High Fidelity Numerical Simulations of Turbulent Combustion

Presented by

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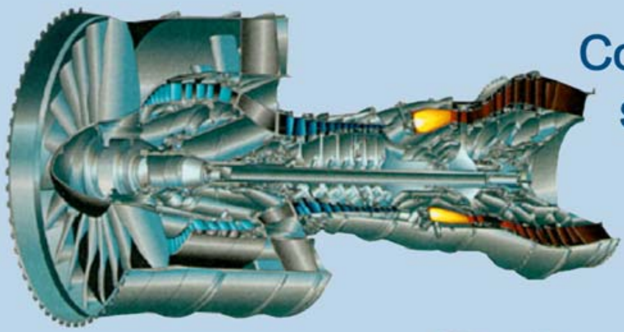
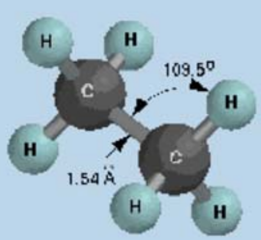
Direct numerical simulation (DNS) of turbulent combustion

Turbulent combustion is a grand challenge

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



Combustor size ~1m



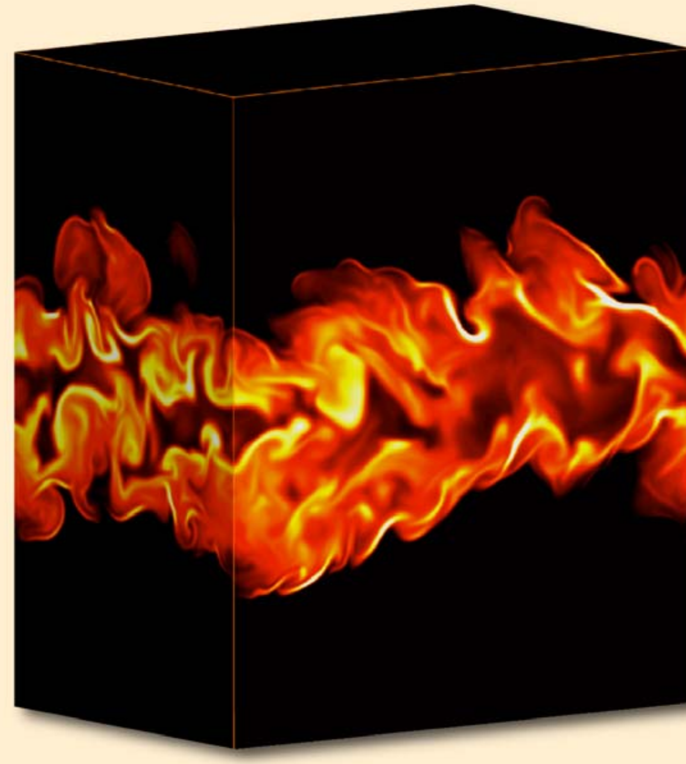
Molecular reactions ~1nm

DNS approach and role

- Fully resolve all continuum scales without using sub-grid 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. Provide numerical benchmark data for predictive model validation and development.

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
- Multi-physics (sprays, radiation and soot) from SciDAC-TSTC
- Ported to all major platforms



DNS provides unique fundamental insight into the chemistry-turbulence interaction

