High Fidelity Direct Numerical Simulations of Turbulent Combustion

Presented by

Jacqueline H. Chen (PI), Chun Sang Yoo, Gaurav Bansal, Hongfeng Yu, Ajith Mascarenhas

Combustion Research Facility
Sandia National Laboratories, Livermore, CA

Ray Grout

National Renewable Energy Lab

Tianfeng Lu

University of Connecticut

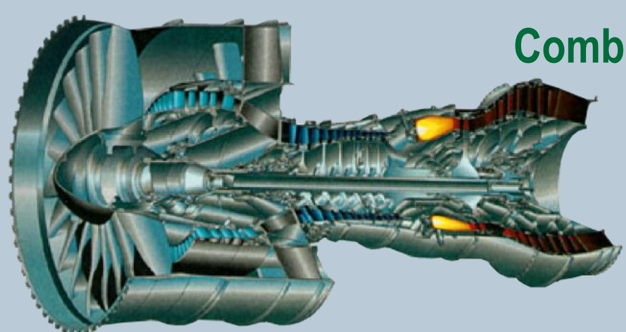
Ramanan Sankaran

National Center for Computational Sciences
Oak Ridge National Laboratory

Direct numerical simulation (DNS) of turbulent combustion

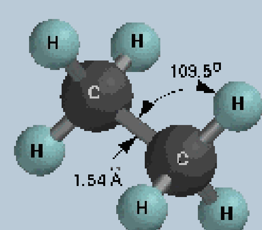
Turbulent combustion is a grand challenge

- Turbulent combustion involves coupled phenomena at a wide range of scales
- O(10^4) continuum scales



Combustor size ~1 m

Molecular reactions ~1 nm

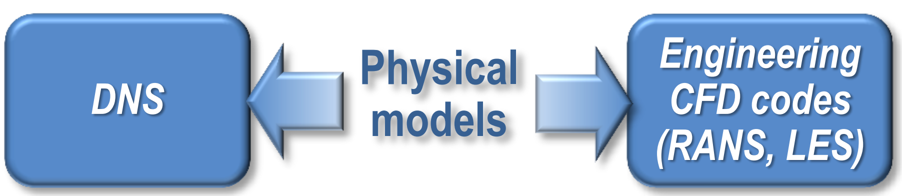


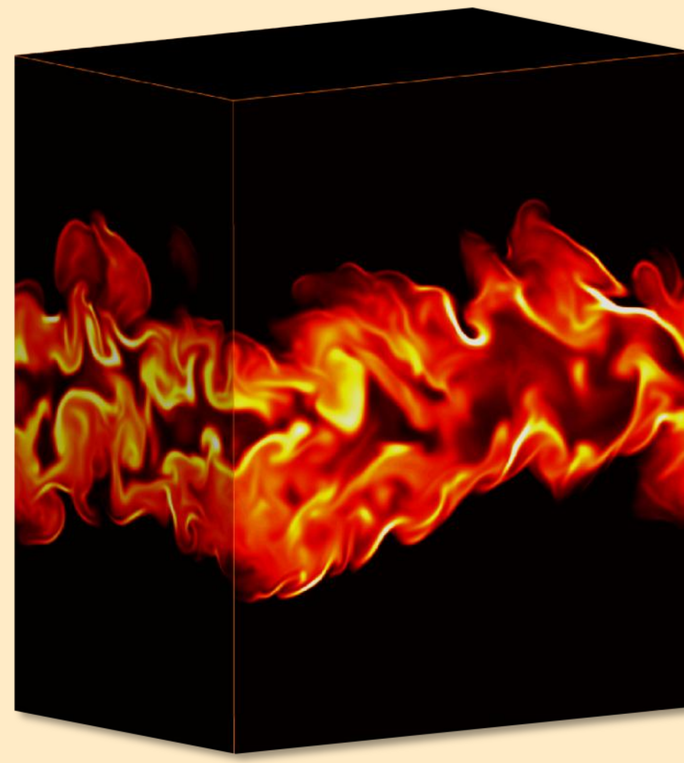
DNS approach and role

- Fully resolve all continuum scales without using subgrid models
- Only a limited range of scales is computationally feasible
  - Petascale computing = DNS with O(10^4) scales for cold flow
- DNS of small-scale laboratory flames
  - Investigate turbulence-chemistry interactions relevant in devices
  - Validate experimental measurement approach (e.g., 2D vs. 3D, surrogate scalars)
  - Provide numerical benchmark data for predictive model development and validation for coarse-grain engineering CFD

S3D—first-principles combustion solver

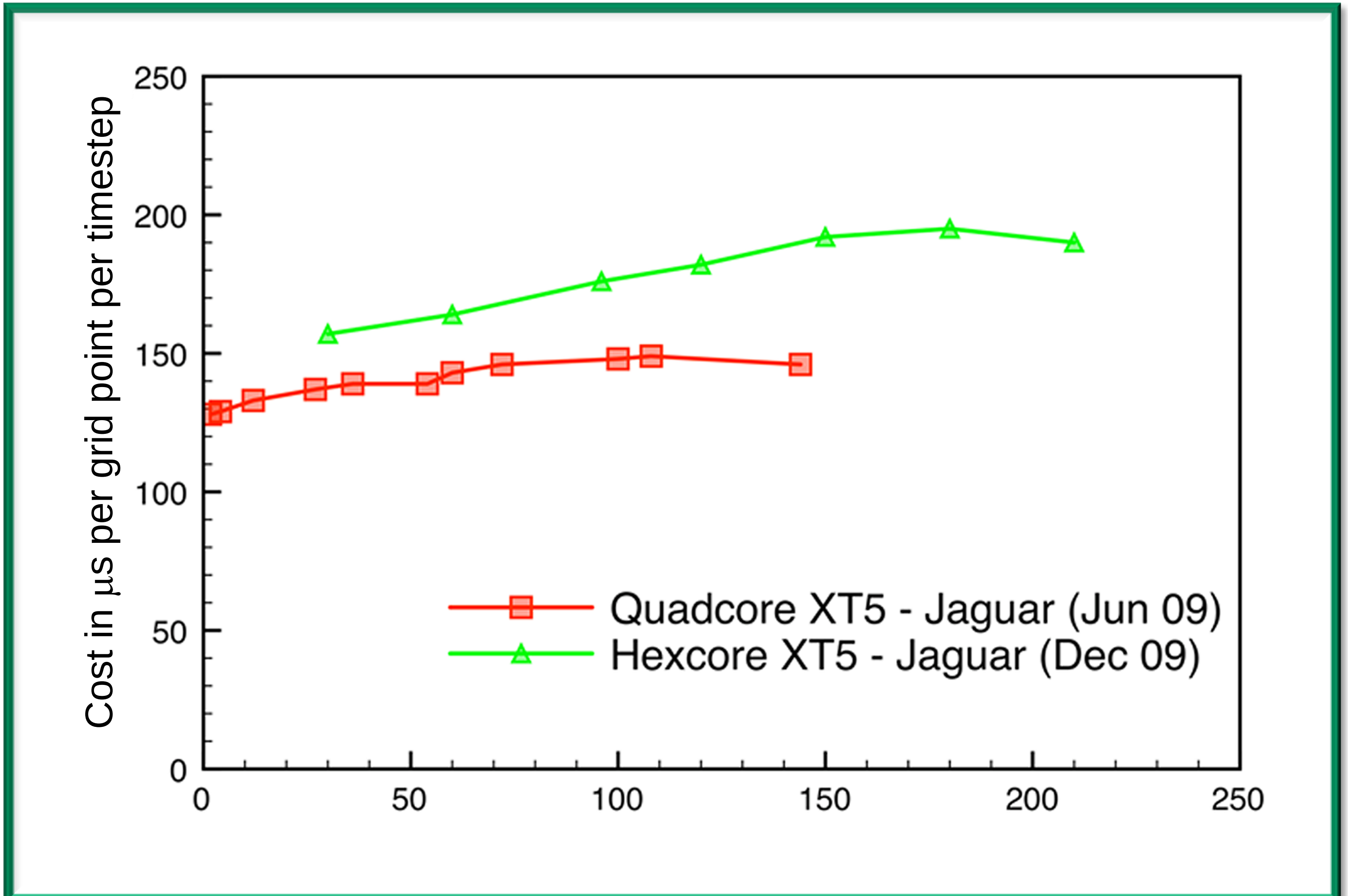
- Used to perform first-principles-based DNS of reacting flows
- Solves compressible reacting Navier-Stokes equations
- High-fidelity numerical methods
- Detailed reaction-kinetics and molecular-transport models
- Multiphysics (sprays, radiation, and soot) from SciDAC-TSTC
- Ported to all major platforms
- Particle-tracking capability



