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

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Project ID: ACE007

Overview

Timeline

- Project provides fundamental research that supports advanced engine development projects
- Focused on development of next generation simulation capabilities using “capability class” computers
- Project scope, directions and continuation evaluated annually

Barriers

- Two sets of barriers addressed
  1 – Development of clean high-efficiency engines using hydrocarbon based fuels (petroleum and non-petroleum) and hydrogen
  – LTC technologies (i.e., understanding effects of fuel-injection, ignition-timing, heat-transfer and engine-geometry on fuel-air mixing, combustion, soot, emissions over broad operating range)
  2 – Requirements for efficient and routine application of high-performance (exascale) computing and advanced simulation/modeling capabilities for advanced engine combustion research

Budget

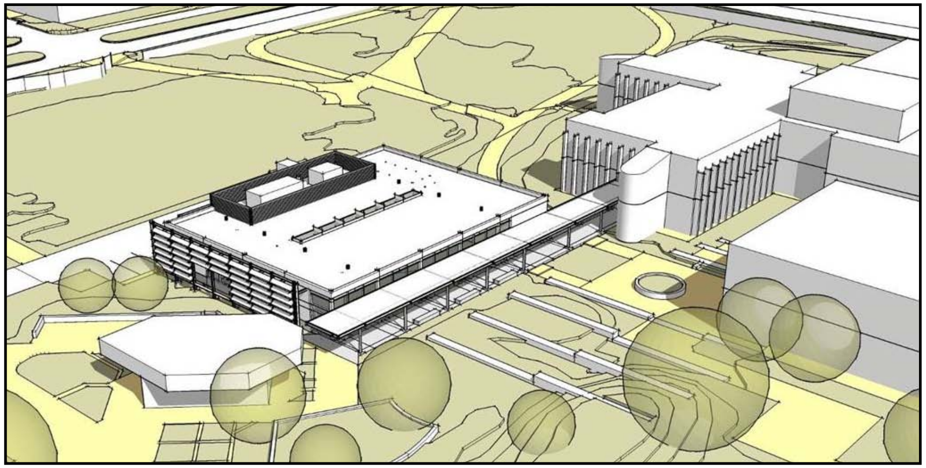
- Project funded by DOE/OVT:
  FY09 – $450K
  FY10 – $450K

Partners

- PI’s in the Engine Combustion Group at Sandia, Wisconsin, Penn State, Michigan, TU Darmstadt, GM (most recent)
- Project lead: Joe Oefelein

Relevance … high performance computing (HPC) and advanced code base offers significant opportunities

- Project objective: Combine unique capabilities to maximize benefits of HPC for advanced engine combustion research
  - Detailed theoretical framework
  - Specialized massively-parallel flow solver
  - Access to full hierarchy of DOE computers
- Provides strong link between DOE Office of Science, related HPC systems and Office of Vehicle Technologies
  - Computational Combustion and Chemistry Laboratory (BES – OVT)
    - Mid-scale computer clusters and storage
    - SISGR mid-scale equipment upgrade (BES)
  - Combustion Research and Computational Visualization Facility (BES – OVT)
    - 9000 sq-ft building for computational combustion
    - Computer room, viz and collaborative space
  - DOE Office of Science Laboratories
    - LBNL NERSC (www.nersc.gov)
    - ORNL NCCS (www.nccs.gov)
  - INCITE Program
    - 25-million CPU hours for LES in 2010 (IC-engines)



Combustion Research and Computational Visualization Facility

Image courtesy of Oak Ridge National Laboratory

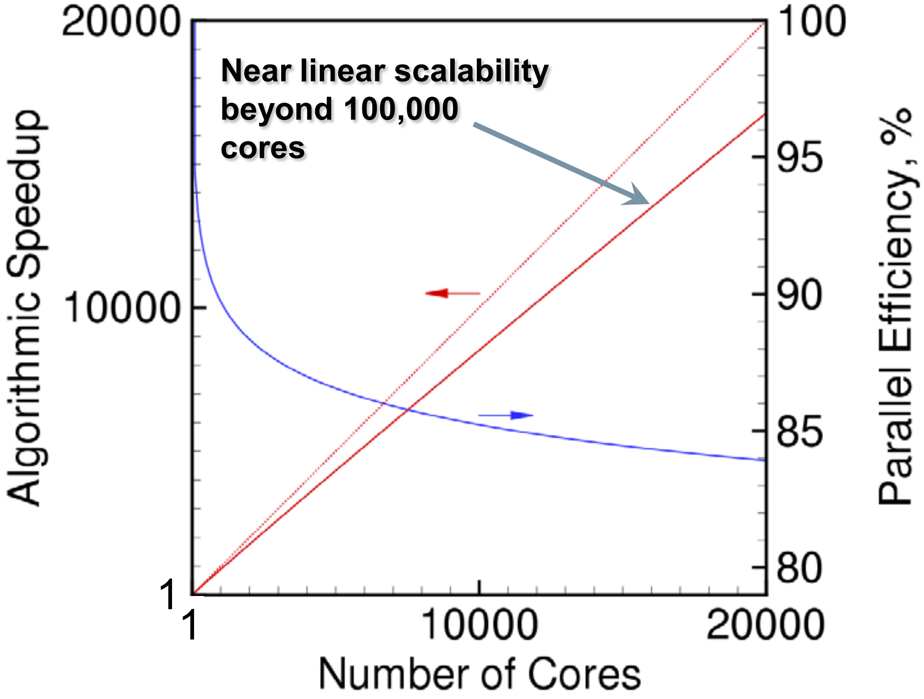
Jaguar, the Cray XT5 at ORNL is the world's fastest computer (2.33-petaflop system, 224,256 processing cores)

Approach … perform unique one of a kind calculations consistent with the role of a national laboratory

- Combine state-of-the-art LES with existing expertise in optical engine (and supporting) experiments
  - High-fidelity simulations that identically match geometry, etc.
  - Computational benchmarks that complement experimental data
- Systematically address barriers associated with advanced modeling and simulation on petascale (and beyond) platforms
  - Access to a hierarchy of computational resources
  - Software that provides highly-scalable performance
  - High-quality grid generation for complex geometries
- Hierarchal model development using benchmarks as additional source of data to address engine related barriers
  - Provide fundamental insights not available anywhere else
  - Establish model performance and implementation requirements
  - Perform collaborative model development for engineering design

Theoretical-Numerical Framework (RAPTOR: A general solver optimized for LES & HPC)

- **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**



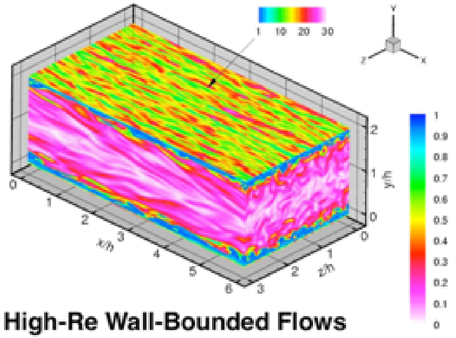
Near linear scalability beyond 100,000 cores

- Strong (fine-grain) scaling attributes exhibited on the ORNL NCCS CRAY XT system (Jaguar)
  - Single block, 1.28-million cells
  - 20,000 blocks with 4^3 cells
- Weak (coarse-grain) scaling on 150,000 cores benchmarked as part of DOE 2009 Joule Code Metric

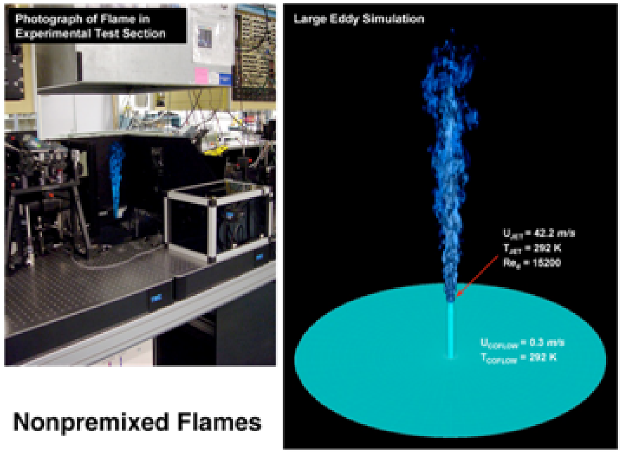
One of the first "capability-class" codes that handles relevant physics & geometry for ICE applications

Verification and validation performed continuously to assess both algorithmic and model accuracy

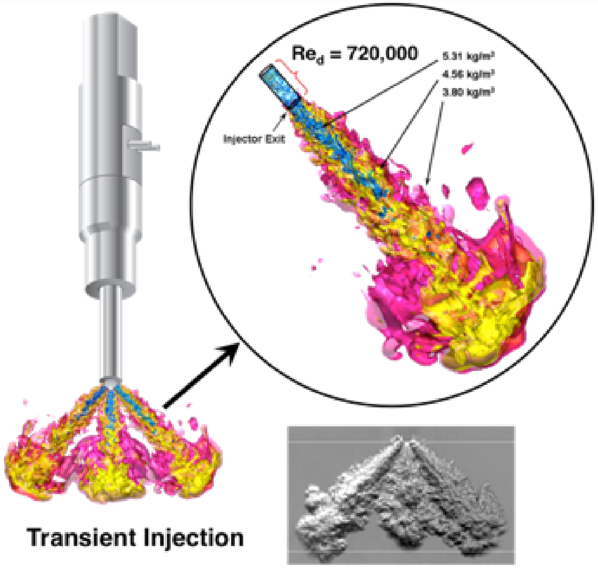
Code framework handles broad range of thermo-physical conditions



