

Direct Numerical Simulations of Turbulent Nonpremixed Combustion: Fundamental Insights Towards Predictive Models

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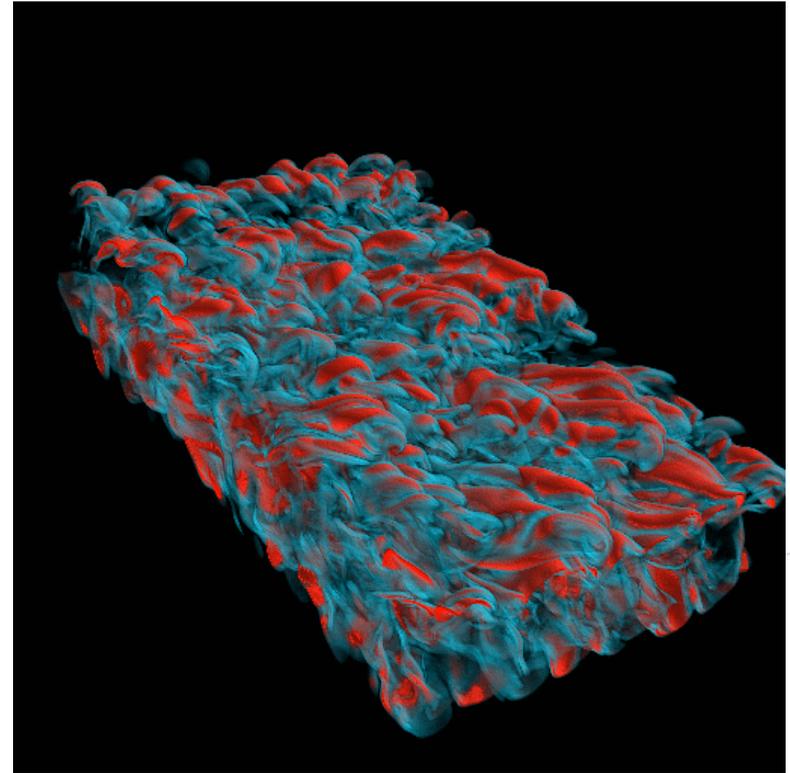
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SciDAC**

***Computing: LBNL NERSC, SNL CRF BES Opteron cluster
Computing Support: David Skinner (NERSC)
Visualization: Kwan-Liu Ma, Hongfeng Yu, Hiroshi Akiba UC Davis***



Outline

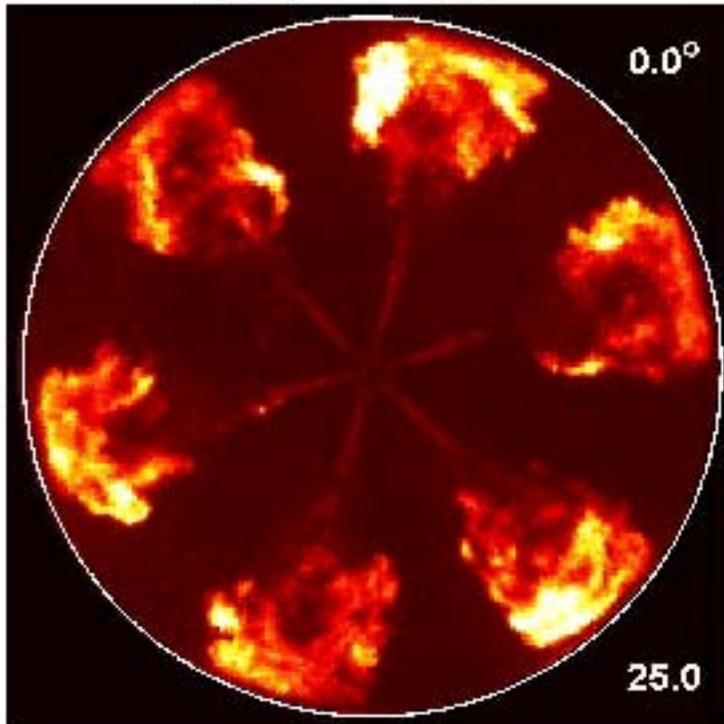
1. Direct Numerical Simulation (DNS) of turbulent combustion – challenges and opportunities
2. Sandia S3D terascale DNS capability
3. INCITE project – 3D simulations of a turbulent CO/H₂ jet flame



Scalar dissipation fields in DNS of a turbulent jet flame
(volume rendering by
Kwan-Liu Ma and Hongfeng Yu)

Turbulent combustion is a grand challenge!

CN45, Glow Plug Off



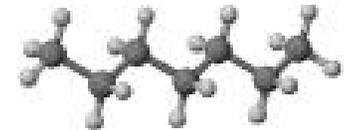
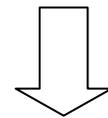
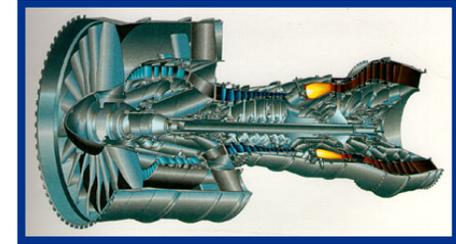
Diesel Engine Autoignition, Soot Incandescence
Chuck Mueller, Sandia National Laboratories

- **Stiffness : wide range of length and time scales**
 - turbulence
 - flame reaction zone
- **Chemical complexity**
 - large number of species and reactions (100's of species, thousands of reactions)
- **Multi-Physics complexity**
 - multiphase (liquid spray, gas phase, soot, surface)
 - thermal radiation
 - acoustics ...
- **All these are tightly coupled**

Several decades of relevant scales

- Typical range of spatial scales

- Scale of combustor: 10 – 100 cm
- Energy containing eddies: 1 – 10 cm
- Small-scale mixing of eddies: 0.1 – 10 mm
- Diffusive-scales, flame thickness: 10 – 100 μm
- Molecular interactions, chemical reactions: 1 – 10 nm



- Spatial and temporal dynamics inherently coupled
- All scales are relevant and must be resolved or modeled

**Terascale computing:
~3 decades in scales
(cold flow)**

Continuum



What is DNS?

- **Complete resolution of all relevant continuum scales.**
- **Does not require any explicit sub-grid scale model** (or implicit sub-grid scale model provided by numerical dissipation).
- CPU limitations imply only a finite range of scales can be tackled – implies restrictions on Reynolds number (ratio of convective to diffusive influences).
- Usually tackle building-block, canonical configurations.
- **Contrast with CFD used in industry** – large scales are handled but **must provide a turbulence or sub-grid scale model.**

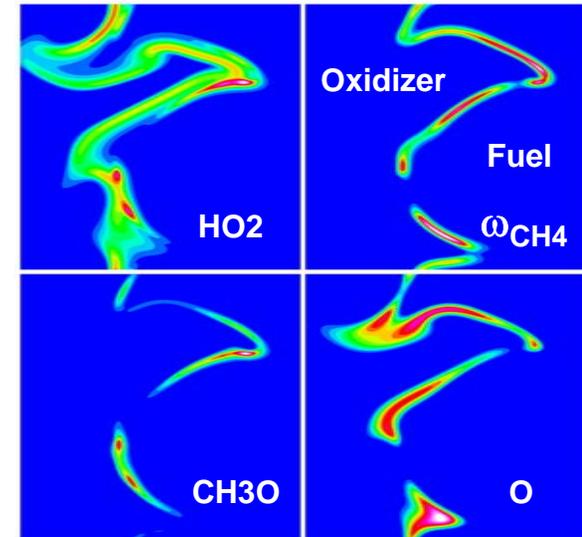
Role of Direct Numerical Simulation (DNS)

- A tool for fundamental studies of the micro-physics of turbulent reacting flows

DNS



- *Physical insight into chemistry turbulence interactions*
- *Full access to time resolved fields*



