Scientific Impacts and Opportunities for Computing

January 9-12, 2008

Wailea, Maui

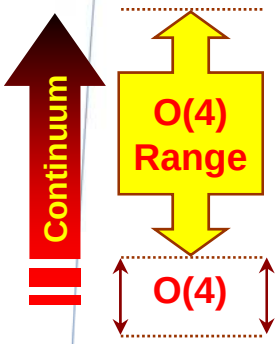
Combustion Session

Moderator: Jackie Chen, SNL

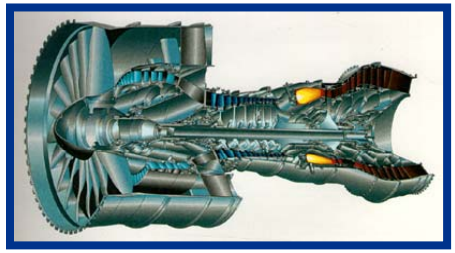
Plenary speaker: Andy McIlroy, SNL

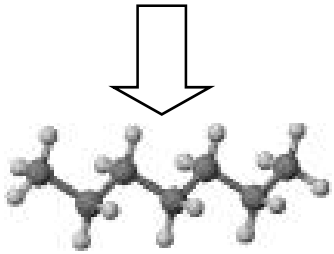
Panelists: Robert Harrison, ORNL, Angela Violi, U. Michigan, Al Wagner, ANL, Sreekanth Pannala, ORNL, Carlos Pantano, UIUC, Jackie Chen, SNL, and Joe Oefelein, SNL

Several decades O(10) 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 μ*m***
  - **Molecular interactions, chemical reactions: 1 – 10 *nm***



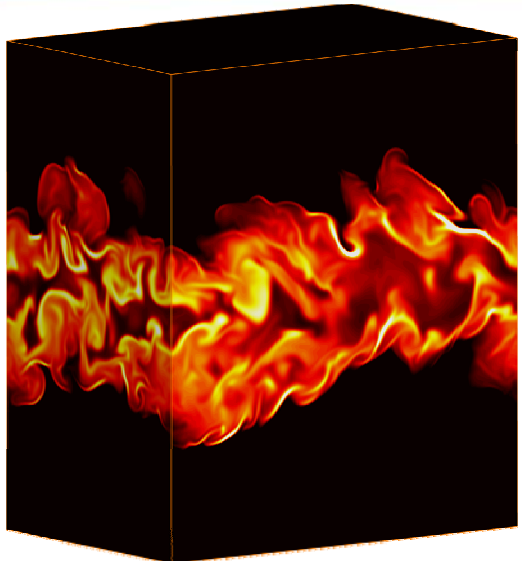


- **Spatial and temporal dynamics <u>inherently coupled</u>**
- **<u>All scales are relevant</u> and must be resolved or modeled**

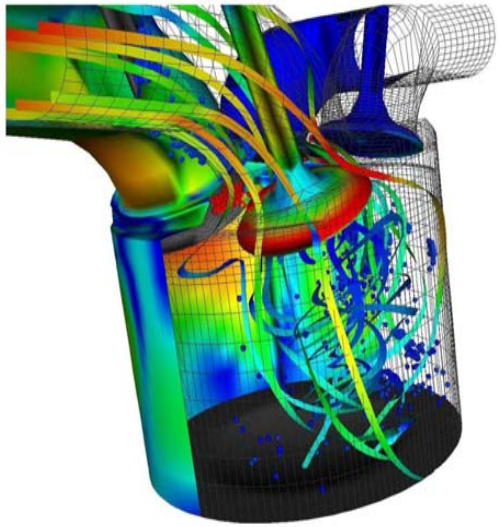
Terascale computing: ~3 decades in scales

Direct Numerical Simulation (DNS)

- **DNS is a tool for fundamental studies of the micro-physics of turbulent reacting flows**
  - **Full access to time resolved 3D fields**
  - **'chemistry-turbulence' interactions**



