Modeling and Simulation for Energy Innovation: Wind Energy

<u>Opportunity/Goals</u> • Delivering Wind Energy at ½ Cost • Transitioning From Turbines to Plants and Facilitating High Penetration Scenarios. • Seamless/Automated Plant to Grid Integration, Transmission & Dispatch Strategy	<u>Approach to overcome Barriers – Actions</u> • Focused effort, e.g., Wind Technology Innovation Hub, to Achieve 50% Cost Reduction & Facilitate High Penetration – integrating across DOE, Industry, and academia • Multi-scale, multi-physics computational solutions • Field observations & validation data at multiple scales and multiple sites
<u>Challenge/Barriers</u> • Increase the current power generation capacity to increase energy capture • Defining the “in-situ” wind plant operating environment driving loads • Forecasting and integrated control of turbines as a plant system to optimize power and performance • Grid integration, dispatch and control of high penetration renewables • Quantification of the potential macro and micro environmental impacts	<u>Impact</u> • Drive cost reduction • Accelerate market deployment to high renewable penetration • Reduced GHG emissions while delivering power in reliable grid • Enable expanded public-private partnerships

Modeling and Simulation for Energy Innovation - Grid

Goals/Opportunity • Dynamically optimize grid operations and resources • Fully integrate dynamic intermittent sources, demand response, and consumer participation into grid resource planning and operations •	***Approach to overcome Barriers*** • Measurement and Controls: Acquire, share, and process data throughout the electric system. • Communication and Security: Establish a secure, resilient information backbone. • Modeling and Analysis: Facilitate system understanding to support better grid operations, planning, markets, and policy decision-making.
Challenge/Barriers • Future grid mix is unknown • The intermittent nature of wind/solar requires new ways to operate the grid ecosystem. • Changes in technologies and policy. • Transforming the grid has been likened to swapping an aircraft engine in flight. • Public perception and acceptance.	***Impact*** • More efficiently match supply and demand. • Improved long term infrastructure planning. • A secure, reliable, and resilient grid. • Recommendation: establish a grid hub with an appropriate focus on utilizing information technology, modeling and simulation, etc. that addresses supply and demand response

Fossil Energy – Carbon Capture

Opportunity/Goals

- Accelerate development & commercial deployment of capture technology.
- Reduce the cost of capture to $10/ton captured.

Approach to overcome Barriers - Actions

- Develop & apply validated multi-scale models for predicting behavior of whole systems at large scales (requires data).
- Develop & apply uncertainty quantification methods for multi-scale models. Identify sources of uncertainty.
- Integrate complex simulations with system-wide, multi-scale optimization (i.e., screening new materials in context of potential processes).

Challenge/Barriers

- Larger scale than ever before deployed resulting in technical and enterprise risk.
- Long scale up period typically required.
- Need for development of materials, equipment and processes.
- Complex processes (chemistry, multi-phase flow, multi-scale phenomena, systems integration).
- Lack of large scale validation data.

Impact

- Reduced time and risk for scale up and deployment.
- Enable cost-effective carbon capture (will allow Enhanced Oil Recovery (EOR), which will facilitate more adoption).
- Enable environmentally responsible use of fossil fuels to support energy security while also mitigating against climate change for both natural gas and coal.

Fossil Energy – Geologic Formations (Fracking, Enhanced Oil Recovery, Carbon Storage)

Opportunity/Goals

- Answer question: Is CO_2 storage safe and permanent?
- Answer question: Is fracking safe?
  - Ensure science-based understanding to build fracking best practices
  - Enable better waste management & disposal practices
- Answer question: Can we design novel, science based technologies for unlocking oil from oil shale/tar sands?

Approach to overcome Barriers - Actions

- Design env. benign “smart” fracking fluids.
- Improved simulation of fracture propagation.
- Better understanding of emission dynamics.
- Develop infrastructure to enable remote execution of simulation codes to answer questions in the field.
- Develop multi-scale approach to simulate kerogen nanoparticle-/clay/rock systems.
- Design methods to quantify uncertainties associated with large-scale geologic simulations.

