

Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry

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Work-in-progress Report – *Period from 03/31/02 to 03/31/03*

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Project Summary

The present project is a multi-institution collaborative effort aimed at adapting an existing high-fidelity turbulent reacting flow solver called S3D for efficient implementation on terascale massively parallel processors (MPP) computers. S3D adopts the direct numerical simulation (DNS) approach: DNS is a unique tool in combustion science proposed to produce both high-fidelity observations of the micro-physics found in turbulent reacting flows as well as the reduced model descriptions needed in macro-scale simulations of engineering-level systems. The new MPP S3D software is enhanced by adding new numerical and physical modeling capabilities, such as: an implicit/explicit additive Runge-Kutta method for efficient time integration; an immersed boundary method to allow for geometrical complexity; an adaptive mesh refinement (AMR) capability to provide flexible spatial resolution; a thermal radiation capability to allow for more realistic heat transfer descriptions; a soot formation capability to enhance pollutant emission predictions; and a liquid spray capability to capture fuel vaporization effects. In addition, the new MPP S3D software is modified to become object-oriented and fit into an advanced software environment based on an adaptive mesh refinement (AMR) framework called GrACE and the Common Component Architecture (CCA).

Program Scope

Direct numerical simulation (DNS) is a mature and productive research tool in combustion science that is based on first principles of continuum mechanics. Because of its high demand for computational power, current state-of-the-art DNS remains limited to small computational domains (*i.e.* weakly turbulent flows) and to simplified problems corresponding to adiabatic, non-sooting, gaseous flames in simple geometries. The objective of this research project is to use terascale technology to overcome many of the current DNS

limitations and allow for first-principles simulations of pollutant emissions (NO_x , soot) from turbulent combustion systems.

The effort leverages an existing DNS capability, named S3D, developed at Sandia National Laboratories and a collaborative effort between Sandia and the Pittsburgh Supercomputing Center for efficient implementation of S3D on massively parallel computers. S3D is a compressible Navier-Stokes solver coupled with an integrator for detailed chemistry (CHEMKIN-compatible), and is based on high-order finite differencing, high-order explicit time integration, conventional structured meshing, and MPI-based parallel computing implementation. The objective here is to both re-design S3D for effective use on terascale high-performance computing platforms, and to enhance the code with new numerical and physical modeling capabilities. The list of numerical developments includes: an implicit/explicit additive Runge-Kutta method for efficient time integration; an immersed boundary method to allow for geometrical complexity; and an adaptive mesh refinement (AMR) capability to provide flexible spatial resolution. The list of physical modeling developments includes: a thermal radiation capability; and a multi-phase capability including soot particles and liquid fuel droplets.

The new MPP S3D software is being modified to be object-oriented and fit into an advanced software framework, known as the Grid Adaptive Computational Engine (GrACE). GrACE is a MPP framework targeted for AMR applications and includes load-balancing capabilities. In addition, S3D will be made compliant to a software interoperability standard, the Common Component Architecture (CCA) developed by the SciDAC ISIC in Ref. [1]. The CCA environment will allow exchanging software components developed by different teams working on complementary tasks. It will allow in particular the re-use of components developed by a separate Sandia-led research project called CFRFS [2]. The CFRFS project is closely related to, and coordinated with, the present effort, and focuses for instance on developing an AMR component. This exchange of software components between different projects is a unique feature allowed by the SciDAC structure that promotes interactions between different teams of application scientists (our project and CFRFS [2]) and between application scientists and computer scientists (our project, CFRFS and the CCA ISIC [1]).

Recent Progress

As explained above, the present developments for S3D include a complete software re-design, new numerical methods and new physical modeling capabilities. We present here a summary of progress made during the first 19 months work period of this project extending from 09/01/01 to 03/31/03.

Software design developments:

- A new Fortran90 version of S3D has been developed and released by SNL (Scott Mason, Jacqueline Chen)
- GrACE has been ported on the PSC TCS computing system (TCS is a Compaq Alphaserver Cluster) and S3D is currently being adapted to the GrACE/CCA framework (PSC/Yang Wang, Roberto Gomez, Raghurama Reddy, Junwoo Lim)

Numerical developments:

- An implicit/explicit (IMEX) additive Runge-Kutta (ARK) time integration scheme has been developed and implemented into S3D (SNL/Christopher Kennedy; PSC/Roberto Gomez, Raghurama Reddy). A separate implicit solver (VODE) has also been implemented into S3D for auto-ignition problems (UWI/Christopher Rutland, [3]).
- A new pseudo-compressibility method has been developed and implemented into S3D (UMD/Arnaud Trouvé, [4]). This method allows for more efficient computations of slow flow problems while still using a fully compressible formulation.
- The S3D inflow boundary scheme (using a characteristic-based analysis) has been modified to allow for injection of laminar/turbulent flow perturbations while minimizing spurious acoustic wave reflections (UMI/Hong Im, [5]).

Physical model developments:

- A new thermal radiation solver (discrete ordinate method, DOM, grey and non-scattering medium) has been implemented into S3D (UMI/Hong Im). A second separate solver based on the discrete transfer method (DTM) is currently under development (UMD/Arnaud Trouvé).
- A phenomenological soot model based on transport equations for the soot volume fraction and particle number density has been implemented into S3D (UMD/Arnaud Trouvé).
- A Lagrangian particle model to describe dilute liquid sprays has been developed and coupled to the gas-phase Eulerian solver in S3D (UWI/Christopher Rutland, [3]).

Note that our strategy is to both work on new developments for S3D and exploit the most recently up-dated version of the solver to produce results and learn about combustion physics. Recent contributions to combustion science based on S3D may be found in Refs. [6-9] (SNL/Jacqueline Chen).

Future Plans

The main focus of the coming work period will be two-fold: (1) to release a CCA/GrACE-based version of S3D; (2) to initiate two pilot demonstration studies. The two pilot studies correspond to: the simulation of compression-ignition of a gaseous or liquid, hydrocarbon fuel in a turbulent inhomogeneous mixture; and the simulation of NO_x and soot emissions from hydrocarbon-air turbulent jet diffusion flames. The generation of these new DNS databases will also be associated with the development of adequate post-processing tools including tools for data visualization, flamelet-based analysis and statistical analysis.

References

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