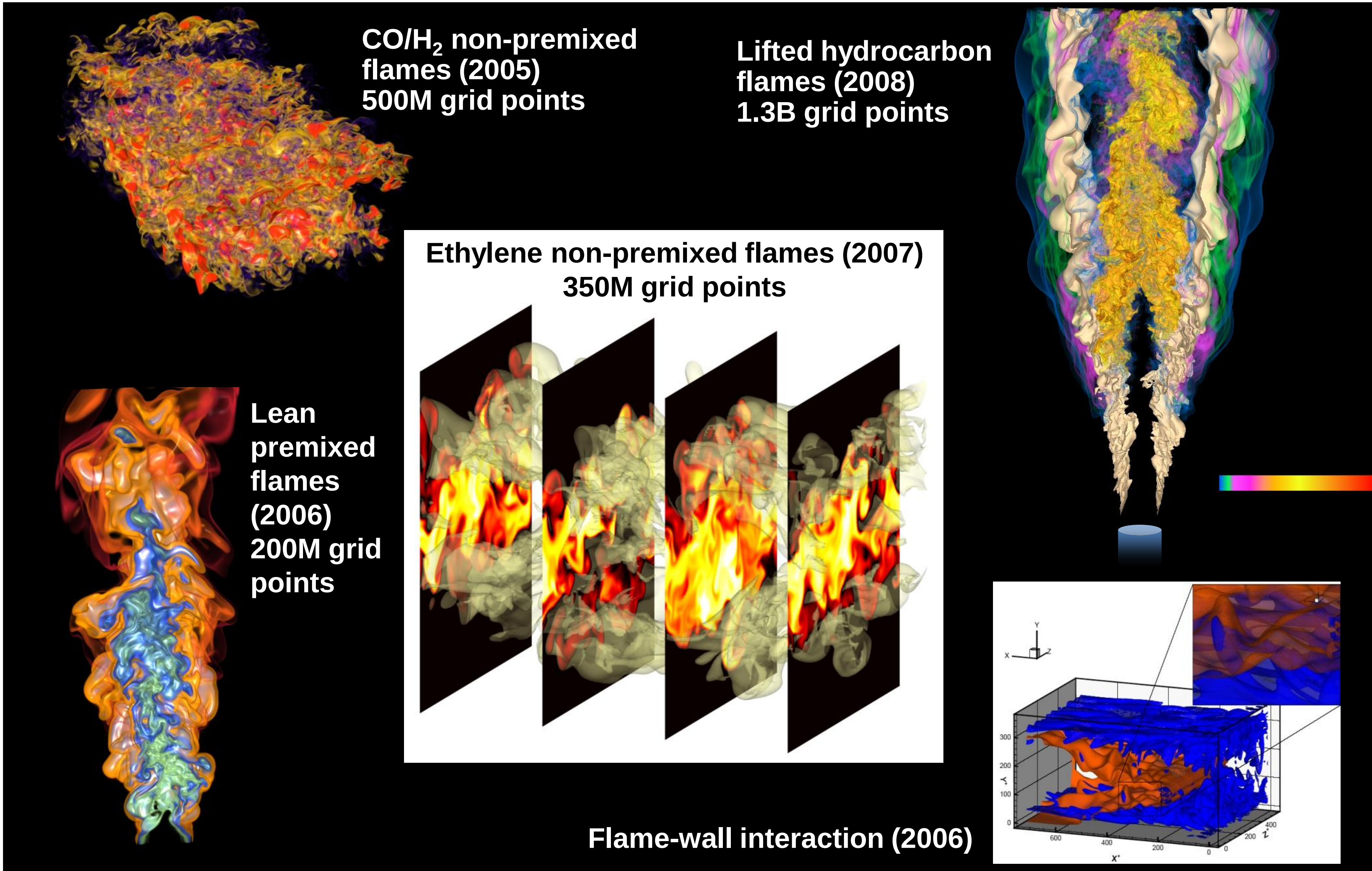


DNS provides unique fundamental insight into the chemistry-turbulence interaction

