Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry

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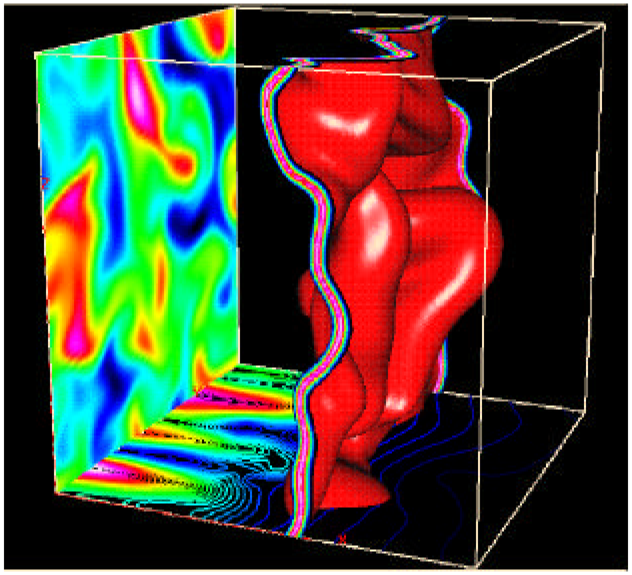
SciDAC: Computational Chemistry

(DOE Office of Science, Basic Energy Sciences: Chemical Sciences, Program Manager: William H. Kirchhoff, Coordinator: Larry Rahn)

PI Meeting - *01/15-16/02, Reston VA*

- Arnaud Trouvé (Univ. Maryland, *atrouve@eng.umd.edu*)
- Jacqueline Chen (Sandia Natl. Lab., *jhchen@ca.sandia.gov*)
- Hong G. Im (Univ. Michigan, *hgim@umich.edu*)
- Christopher J. Rutland (Univ. Wisconsin, *rutland@engr.wisc.edu*)
- Raghurama Reddy, Sergiu Sanielevici (PSC-Carnegie Mellon Univ., *rreddy@psc.edu*, *sergiu@psc.edu*)

Direct Numerical Simulation (DNS) of Turbulent Combustion

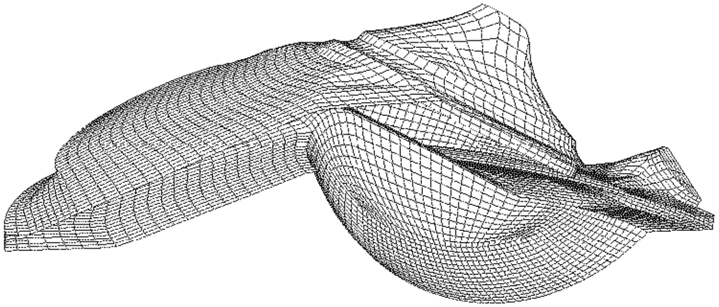


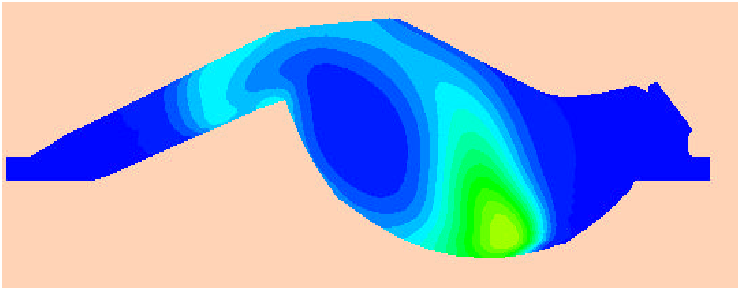
- A tool for fundamental studies of the micro-physics of turbulent reacting flows

DNS ⟷ *Answer basic questions; Detailed comparisons with experimental studies*

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

DNS ⟷ *Physical Models* ⟷ *Engineering-level CFD codes*





Objectives

Develop a terascale DNS capability for turbulent combustion:

- To leverage previous work in high-order Navier-Stokes and stiff chemistry numerical integrators, an existing collaboration between SNL and PSC for DNS implementation on MPP computers, and software/hardware infrastructures developed within SciDAC

- To adopt an object-oriented, component-based software design approach

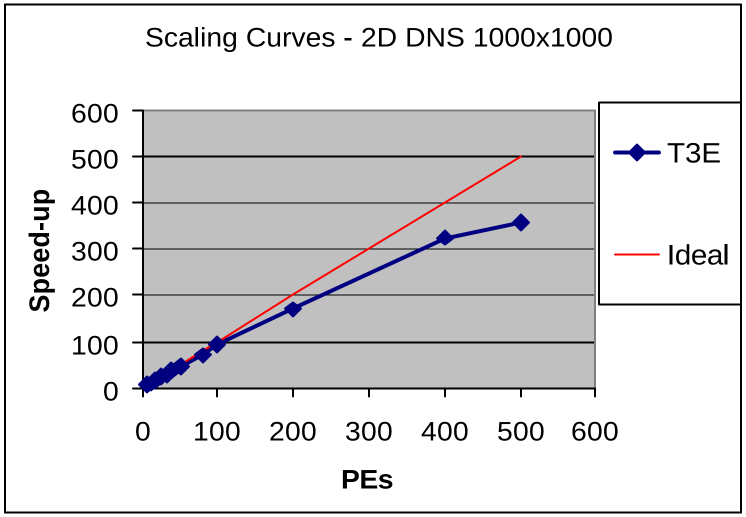
  ➡ enforce compliancy to the Common Component Architecture (CCA) developed by the SciDAC ISIC "*Center for Component Technology for Terascale Simulation Software*"

