High Fidelity Terascale Simulations of Turbulent Combustion

Ramanan Sankaran, Evatt R. Hawkes
and Jacqueline H. Chen

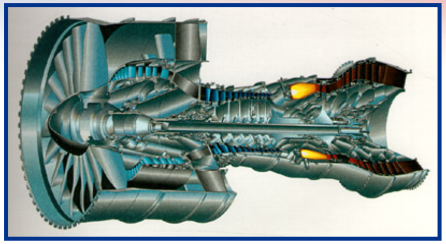
Combustion Research Facility
Sandia National Laboratories
Livermore CA

Supported by
Division of Chemical Sciences, Geosciences, and Biosciences,
Office of Basic Energy Sciences, and DOE SciDAC

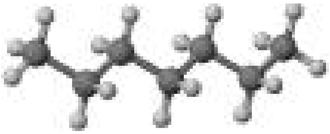
Sandia National Laboratories

CRF

Turbulent Combustion is a Grand Challenge!



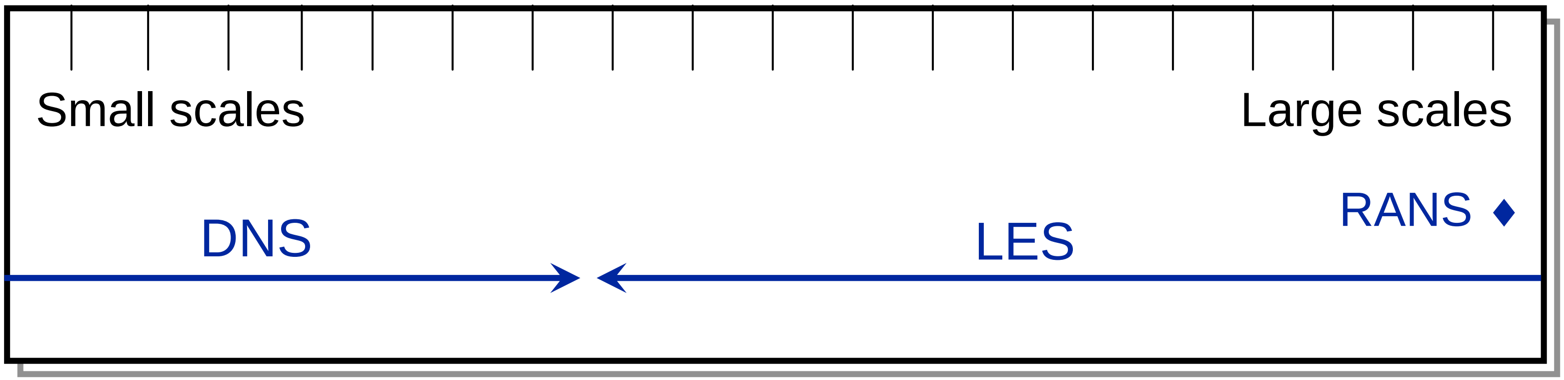
- **Stiffness: wide range of length and time scales**
  - Scale of combustor: 10 – 100 cm
  - Energy containing eddies: 1 – 10 cm
  - Small-scale mixing of eddies: 0.1 – 10 mm
  - Diffusive-scales, flame thickness: 10 – 100 μm
  - Molecular interactions, chemical reactions: 1 – 10 nm



- **Chemical complexity**
  - 100's of species, 1000's of reactions
- **Multi-physics interaction**
  - Multiphase (liquid spray, gas phase, soot, surface)
  - Thermal radiation
  - Acoustics
- **All scales and physics are relevant and coupled**
  - Must be resolved or modeled
- **Terascale computing $\rightarrow$ cold flow with O(10^3) scales**

DNS Approach and Role

- **No sub-grid modeling required. Fully resolves all scales. Limited on range of scales.**
- **A tool for fundamental studies of turbulent reacting flows**
  - Physical insight into chemistry turbulence interactions
  - Full access to time resolved fields
- **Validate models used in device-scale simulations.**
  - **Engineering CFD codes (RANS) and LES.**