Challenge/Barriers

- Tie physics and chemistry of fluids (fracking and CO_2) with geomechanics – multi-scale/multiphysics.
- Validation of codes.
- Need to characterize and understand failure mechanism of the well bore.
- Geological formations have diverse characteristics.
- Interaction of hydrocarbon nanomoyeties (e.g. in kerogen) with minerals.
- Oil/gas industry not broadly participating in HPC.

Impact

- Ensure the long term viability of shale gas/oil resources
  - Kerogen is an abundant source of hydrocarbons in the US.
- Ensure safety and viability of carbon storage.
- Provide scientific foundations for regulations of fracking, carbon storage, etc.

Specific Recommendations for FE

- Create new initiatives or expand existing initiatives (Carbon Capture Simulation Initiative (CCSI), National Risk Assessment Partnership (NRAP)) to specifically focus on applying advanced computing and model validation to these problems:
  - $10/ton capture
  - Determining safe fracking practices, understanding down hole behavior, assessing risks, improved (safer) fracking fluids
  - Determining fracking water disposal practices
  - Unlocking oil from shale & tar sands in environmentally sustainable manner
- Create advanced modeling & simulation component for DOE FOAs/grants for capture technology development & demonstration projects.
  - Will provide capability to develop & demonstrate advanced computing capabilities and provide access to validation data (i.e., capture technology, CO_2 injection, Marcellus shale) for portfolio of FE projects at Strategic Center for Coal (SCC) & Strategic Center for Natural Gas & Oil (SCNGO)
  - Opportunity to tie experimental projects with simulation for mutual benefit
- Develop program to improve and optimize fossil energy "carbon" life cycle from production (e.g., fracking) to transport to use (e.g. power generation) to recovery (e.g. carbon capture) to utilization or storage of CO_2 (e.g. Enhanced Oil Recovery (EOR).

Grand Challenges of Advanced Computing for Energy Innovation: Vehicles (combustion)

