics throughout domain using validated solution
  - Extract information that cannot be measured (i.e., physics, models)
- Issues:
  - Boundary conditions applied with one-to-one correspondence
  - Spatial resolution of PIV and LES results must match (i.e., be filtered with identical cutoff values)
  - Consider only planar components (neglect out of plane component)
  - Converged phase-locked statistics (mean, RMS, higher-order moments)

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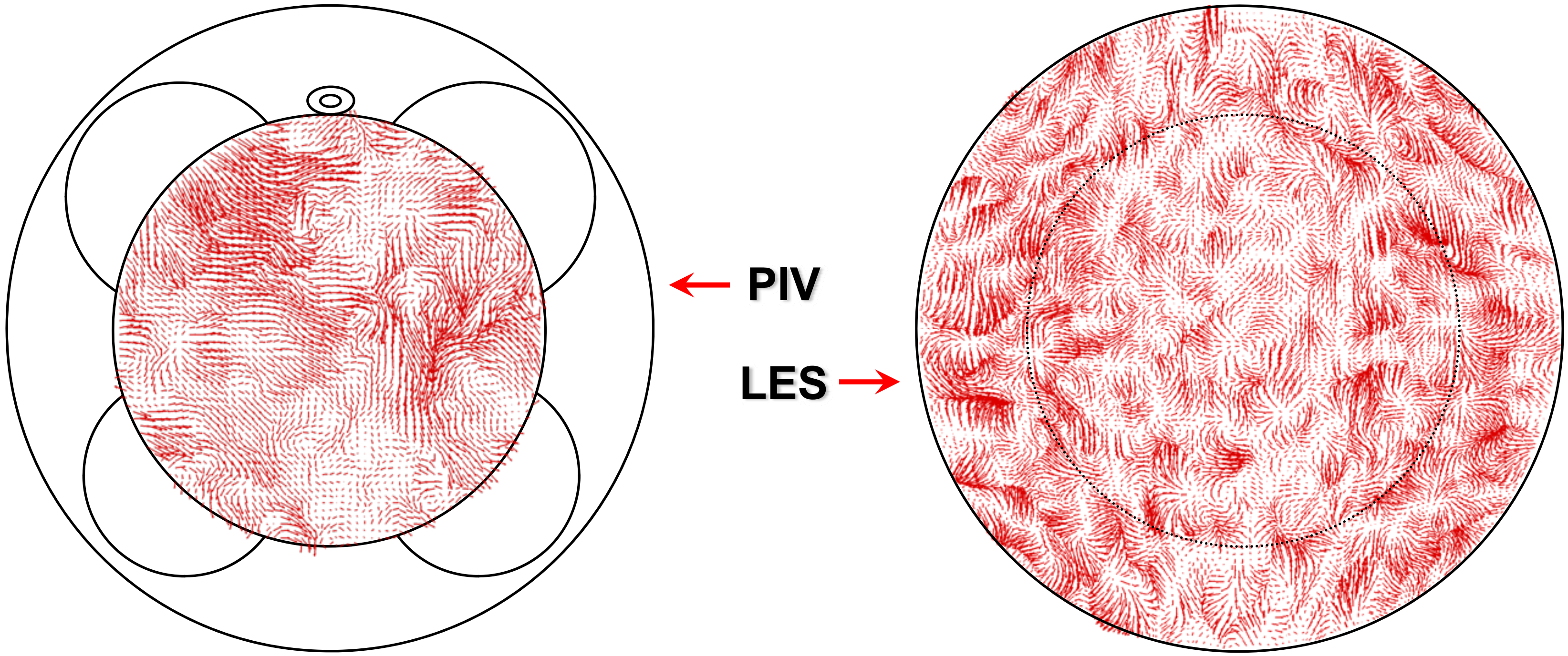
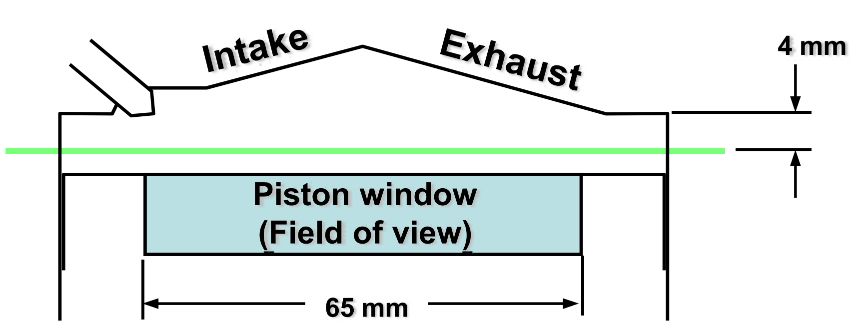
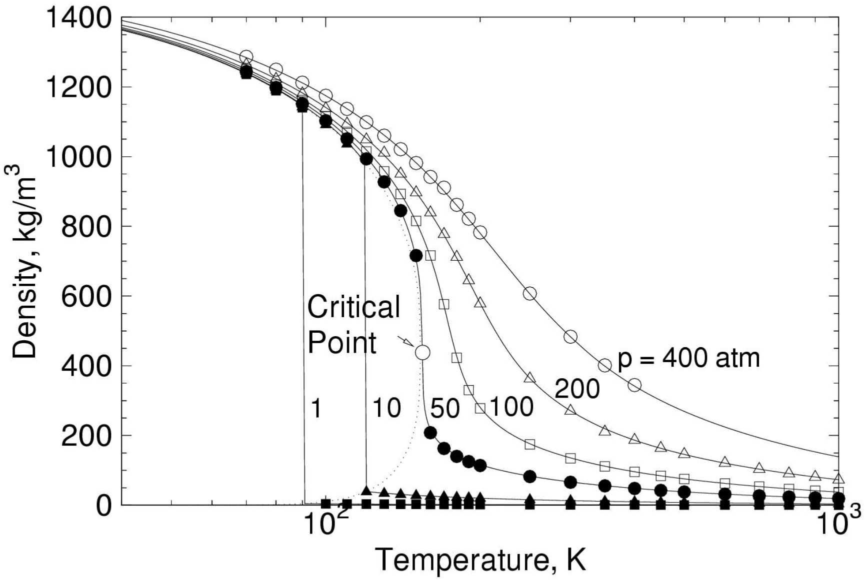