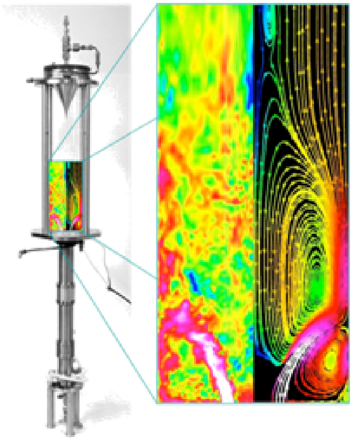
High-Re Wall-Bounded Flows



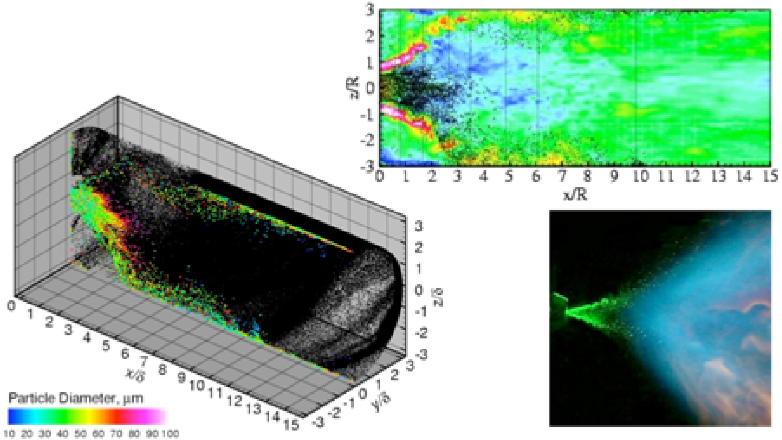
Nonpremixed Flames



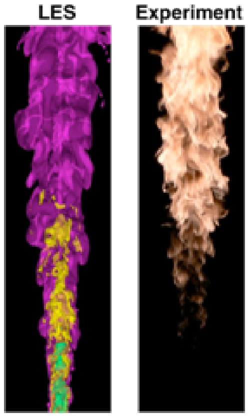
Transient Injection



Premixed Flames



High-Pressure Multiphase Flows



Soot and Emissions

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)
  - Currently focused on liquid hydrocarbon injectors (collaboration with Musculus, Pickett (www.ca.sandia.gov/ECN))
- Continue high-fidelity simulations of 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)
- Begin simulations of HCCI engine experiments (Dec *et al.*)
  - Detailed studies of low temperature combustion processes
  - Current focus on natural thermal stratification

Technical accomplishments achieved in all three areas as follows

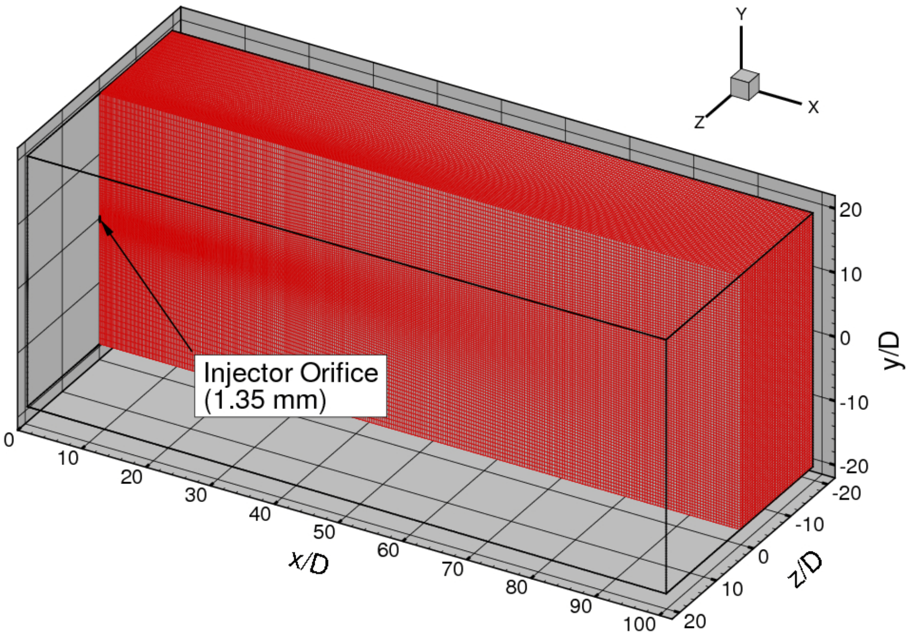
Accomplishment 1: Analysis of transient jet dynamics and entrainment with emphasis on Diesel injection

- Diesel jets involve quasi-steady and transient (decelerating) phases
- Decelerating phase important for design of LTC engines due to greater mixing
  - Lean mixture decreases tendency for soot formation … desirable
  - Over-lean mixture increases tendency for UHC emissions … undesirable
- Entrainment is rate-controlling process

- **Objective**: Understand entrainment processes in transient jets at Diesel like injection conditions
  - Quantify unsteady characteristics as function of entrainment coefficients
  - Understand governing mechanisms during jet deceleration

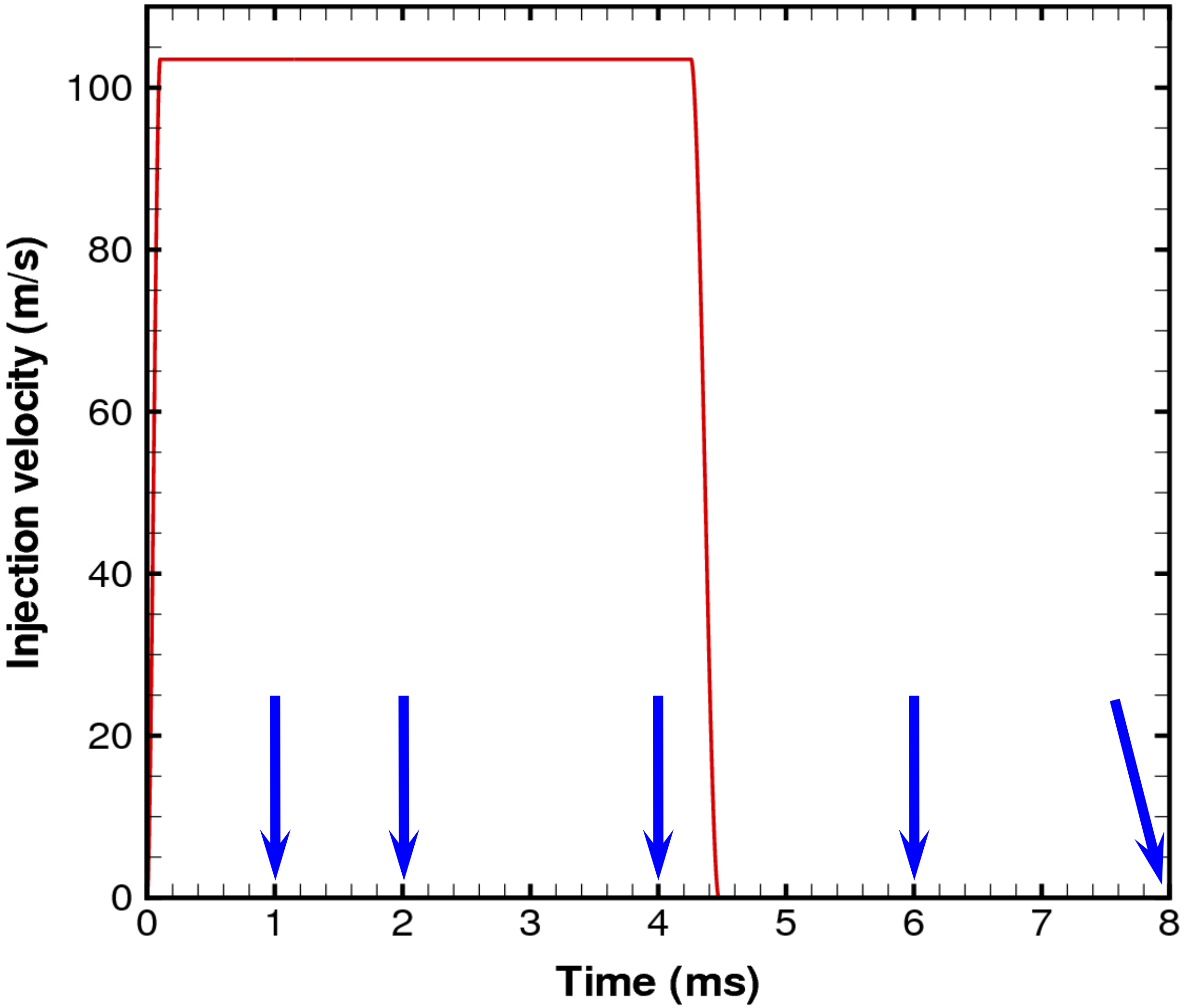
B. Hu, M. P. Musculus, and J. C. Oefelein. Large eddy simulation of a transient gas jet with emphasis on entrainment during deceleration. SAE World Congress, Paper 2010-01-1133, April 13-15 2010.

