Reacting Flow Simulation Framework for High Fidelity Simulations of Turbulent Combustion

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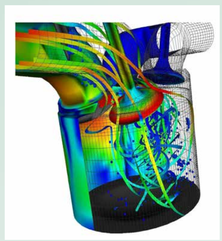
Abstract

We present a new reacting flow simulation software being developed to enable high fidelity direct numerical simulations of turbulent combustion using massively parallel computers. Initial applications of the software will enable direct numerical simulations (DNS) of compressible reacting flows with detailed chemical kinetics on a structured Cartesian mesh.

Direct Numerical Simulation (DNS)

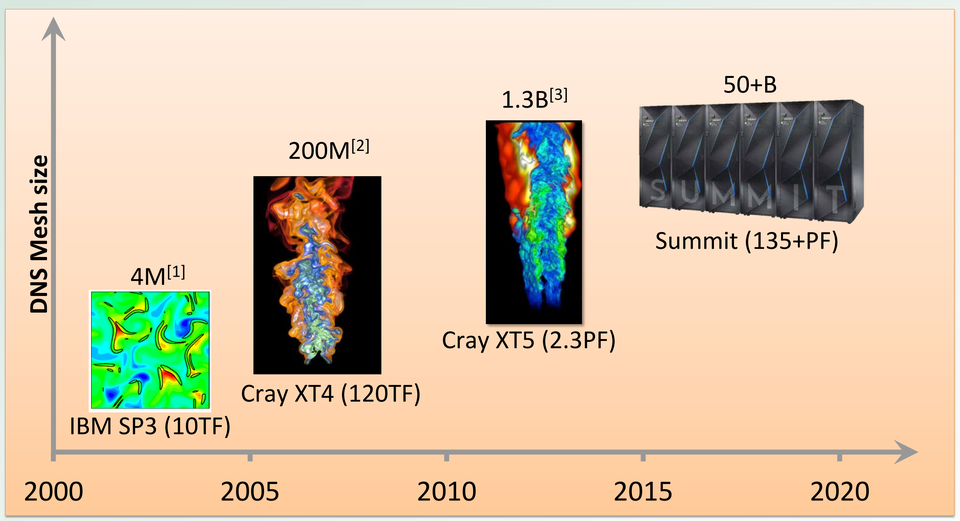
DNS is a tool for fundamental studies of the micro-physics of turbulent reacting flows. Our DNS approach fully resolves all continuum scales without using subgrid models. Device scale conditions are beyond reach due to the wide range of scales and computational complexity. DNS of small-scale laboratory flames and canonical configurations have immense potential for (1) investigating turbulence-chemistry interactions relevant for engineering scale devices (2) validating experimental measurement approach and (3) provide numerical benchmark data for predictive model development.

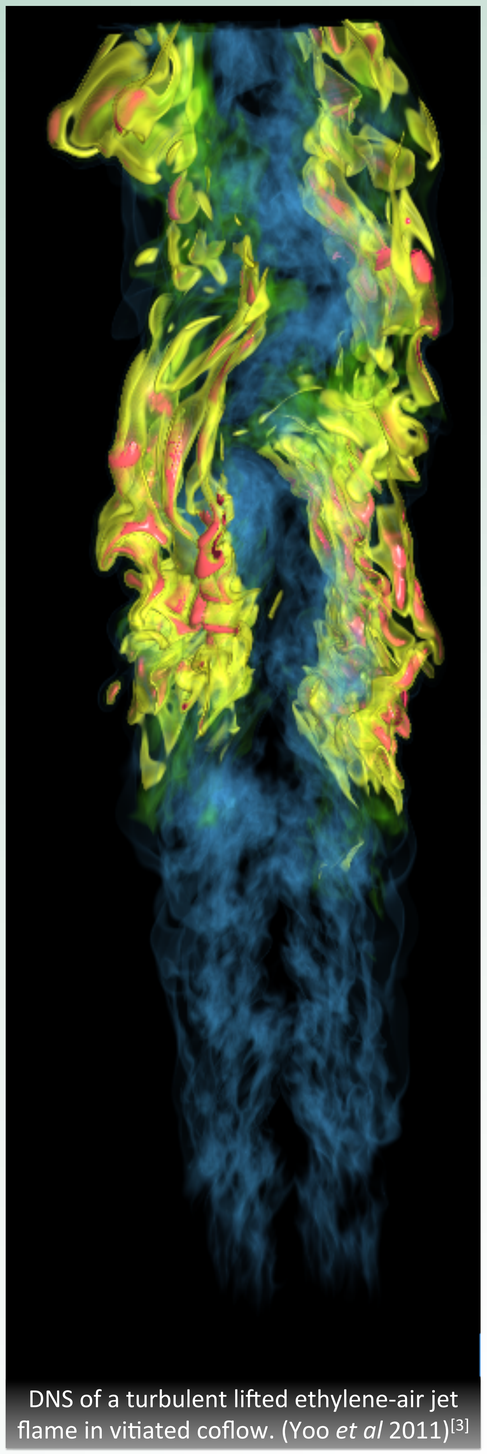
DNS ⟷ **Physical Models** ⟷ **Engineering CFD codes (RANS, LES)**