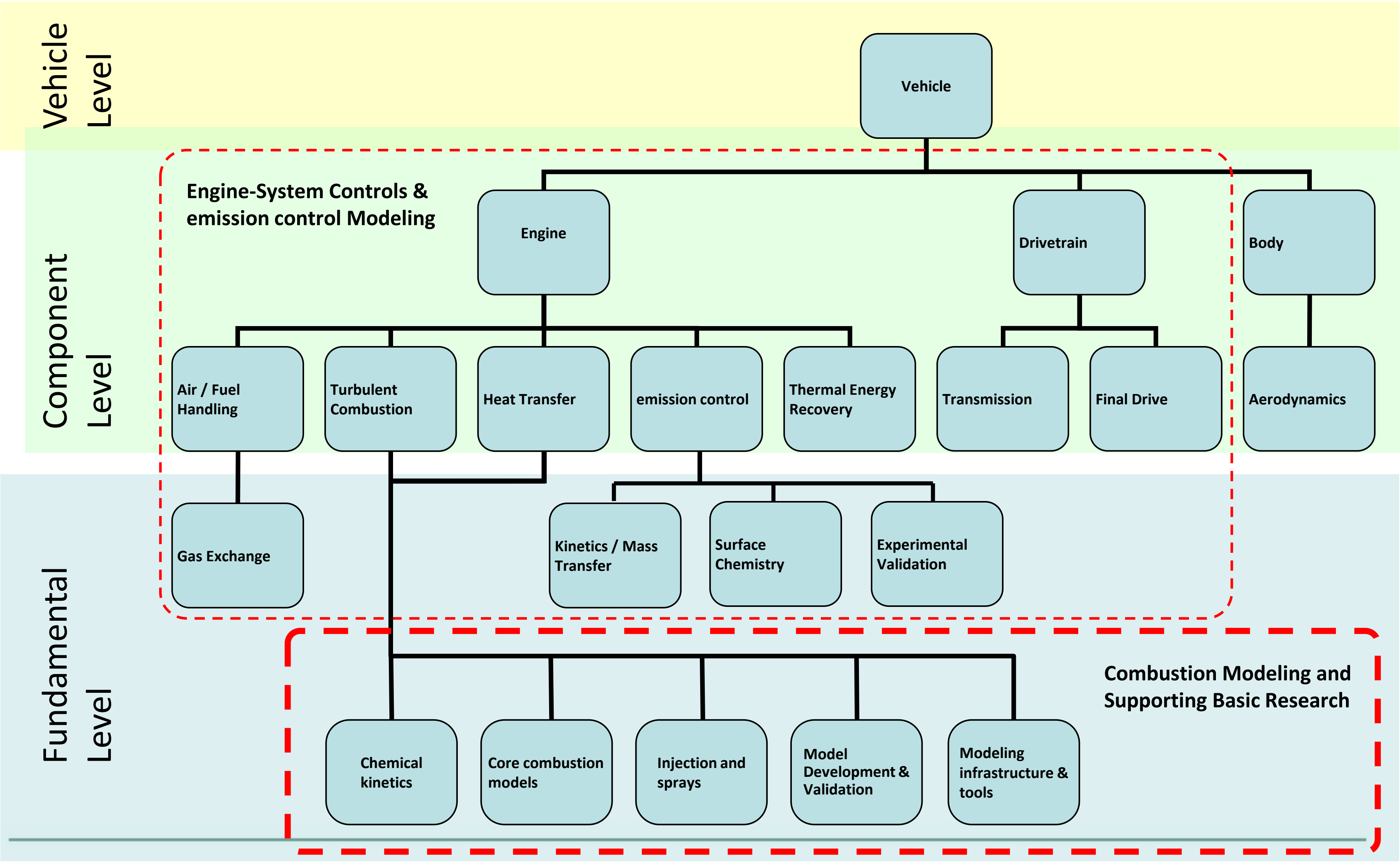
Utilizing HPC to:

- Reduce U.S. oil use by 4M barrels per day
- Dramatically decrease product time to market

Modeling and Simulation for Vehicle Innovation

Opportunity/Goals • Combustion engines • Materials: catalysis, hydrogen storage, batteries, structural • End-to-end batteries, fuel cell systems, total vehicle •Alternative fuels	**Approach to overcome Barriers - Actions** • Develop the infrastructure, both hardware and software, to implement the next generation of advanced multi-physics models •Integrated experimental and mod/sim program •Coordinated vehicle industry, DOE Lab, and software vendor effort
Challenge/Barriers • Breadth of length/time scales, complexity • Understanding of underlying physics/chemistry/kinetics • Mod/Sim development "ecosystem" inefficient •High experimental costs	**Impact** • Improved vehicle efficiency •Shorter, cheaper development times •Reduced petroleum use •Enable alternative vehicles •Lower environmental impact