Computational Domain

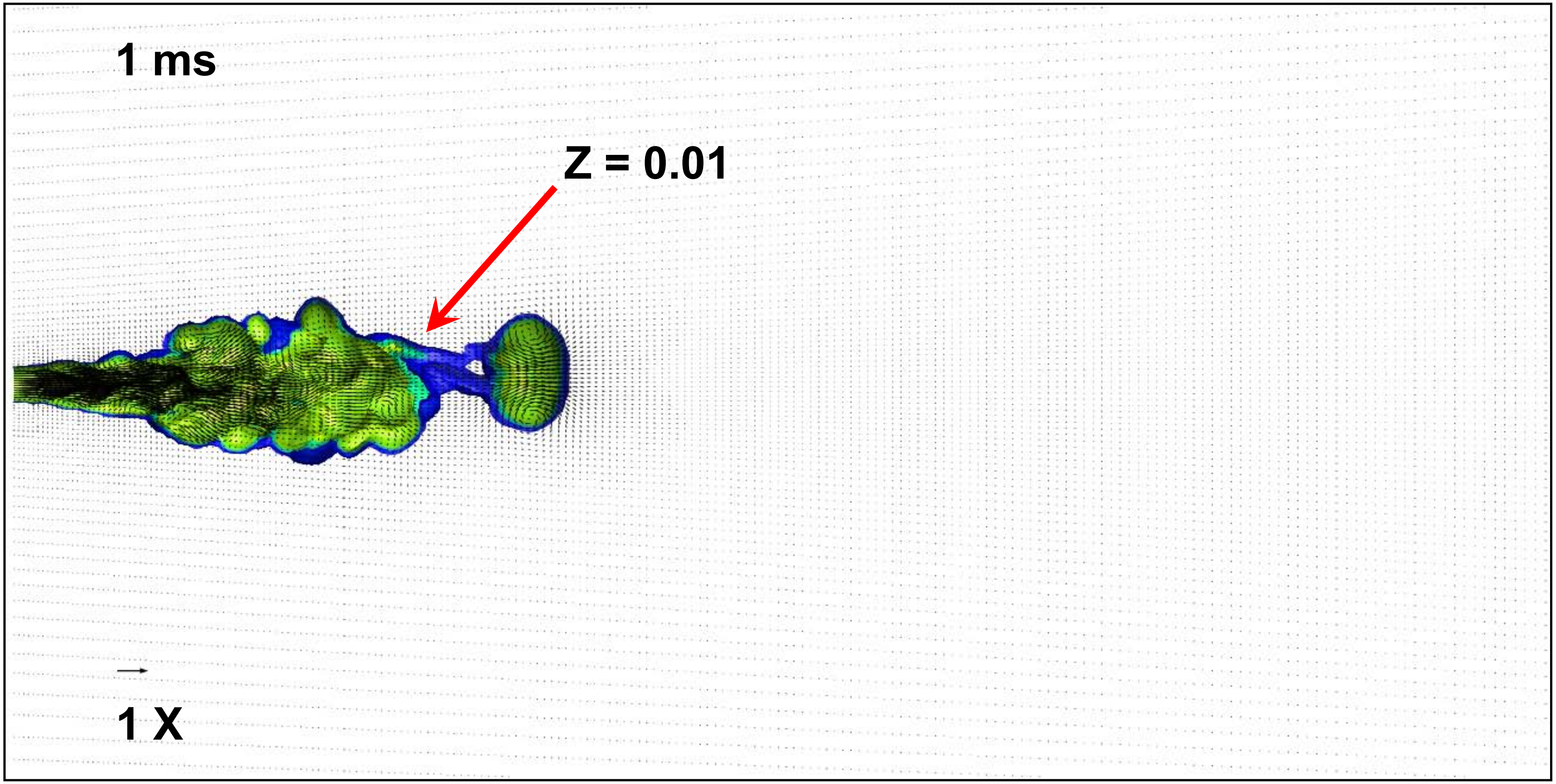


- Multiblock grid with 3-million cells and optimal stretching (130-million CPU hrs)
- Time step 160 ns, correlated fluctuations imposed at orifice inflow boundary
- Injected fluid marked using passive scalar ($Z_{JET} = 1$)

Mean injection profile designed to match experiment of Witze (AIAA Journal, Vol. 21, 1983)

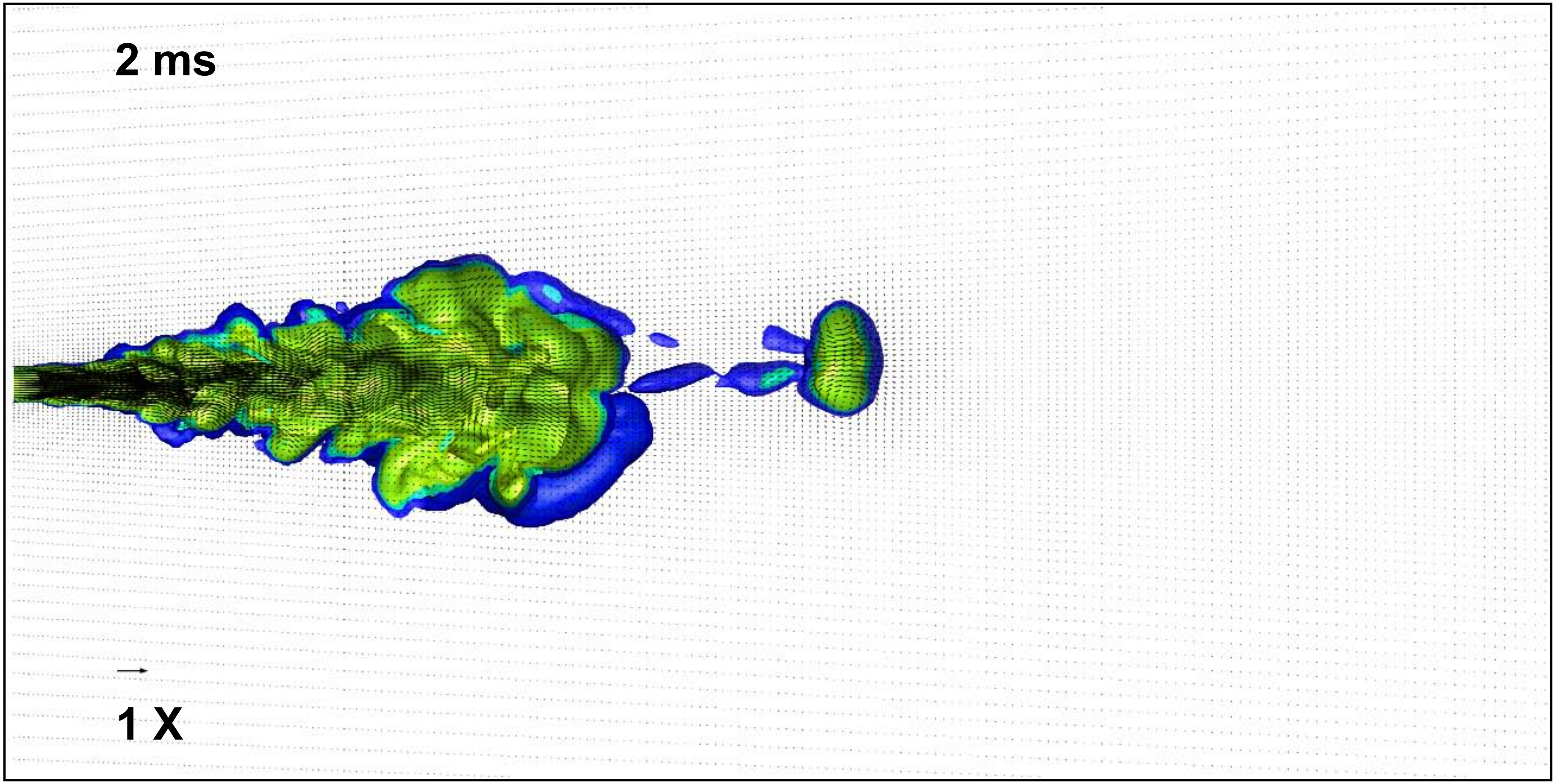


Spatial and temporal evolution



Iso-surfaces of passive scalar with the corresponding velocity vectors

Spatial and temporal evolution



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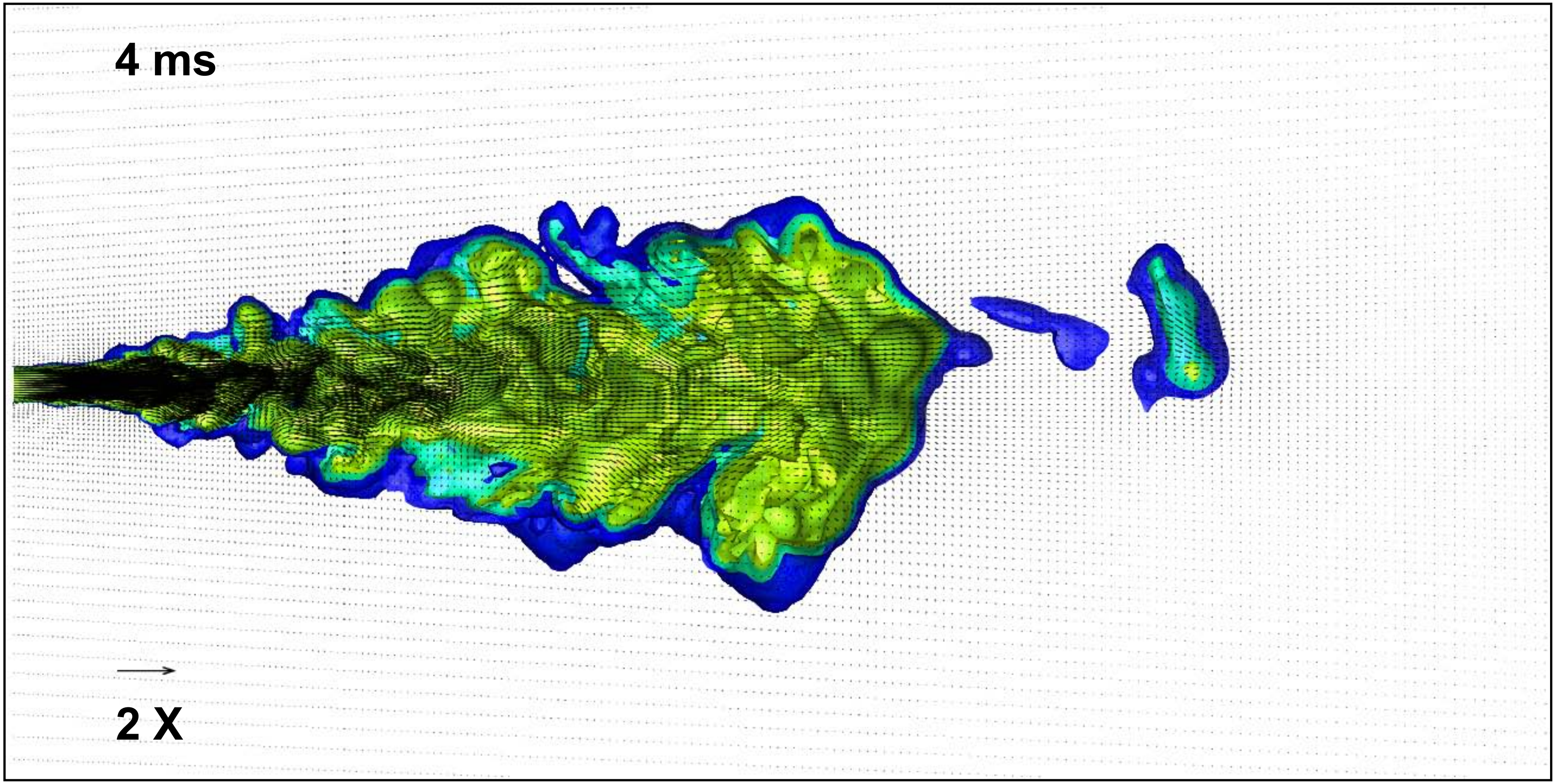