DNS ⟷ *Physical models* ⟷ *Engineering CFD codes (RANS, LES)*

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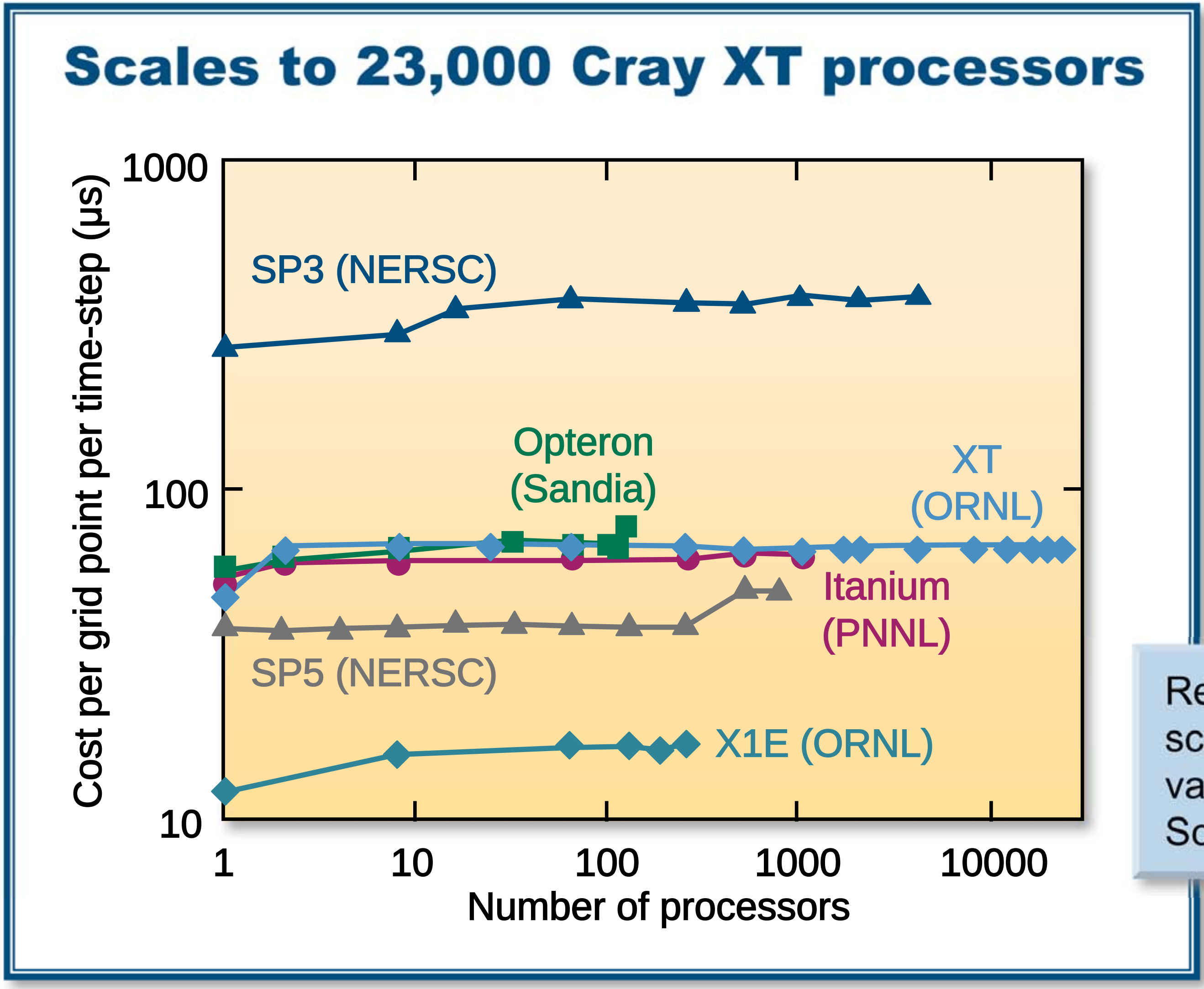
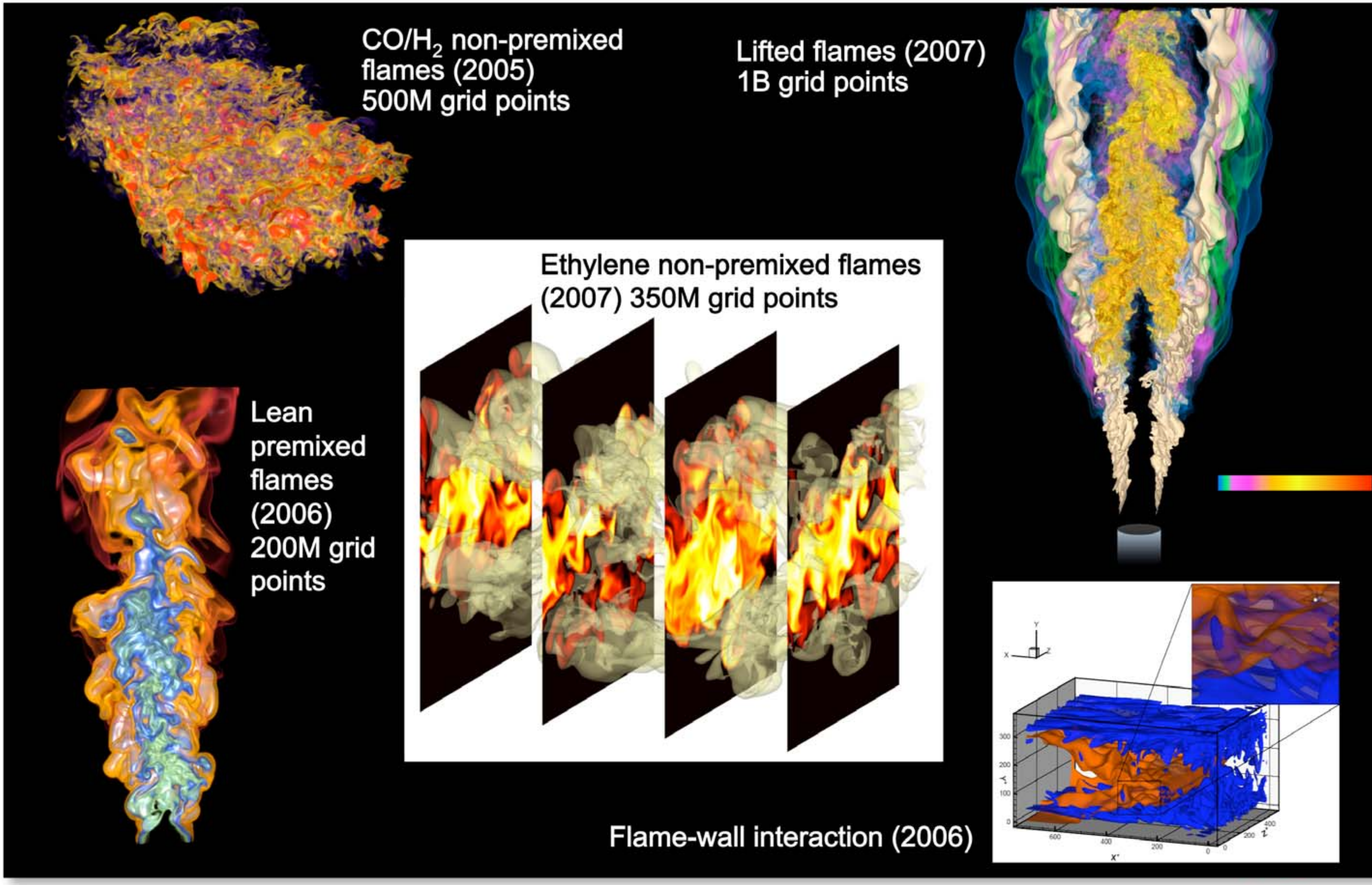
Efficient parallel scaling