Software Objectives

- **Scalability and Portability** - Needs to efficiently utilize HPC resources at multiple sites including future systems such as Shaheen-II (KAUST) and Summit (OLCF).
- **Extensibility** - Future applications beyond Cartesian mesh DNS.
- **Leverage** open source libraries for combustion models and programming abstractions





DNS of a turbulent lifted ethylene-air jet flame in vitiated coflow. (Yoo *et al* 2011)[3]

DNS Numerical Method

- Solves the fully compressible governing equations for reacting flows. Navier-Stokes, energy, chemical species and mass conservation equations.
- Explicit 8th order finite differencing on a 9 point stencil.
- 4th order Runge-Kutta time integration.
- Nearest-neighbor MPI communication.

Challenges

- **Treatment of multi-species fluid properties adds computational complexity, communication and synchronization overheads.**
- **The continuous development of multi-physics models and ensuring their scalability requires a high level programming approach.**

Cantera library

We leverage Cantera for computing the chemical kinetics, thermodynamic and transport properties. We develop our own implementations of the performance critical kernels for performance and portability to GPU accelerators.

Kokkos programming model

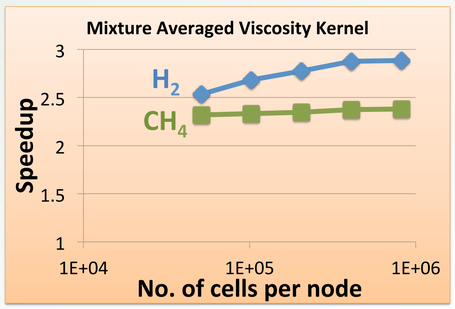
Kokkos, a Trilinos package, provides performance portability. It abstracts the device and memory layout. Here, we use a MPI+Kokkos model. Performance critical kernels are programmed as C++ functors that are dispatched to the device.

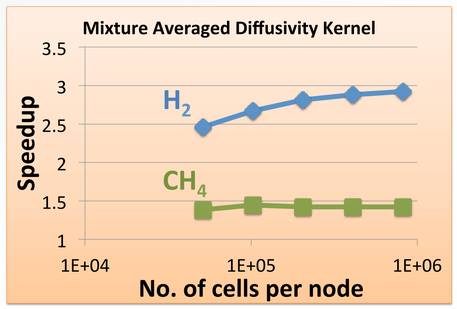
GPU Performance Results

Cray XC30 node with dual Intel Xeon E5-2670. 16 physical cores, 32 logical.

VS

Cray XK7 node with Tesla K20x accelerator.





- Performance and scalability are tested for two chemical models (i) 9 species Hydrogen (H_2) model and (ii) 53 species natural gas (CH_4) model.
- Viscosity kernel shows good speedup for problem sizes from 50k to 1M cells per node.
- Mixture averaged diffusivity shows performance issues for the large CH_4 chemical model. Nvprof results indicate register pressure and contention for memory bandwidth.
- Further work is needed to improve performance and to accelerate additional kernels.

References

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3. C. S. Yoo, E. S. Richardson, R. Sankaran, and J. H. Chen. 2011. doi:10.1016/j.proci.2010.06.147.

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