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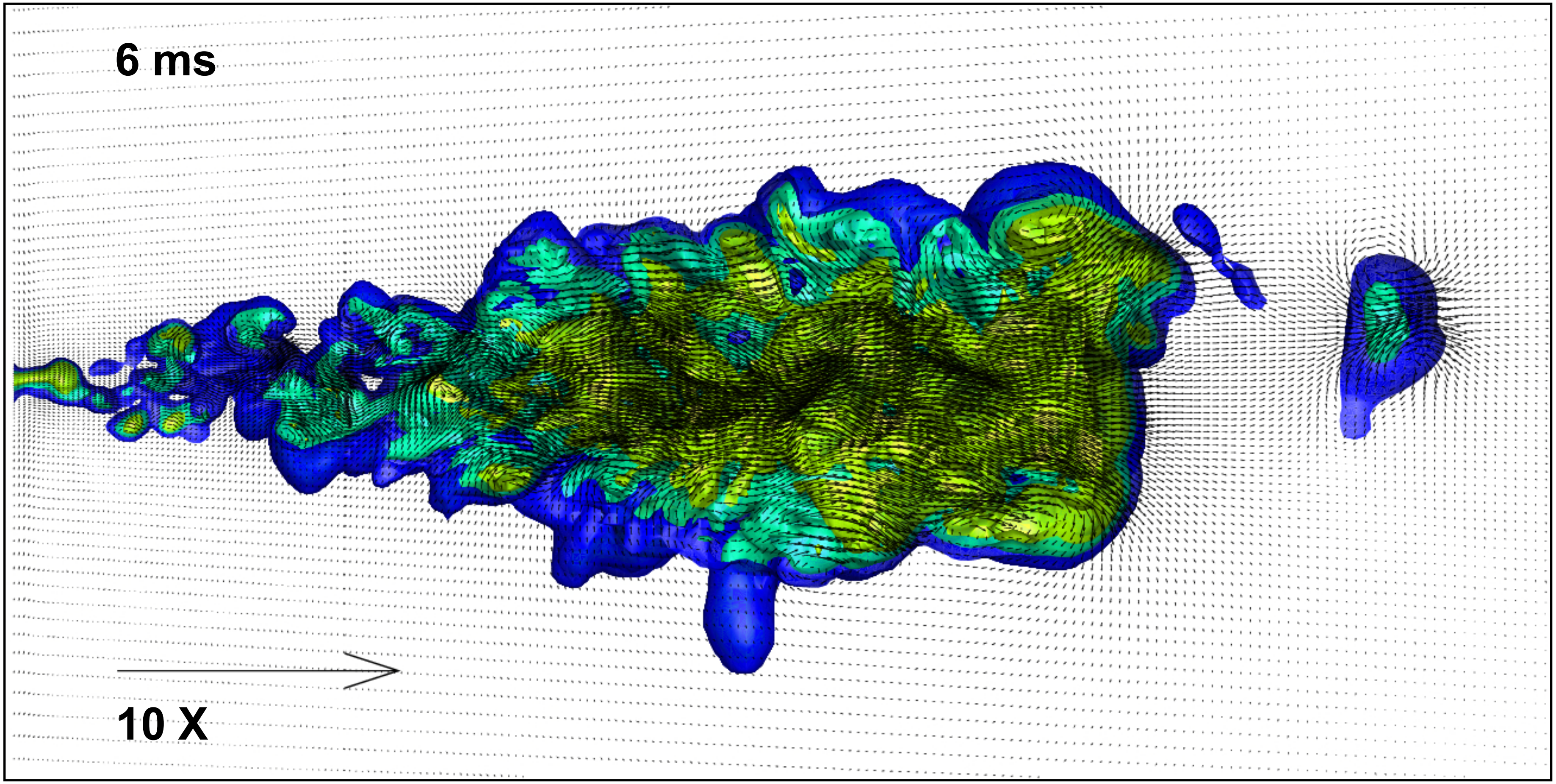

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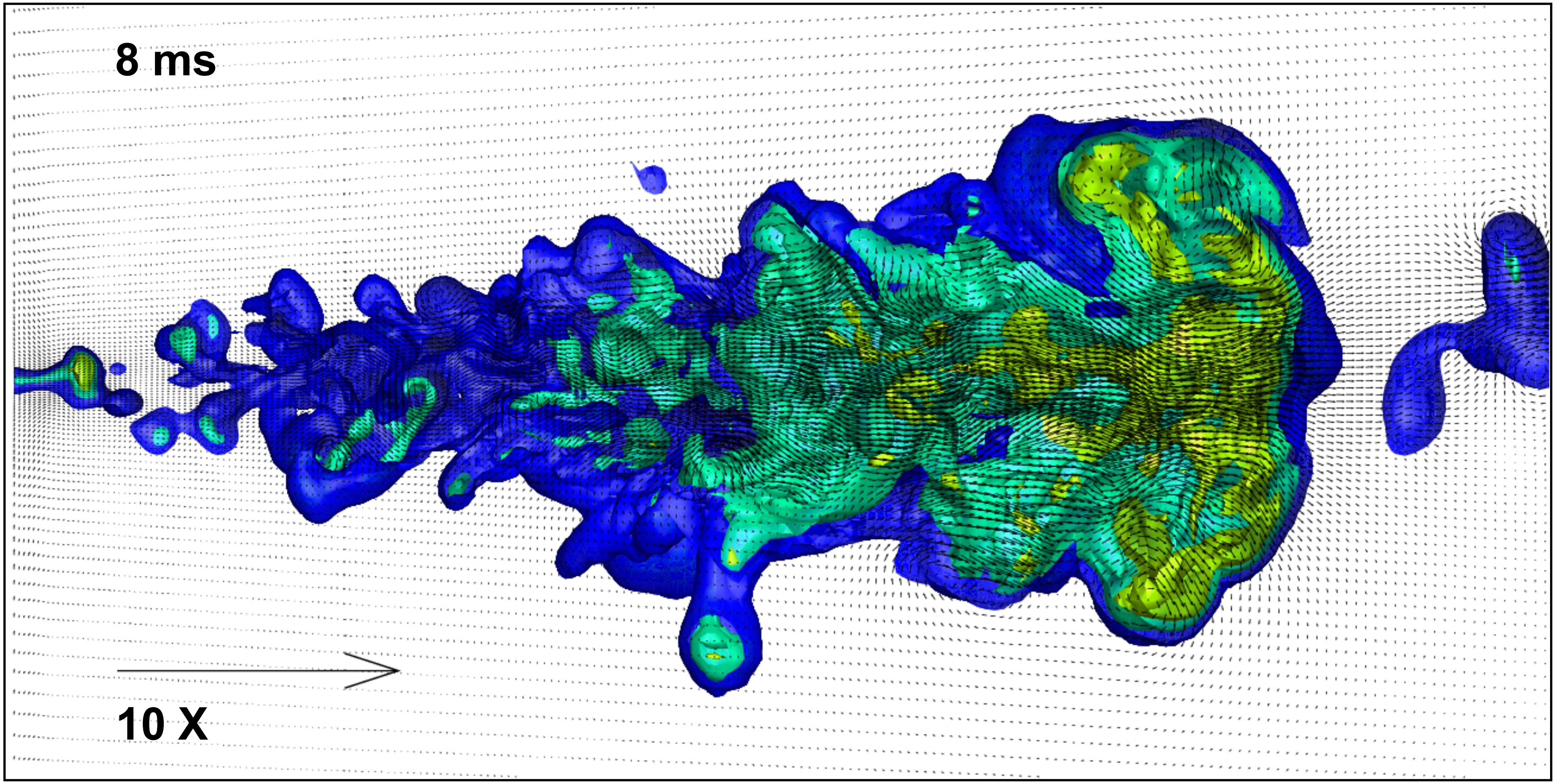
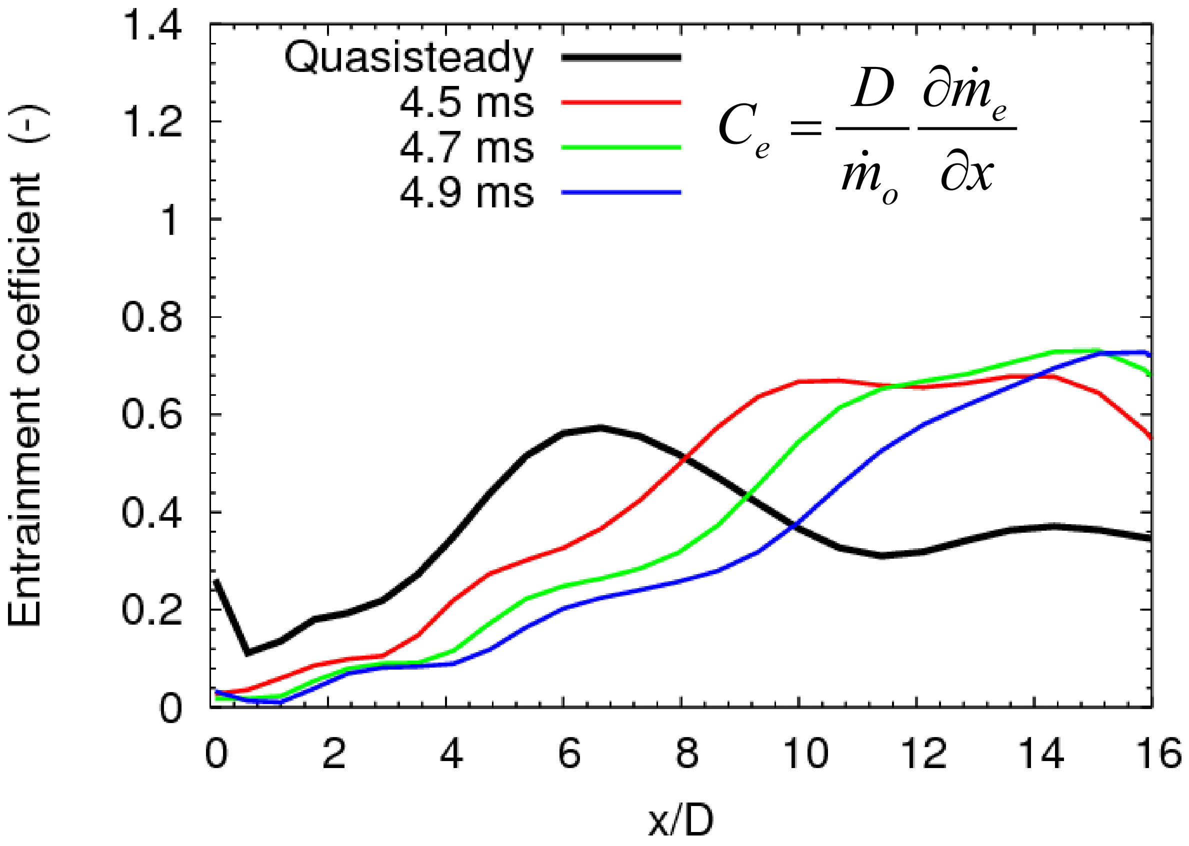