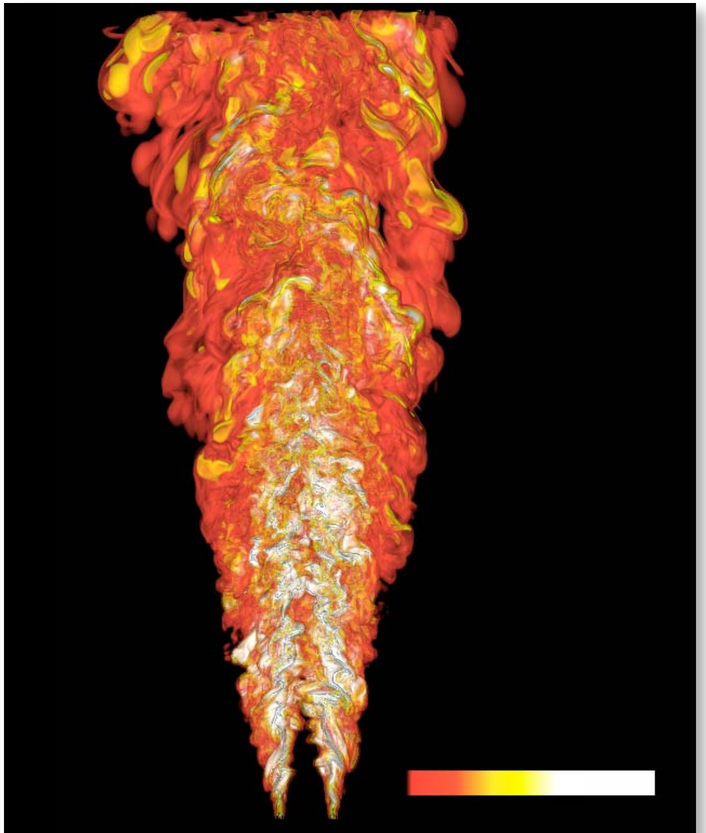
Results from weak scaling test on various Office of Science platforms

