High Fidelity Direct Numerical Simulations of Turbulent Combustion

Presented by

Jacqueline H. Chen (PI)
Chun Sang Yoo
Ed Richardson
Ray Grout
Hongfeng Yu

Combustion Research Facility
Sandia National Laboratories, Livermore, CA

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

**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. 2-D vs. 3-D, surrogate scalars)
- Provide numerical benchmark data for predictive model development and validation for coarse-grain engineering CFD

---

Molecular reactions \( \sim 1 \text{nm} \)

Combustor size \( \sim 1 \text{m} \)
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
Efficient parallel scaling

Results from weak scaling test on various Office of Science platforms
Combustion science enabled by the NCCS

- CO/H₂ non-premixed flames (2005) 500M grid points
- Lifted hydrocarbon flames (2008) 1.3B grid points
- Ethylene non-premixed flames (2007) 350M grid points
- Lean premixed flames (2006) 200M grid points
- Flame-wall interaction (2006)
DNS of turbulent lifted ethylene/air jet flames in heated coflow

- Determine stability characteristics of a lifted hydrocarbon flame
- Understand flame stabilization mechanism
  - Effect of degree of fuel–air premixing
  - Effect of turbulent flow
  - Effect of preheating and autoignition
- Simulation performed on Jaguar on 30,000 cores and 7.5 million cpu-hrs
  - ~1.3 billion grid points, 120 TB field data, 25 TB particle data
  - Detailed C₂H₄/air chemistry, 22 resolved species, 18 global reactions, 167 steps
  - Jet Reynolds number = 10,000
  - 18% C₂H₄ + 82% N₂ at 550 K, jet velocity 204 m/s, jet width H = 2.0 mm, 1550 K air coflow at 20 m/s, 1 atm

Formaldehyde mass fraction, rendering by H. Yu and K. L. Ma of SciDAC Ultrascale Visualization Institute
Lifted flame stabilization due to upstream autoignition

- Flame stabilizes in fuel-lean mixture where the temperature is high (toward the heated air coflow) and scalar dissipation rate (i.e., mixing rate) is low.
- Flame is stabilized by autoignition upstream of the flame; hydroperoxy, methyl, and formaldehyde are chemical markers of ignition.

**Sequential autoignition kinetics**

Upstream of the flame base, HO\(_2\) and CH\(_3\) accumulate in hot, fuel-lean mixtures:

\[
\text{C}_2\text{H}_4 + \text{O} \rightarrow \text{CH}_3 + \text{HCO}; \quad \text{HCO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CO}
\]

Near the flame base, radical explosion induces thermal runaway:

\[
\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{O} + \text{OH}; \quad \text{CH}_3\text{O} \rightarrow \text{CH}_2\text{O} \rightarrow \text{HCO} \rightarrow (\text{H, CO, HO}_2)
\]

Conditional temperature, mixing rate, and heat-release rate at varying axial positions, x/H, in the jet.
Comparison of dissipation-layer thickness between DNS and experiment

- Mixture fraction scalar dissipation rate
  - A characteristic mixing time-scale
  - Key parameter in models to characterize extinction, burning rate, and ignition
- Direct measurement of dissipation-layer thickness, $\lambda_D$
  - Determine morphology of dissipation layers
  - Assess validity of surrogate 2-D thermal dissipation measurements
  - Provide turbulence scaling for non-premixed turbulent flame modeling
- DNS statistics
  - Near the lifted flame base, peak PDF occurs at $\lambda_D \approx 5.6\eta$ (\(\eta\) Kolmogorov scale)
  - Downstream of the lifted flame base, peak PDF occurs at $\lambda_D \approx 6.7\text{--}7.4\eta$, consistent with experimental results
- Measuring 3-D-layer thickness is under progress; provides correction to 2-D experimental measurement

Snapshots of thermal dissipation rate and its layer centers with the tracers out to 20%-width in experiments (left, from Kaiser and Frank, *Proc. Combust. Inst.* 31) and from DNS of lifted autoignitive jet flame (right)

PDF of scalar ($\chi$) and thermal ($\chi_T$) dissipation-layer thickness from DNS of lifted autoignitive jet flame, linear scale (left) and log-log scale (right)
Segmentation of dissipation elements

- Dissipation elements are 3-D; estimation of the thickness from a 2-D projection is an incomplete representation.

- Topology-based analysis (collaboration with V. Pascucci, P.-T. Bremer, A. Mascarenhas of SciDAC VACET) produces a full 3-D representation and time tracking.

- Combinatorial method guarantees consistency and facilitates discarding insignificant local extrema based on physically sensible criteria.

These features are topologically equivalent to a portion of the Morse complex and also closely related to the previous method of measuring the dissipation elements: full 3-D representation + consistency with prior methods.
Lagrangian particle tracking

- New software module was implemented in S3D for Lagrangian particle tracking
- New scalable particle queries
  - Track time history of tracer particles while advected by turbulent flow
  - parallel, efficient, and scalable
- Lagrangian statistics of unsteady ignition and micromixing processes
- Validation data for stochastic micromixing and ignition models

30 million particles in lifted jet flame
DNS colored by temperature
Contacts

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