Iso-surfaces of passive scalar with the corresponding velocity vectors

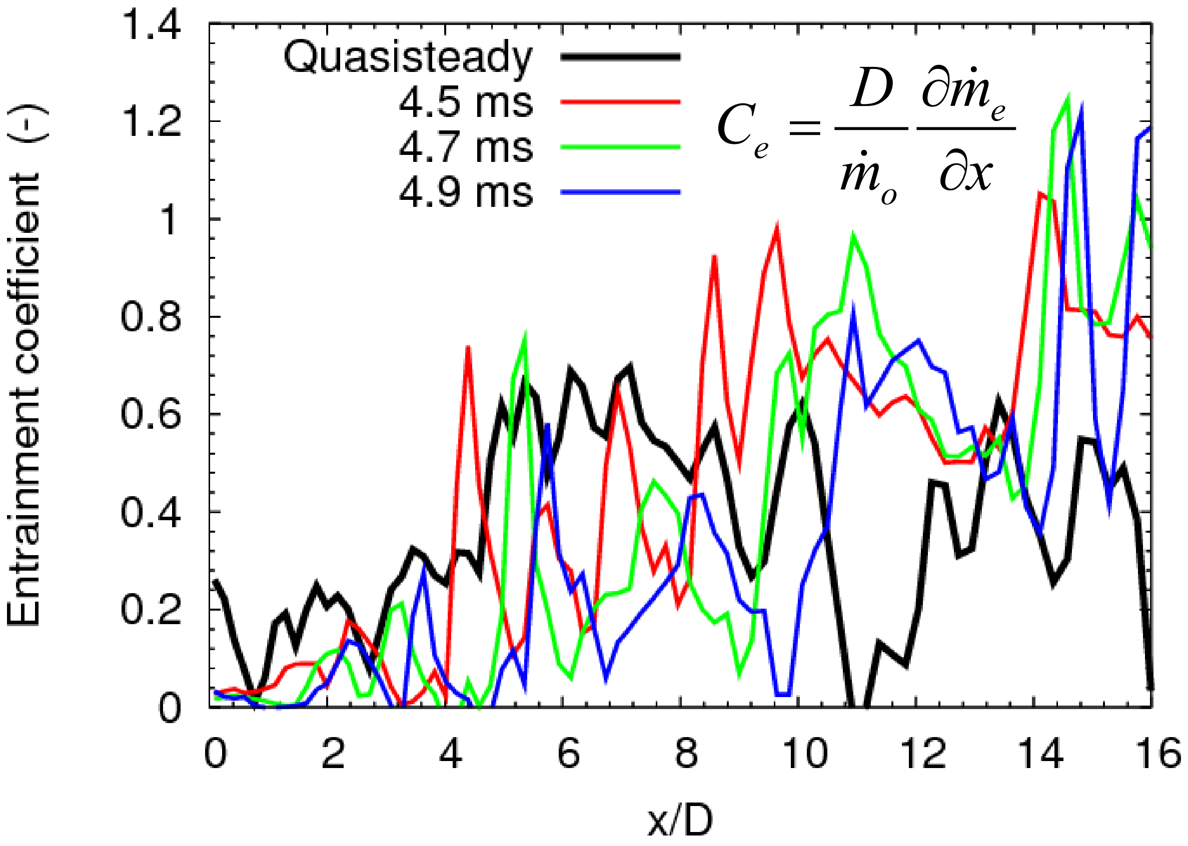
The decelerating jet shows increased entrainment compared with the quasi-steady jet



$$C_e = \frac{D}{\dot{m}_o}\frac{\partial \dot{m}_e}{\partial x}$$

- **Entrainment coefficient describes entrained mass per unit axial distance**
- **Decelerating jet shows increased entrainment in downstream region**
- **Increased entrainment leads to a much leaner mixture**

Conventional analysis only considers bulk effects, with LES we can study the unsteady broadband dynamics



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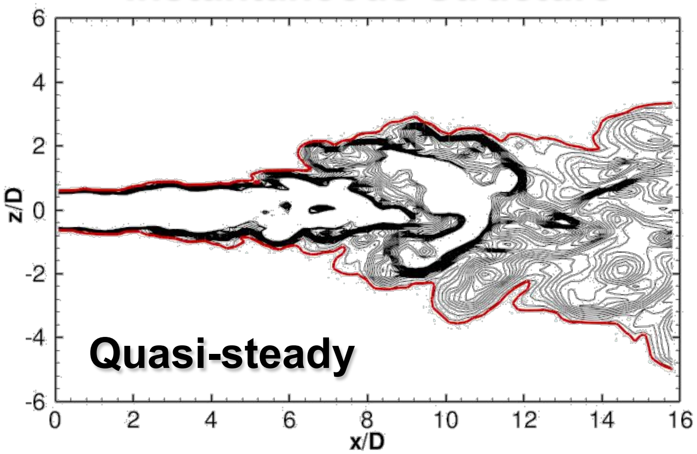
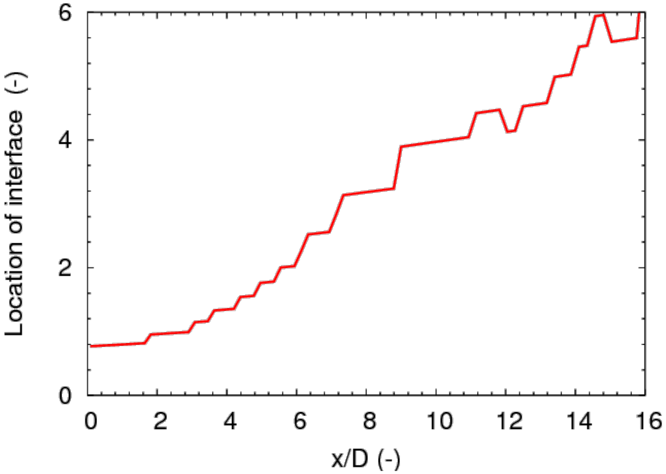
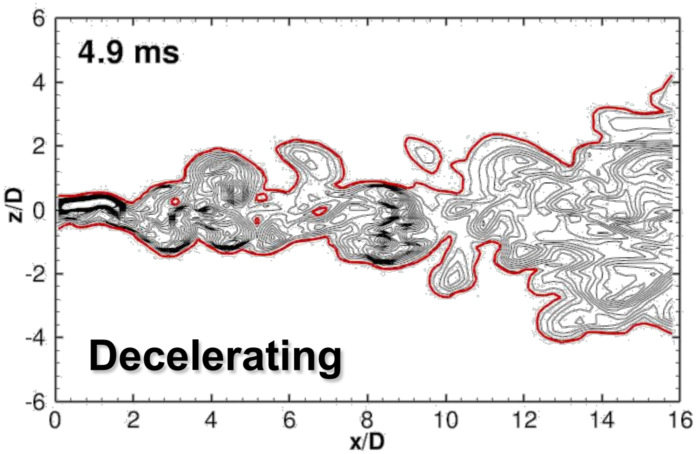
Structural differences between steady and unsteady jets is reason for difference in entrainment