Efficient parallel scaling on Jaguar



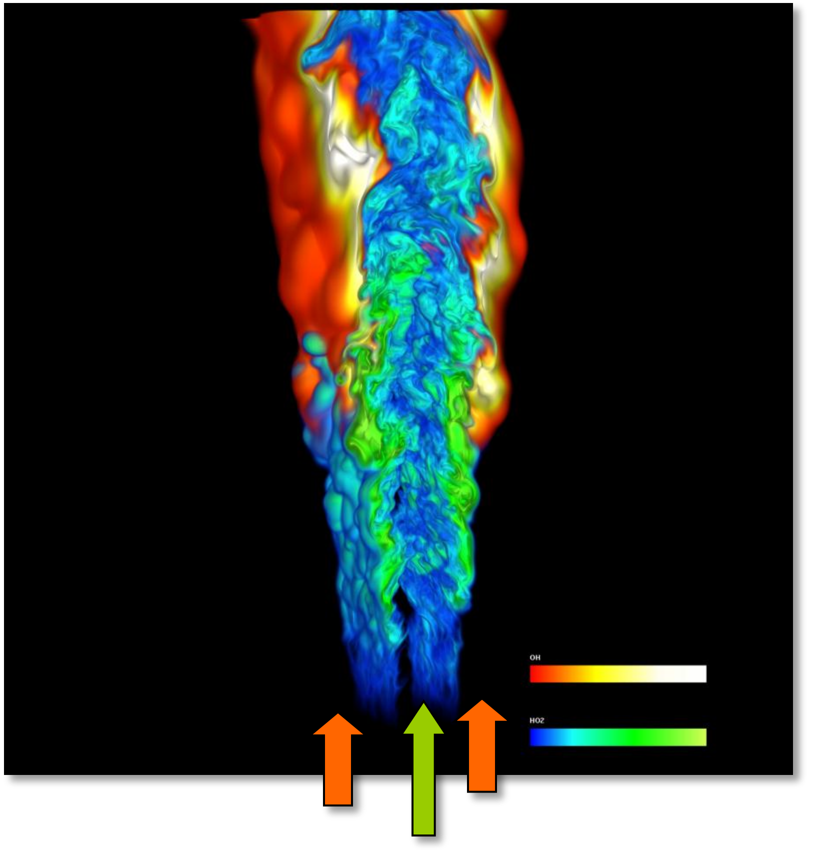
Combustion science enabled by NCCS



DNS of lifted ethylene-air jet flame in a heated coflow

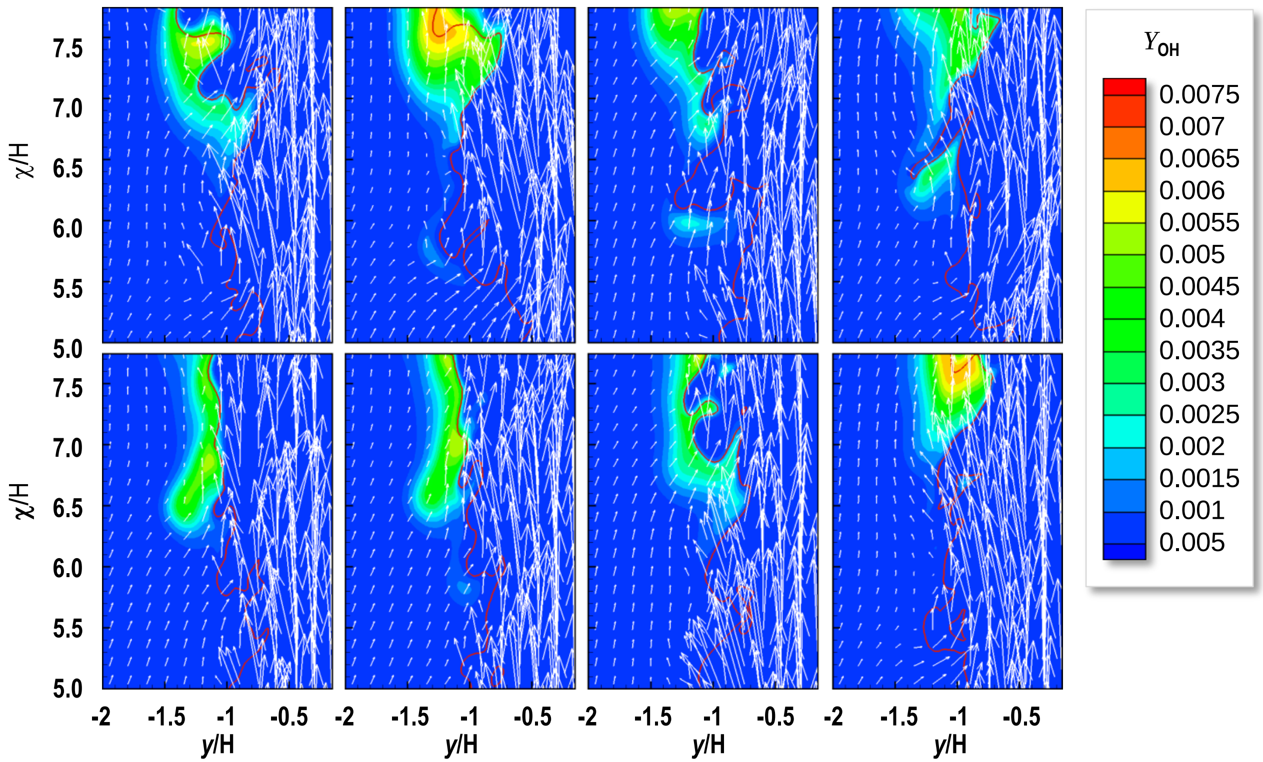
- 3D slot burner configuration:
  - $L_x \times L_y \times L_z$ = 30 × 40 × 6 mm^3 with 1.28 billion grid points
  - High fuel jet velocity (204 m/s); coflow velocity (20 m/s)
  - Nozzle size for fuel jet, H = 2.0 mm
  - Re_{jet} = 10,000; τ_j = 0.15 ms; 3 flow-through times
  - Cold fuel jet (18% C_2H_4 + 82% N_2) at 550 K, $\eta_{st} \approx 0.27$
  - Detailed C_2H_4/air chemistry, 22 species, 18 global reactions, 201 steps
  - Hot coflow air at 1,550 K
- Performed on CrayXT4 at ORNL on 30,000 cores and 7.5 million cpu hours
  - 240 TB field data, 50 TB particle data

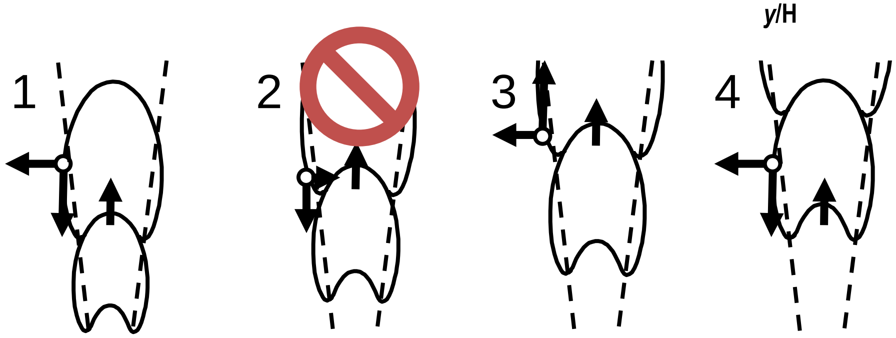
Ethylene-air lifted jet flame at Re = 10000



Conceptual stabilization mechanism

Temporal evolution of OH mass fraction showing ignition kernel growth and convection with jet mixing structure at t/τ_j = 0.227 ~ 1.160, black line stoichiometric mixture fraction, arrows are velocity vectors