  ➡ use CCA to exchange components with the SciDAC project "*Computational Facility for Reacting Flow Science*"

- To enhance the DNS code with new numerical (implicit/explicit time integration; immersed boundary method; adaptive mesh refinement) and physical modeling (thermal radiation; soot particles; liquid droplets) capabilities

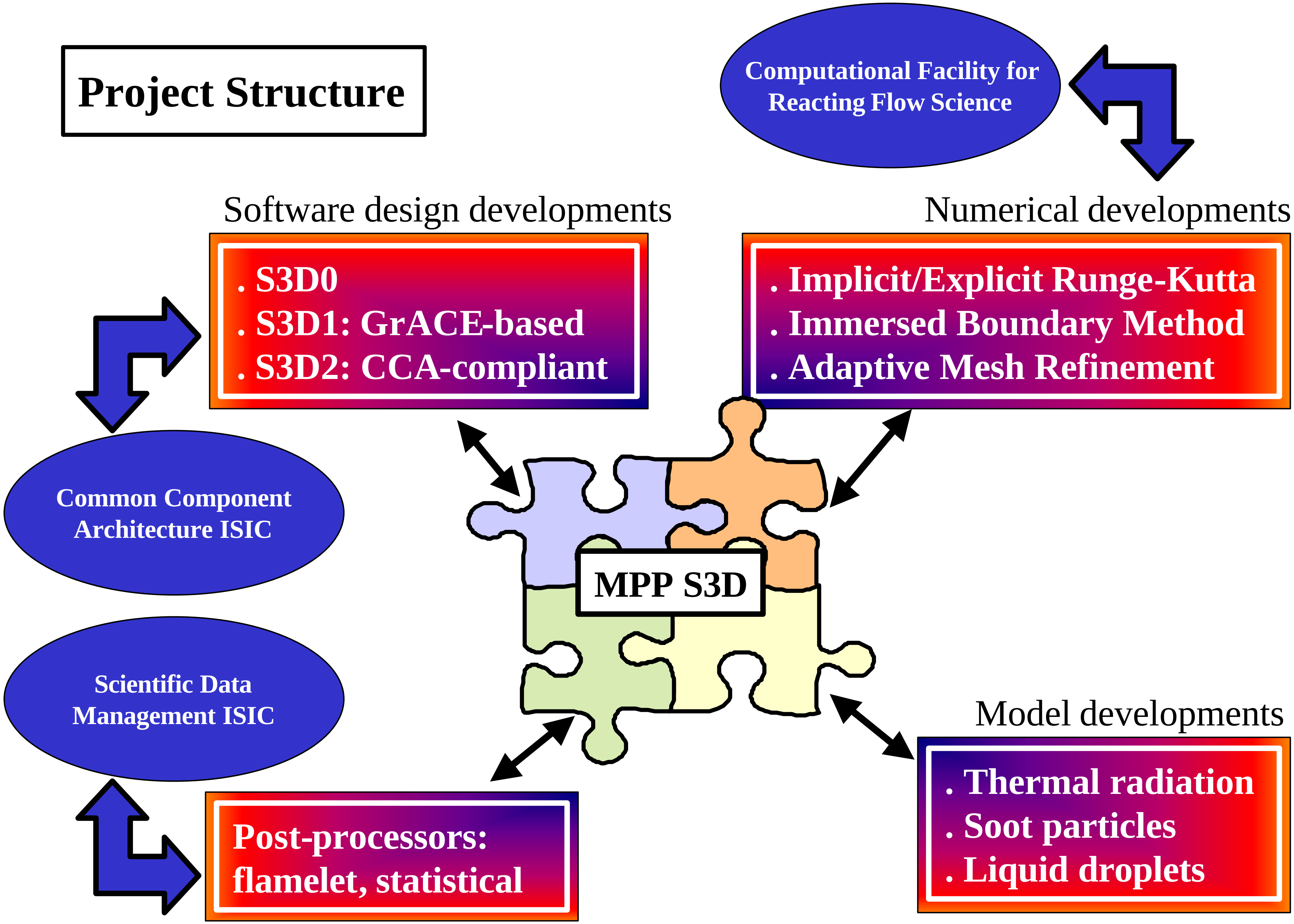
Current Direct Numerical Simulation Software

- S3D: S3D is a MPP-scalable, MPI-based, f77/f90, DNS solver developed by Sandia National Laboratories (SNL) and Pittsburgh Supercomputing Center (PSC)