- A tool for the development and validation of reduced model descriptions used in macro-scale simulations of engineering-level systems

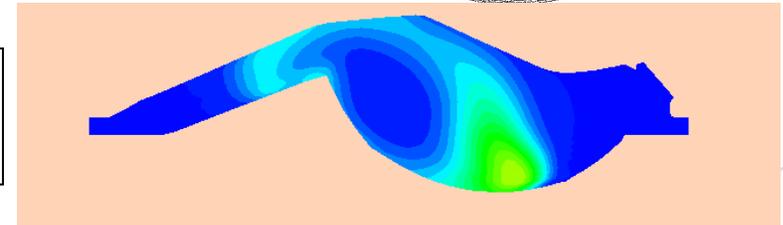
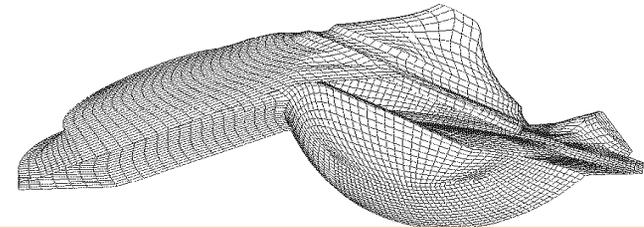
DNS



Physical Models



Engineering-level CFD codes



Piston Engines

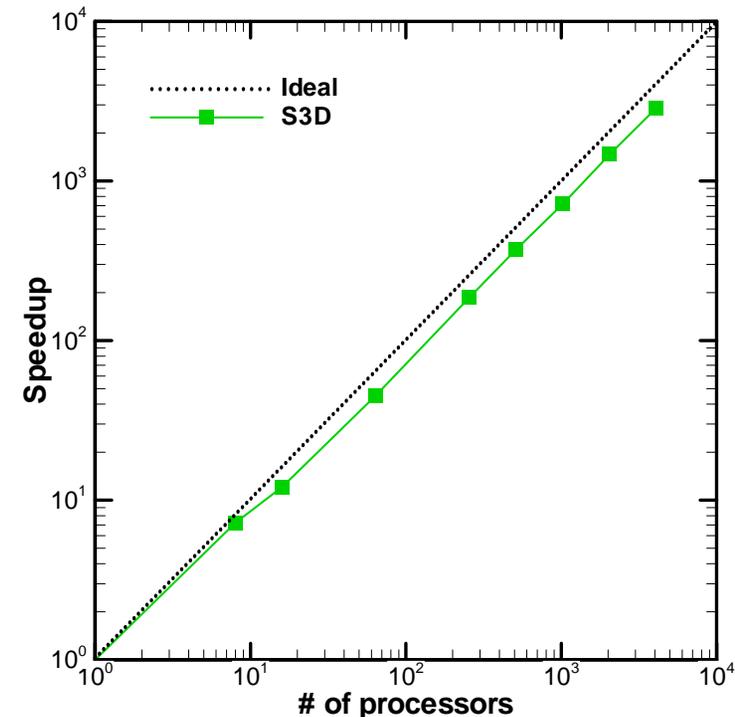


S3D MPP DNS capability at Sandia

S3D is a state-of-the-art DNS code developed with 13 years of BES sponsorship.

- **S3D code characteristics:**
 - Solves compressible reacting Navier-Stokes
 - F90/F77, MPI, domain decomposition.
 - Highly scalable and portable
 - 8th order finite-difference spatial
 - 4th order explicit RK integrator
 - hierarchy of molecular transport models
 - detailed chemistry
 - multi-physics (sprays, radiation and soot) from **SciDAC TSTC**
- **70% parallel efficiency on 4096 processors on NERSC (weak scaling test)**

S3D scales up to 1000s of processors... and beyond?



Performance improvements on Seaborg

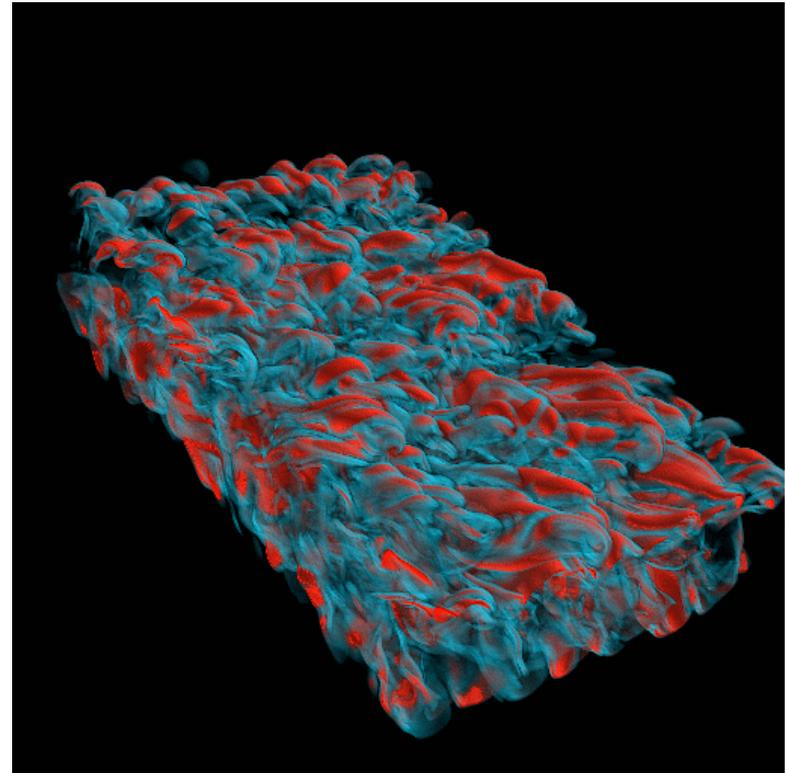
- Terascale computations – need optimizations customized to architecture
- Lots of assistance from NERSC consultant David Skinner
- Used Xprofiler, IPM
- Scalar improvements:
 - used vector MASS libraries for transcendental evaluations
 - re-structured loops in legacy code (eg vectorize)
 - eliminated unnecessary memory allocation introduced by compiler
 - flops reductions: tabulate thermodynamic quantities, minimize unit conversions, eliminate unimportant reactive species.
- Parallel improvements:
 - removed non-contiguous MPI data-types
 - re-wrote parts of communication to decouple communication ‘directions’, removing possible blocking
 - removed all unnecessary barriers

= net 45% reduction in execution time!