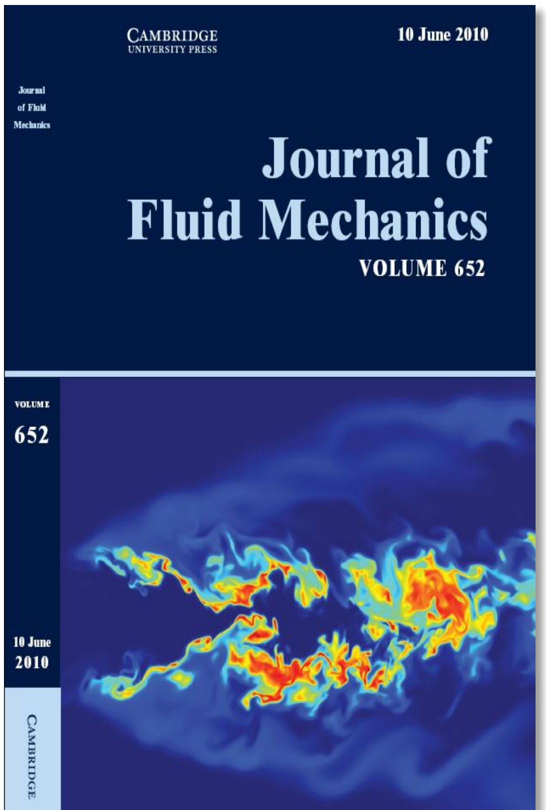


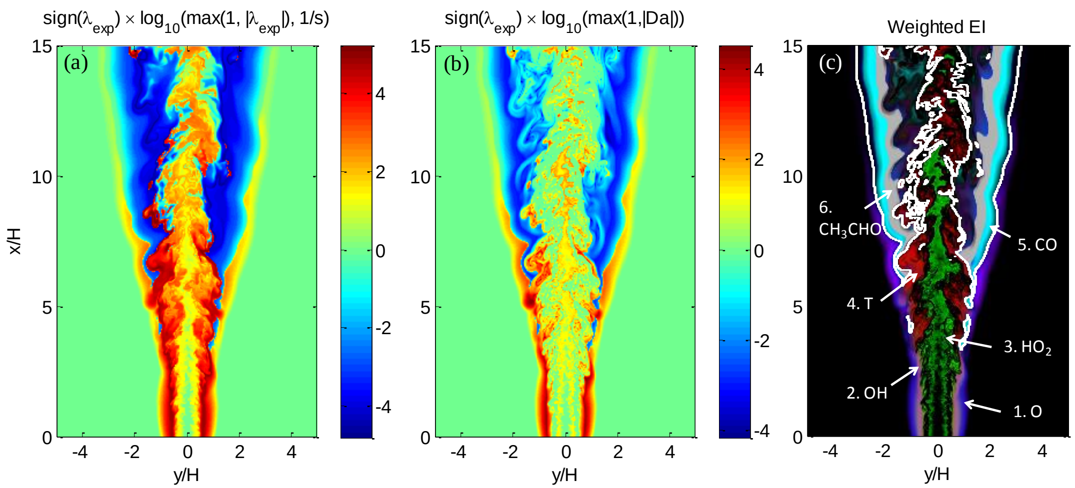


Convective velocity greater than displacement speed for η_{st} = 0.27

1. Ignition occurs in lean mixtures with low χ
2. No self-propagation upstream with mixing structure
3. Local extinction occurs by high χ, or flame shortening occurs as the point is convected downstream
4. Ignition occurs in another coherent jet structure

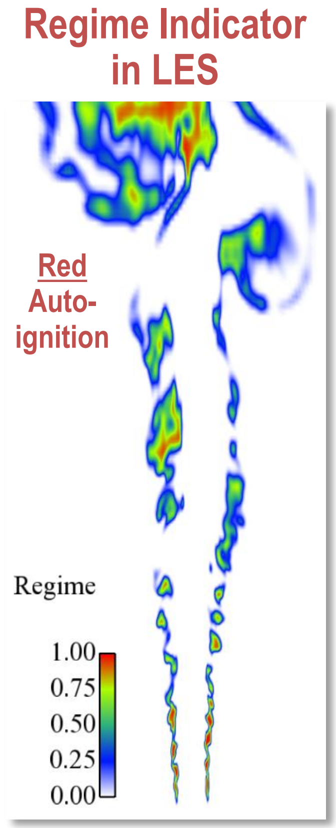
DNS of lifted jet flames in hot coflow – chemical explosive mode analysis (Lu et al. 2010)