DNS Capability at Sandia

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

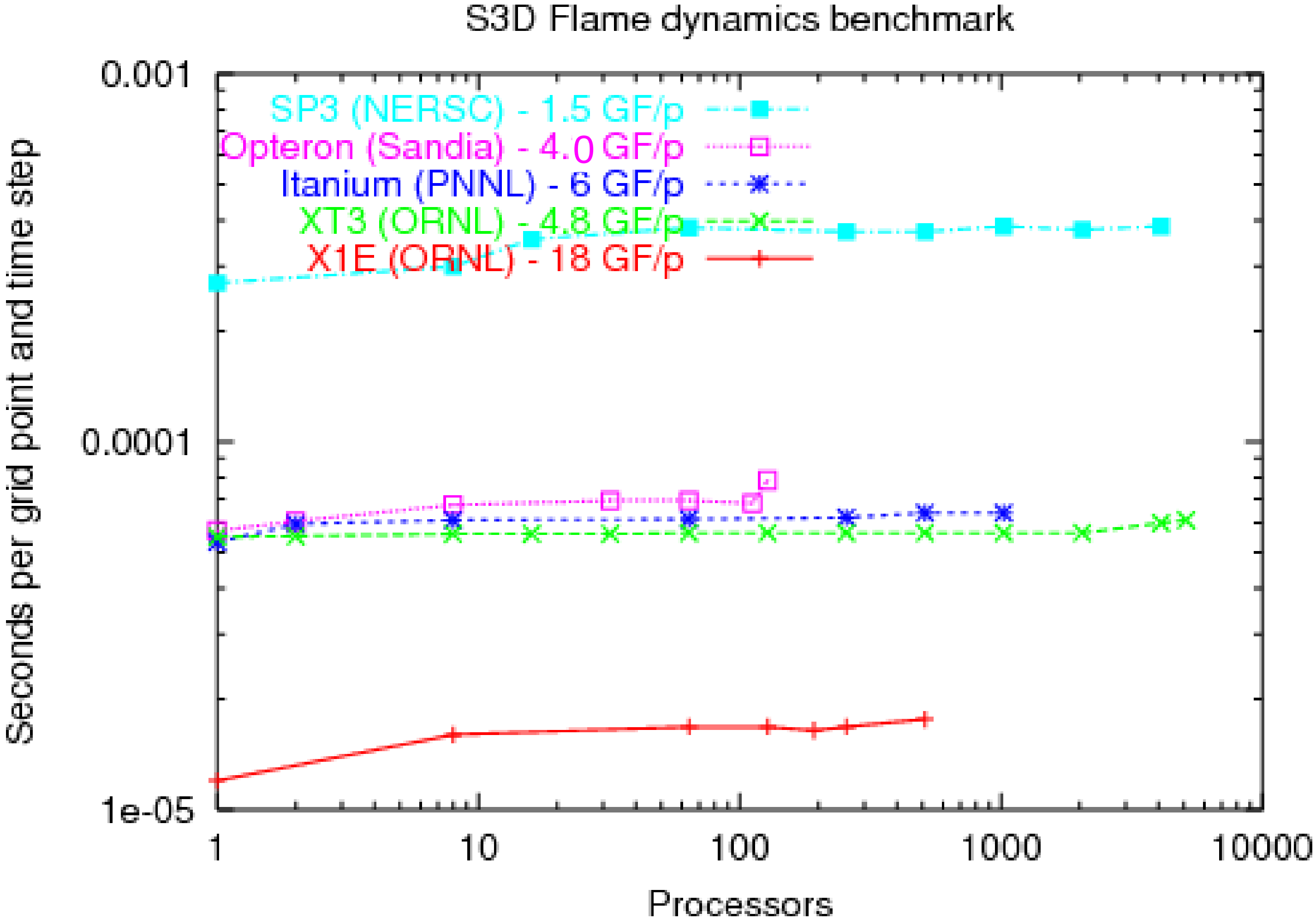
- Solves compressible reacting Navier-Stokes equations.
- High fidelity numerical methods.
  - 8th order finite-difference.
  - 4th order explicit RK integrator
- Hierarchy of molecular transport models
- Detailed chemistry
- Multi-physics (sprays, radiation and soot)
  - From SciDAC-TSTC (Terascale Simulation of Turbulent Combustion)
- Fortran90 and MPI
- Highly scalable and portable

Recent Performance Improvements

- INCITE award – 2.5 Million hours on IBM SP at NERSC
- Cray X1E award – 300,000 hours.
- Matrix Joule goal - Application Software Case Studies in FY05 for MICS
- Vectorization on X1E with help from CCS consultants.
  - Chemistry and Transport modules rewritten to enable vectorization
    - Use F90 explicit array syntax
    - Manually inline functions that compiler could not inline.
  - Co-array communication
- Improvements on all platforms
  - Minimize unit conversions
  - Tabulate thermodynamic properties
  - Eliminate MPI-derived data types for sending non-contiguous data
- Code runs **36 times faster!**

Performance on Various Platforms

90% Efficiency on 5120 XT3 processors



Non-premixed Flames

- Fuel and Air are separate – 'non-premixed'
  - Example – aircraft gas turbine combustor
    - Separated for safety reasons
  - Fuel and air have to mix at molecular scale for reaction to occur
  - Combustion depends on mixing rate.