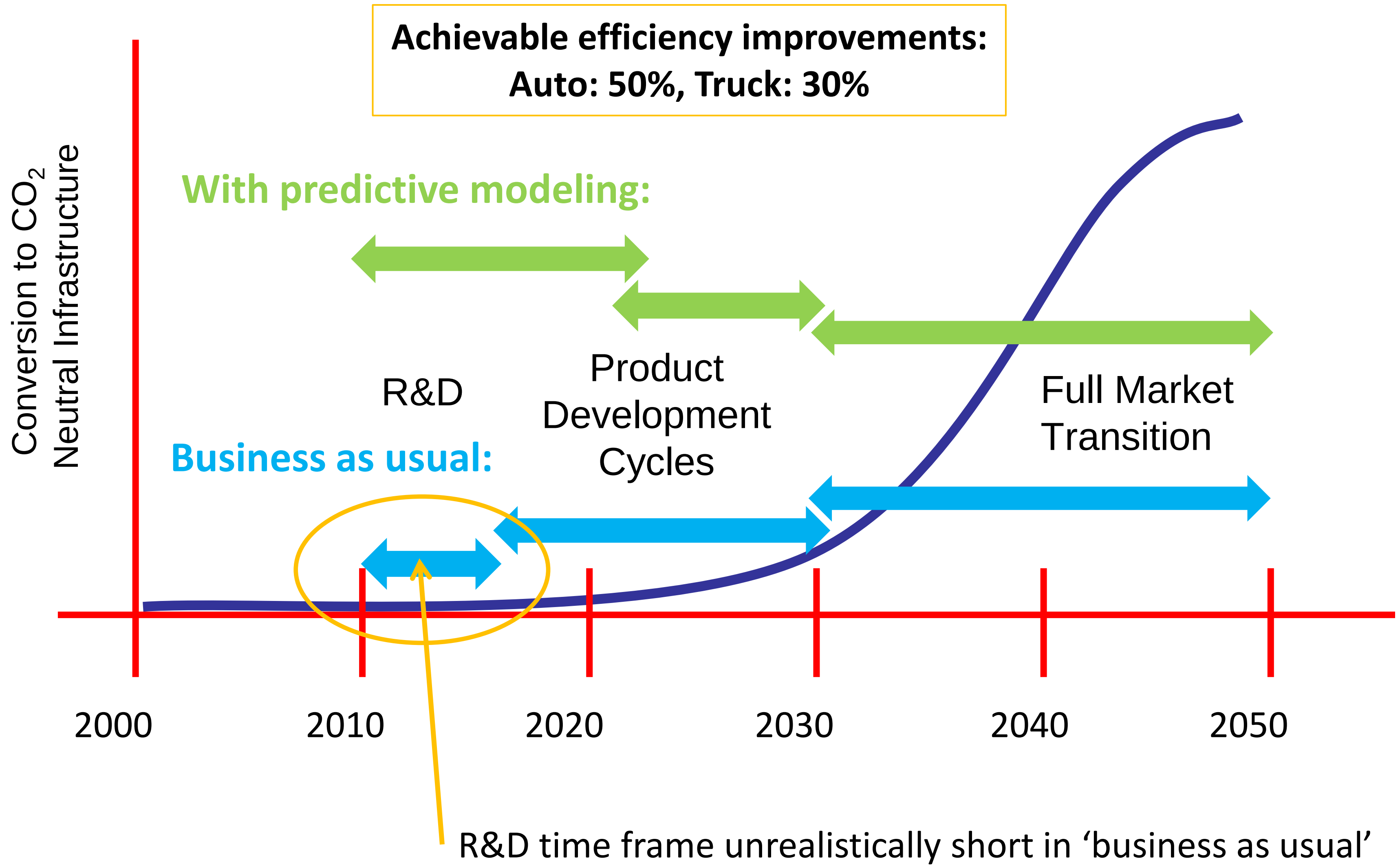
Vehicle Model Hierarchy



Combustion modeling overview

- **Integration of combustion models with vehicle-level simulation is achievable.**
- **The program approach must focus on**
  - key technical targets (identified by critical needs and model shortcomings)
  - well-defined benchmark configurations (for both experiments and simulations)
- **A hierarchy of combustion models is needed:**
  - Full drive-cycle simulations and system-level optimizations
  - Multi-dimensional engineering models
    - fine-tune system optimizations
    - optimize engine geometry
    - capture fuel effects
    - can be used to develop efficient low-order models
  - High-fidelity LES simulations and experiments
    - develop the physical foundation for engineering models
    - tune them for accuracy
    - establish their range of applicability