Combustion science enabled by NCCS



DNS of turbulent lifted H_2/air jet flames in heated coflow

- Determine stability and characteristics of a lifted flame
- Understand flame stabilization mechanism
  - Effect of degree of fuel-air pre-mixing
  - Effect of turbulent flow
  - Effect of preheating and auto-ignition
- Simulation performed on Jaguar on 9000 cores and 2.5 million cpu-hrs
  - ~1 billion grid points
  - Detailed H_2/air chemistry with 14×10^9 DOF
  - 9 resolved species and 21 elementary reaction steps
  - Jet Reynolds number = 11,000



Instantaneous volume rendering of the local mixing rate, by H. Yu and K. L. Ma of the SciDAC Institute for Ultrascale Visualization

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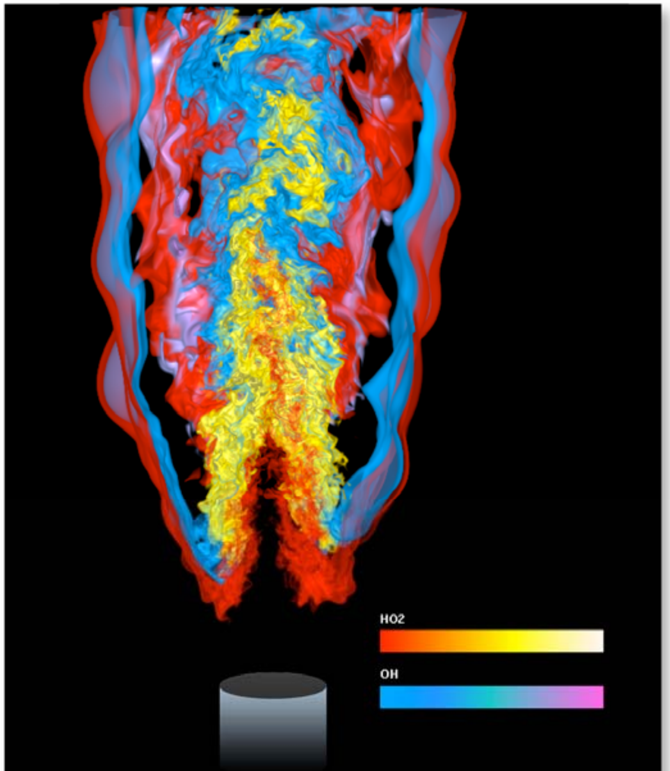
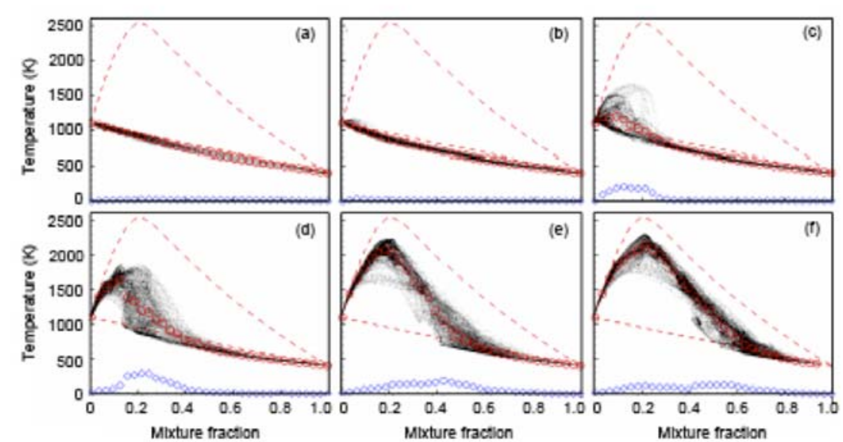
Flame stabilization primarily due to autoignition