Outline

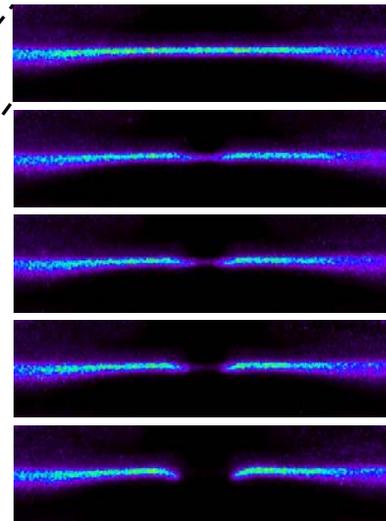
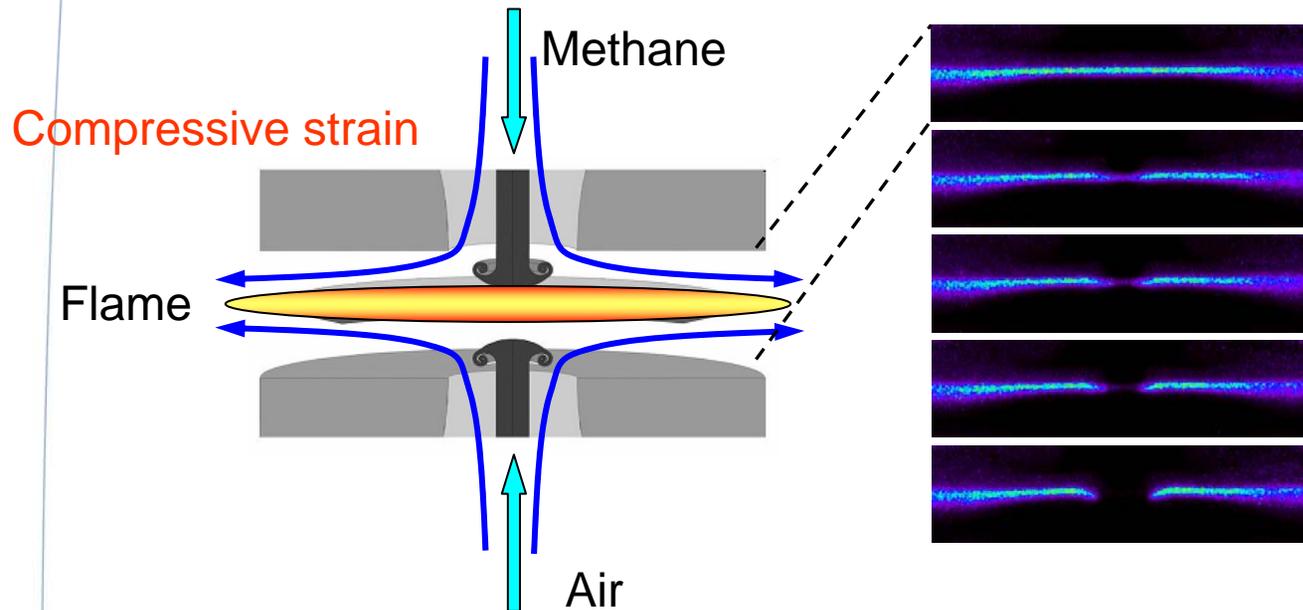
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Scalar dissipation fields in DNS of a turbulent jet flame
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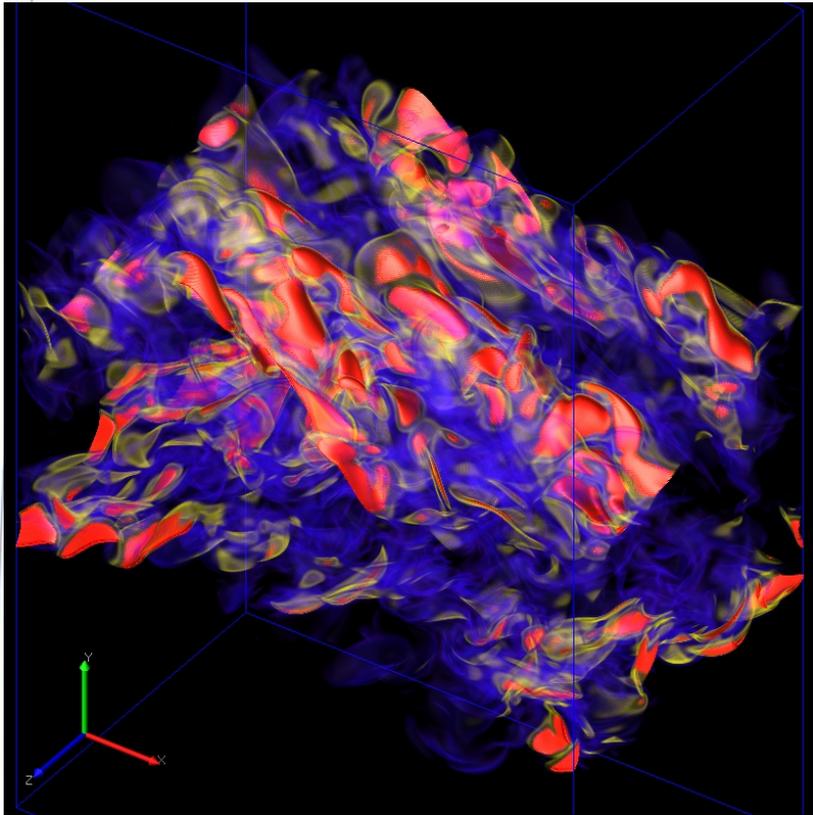
Understanding turbulence-chemistry interactions in non-premixed flames

- Fuel and Air are separate – ‘non-premixed’
 - Example – aircraft gas turbine combustor
 - Separated for safety reasons
 - Molecular mixing of fuel and air is needed for reaction to occur
 - Combustion depends on mixing rate (burning intensity, emissions, extinction, flame stabilization)



CO reaction rate
imaging experiment
J. H. Frank et al.

INCITE project: Direct simulation of a 3D turbulent CO/H₂/air jet flame with detailed chemistry

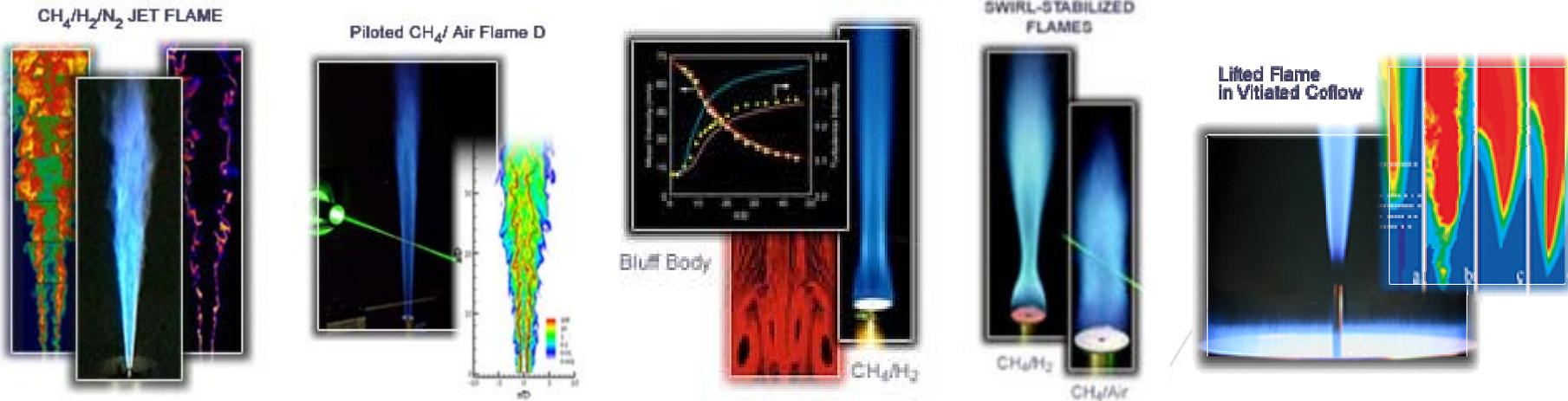


Scalar dissipation rate,
100 million grid point run

- Understand the dynamics of extinction and re-ignition in turbulent nonpremixed flames
- Find ways to parameterize local chemical states with lower-dimensional manifolds
- Understand the influences of differential diffusion on combustion
- Contribute to the interpretation of experimental data
- Develop and validate modeling approaches
- Understand how the details of molecular transport and reactions can interact with turbulent mixing.