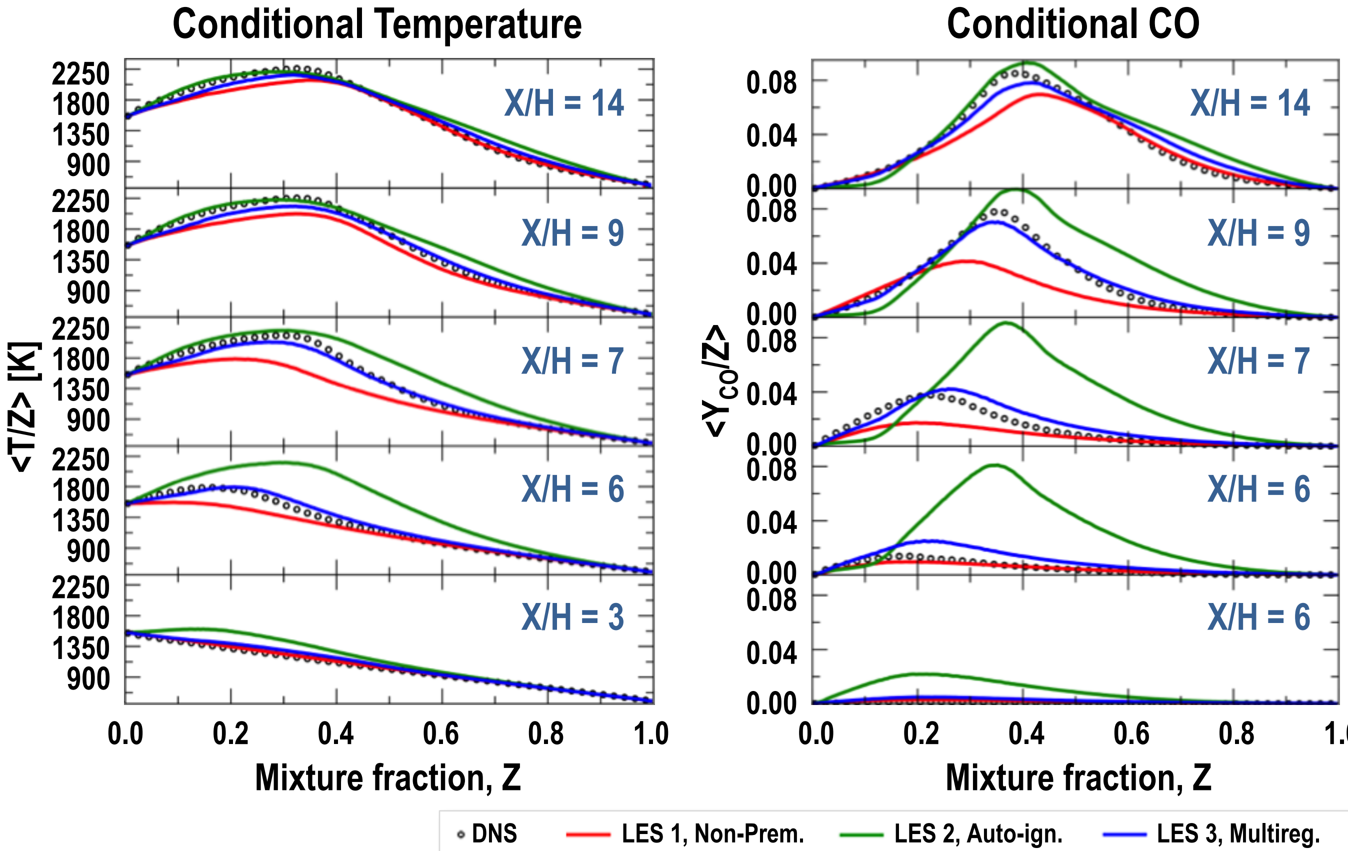




- **Chemical explosive mode (CEM) diagnostic developed as a chemical diagnostic to delineate explosive regions from normal flames**
- **A chemical mode is defined as the eigenmode of the Jacobian matrix of the chemical source terms in the species and temperature equations. CEM is a chemical mode whose eigenvalue is positive, and hence, large eigenvalues of the CEM at a given location indicate that the mixture is highly autoignitive**
- **A Damkohler number based on the ratio of CEM to local mixing rate determines whether the region is autoignitive or a normal flame**
- **Explosive index (EI) reveals important species aligned with CEM**

A posteriori evaluation of LES/Flamelet model with DNS of lifted ethylene jet flame
(Knudsen, Pitsch, Richardson, Chen)

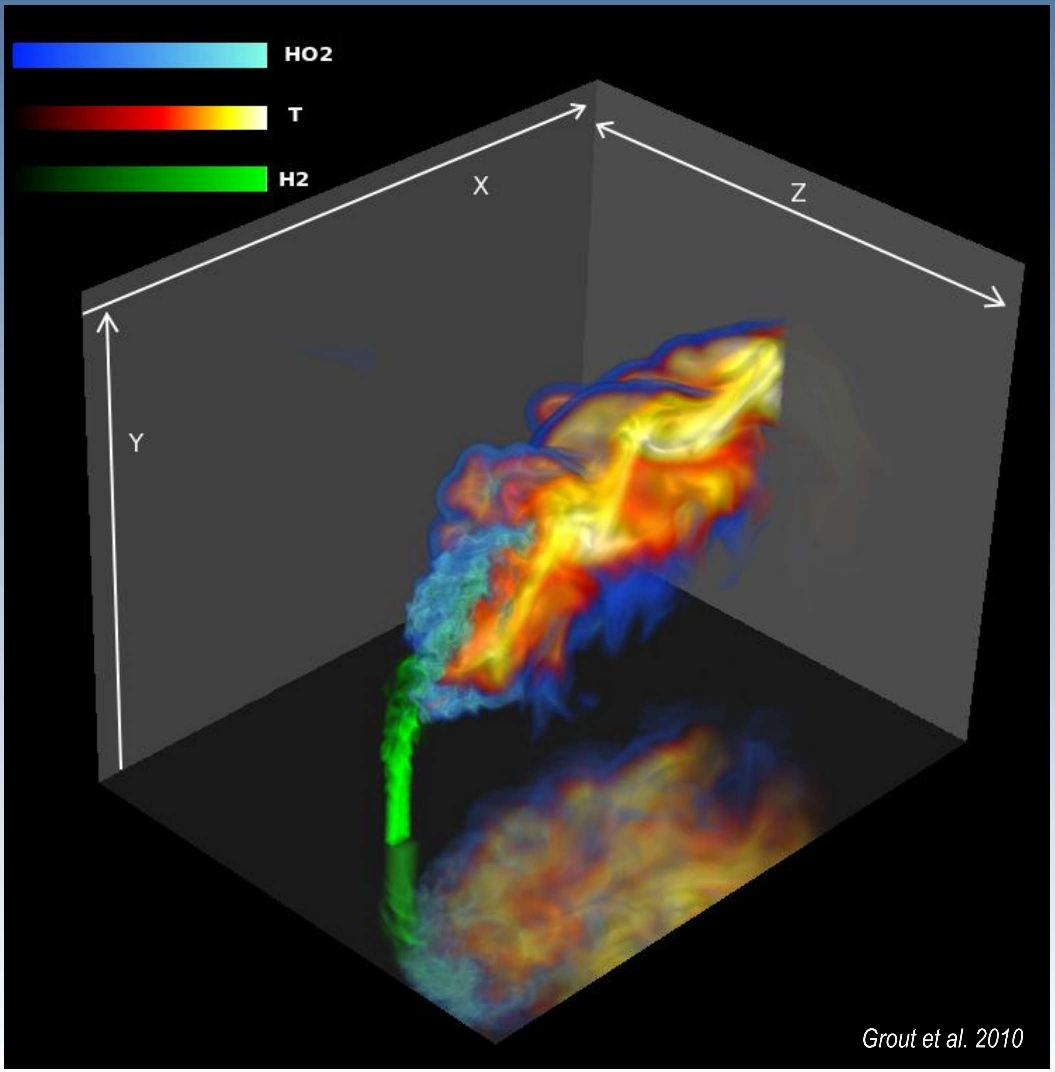




- Universal auto-ignition underpredicts liftoff
- Steady burning overpredicts liftoff
- Multiregime approach promising for efficiently describing turbulent ignition
- Continuing work: using DNS to understand model shortcomings

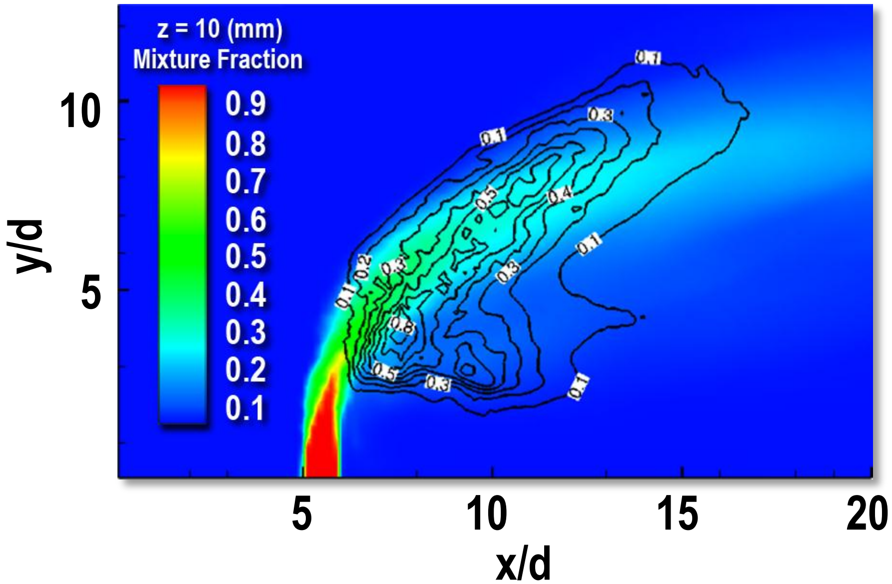
Reacting H_2 jet in heated air cross flow (JICF)