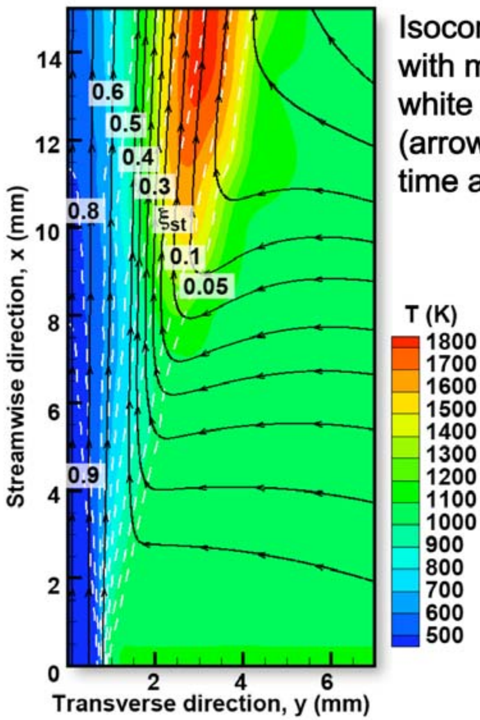
Instantaneous volume rendering of HO_2 (ignition marker) and OH (flame marker) by H. Yu and K. L. Ma of the SciDAC Institute for Ultrascale Visualization

- Flame stabilizes in fuel-lean mixture where the temperature is high (toward the heated air coflow) and mixing rates are low.
- Hydroperoxy radical (HO_2):
  - Precursor of auto-ignition in hydrogen-air chemistry.
  - Builds up upstream of OH and other intermediate radicals (H and H_2O_2).
  - Indicates auto-ignition should be primary stabilization mechanism.

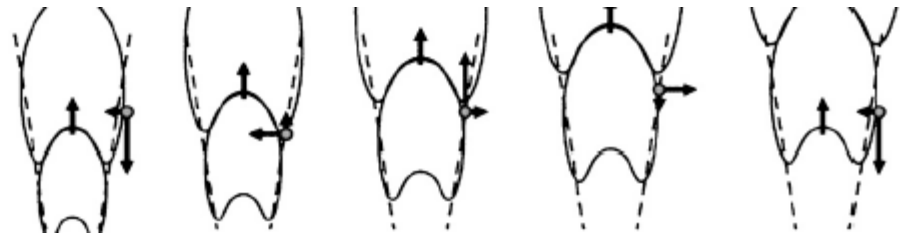
Temperature versus mixture fraction at various axial positions

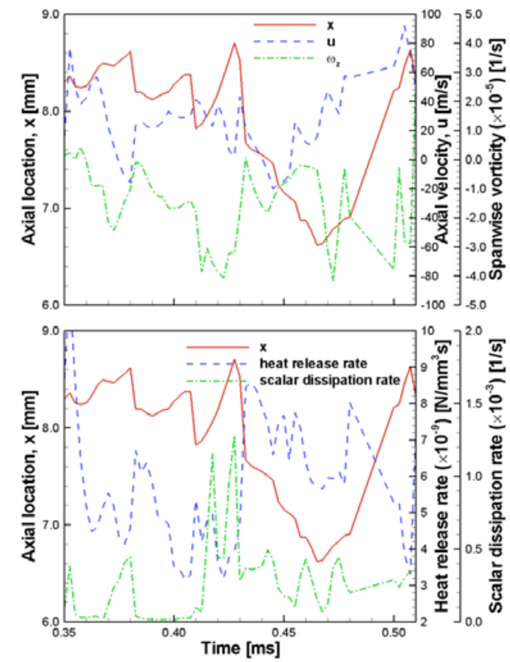


Stabilization depends on competition between autoignition and large-scale eddy passage