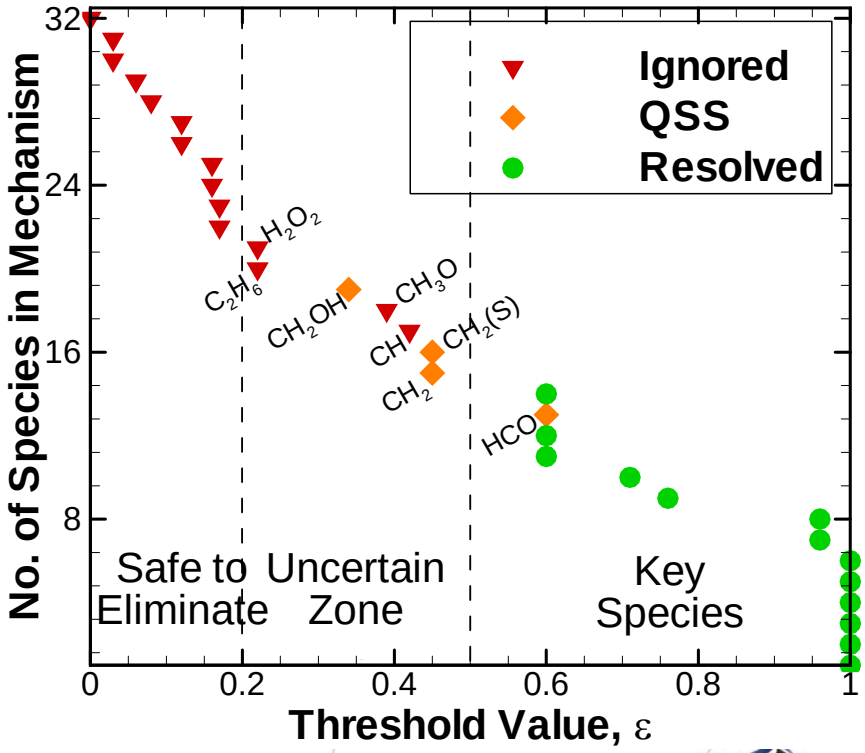
- **Develop and validate reduced model descriptions used in macro-scale simulations of engineering-level systems**



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

Chemistry Models for DNS

- Usual CH_4-Air mechanisms are not suitable for DNS
- Custom chemistry for DNS
  - By T. Lu and C.K. Law (Princeton U.)
- Starting with GRI1.2
  - 32 species, 177 reactions
- Identify species for elimination
  - Directed relation graph (DRG)
  - Sensitivity analysis
- Eliminate unimportant species
- Quasi-steady state assumption for CH_2OH, CH_2, $CH_2(s)$, HCO
  - Explicit algebraic relations
  - No costly iterations
- Ethylene-air and n-heptane-air (high pressure, low temperature)