Volume rendering of HO_2, temperature, and H_2 with a Z cutting plane through the center of the counter-rotating vortex pair

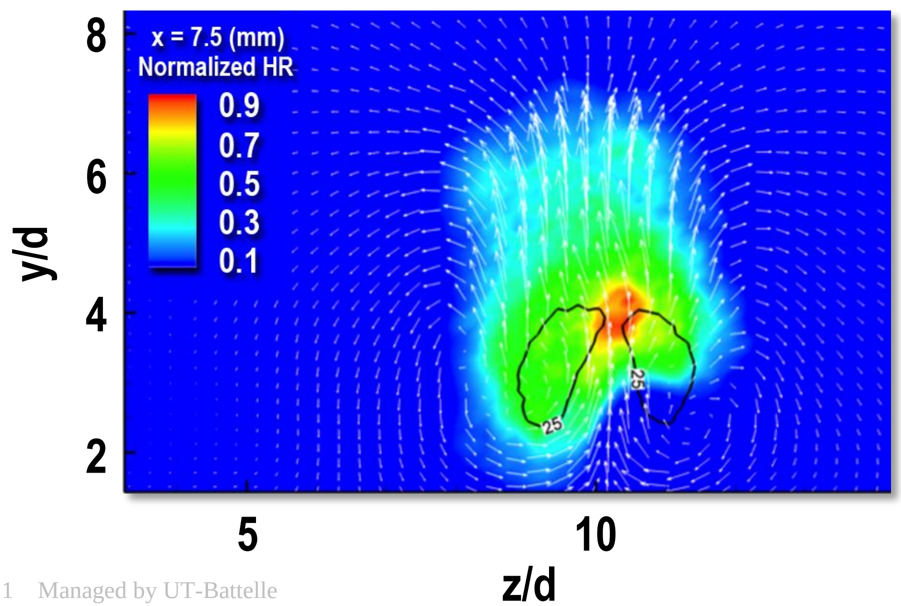


- Canonical configuration useful for studying fuel injection/flashback safety in stationary gas turbines
- H_2/N_2 jet, O_2/N_2 boundary layer flow
- 1 mm jet,
  25 mm x 20 mm x 20 mm domain
- Mass, momentum, energy, species balance equations solved using 'S3D'
- FD grid (1408 x 1080 x 1100), 9 species
  ~8M cpu hours on Jaguar, 1.6 billion grids, ADIOS used for fast I/O on 94,000 cores

Mean jet trajectory and stabilization location



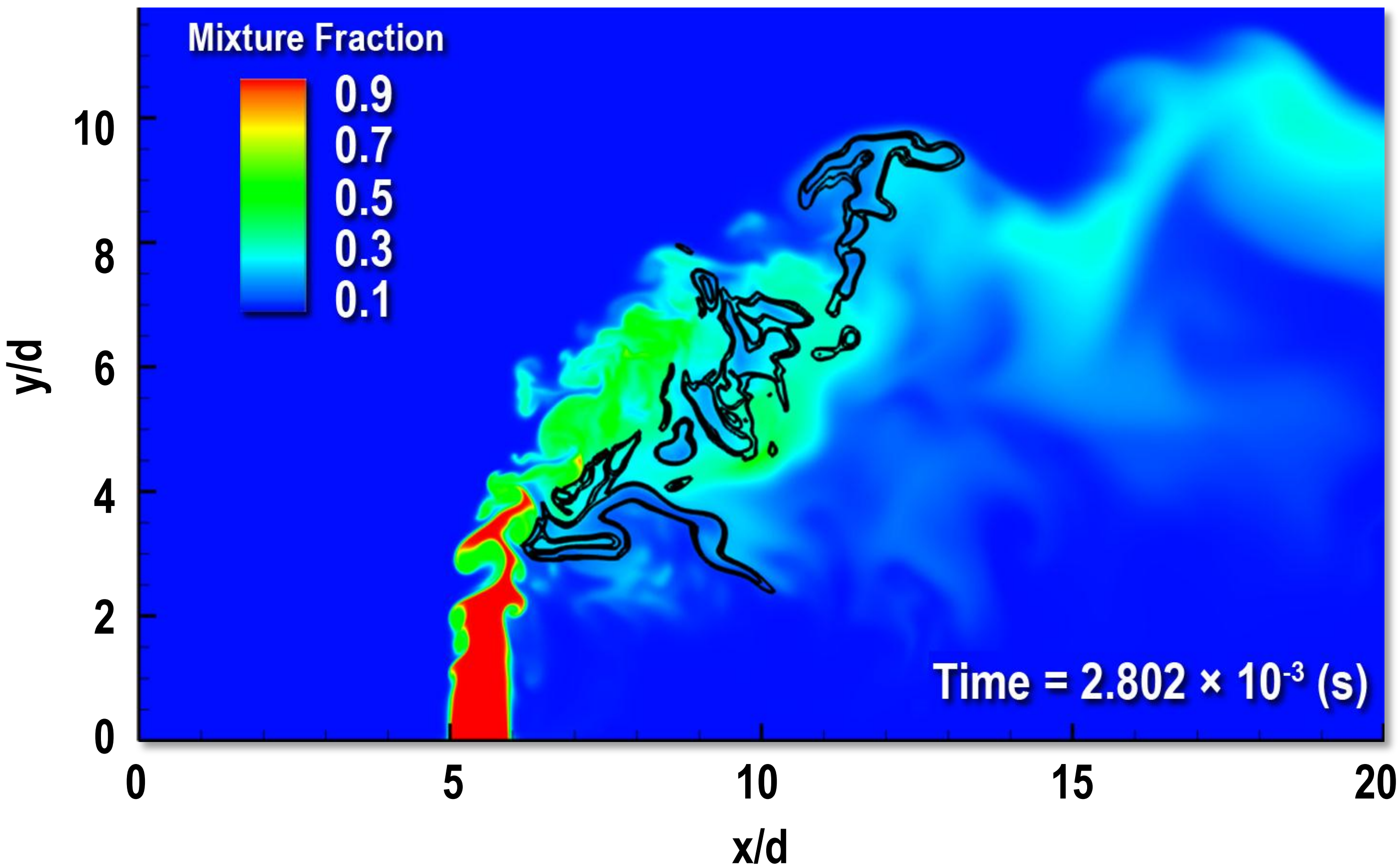
RANS heat release rate (black isocontour lines) in a spanwise slice showing stabilization point is near stoichiometric mixture fraction and low velocity region in between counter-rotating vortex pair (CVP), a recirculation region with hot products of combustion



RANS low velocity region (<25 m/s denoted by black isoline) in streamwise slice superimposed on heat release color isocontours showing peak heat release at stabilization location is in between the CVP