Product Development Must Be Accelerated To Meet Energy Goals



Identified Industry Barriers For Advanced Engines

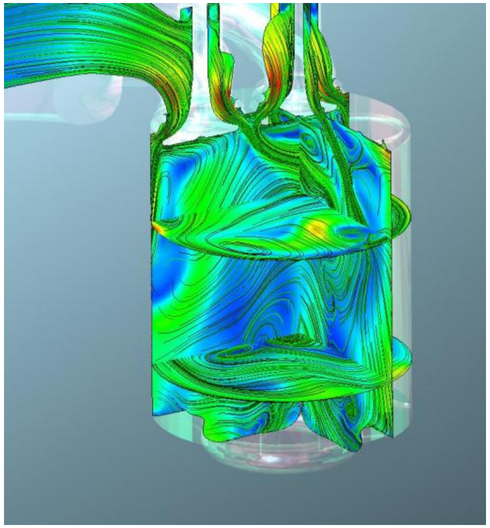
Highest priorities – PreSICE workshop focus

1. Effect of stochastic nature of in-cylinder flow on engine combustion, performance and emissions
2. Spray modeling and experimentation in dense spray and nozzle internal flow regions, including physics like cavitation and flash boiling
3. Surface chemistry and physics for high-efficiency, low-temperature catalysis and filtration
4. Fundamental understanding of near-wall processes (e.g., flow, heat transfer, diffusion, chemistry, wall films)
5. High-pressure, dilute combustion including turbulence-chemistry interaction and extremes of equivalence ratio, dilution, and turbulence

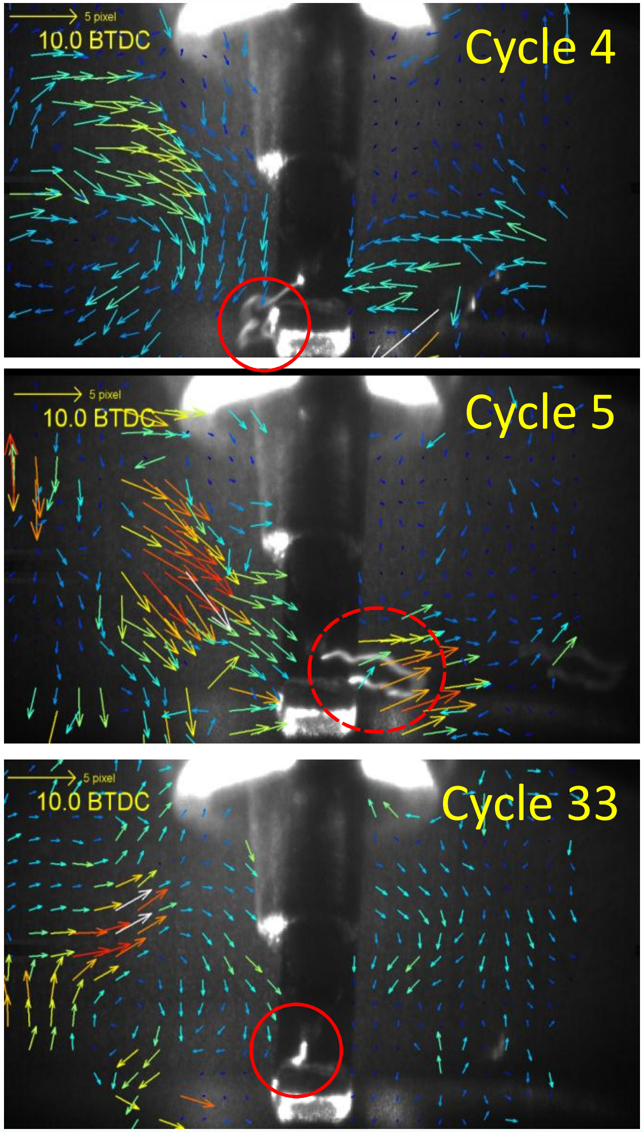
All can be mitigated or overcome through science-based modeling