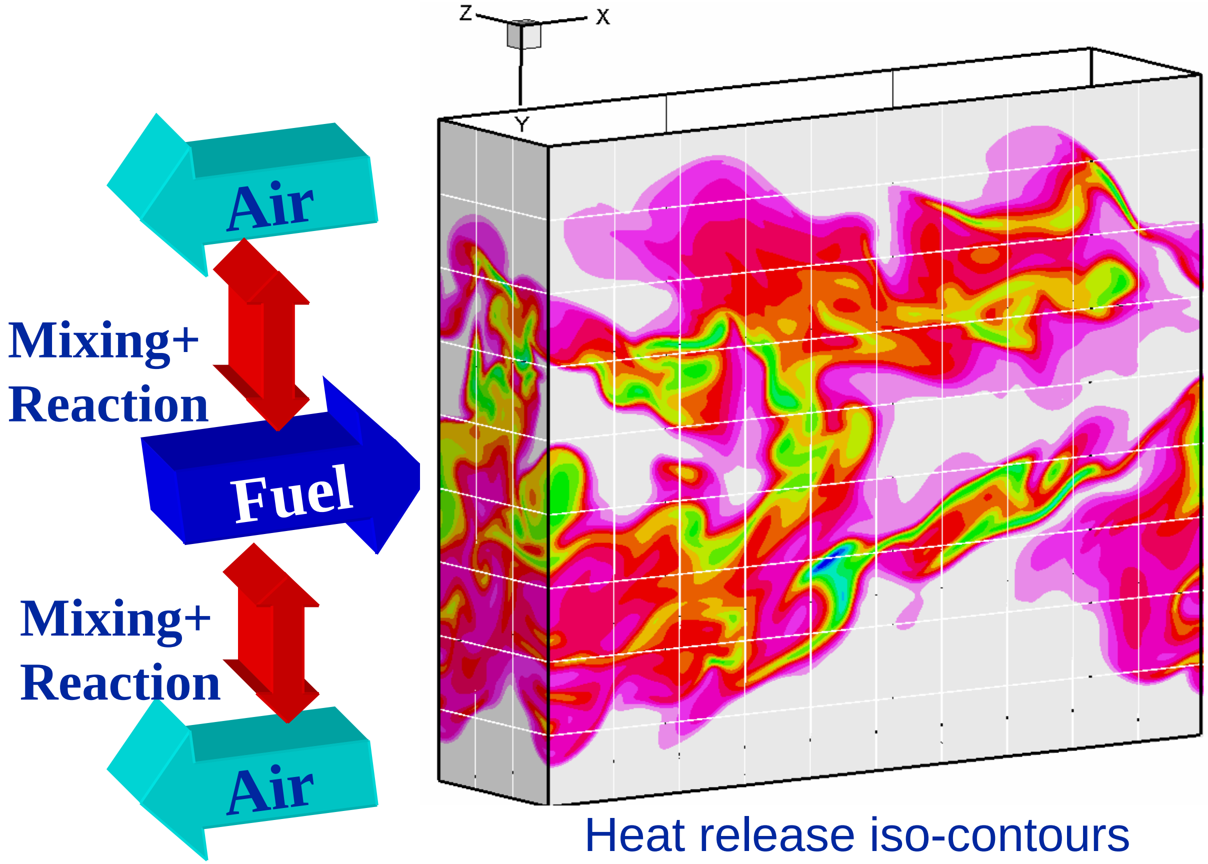
- "The effect of chemistry-turbulence interactions in turbulent non-premixed jet flames: mixing of passive and reacting scalars".

  E. R. Hawkes, R. Sankaran, J. C. Sutherland and J. H. Chen.

  (To be submitted to 31st combustion symposium.)