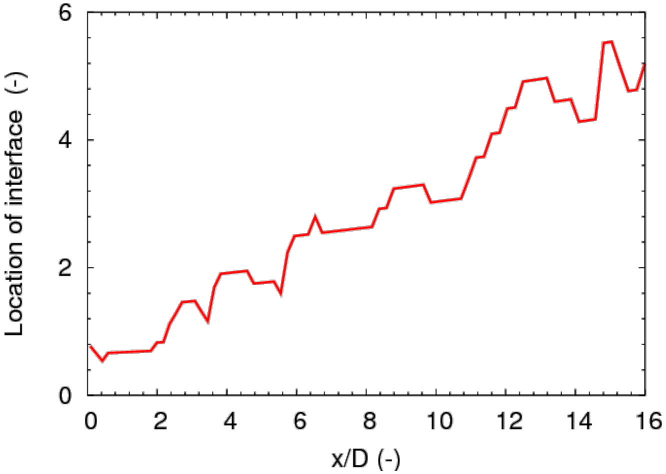
Instantaneous Structure

Location of Interface



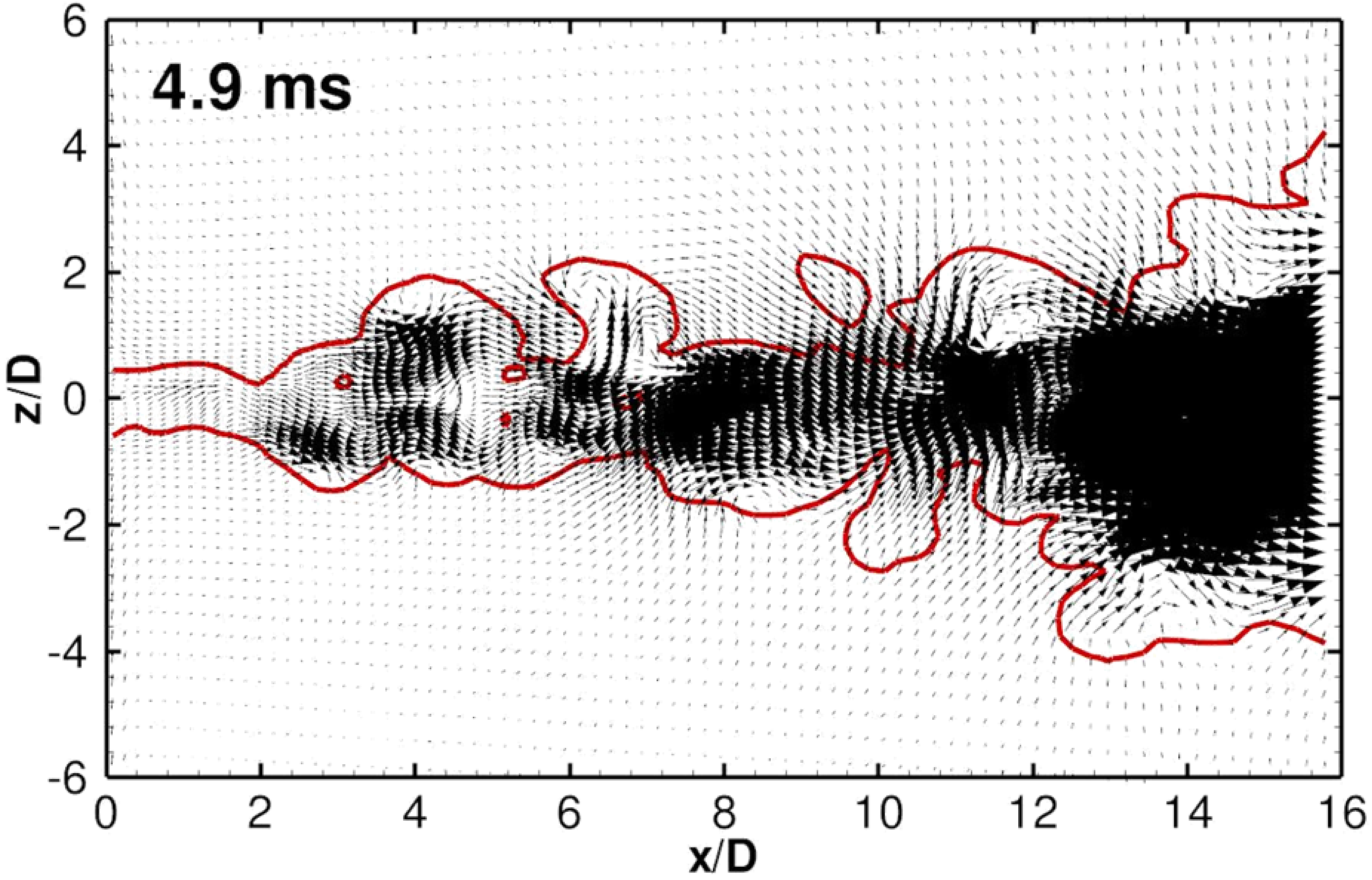






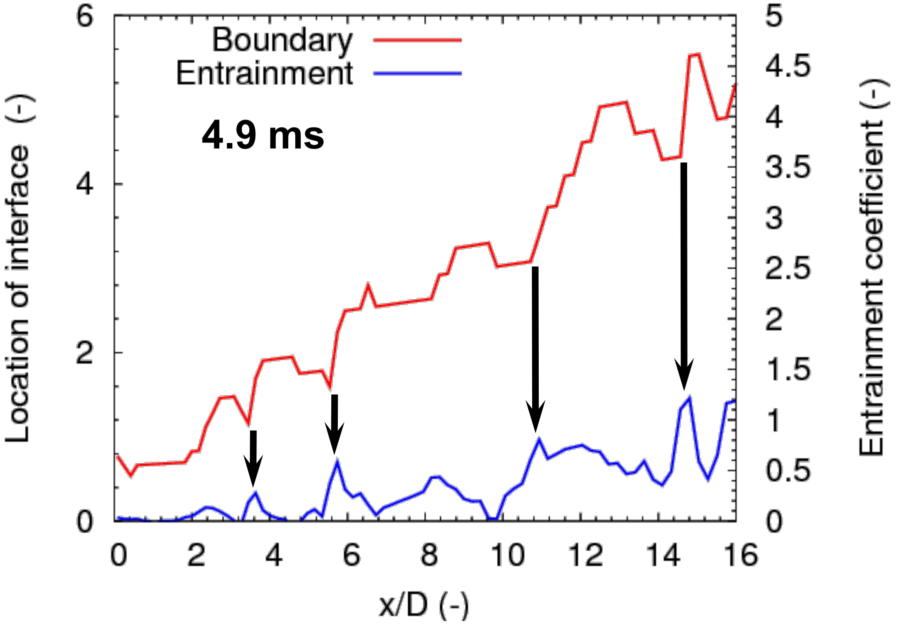
Decelerating jet exhibits more indentations on the interface

Does the formation of interface indentations induce increased entrainment?



Decelerating jet exhibits more indentations on the interface

Analysis of unsteady dynamics reveals a correlation between interface indentations and entrainment



- Each indentation accompanies increased entrainment
  - Indentations form engulfment regions
  - Engulfment regions contain large packets of ambient fluid
  - These fluids have higher probability to cross jet boundary (to be entrained)

Summary

- Region of increased entrainment forms and propagates during deceleration
  - Interface indentations are induced by flow instabilities
  - Appears to be key mechanism of enhanced entrainment
  - Has implications on fuel injection strategy and control
- Manipulation of jet instability as part of injection strategy can be used to control downstream mixing in diesel engines

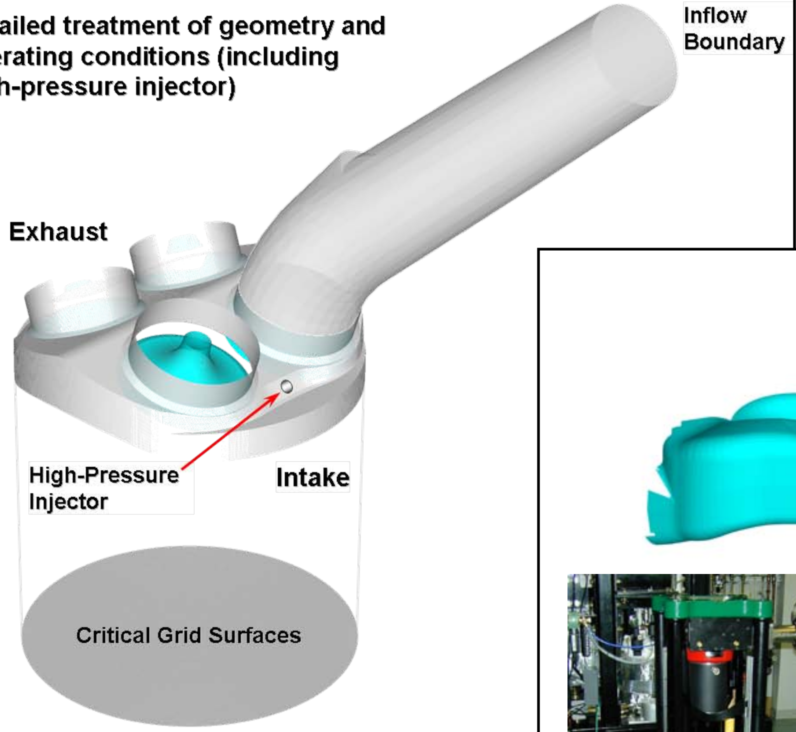
Next Steps

- Refined analysis focused on control in collaboration with Musculus et al.
- Model reduction for industry design codes in collaboration with Rutland et al.
- Extension to n-heptane combustion using ECN target cases in collaboration with Pickett et al.

Accomplishments 2, 3: In-cylinder flow dynamics and combustion in the CRF hydrogen and HCCI engines

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)

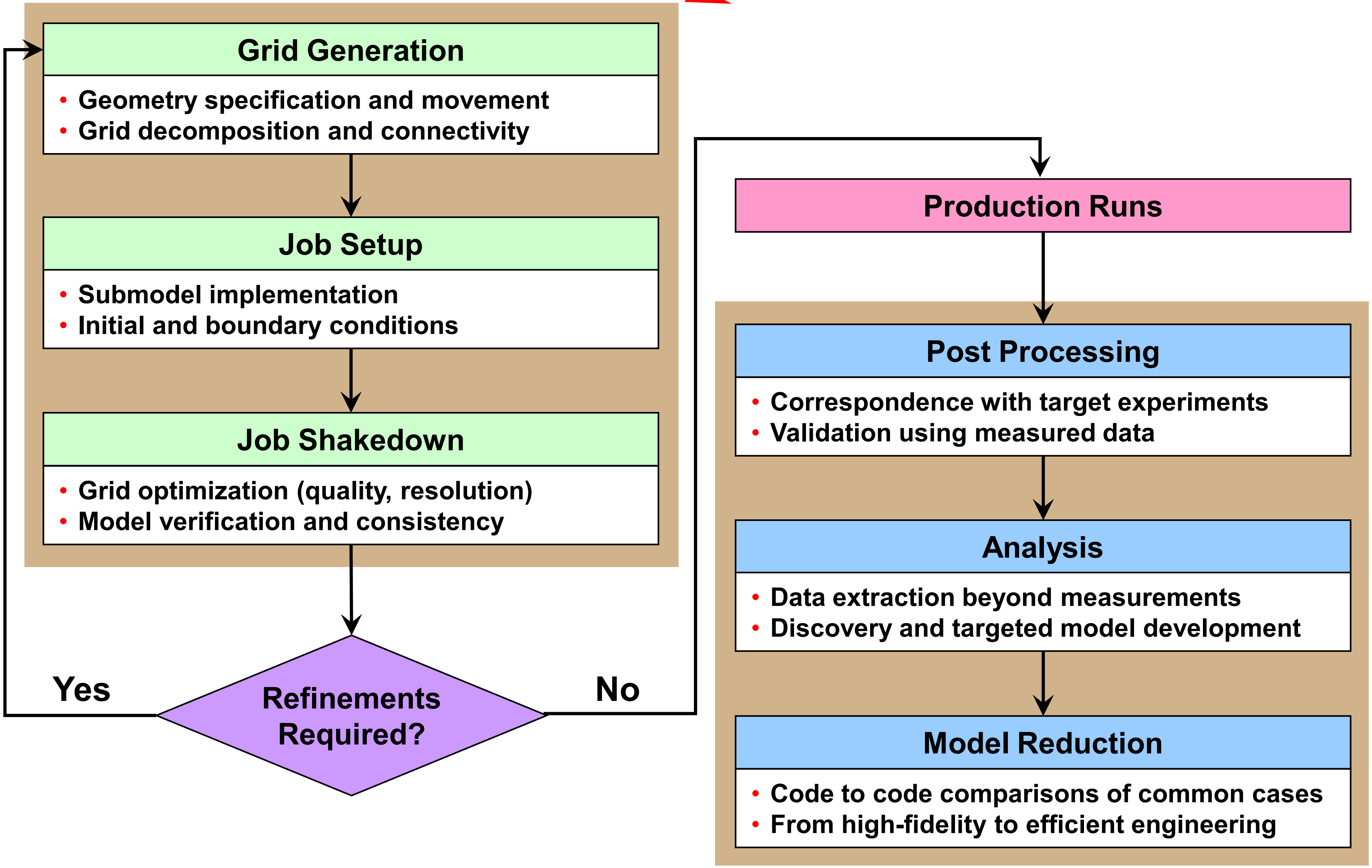


Direct-Injection Hydrogen-Fueled IC-Engine (Kaiser et al.)