Isocontours of temperature with mixture fraction (dotted white line) and streamlines (arrowed line) averaged in time and z-direction





Correlation of stabilization point and axial velocity and ignition

- Near flame base, slightly negative or small positive axial velocity is observed (recirculation assists stabilization of flame base).
- Stabilization point movement is cyclic with passage of large-eddies

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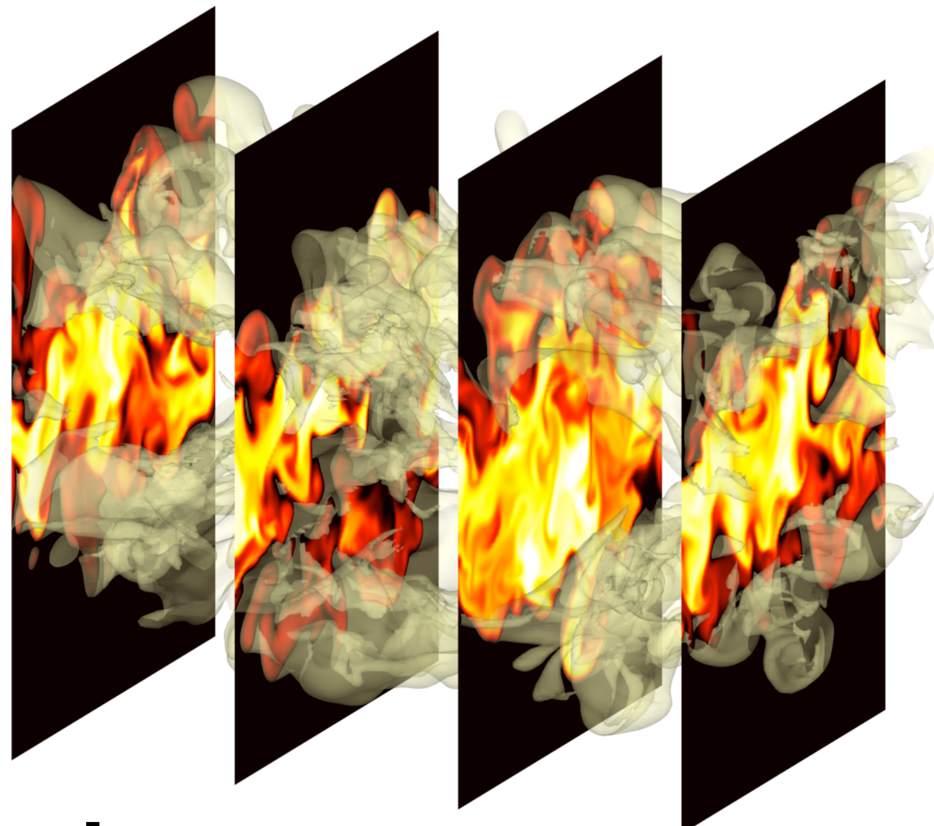
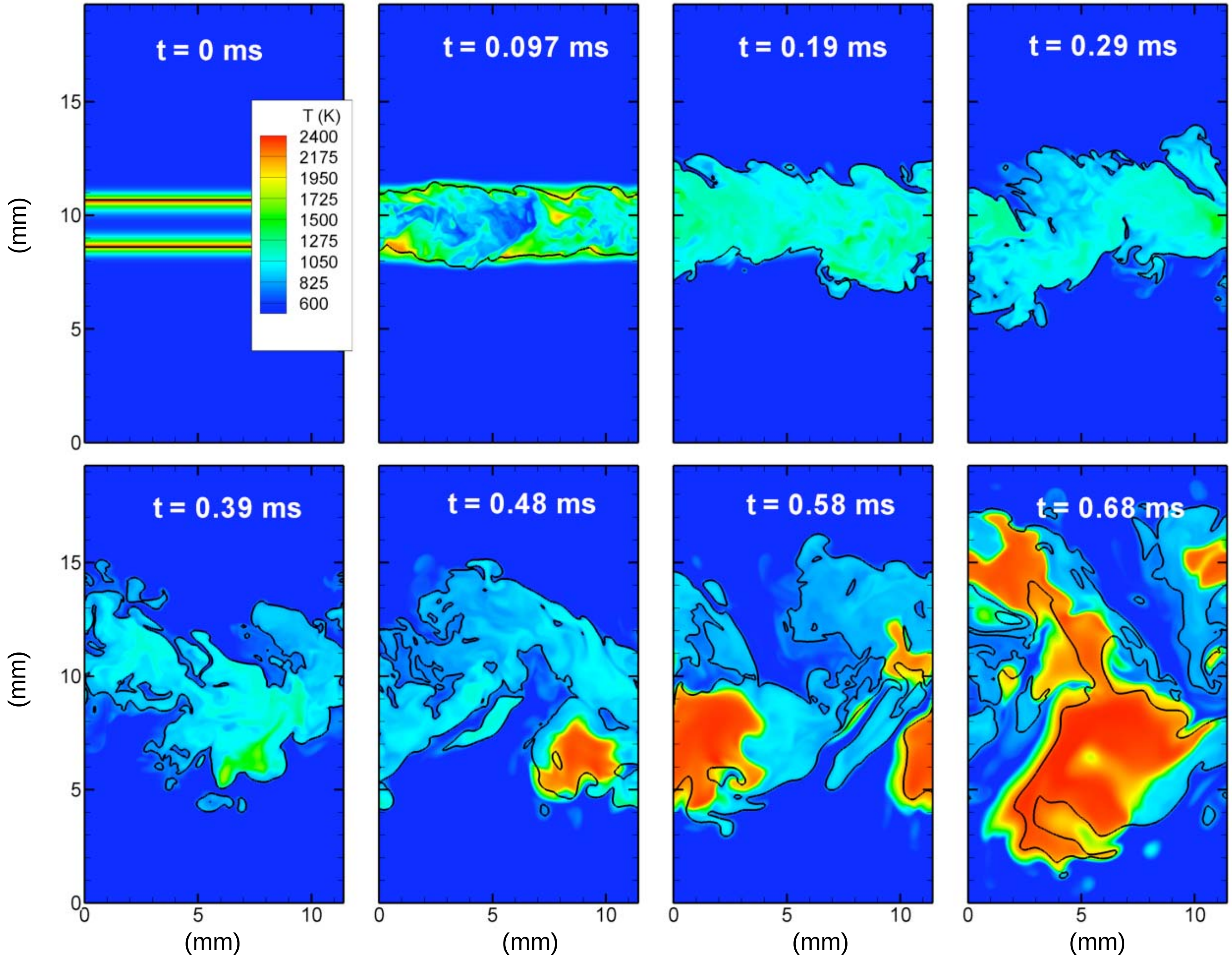
Extinction and reignition in a nonpremixed ethylene/air turbulent jet flame