Description of Runs

- Temporally evolving non-premixed plane jet flames
- Canonical flow with shear-driven turbulence
- Detailed H_2/CO chemistry (17 d.o.f., Li et al. 2005)



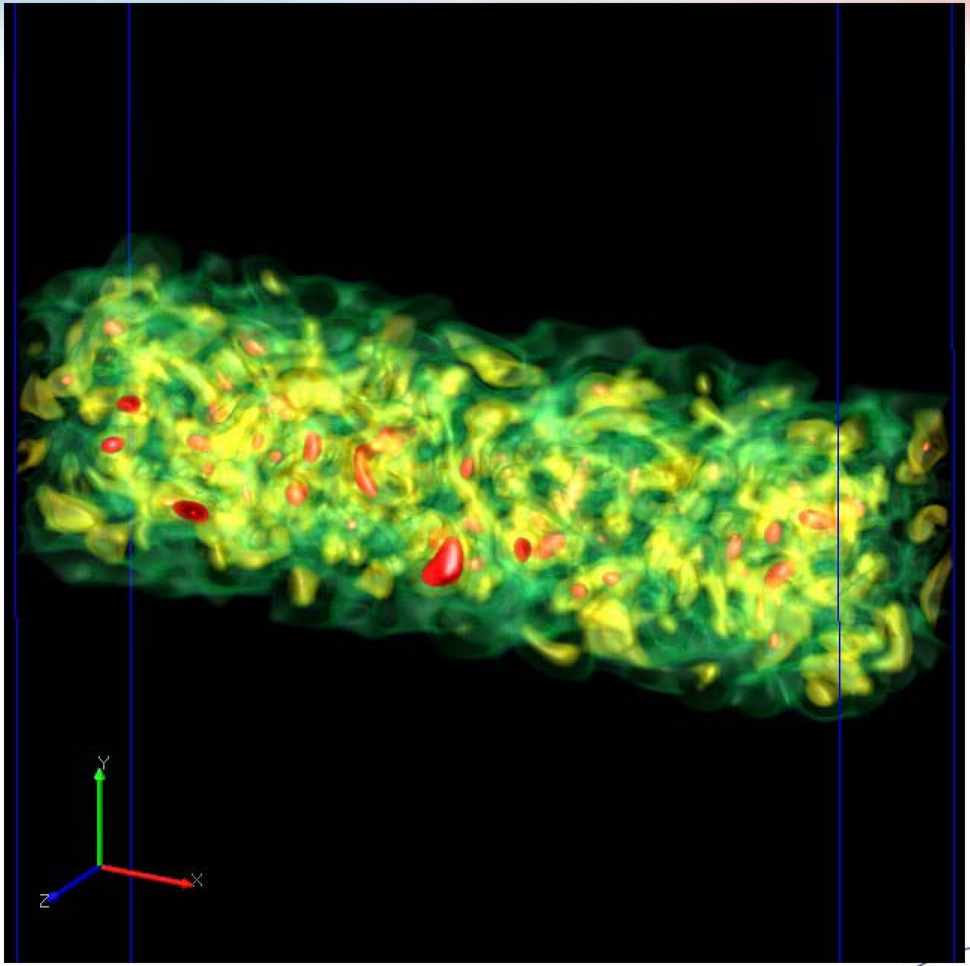
Heat release iso-contours

DNS Data Sets

- **Case A:**
  - Re = 6000
  - 40 million grid points
  - 480 processors on PNNL MPP2
  - ~ 1 TB data
- **Case B:**
  - Re = 8000
  - 100 million grid points
  - 1728 processors on NERSC Seaborg
  - 192/240 processors on ORNL Cray X1E
  - ~ 2.5 TB data
- **Case C: INCITE calculation**
  - Re = 4500
  - Running on Seaborg
    - 4096 procs
  - 350 million grid points
  - 3 million hours. 9TB raw data.
- **Case D:**
  - Re = 2500
  - Running on XT3
    - 2016 procs
  - 150 million grid points
- **Case E:**
  - Re = 9000
  - Running on X1E
    - 512 procs.
  - 500 million grid points