HCCI Engine (Dec et al.)

Process for in-cylinder calculations

Grid generation currently a huge bottleneck



Grid Generation

- Geometry specification and movement
- Grid decomposition and connectivity

Job Setup

- Submodel implementation
- Initial and boundary conditions

Job Shakedown

- Grid optimization (quality, resolution)
- Model verification and consistency

Refinements Required?

Yes

No

Production Runs

Post Processing

- Correspondence with target experiments
- Validation using measured data

Analysis

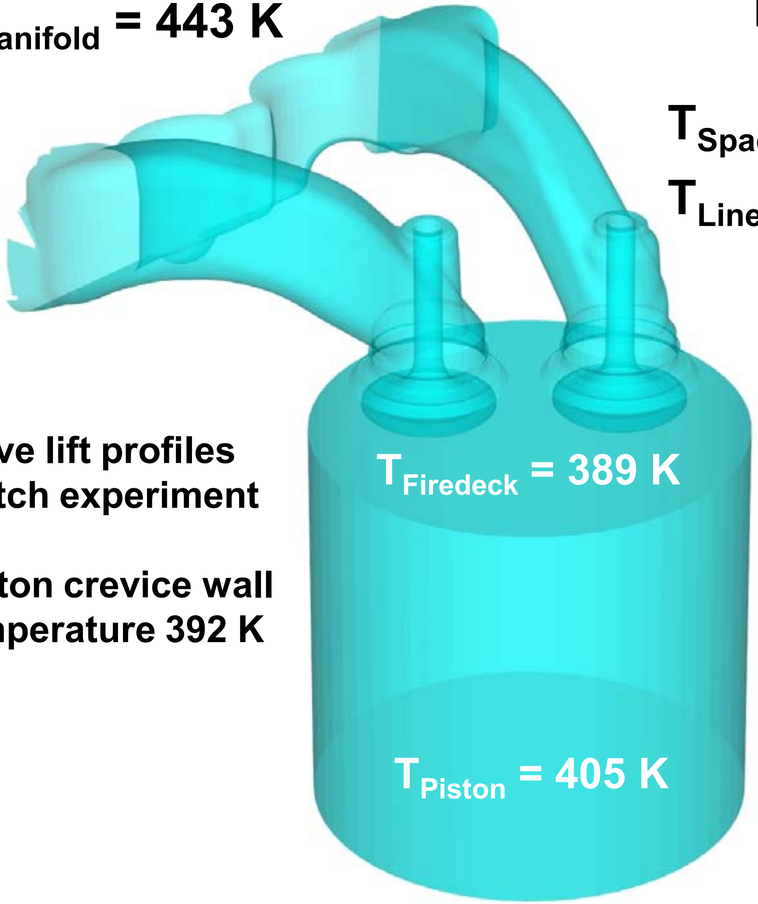
- Data extraction beyond measurements
- Discovery and targeted model development

Model Reduction

- Code to code comparisons of common cases
- From high-fidelity to efficient engineering

Preliminary simulation of natural thermal stratification processes in HCCI engines

$T_{Manifold}$ = 443 K



$T_{Firedeck}$ = 389 K

T_{Piston} = 405 K

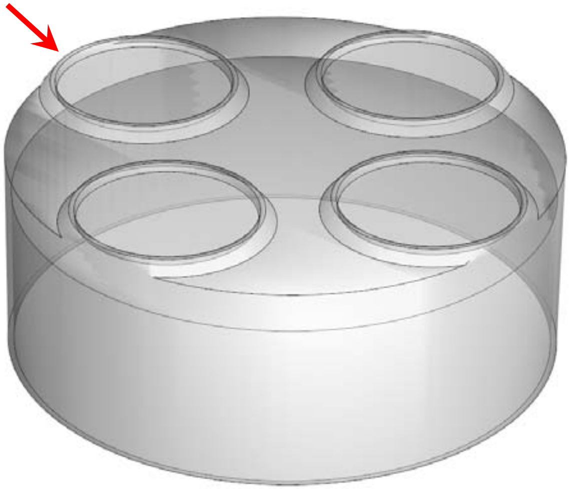
Valve lift profiles match experiment

Piston crevice wall temperature 392 K

Valve seat indentations must be accounted for

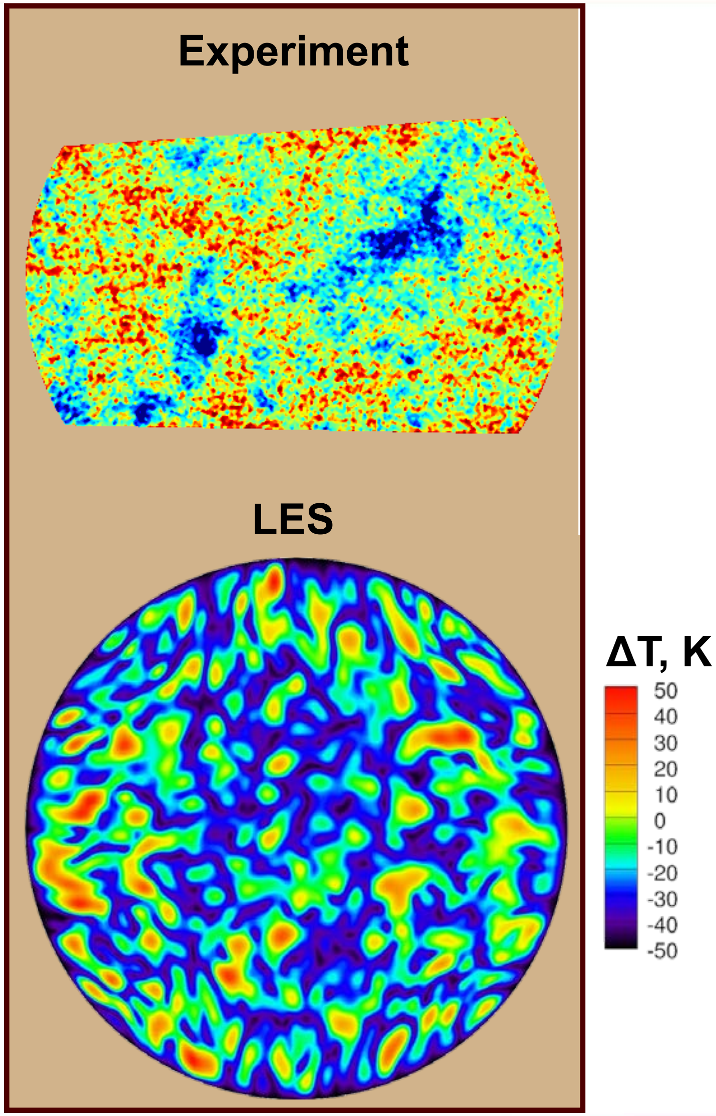
T_{Spacer} = 401 K

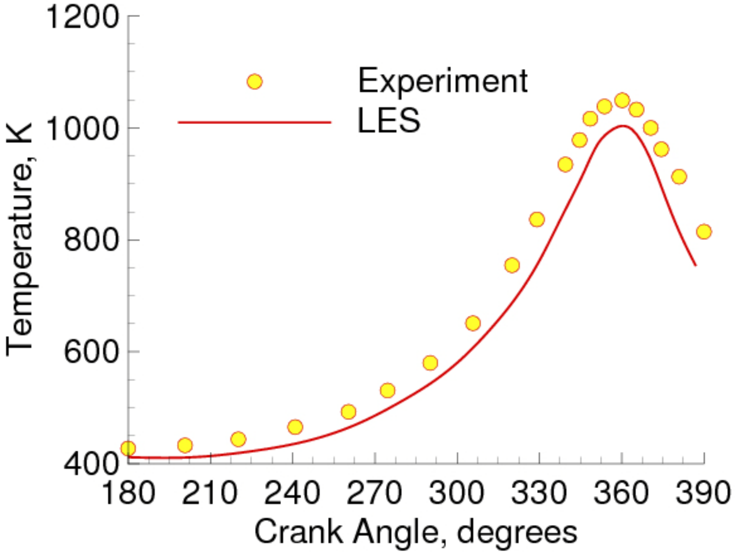
T_{Liner} = 378 K



Bore	102 mm
Stroke	120 mm
Connecting Rod Length	192 mm
Compression Ratio	14:1
Engine Speed	1200 rpm
Intake Pressure	100 kPa (absolute)
Intake Temperature	170 C (443 K)
Coolant Temperature	100 C

Initial qualitative comparisons with data from Dec et al. in progress





- Images at left show temperature fields at 360° CA, 4 mm below firedeck.
- Plot above shows bulk temperature in cylinder during compression
- Simulations produce similar temperature variations as a function of crank angle
- Detailed treatment of flow boundary conditions and swirl must be added

Supporting model development with emphasis on combustion and multiphase flows at high-pressures

- Turbulence-chemistry interactions
  - Continued development of combustion closures, emphasis on hydrocarbons
  - Reduction from high-fidelity models to affordable engineering-based models
- Extension to variety of fuels

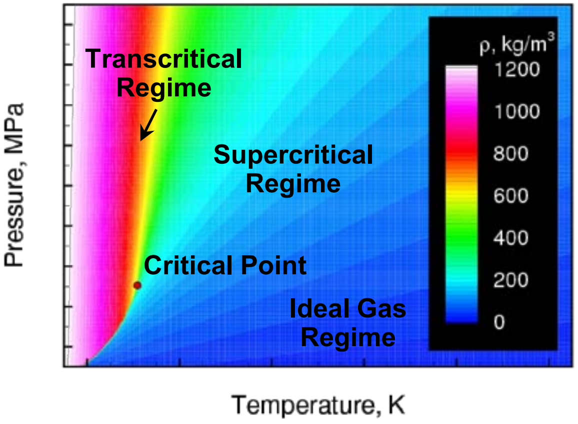
BES ⇨ – Dimethyl-ether, ethane, propane, ethylene

OVT ⇨ – Ethanol, dodecane, n-heptane, iso-octane

Thermophysical Properties

High-pressure, low-temperature multiphase combustion processes require treatment of non-ideal gases and liquids at near-critical and supercritical conditions.