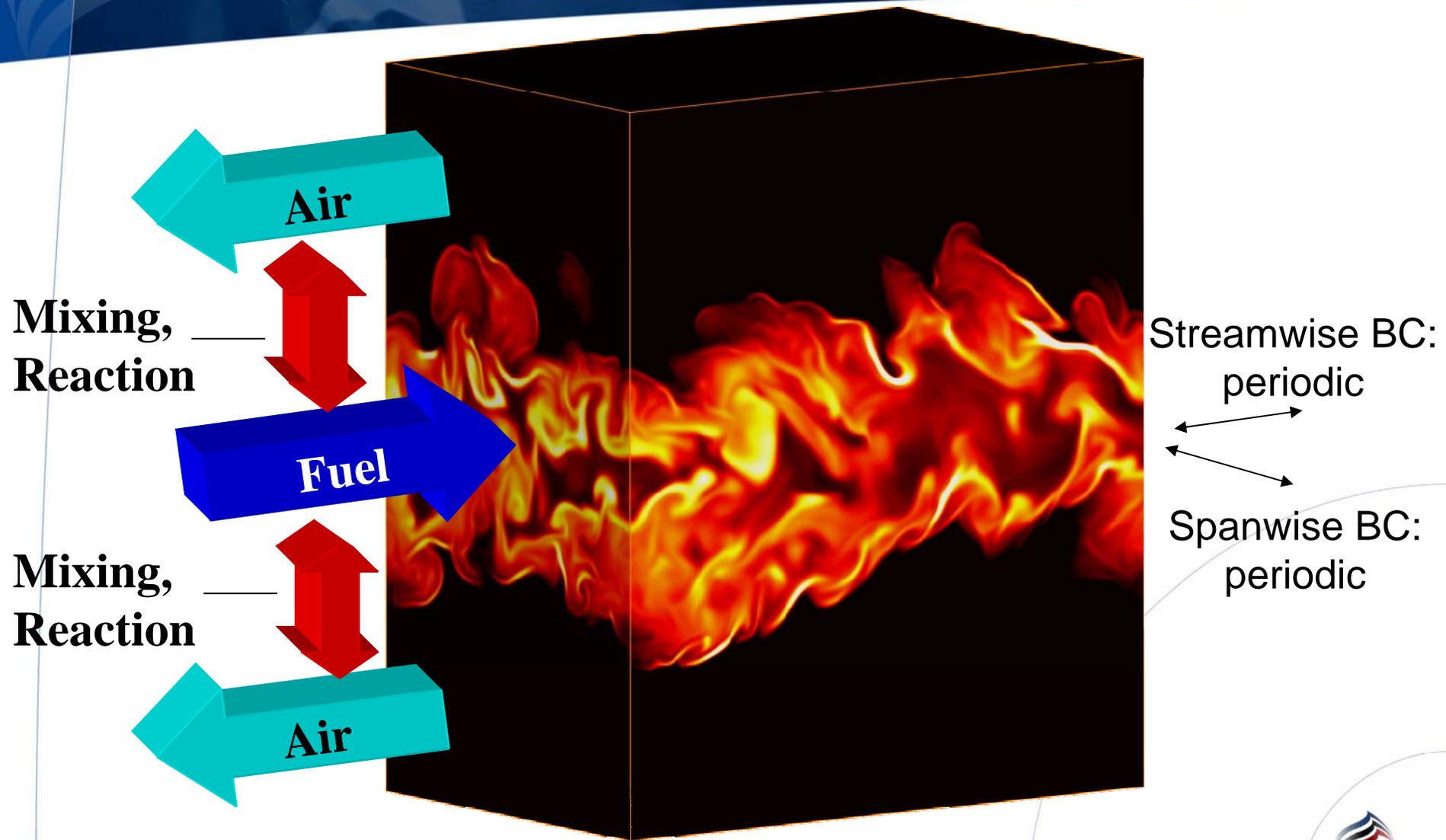
Community data sets

- How to maximize the impact of these large data-sets?
- TNF workshop (1996-present): International Collaboration of Experimental and Computational Researchers



Description of Run

- Temporally Evolving Non-premixed Plane Jet Flame



DNS data-sets of turbulent nonpremixed CO/H₂ flames

- **INCITE allocation enables extension to 3D, and hence realistic turbulence**
- Detailed CO/H₂ chemistry (16 d.o.f., Li et al. 2005)
- Parameters selected to maximize Reynolds number, Re (largest range of scales)
- ~40 small calculations prior to main run (mostly, on our local cluster)

- **INCITE calculation:**
 - 90% completed
 - Re 4500
 - 350 million grid points
 - **2048, 3072 or 4096 Seaborg processors**
 - **(most efficient on 4096!)**
 - 3.0 million hours total
 - ~ 10TB raw data

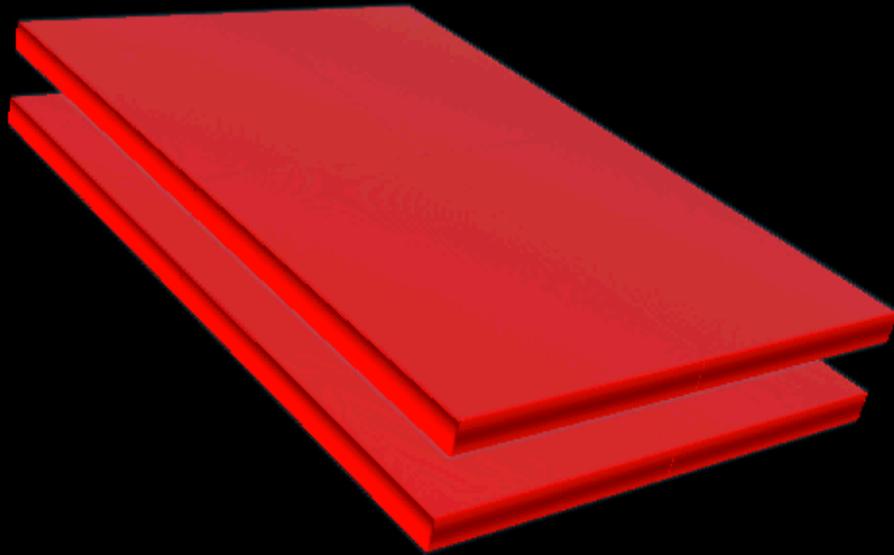
- Plan to complement the INCITE calculation with additional runs at different Re

Non-premixed combustion concepts

- Mixture fraction Z : the amount of fluid from the fuel stream in the mixture
- Z is a conserved (passive) scalar – (no reactive source term)
- Scalar dissipation, a measure of local molecular mixing rate:

$$\chi = 2D\nabla Z \cdot \nabla Z$$

Volume rendering of scalar dissipation



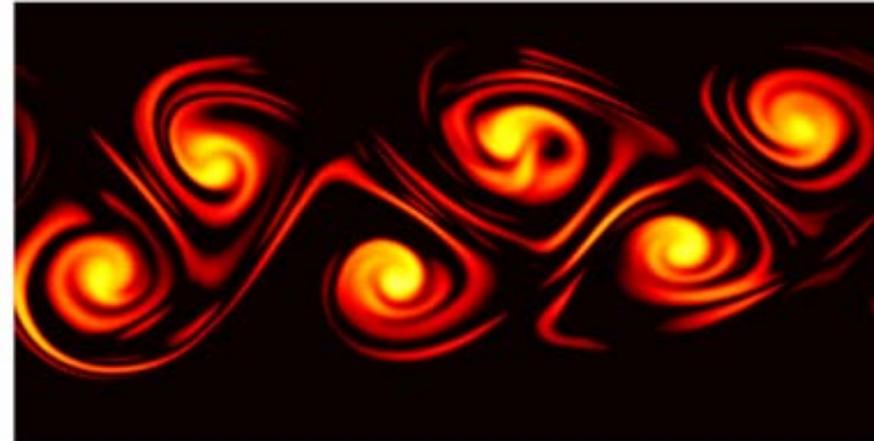
- Scalar dissipation exists in thin, highly intermittent layers
- Initially fairly organized structures aligned across principal strain directions.
- Later, jet breaks down and a more turbulent, isotropic structure exists.