- Typical Result
  - Single shot PIV at -60 CAD BTDC compared to corresponding LES
  - 1200 rpm, 0.5 bar intake pressure
  - LES filtered to match resolution of PIV
- Good agreement between measured and modeled fields (instantaneous & average)

Toward HCCI and Diesel Engines …

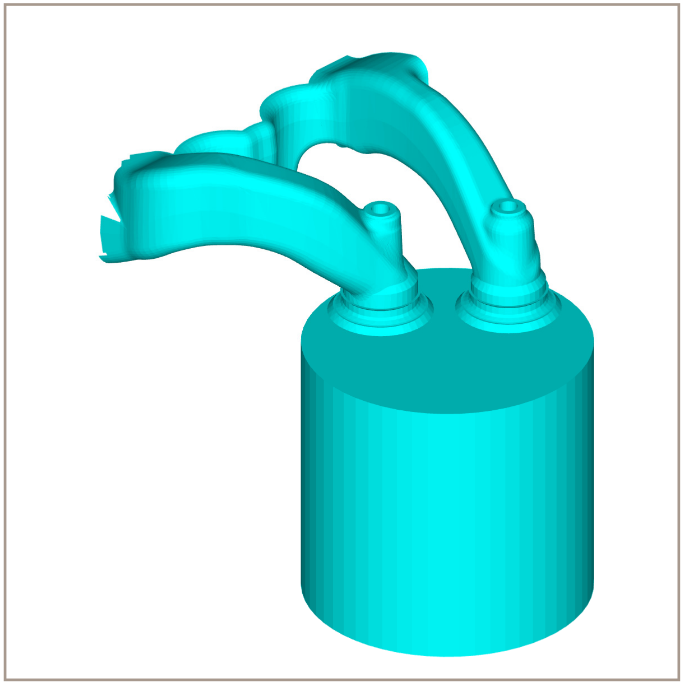
- **Detailed Thermodynamics and Transport for High-Pressure Hydrocarbon Mixtures**



J.C. Oefelein (2009). General package for evaluation of multicomponent real-gas and liquid mixture states at all pressures. SAND report in print.

- **Transient Injection with Emphasis on Entrainment**
  - **Collaboration with Bing Hu (new LES post-doc from U. Wisconsin) and Mark Musculus**

- **Grid Development for Analysis of CRF Optical/Metal HCCI Engines (Dec et al.)**



Future Work

- Continue high-fidelity simulations of optical H_2-ICE
  - Detailed analysis of in-cylinder direct-injection processes
  - Validation through comparison of measured, modeled results
  - Joint analysis of data from validated simulations
- Systematically extend to HCCI engine experiments
  - Detailed studies of low temperature combustion processes
  - Treatment of complex hydrocarbon processes
- Continue canonical calculations of direct-injection processes for high-pressure, low-temperature engine applications
  - Collaboration with Musculus, Pickett's "Engine Combustion Network" for validation (www.ca.sandia.gov/ECN)
- Continue leveraging between DOE Office of Science and Energy Efficiency and Renewable Energy activities
  - Access to DOE high-performance "capability-class" computers
  - Development and validation of turbulent combustion models

Summary

- **Project provides significant link between DOE Office of Science and Office of Vehicle Technologies**
  - Objective: Merge state-of-the-art LES capability with key experiments
  - Benefits: Moves beyond current models, additional source of detailed data
  - Focus: Barriers related to both Advanced Engine R&D and Development of Advanced Simulation Capabilities using high-performance computing
- **Four major accomplishments since last review**
  - INCITE grant on DOE capability class computers (30-million CPU hours)
  - Developed and validated detailed model for high-pressure fuel injection
  - Detailed simulations of H_2-ICE, comparisons with experiments ongoing
  - Detailed analysis of transient injection and entrainment processes
- **Have begun to establish technology transfer through collaborations with industry and academia with emphasis on**
  - Developing a validated suite of benchmark simulations and sub-models
    - High-pressure phenomena (chemistry, thermodynamics, transport …)
    - Multiphase flow and combustion (atomization, jet breakup …)
    - Clean and efficient combustion of alternative fuels …