Stochastic Processes Priority Research Direction

- **Development and validation of models to enable simulation of stochastic processes**
  - Sub-grid scale models for unresolved processes
  - Reduced chemical kinetic mechanisms
  - New theoretical frameworks / efficient numerical approaches



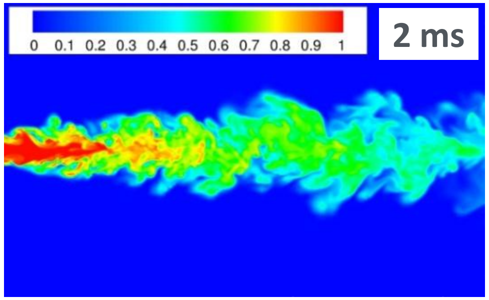
Complex in-cylinder flow during intake stroke in diesel engine



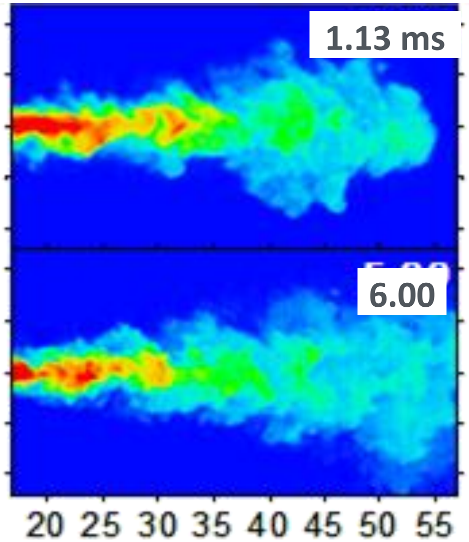
Providing New Breakthroughs with HPC: High-fidelity, Large Eddy Simulation (LES) Coupled with Engine Experiments

- ❑ **Currently simulating a progression of fuel injection sprays for direct injection engines.**
  - Validated high-fidelity LES is run on DOE supercomputer platforms
  - Results providing insights for improving engineering CFD models

Large Eddy Simulation of fuel concentration

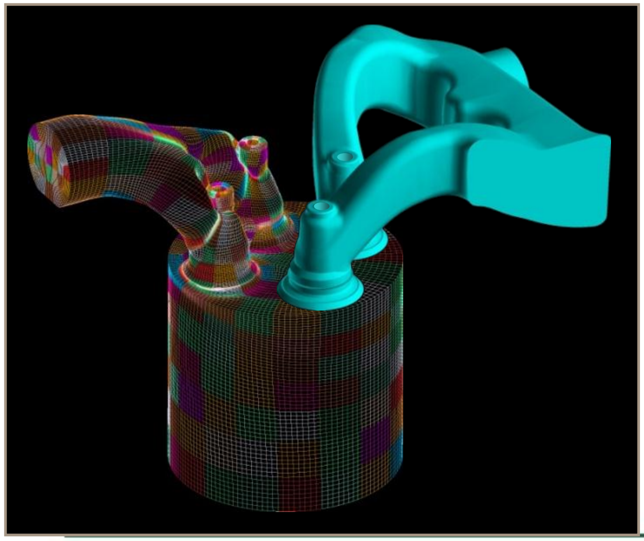


Rayleigh Scattering images of fuel concentration



Axial Distance, mm

Sandia HCCI Engine grid for LES



- ❑ **HCCI engine LES in progress:**
  - Demonstrated LES can capture physics
  - Now focused on improving grid fidelity (advanced gridding)
    - Intake flow with anti-swirl plate
    - Valve seat indentations and piston crevice
    - Detailed heat transfer model for walls
  - Simulations will explore thermal stratification effects on heat release rate to improve understanding and engineering models

What is the impact ***if*** new 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 60% limit on thermodynamic efficiency**

Potential for saving 4 M barrel of petroleum per day

A program based on PreSICE workshop results will enhance U.S. competitiveness and the future workforce for industry, improve energy security, and promote global environmental security.