Comparison with 2D simulation

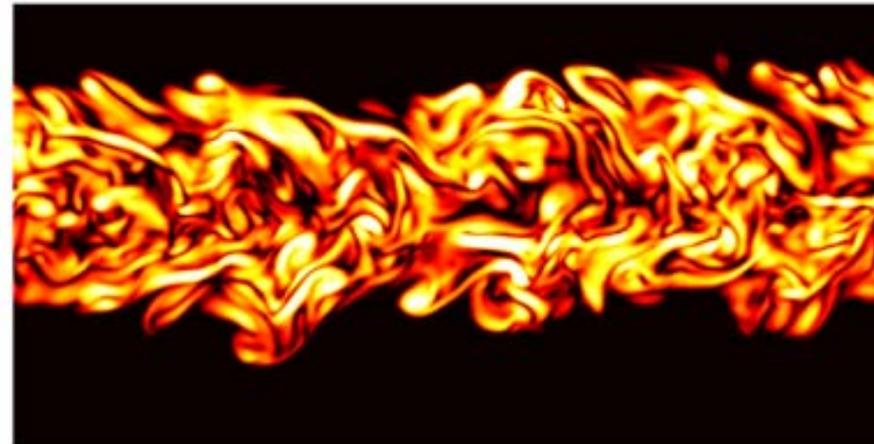
Vorticity fields

- **2D and 3D flows are qualitatively different ...**
- Stanley, Sarkar et al. 1998
 - nonreacting 2D and 3D DNS
 - 2D jet is dominated by a large scale vortex dipole instability, which does not occur in 3D
 - 3D, more small-scale structures

2D



3D

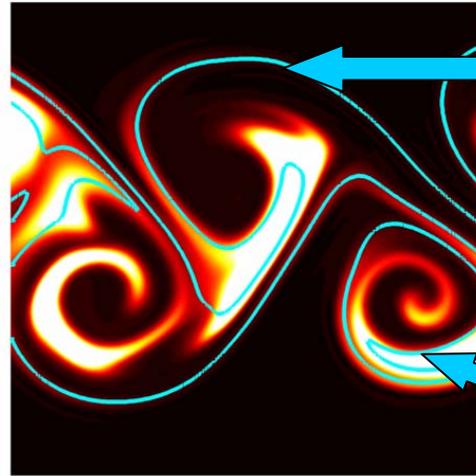


Comparison with 2D simulation

- In 2D, see large coherent structures
 - high dissipation regions very persistent
 - allows mixing with non-reacting pure air and fuel streams
 - leads to over-prediction of extinguished states
- In 3D, see considerable generation of small scale energy
 - high dissipation structures are more transient
 - smaller structures – mixing occurs with reacting states

OH mass fractions Stoichiometric mixture fraction

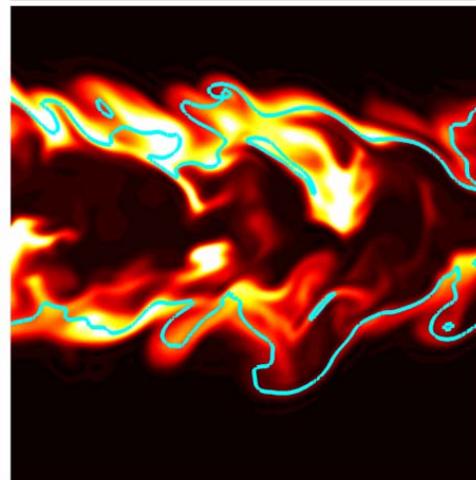
2D



Under-prediction in 'braids'

Over-prediction in vortex cores

3D



Mixing timescales

- Models for molecular mixing are required in the PDF approach to turbulent combustion (Pope 1985), a sub-grid model used in engineering CFD approaches.
- TNF workshop – CFD predictions are dependent on mixing timescale choice.
- Models assume that scalar mixing timescales are identical for all scalars and determined by the turbulence timescale.
 - scalars with different diffusivities?
 - reactive scalars?

Definitions

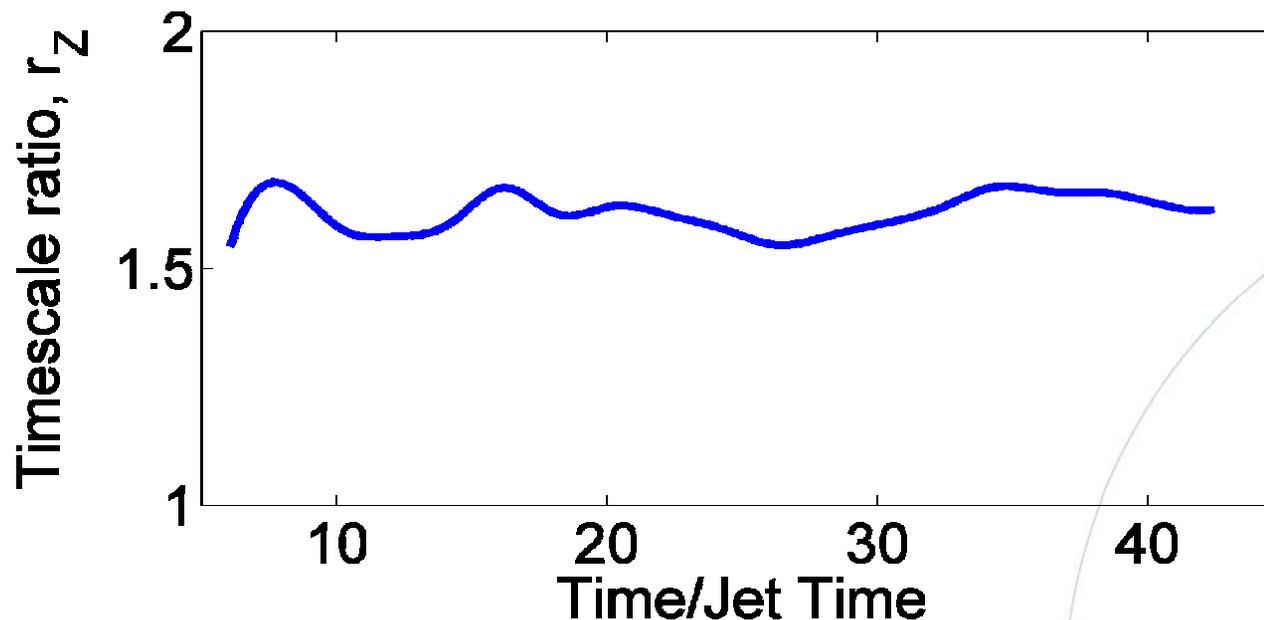
- Mechanical time-scale: $\tau_u = \frac{\bar{k}}{\varepsilon}$
- Scalar time-scale: $\tau_\varphi = \frac{\overline{\varphi'^2}}{2D\nabla\varphi \bullet \nabla\varphi}$
- Time-scale ratio: $r_\varphi = \frac{\tau_u}{\tau_\varphi}$