Instantaneous behavior of JICF

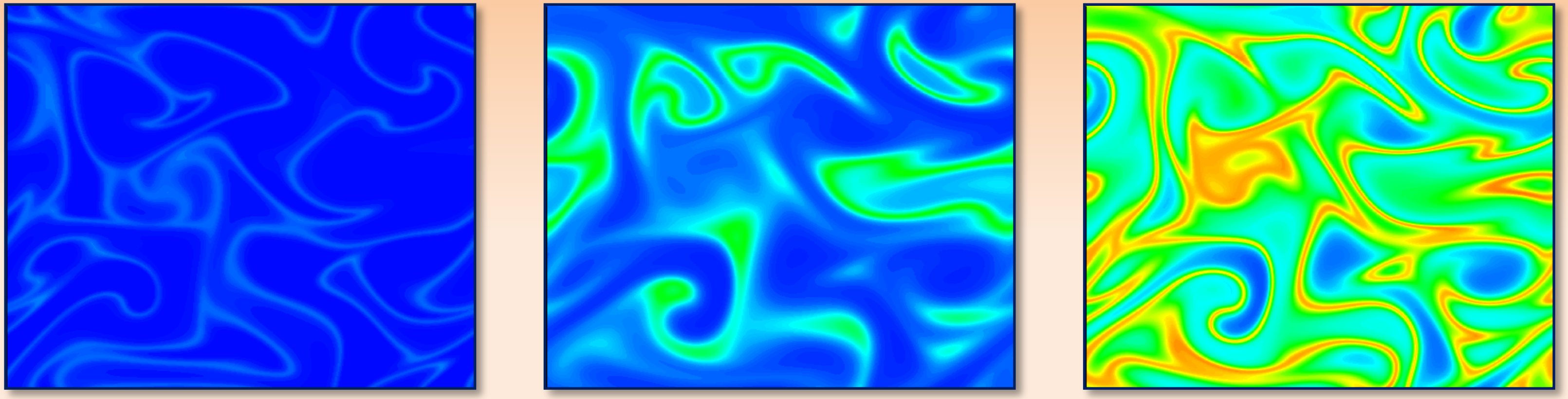
- Stabilization picture is much more complex than mean fields suggest
- Key issues
  - Burning mode – non-premixed or premixed?
  - Interaction between flame and turbulence?



Instantaneous z slice showing heat release (black isocontours) and mixture fraction

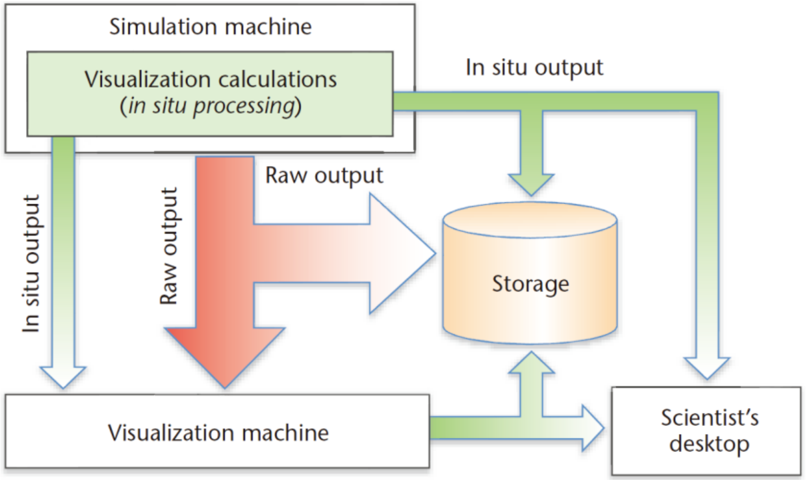
HCCI combustion with stratification

- Motivation: next generation internal combustion engine concept
  - Strategy: Operate engines lean and at low temperatures
  - Benefits: Less NO_x, fewer particulates, high efficiency
  - Challenges: High rates of pressure rise, ignition control difficult
- Fundamental DNS study of turbulence-autoignition interaction in nonhomogeneous mixtures at high pressures (~30 atm)
- Detailed dimethyl-ether (DME) chemistry – 30 chemical species; DME proposed as good biofuel substitute to diesel
- Key Results
  - Three stages of heat release in DME-air mixtures
  - 2nd and 3rd stage waves are simultaneously present
  - 2nd stage predominantly spontaneous ignition front; 3rd stage predominantly deflagration wave
  - Twin-ringed structure of heat release rate for both thermal and composition stratification case

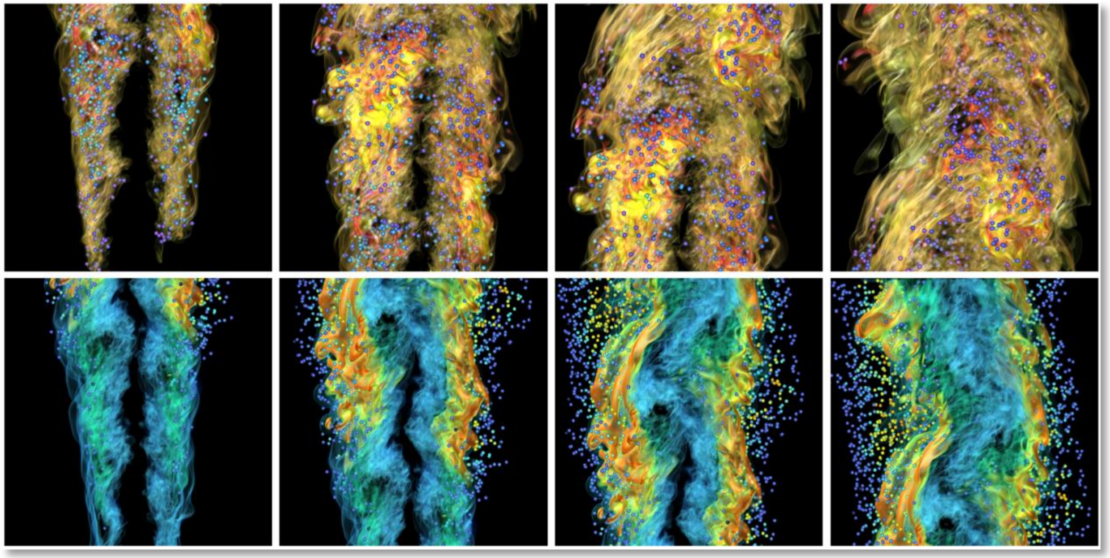


Heat release rate field (colormap inverted) at 1.4, 2.075, and 2.135 ms

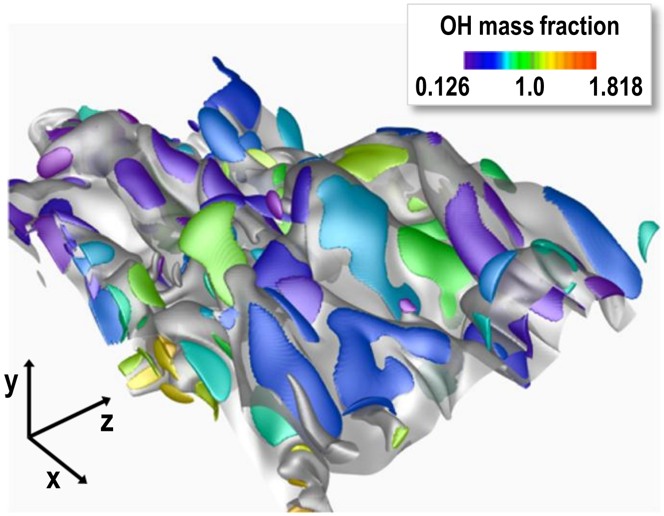
In situ visualization and analysis in S3D