- Goal: study extinction reignition processes in hydrocarbon flames
  - Autoignition
  - Premixed flame propagation
  - Edge flame propagation
- 3D DNS of a slot jet at Re = 5120
- Reduced ethylene mechanism consisting of 19 transported and 10 quasi-steady state species, with 167 reactions (Lu and Law 2007)
- 340 million grid points (8.16×10^9 DOF)
- 2.0 million cpu-hours; 14,112 cores on Jaguar

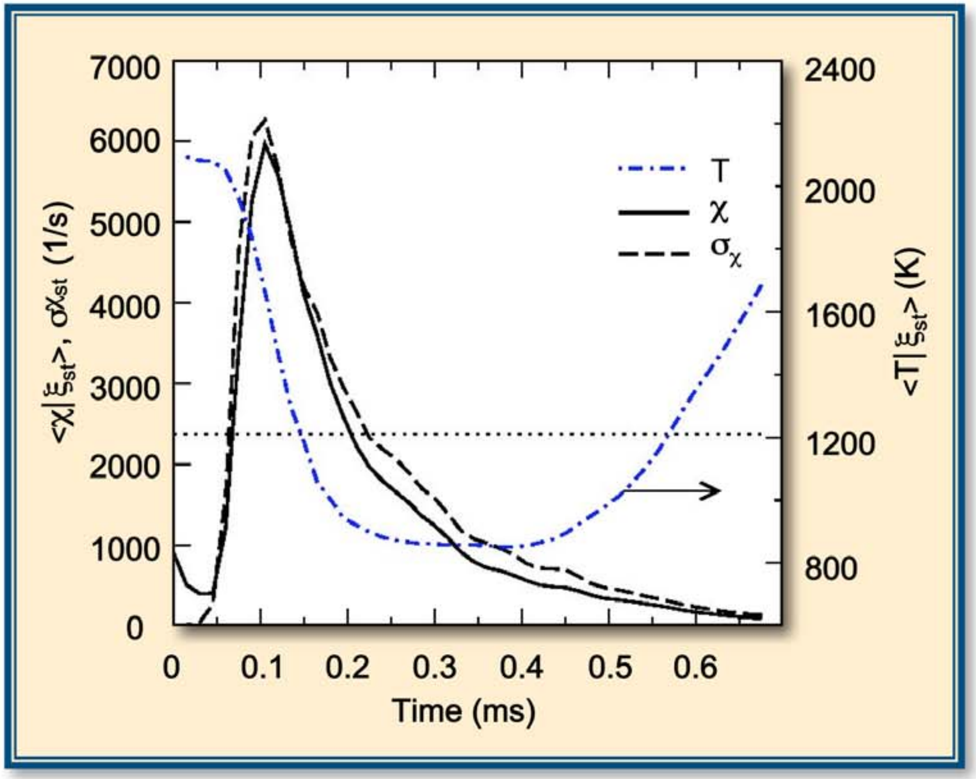


Temperature history in a spanwise slice reveals extinction and reignition

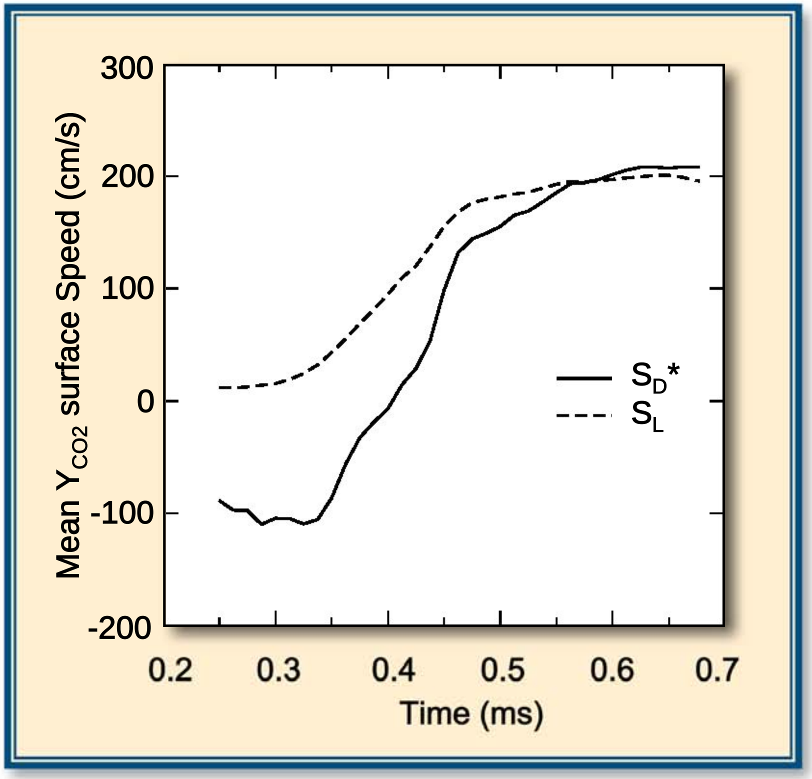


Stoichiometric mixture fraction (black line)

Excessive mixing quenches the flame and flame reignites by premixed flame propagation



Conditional mean and variance of scalar dissipation rate (mixing rate) and temperature at the flame



Propagation speed of ignition front compared with laminar flame speed

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