r_φ is assumed to be order unity in most models

r_φ is assumed to be the same for all scalars

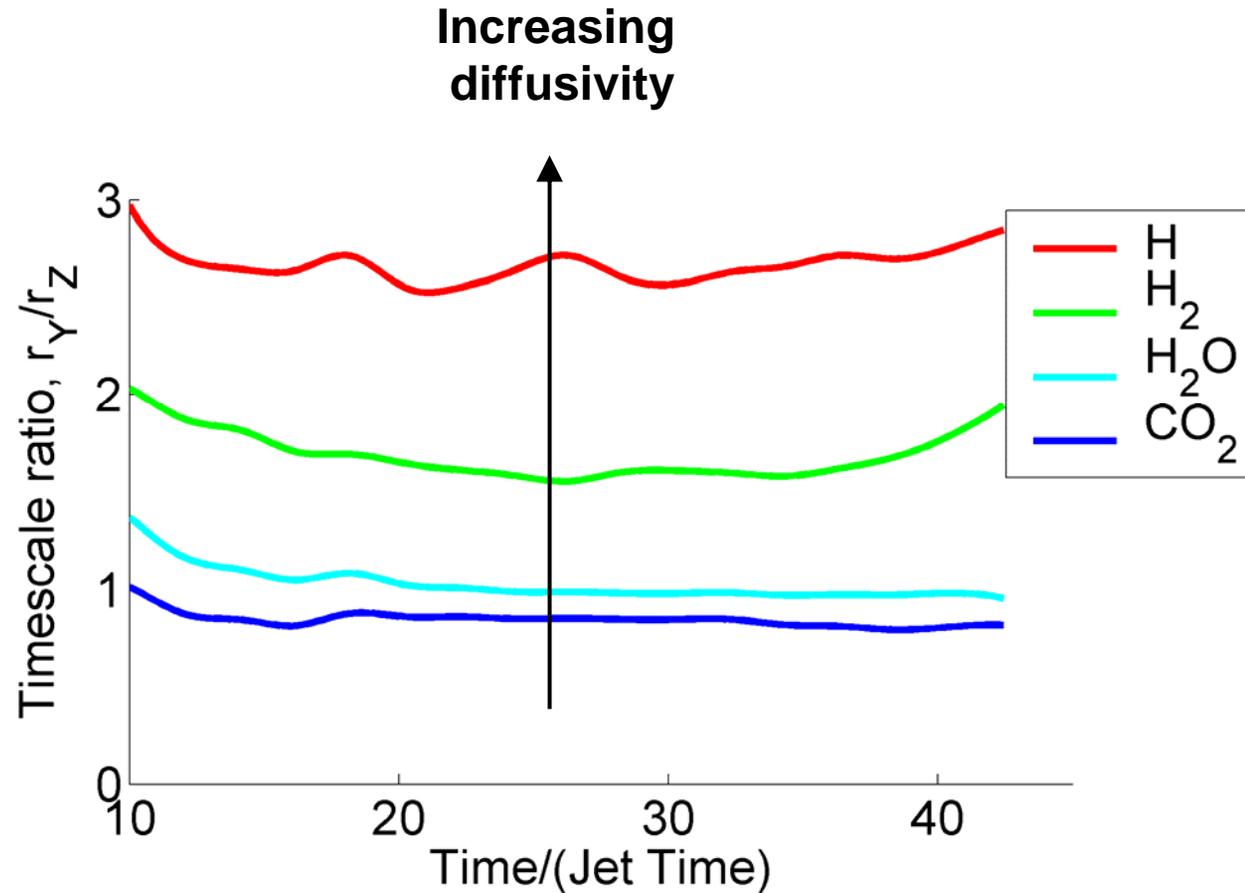
Mixture fraction to mechanical timescale ratio

- Confirmation that mixture fraction to mechanical time scale ratio is order unity.
- Average value about 1.6, similar to values reported by experiments, simple chemistry DNS, and used successfully in models.



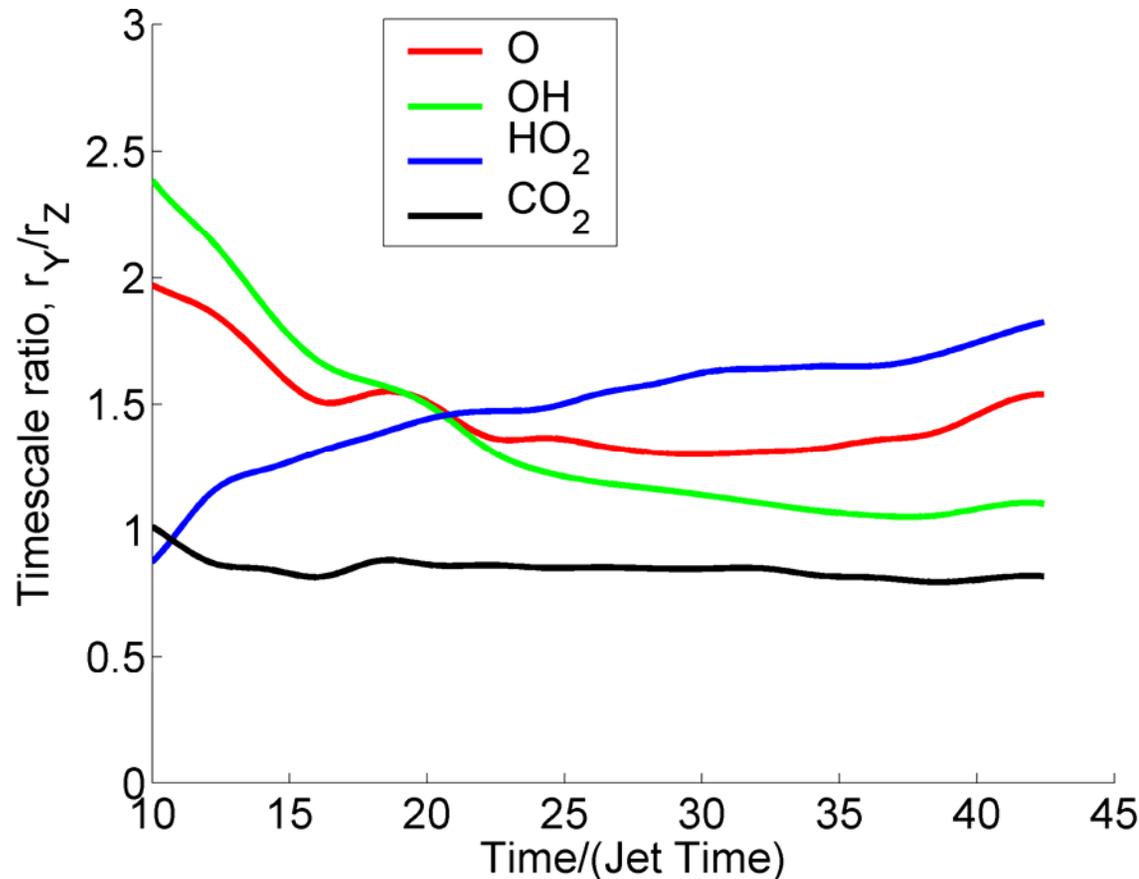
Effect of diffusivity

- Smaller, more highly diffusive species do have faster mixing timescales
- Ratio is not as large as the ratio of diffusivities – indicates a partial balance of production and dissipation exists.
- Future work: compare with models in literature.



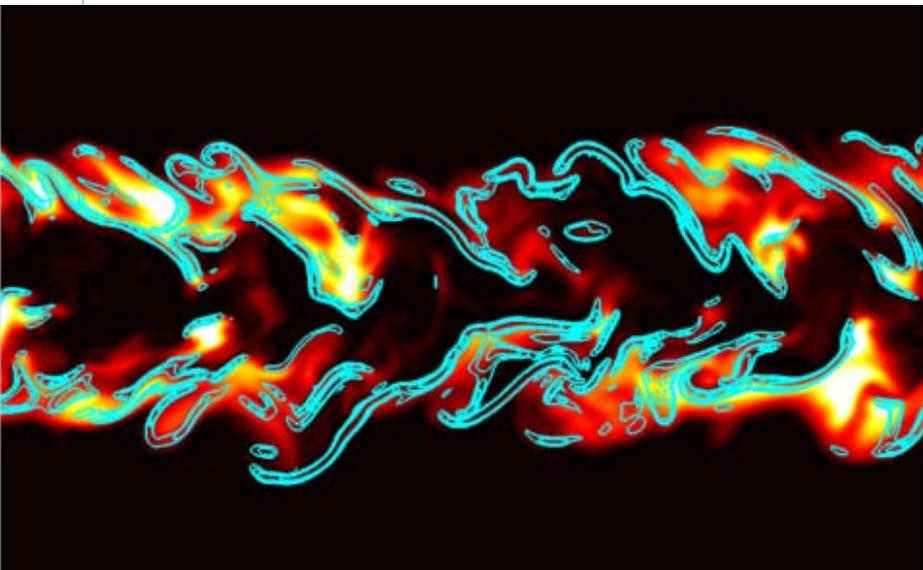
Chemistry effects on mixing?