- Capability: S3D is a fully compressible Navier-Stokes solver coupled with a solver for detailed, gas-phase chemical kinetics (based on the standard CHEMKIN package)
- High-fidelity: S3D is based on high-order finite difference methods (6^{th}-8^{th} order spatial discretization, 3^{rd}-5^{th} order explicit time integration with error controllers, characteristic-based inflow/outflow boundary conditions treatment, structured computational mesh)

Project Structure



Numerical Developments

- Implicit/Explicit Additive Runge-Kutta Method: explicit time integration of convective and diffusive transport (*Dt* determined by CFL/Fourier stability conditions); implicit treatment of stiff chemistry (*Dt* determined by error controllers)

⇒ Collaboration with C. Kennedy (SNL)

- Immersed Boundary Method: model geometrical complexity (multi-bodies, curved wall boundaries, moving wall boundaries) using a body-forcing approach embedded in a conventional cartesian computational mesh

⇒ Collaboration with C. Kennedy (SNL)

- Adaptive Mesh Refinement: develop a wavelet-based grid refinement/coarsening strategy coupled to high-order centered finite differencing

⇒ Collaboration with SciDAC project *"Computational Facility for Reacting Flow Science"* (H. Najm, J. Ray, SNL)

Physical Model Developments

- Themal Radiation: develop a tractable model based on the radiative transfer equation (RTE) to treat gray/non-gray gas radiative properties; solve the RTE using a discrete ordinate (DOM) or discrete transfer (DTM) method
- Soot Particles: develop a cost-effective phenomenological model based on transport equations for the soot volume fraction and particle number density (detailed gas-phase chemistry; no soot precursor chemistry; monodispersed soot particle size distribution)
- Liquid Droplets: develop a Lagrangian particle model to describe dilute liquid sprays (full gas/liquid phases interactions using sub-models for droplet drag and evaporation; allow for non-spherical droplet geometries; no description of break-up and droplet collisions)

Software Design Developments

- S3D0: enhance existing MPP version of S3D by including new numerical (implicit/explicit Runge-Kutta; immersed boundary method) and physical modeling capabilities (thermal radiation; soot particles; liquid droplets)
- S3D1- GrACE-based: adopt an object-oriented design and fit S3D into the Grid Adaptive Computational Engine (GrACE) framework. GrACE is a MPP framework targeted for adaptive mesh refinement (AMR) applications and includes load-balancing capabilities

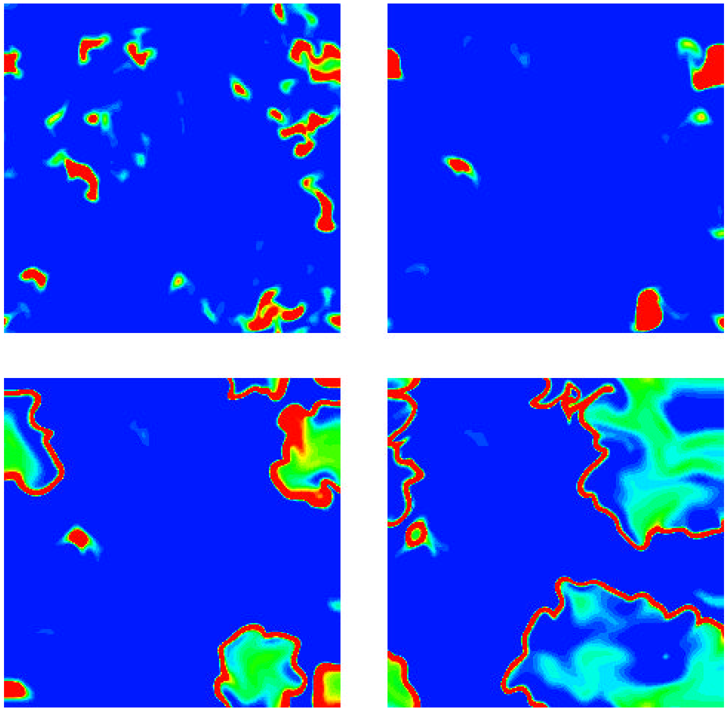
➡ Collaboration with SciDAC project "*Computational Facility for Reacting Flow Science*" (CFRFS, H. Najm, J. Ray, SNL)

- S3D2- CCA compliant: adopt a software interoperability standard, the Common Component Architecture (CCA); exchange software components (structured AMR component) with CFRFS project

➡ Collaboration with SciDAC CFRFS project (H. Najm, J. Ray, SNL) and SciDAC ISIC "*Center for Component Technology for Terascale Simulation Software*" (R. Armstrong)

Pilot Demonstration Studies

- DNS of compression-ignition in a liquid hydrocarbon fuel and air turbulent mixture: requires stiff time integrator and liquid spray modeling capability; applications to homogeneous-charge compression-ignition (HCCI) IC engines



- DNS of NOx emissions from turbulent jet flames: requires adaptive mesh refinement and thermal radiation/soot particles modeling capabilities; canonical problem to study pollutant emissions from non-premixed combustion systems