Scope of Study

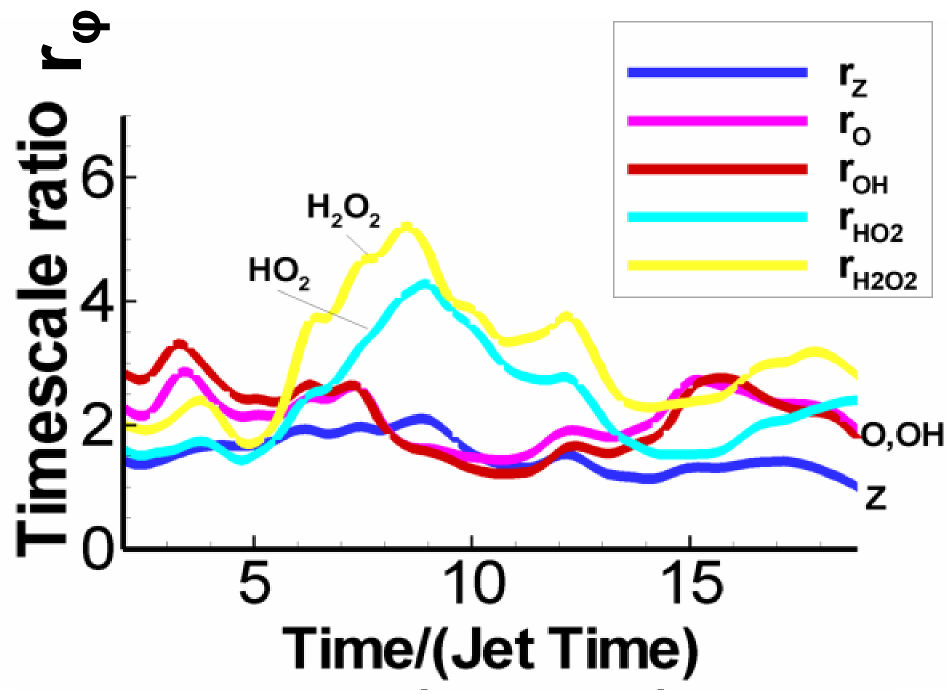
- Fundamental understanding of modes of extinction and re-ignition
- Study mixing of passive vs. reactive scalars
- Explore reduced descriptions of chemical states
- Study the effects of differential diffusion of radicals
- Develop and validate engineering CFD models for turbulent combustion



Case A - 40 Million Grid PNNL Run
Viz. by Akiba and Ma (UC Davis)

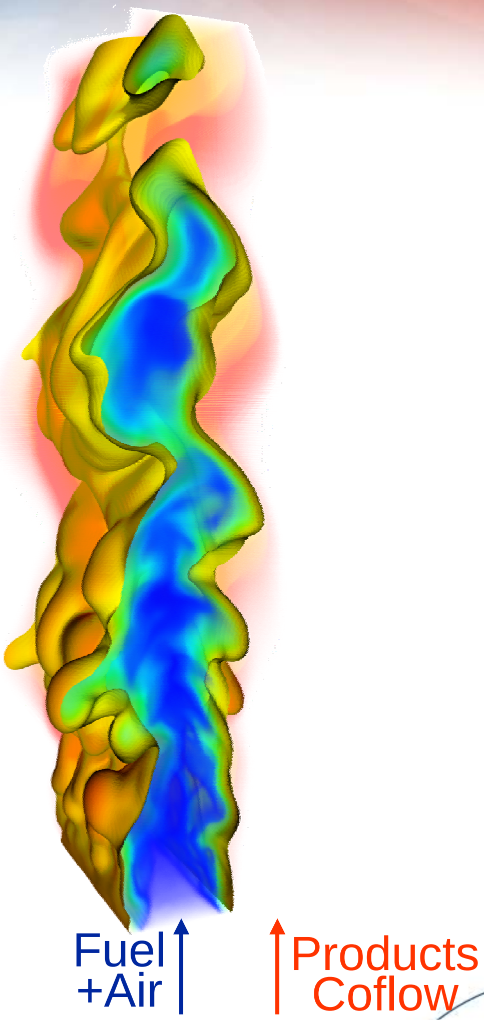
Diffusivity and Chemistry Effects on Mixing Timescale

- Mixing time scale is key element of combustion models (transported PDF method)
- Most models assume mixing time scale same as mechanical time scale for all species
- Detailed transport and chemistry effects can alter the observed mixing timescales



Premixed Flames

- Lean premixed combustion for natural-gas based stationary gas turbines.
  - Improved efficiency and reduced emissions
  - Combustion instability due to flammability limit
- DNS of turbulent premixed flame in a high turbulence regime
  - Detailed CH4/Air chemistry by T. Lu and C. K. Law (Princeton)
  - Work in progress on Cray X1E.