- Major species such as CO_2 are relatively constant while minor radicals O , OH and HO_2 are time varying.
- At late times, the diffusivity trend does not appear to hold for HO_2 versus O and OH .
- Theory: somehow chemistry effects are causing these different behaviors.

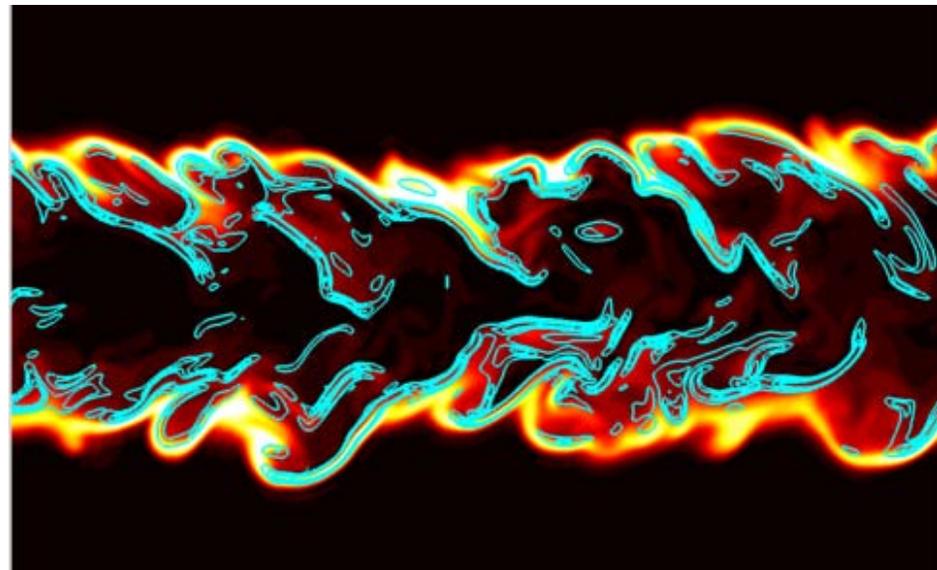


Radical production and destruction in high dissipation regions

OH



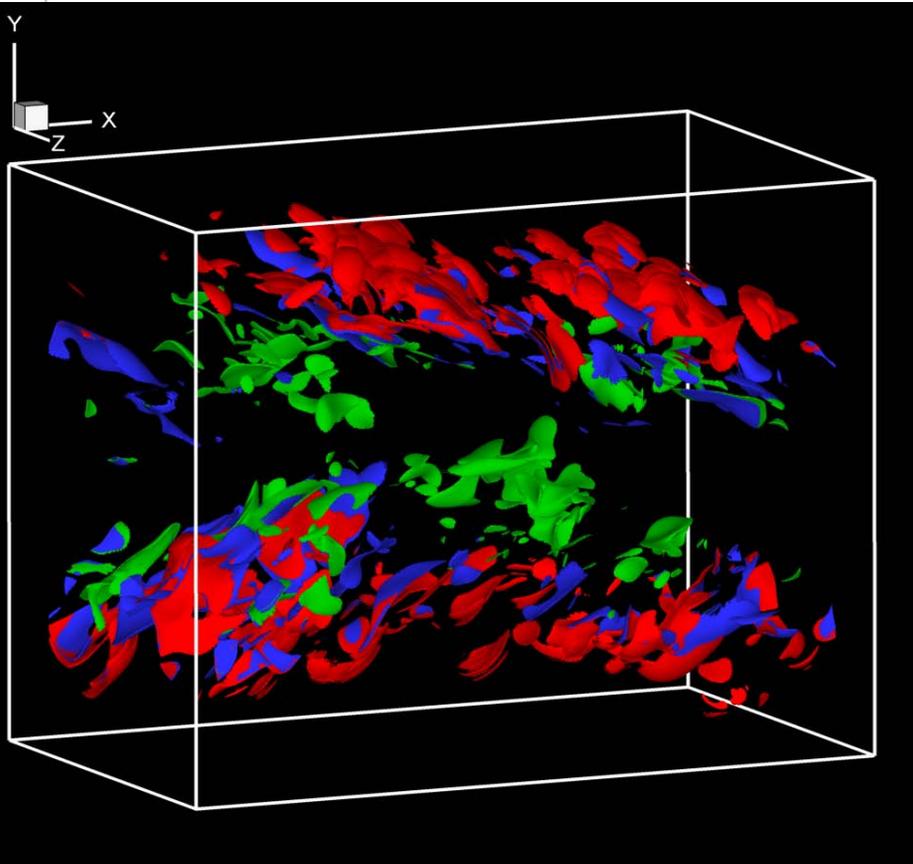
HO₂



Color scale: mass fraction
Blue contours: χ

- OH is destroyed while HO₂ is produced in high dissipation regions

Dissipation of passive and reactive scalars



- Blue: χ_Z , Green: χ_{OH} , Red: χ_{HO_2}
- Dissipation fields of Z and HO₂ are co-incident and aligned with principal strain directions
- OH dissipation occurs elsewhere, more in the centre of the jet
- These fundamentally different structures are due to the different chemical response of the species
- Future work – how does this affect the mixing timescales?

Conclusions - mixing timescales

- New finding: detailed transport and chemistry effects can alter the observed mixing timescales
- Models may need to incorporate these effects
 - a poor mixing model could lead to incorrectly predicting a stable flame when actually extinction occurs
- This type of information cannot be determined any other way at present
 - ambiguities in a-posteriori model tests
 - too difficult to measure
 - need 3D and detailed chemistry to see this

Summary

- We used a state-of-the-art DNS capability to perform some very challenging turbulent combustion simulations, utilizing up to 4096 IBM SP3 processors at NERSC.
- INCITE Award enabled extension to 3D and correct representation of the turbulence dynamics
- 3D DNS of detailed finite-rate chemistry effects in turbulent jets provides new insights and data for combustion modeling.
 - First glimpse of results reveals mixing of reactive and differentially diffusing scalars can be very different from conserved scalars.
 - More to come...!

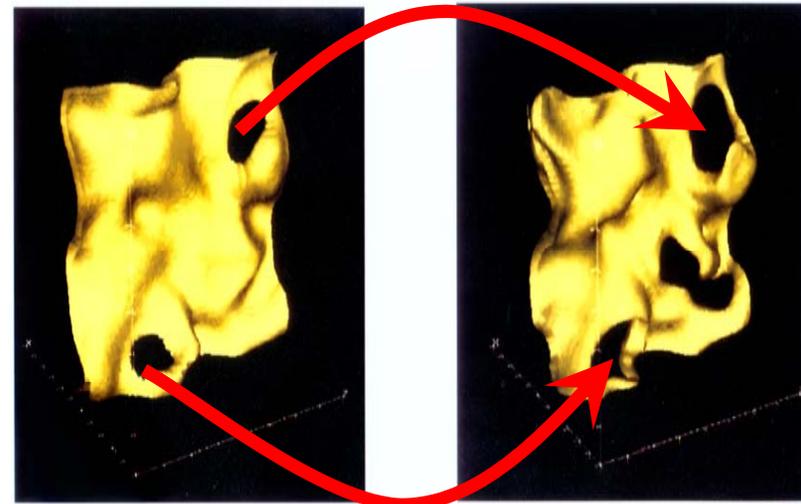
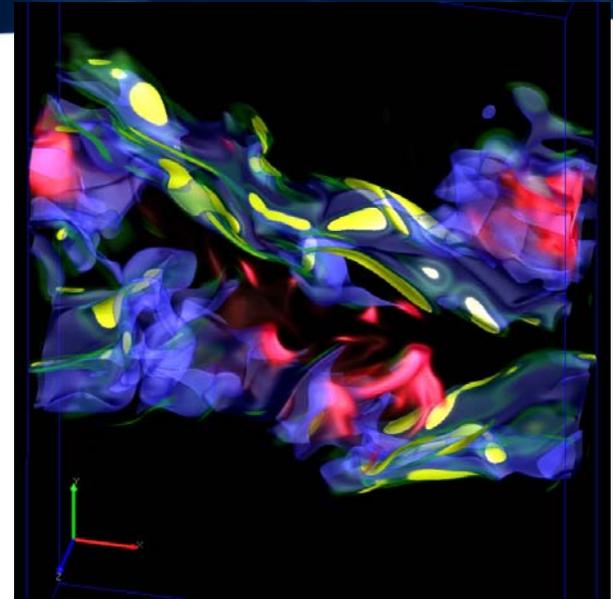
Knowledge Discovery From Terascale Datasets