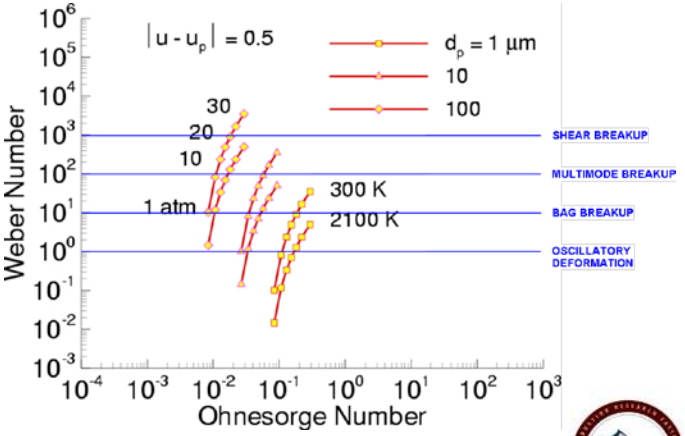
Our existing capabilities in this area will be further generalized over the next review cycle.



J.C. Oefelein (2010.). General package for evaluation of multicomponent real-gas and liquid mixture states at all pressures. SAND report.

- Progressive treatment of sprays
  - Research issues are well known
    - Atomization and treatment of interfaces
    - Near-critical, supercritical jet disintegration
    - Secondary breakup, dense spray dynamics
    - Dilute drop dynamics and combustion
  - Adopt hierarchal approach
    - Past work has demonstrated baseline accuracy for dilute particle-laden flow
    - Extend findings for case of dilute vaporizing flow (e.g., Masri et al.)
    - Work toward treatment of secondary breakup and incorporation of combustion
    - Concurrent efforts on jet atomization and interface dynamics (Herrmann et al.)

Past studies have facilitated mapping of key secondary breakup phenomena over typical device scale conditions.



Collaborators … Special thanks to Dr. Bing Hu, Postdoctoral Appointee funded under this project

- CRF Departments 8351, 8353, 8362, 8367, 8963 (Barlow, Chen, Dec, Frank, Kaiser, Keller, Kerstein, Mayo, Miles, Musculus, Najm, Pickett, Rouson, Settersten, Shaddix, Siebers, Steeper).
  - 8353: Combustion Chemistry
  - 8362: Engine Combustion
  - 8367: Hydrogen & Combustion Technology
  - 8963: Scalable Modeling & Analysis

- Professor W. Anderson, Purdue University.
- Professor J.-Y. Chen, University of California, Berkeley.
- Professor A. Dreizler, Technical University of Darmstadt, Germany.
- Professor B. Geurts, University of Twente, The Netherlands.
- Professor D. Haworth, The Pennsylvania State University.
- Professor J. Janika, Technical University of Darmstadt, Germany.
- Professor A. Kempf, Imperial College London, UK.
- Professor T. Lieuwen, Georgia Institute of Technology.
- Professor K. Mahesh, University of Minnesota.
- Professor S. Menon, Georgia Institute of Technology.
- Professor C. Merkle, Purdue University.
- Professor M. Modest, University of California, Merced.
- Professor C. Pantano, University of Illinois at Urbana-Champaign.
- Professor T. Poinsot, CERFACS, France.
- Professor S. Pope, Cornell University.
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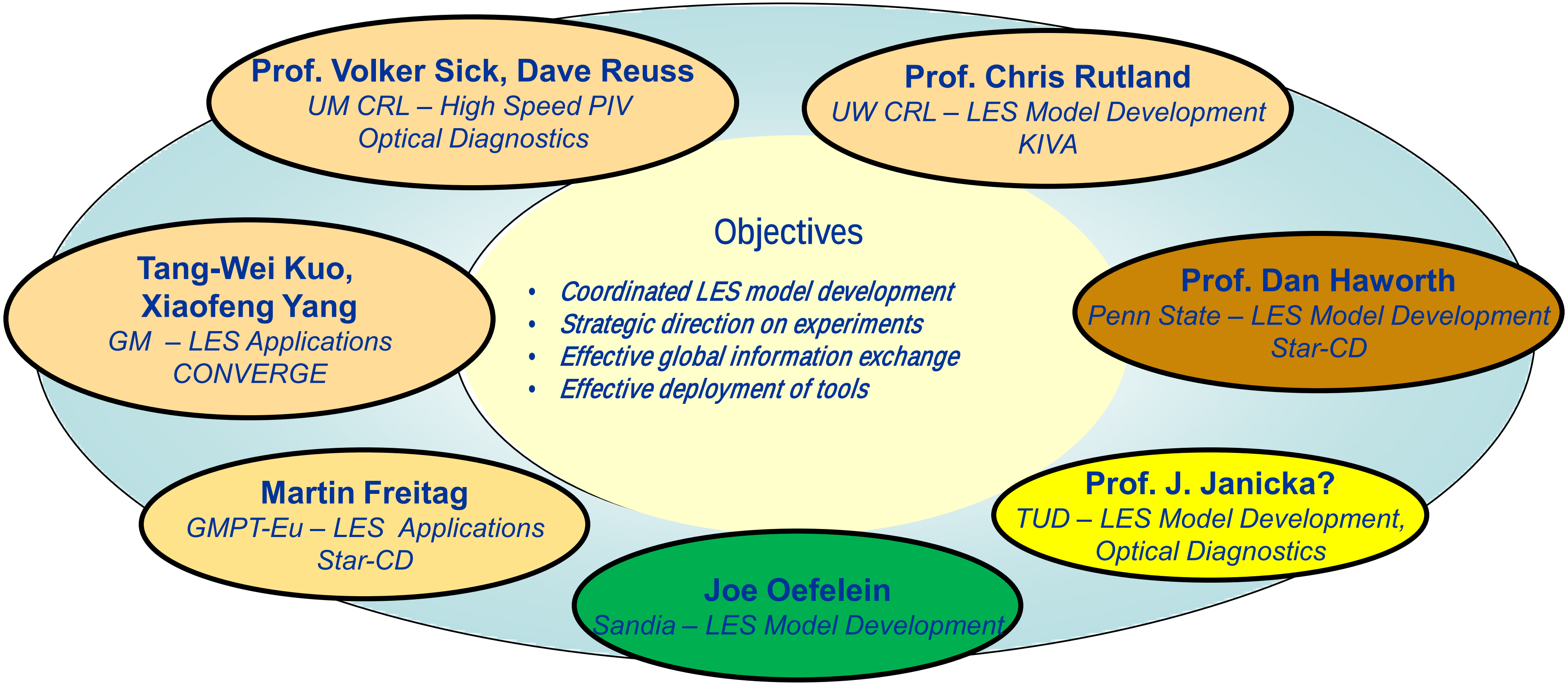
- Professor R. Santoro, The Pennsylvania State University.
- Professor V. Sick, University of Michigan.
- Professor H. Wang, University of Southern California.
- Professor V. Yang, Georgia Institute of Technology.

- Dr. J. Bell, Lawrence Berkeley National Laboratory.
- Dr. J. Bellan, NASA Jet Propulsion Laboratory.
- Dr. C. Carter, Air Force Research Laboratory, WPAFB, OH.
- Dr. T. Drozda, Rolls Royce Aircraft Engines.
- Dr. O. Haidn, The German Aerospace Center (DLR).
- Dr. D. Kothe, Oak Ridge National Laboratory.
- Dr. T.-W. Kuo, General Motors R&D Center.
- Dr. M. Oschwald, The German Aerospace Center (DLR).
- Dr. S. Rahman, NASA Stennis Space Center.
- Dr. M. Roquemore, Air Force Research Laboratory, WPAFB, OH.
- Dr. R. Sankaran, Oak Ridge National Laboratory.
- Dr. V. Sankaran, United Technologies Research Center.
- Dr. K. Tucker, NASA Marshall Space Flight Center.
- Dr. D. Talley, Air Force Research Laboratory, EAFB, CA

- Postdoc's and Students
- Tomasz Drozda, University of Pittsburgh, Oct 2005 – Oct 2008.
- Victoria Lee, Cal. Polytechnic State University, Summer 2006, 2007.
- Vaidyanathan Sankaran, Georgia Tech., Feb 2006 – Oct 2008.
- Robert Knaus, UIUC, Summer 2007, 2008.
- Joshua Smith, University of Adelaide, Australia, 2007.
- Bing Hu, University of Wisconsin, Madison, Jan 2009 – Present.
- Jeffrey Doom, University of Minnesota, Jan 2009 – Present.
- Guilhem Lacaze, CERFACS, Toulouse France, Aug 2009 – Present.
- Ville Vuorinen, Helsinki University of Technology, Finland, 2009.
- Rainer Dahms, Aachen University, Germany, Starting Jun 2010.
- Matthieu Masquelet, Georgia Tech., 2010.

*Names in red are Postdoctoral Appointees assigned to this project

Collaborators … LES working group established for joint model development using common experiments



Prof. Volker Sick, Dave Reuss
UM CRL – High Speed PIV
Optical Diagnostics

Prof. Chris Rutland
UW CRL – LES Model Development
KIVA

Tang-Wei Kuo, Xiaofeng Yang
GM – LES Applications
CONVERGE

Objectives

- *Coordinated LES model development*
- *Strategic direction on experiments*
- *Effective global information exchange*
- *Effective deployment of tools*

Prof. Dan Haworth
Penn State – LES Model Development
Star-CD

Martin Freitag
GMPT-Eu – LES Applications
Star-CD

Prof. J. Janicka?
TUD – LES Model Development,
Optical Diagnostics

Joe Oefelein
Sandia – LES Model Development

Future Work

- 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 high-fidelity simulations of optical H_2-ICE (Kaiser et al.)
  - Validation through comparison of measured, modeled results
  - Joint analysis of data from validated simulations
- Continue simulations of HCCI engine experiments (Dec et al.)
  - Current focus on natural thermal stratification
  - Extend to reacting flow over full engine cycles
- 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
- **Major accomplishments since last review**
  - INCITE grant on DOE capability class computers (25-million CPU hours)
  - Contributions toward establishing collaborative resources and facilities
  - Detailed analysis of transient injection and entrainment processes
  - In-cylinder calculations of CRF hydrogen and HCCI engines ongoing
- **Have begun to establish technology transfer through collaborations with industry and academia with emphasis on**
  - Model reduction for industry design codes, validated suite of sub-models
    - High-pressure phenomena (chemistry, thermodynamics, transport …)
    - Multiphase flow and combustion (atomization, jet breakup …)
    - Clean and efficient combustion of using a variety of fuels …
  - Establishing model implementation and performance criteria for LES and RANS (i.e., maximize accuracy, minimize cost)