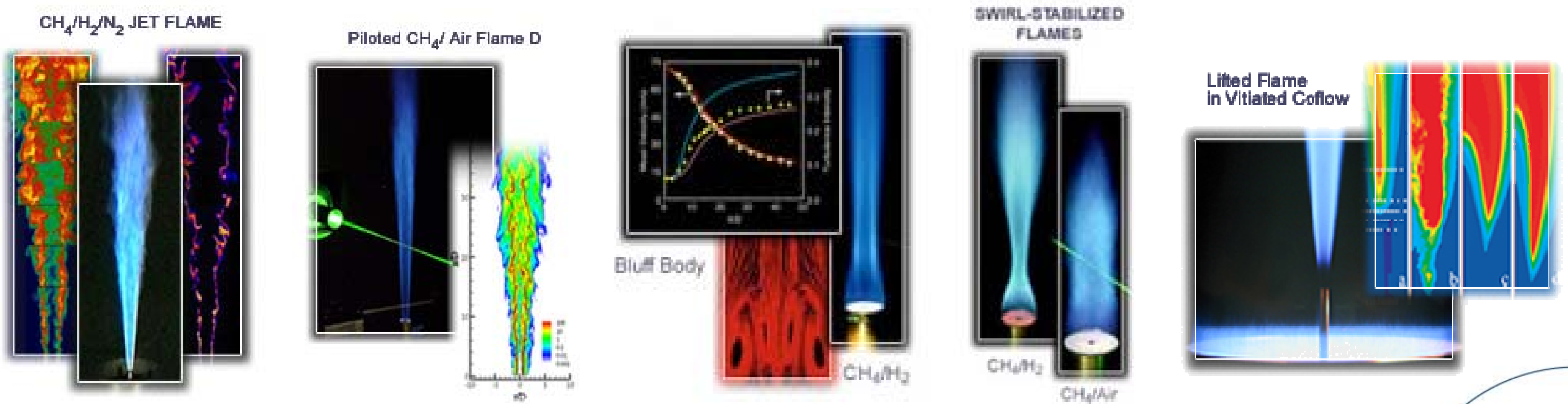
Viz. by D. Thompson and P. Pebay using Paraview

Sandia National Laboratories

CRF

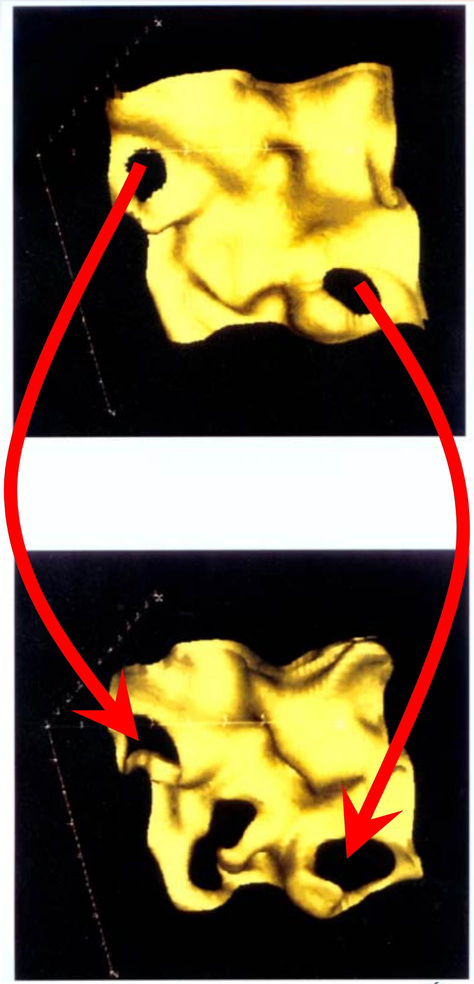
Community Data Sets

- TNF workshop (1996-2004): International Collaboration of Experimental and Computational Researchers
  - Framework for detailed comparison of measured and modeled results (http://www.ca.sandia.gov/TNF/abstract.html)
- New opportunities for numerical benchmarks – highly resolved LES and DNS