- Challenge:

- Large data size, complex physics
- Lots of researchers with different questions – flexible workflow
- Post-processing needs to be interactive
- Remote archives and slow network

- Solution:

- Need interactive knowledge discovery software
- Multi-variate visualization
- Feature extraction/tracking
- Scalable transparent data sharing and parallel I/O across platforms



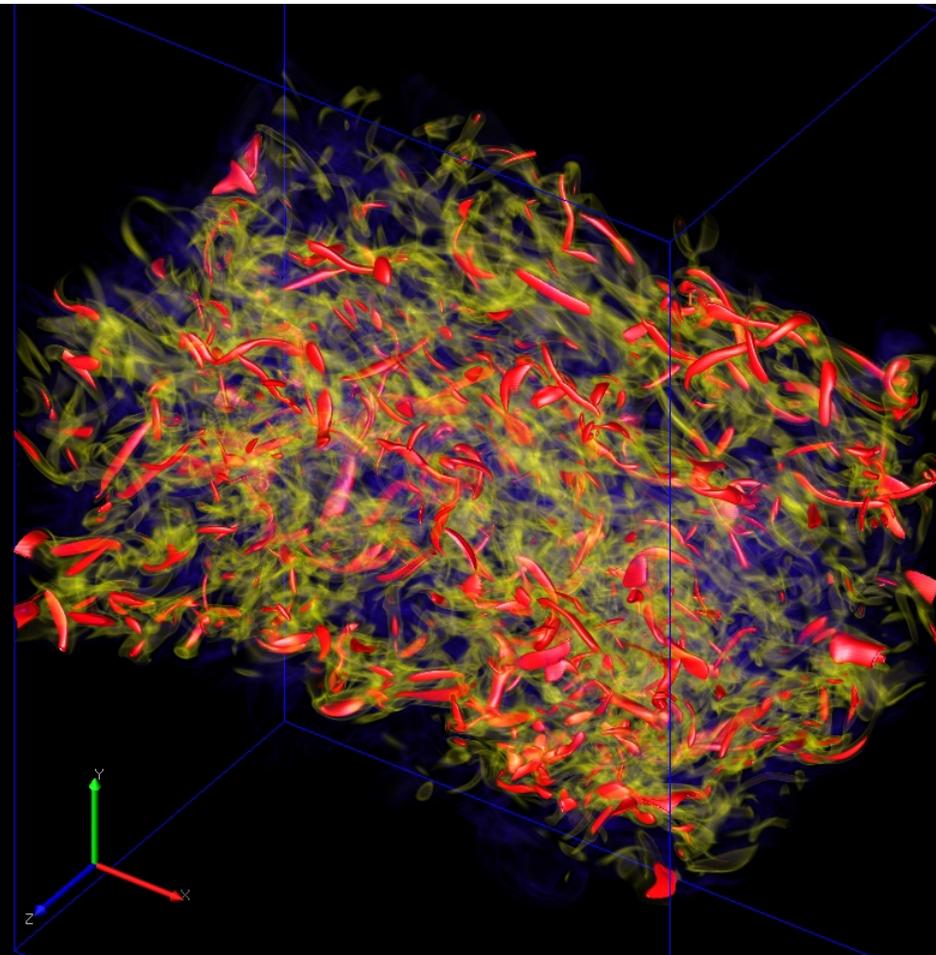
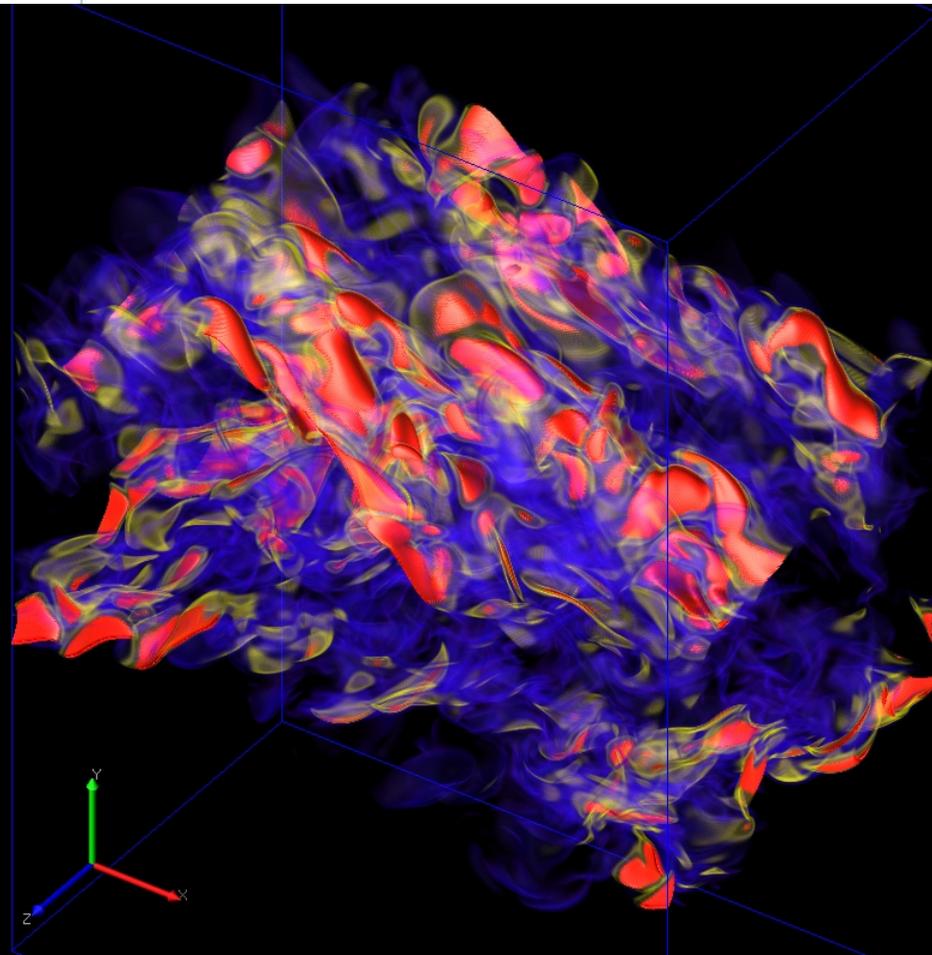
100 million grid run

Scalar Dissipation

$$\chi = 2D\nabla Z \bullet \nabla Z$$

Vorticity

$$|\omega| = |\nabla \times u|$$



100 million grid run

HO₂ dissipation

$$\chi_{HO_2} = 2D_{HO_2} \nabla Y_{HO_2} \bullet \nabla Y_{HO_2}$$

OH dissipation

$$\chi_{OH} = 2D_{OH} \nabla Y_{OH} \bullet \nabla Y_{OH}$$