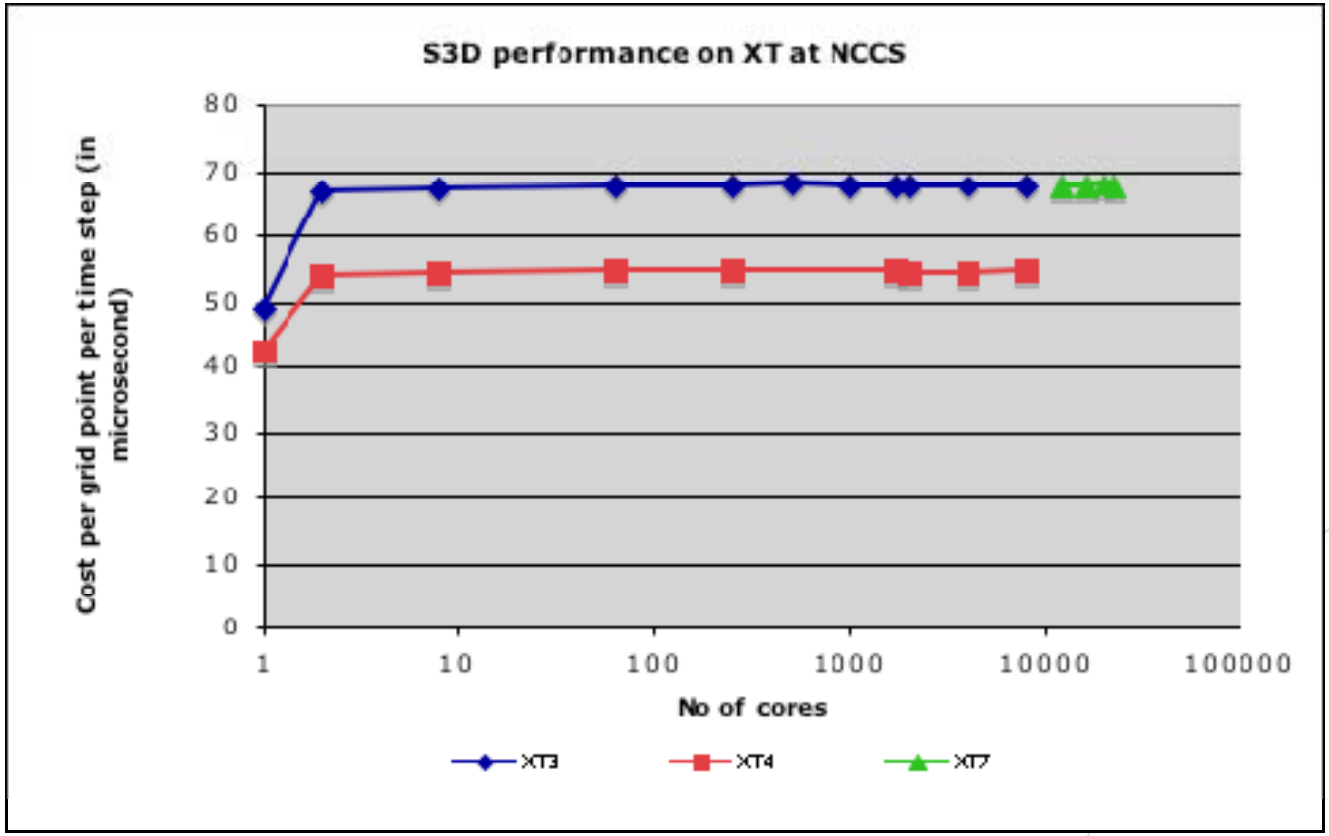


Partnerships with HPC Community

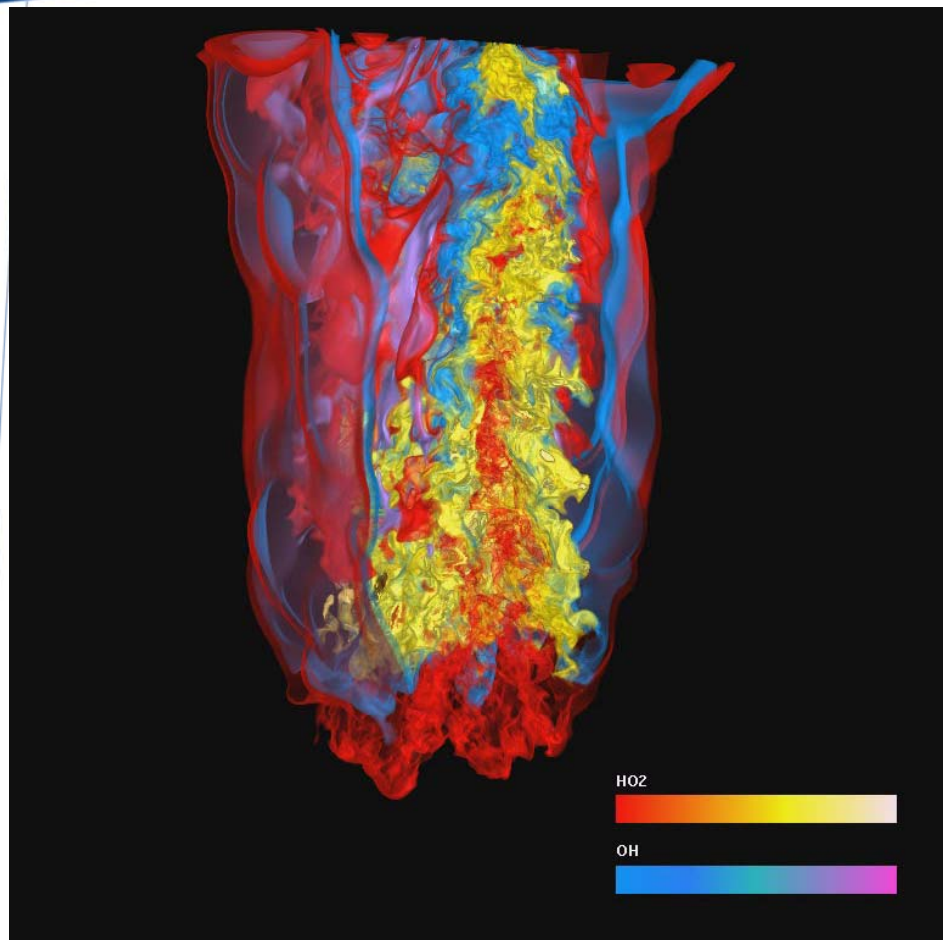
- Scalar and vector optimization of S3D (Mark Fahey, Ramanan Sankaran, ORNL, David Skinner, LBNL, SciDAC PERI Institute, David Bailey LBNL)
- Collective I/O (M. Fahey, ORNL, Choudhary and Liao, Northwestern U.)
- Multi-core programming paradigm (Fahey, Cray)
- Parallel Viz. (Ahern, ORNL, Ma, UC Davis)
- Topological Feature Segmentation and Tracking (Pascucci, LLNL)
- Combustion workflow in Kepler (Scott Klasky, ORNL)

S3D Parallel Performance

- S3D scales with 90% parallel efficiency on 20000 cores on CrayXT3 (ORNL)



Stabilizing an autoignitive turbulent jet flame



1 billion grids, 13 transported variable, 3.5 M cpu-hr, 35 TB data, 2007

- **Objective:How is a lifted autoignitive turbulent flame stabilized? What Is the structure of the flame and how are emissions affected? What is the effect of fuel dilution, turbulence, and coflow temperature?**

Numerical experiments:
Slot turbulent lifted jet flame in a vitiated coflow

- **Ambient pressure (experiments)**
  - **Fuel effects: H2, ethylene**
- **High pressure**
  - **n-heptane, bio-fuels**
  - **Multi-stage ignition**
- **Unique benchmark data used to evaluate and develop models**