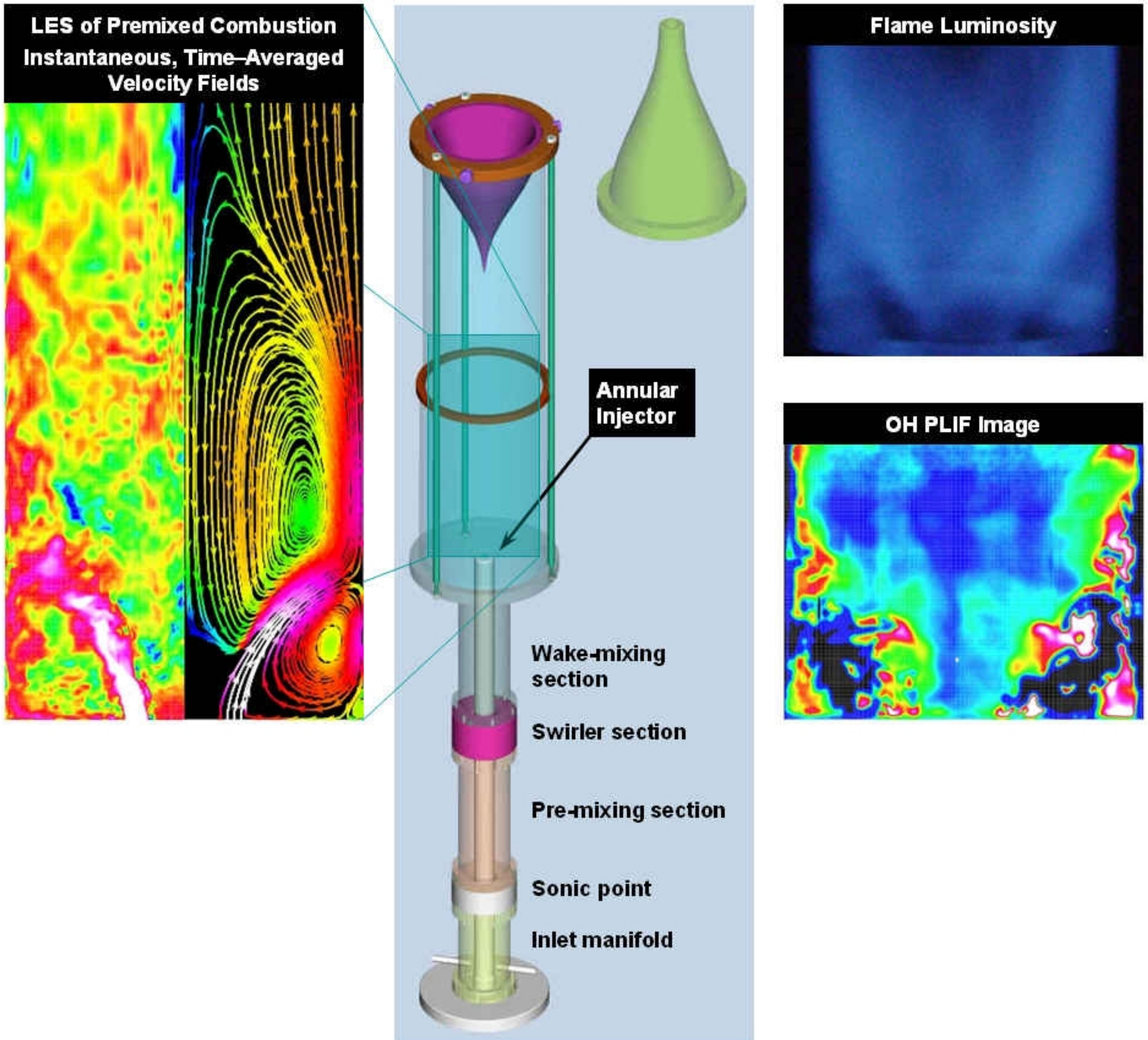


Knowledge Discovery from Terascale Datasets

- **Challenge**:
  - Large data size, complex physics
  - Lots of people with different questions
  - Post-processing needs to be interactive
  - Remote archives and slow network
- **Solution**:
  - Need interactive knowledge discovery software
  - Intelligent feature extraction/tracking
  - Scalable transparent data sharing and parallel I/O across platforms



LES Capability at Sandia



- LES treats the large scales directly
- Large scales are geometry dependent
- LES can couple directly with high Re experiments
- But – LES needs sub-grid models

Future Directions

- Current runs
  - Re=9,000, CO/H2 air chemistry, is in production on X1E.
    - 512 MSPs, 20 days
- What is possible with 100TF?
  - Re=20,000
    - Closer to parameter space of practical applications
    - Reynolds number invariance can be anticipated
  - Higher hydrocarbons
  - Multi-physics