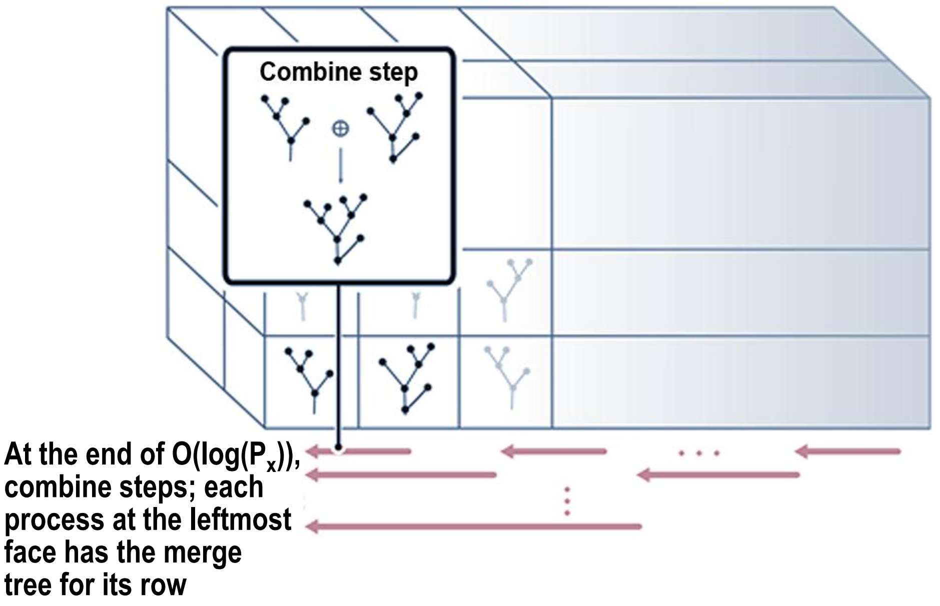
- In situ processing
  - Execute on the same processors
  - Avoid intermediate file I/O
  - Runtime monitoring, interpreting, and steering
  - Access the full resolution simulation data and perform data analysis in a more accurate fashion
- Challenges
  - Optimize memory usage: make data processing code interact directly with the simulation code and share the same data structures and optimize memory usage
  - Balance workload: difficult to achieve as data partition and distribution are dictated by the simulation code
  - Lower data processing calculations cost: lower the cost without hardware acceleration
  - Implement highly scalable parallel volume rendering, particle rendering, and image compositing
  - Visualization cost is less than 1% of simulation time



Topological methods for extracting and tracking combustion and flow features



Segmentation of conditional mixing rates in a turbulent jet flame

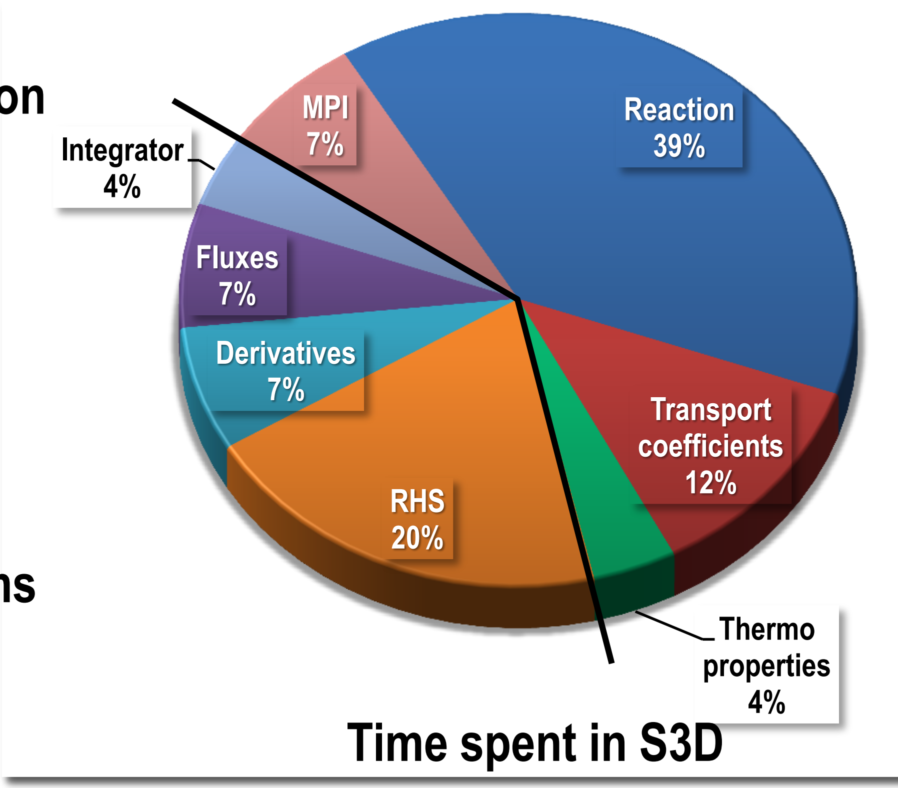


- Topological methods allow robust segmentation, simplification, and quantification of important features in scalar fields
- Parallel computation of merge tree will enable analysis of massive data sets
  - We compute the merge tree in parallel for each piece of the domain
  - We combine the merge trees of the pieces into the global merge tree using a binary reduction along the 3 axes

Refactoring S3D for hybrid multicore architectures

Programming for the hybrid multicore architectures

- Generate hybrid (MPI+threads) multicore software for heterogeneous architectures
- Improve performance through better utilization of memory hierarchy and bandwidth
- Ensure scalability of MPI parallelism to $O(10^6)$ nodes



Strategy

- Identify key computational kernels that consume 90% of the time
- Extract kernels to stand-alone serial programs
- Reprogram kernels for multiple options for heterogeneous computing
  - OpenMP threading
  - Compiler directive assisted porting to accelerator hardware
  - Reprogram in CUDA

Contact

Jacqueline H. Chen

Principal Investigator
Combustion Research Facility
Sandia National Laboratories
Livermore, CA 94550
jhchen@sandia.gov

Ramanan Sankaran

Scientific Computing liaison
National Center for Computational Sciences
Oak Ridge National Laboratory
sankaranr@ornl.gov