Final Report (Project Period 2004-2008)
Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry (TSTC)

SciDAC: Computational Chemistry
DOE Office of Basic Energy Sciences, Chemical Sciences
Program Manager: Dr. Mark Pederson
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Principal Investigators

• Hong G. Im (University of Michigan, *hgim@umich.edu*)
• Arnaud Trouvé (University of Maryland, *atrouve@umd.edu*)
• Christopher J. Rutland (University of Wisconsin, *rutland@engr.wisc.edu*)
• Jacqueline H. Chen (Sandia National Laboratories, *jhchen@ca.sandia.gov*)

Project Summary

The TSTC project is a multi-university collaborative effort to develop a high-fidelity turbulent reacting flow simulation capability utilizing terascale, massively parallel computer technology. The main paradigm of our approach is direct numerical simulation (DNS) featuring highest temporal and spatial accuracy, allowing quantitative observations of the fine-scale physics found in turbulent reacting flows as well as providing a useful tool for development of sub-models needed in device-level simulations. The code named S3D, developed and shared with Chen and coworkers at Sandia National Laboratories, has been enhanced with new numerical algorithms and physical models to provide predictive capabilities for spray dynamics, combustion, and pollutant formation processes in turbulent combustion. Major accomplishments include improved characteristic boundary conditions, fundamental studies of auto-ignition in turbulent stratified reactant mixtures, flame-wall interaction, and turbulent flame extinction by water spray. The overarching scientific issue in our recent investigations is to characterize criticality phenomena (ignition/extinction) in turbulent combustion, thereby developing unified criteria to identify ignition and extinction conditions. The computational development under TSTC has enabled the recent large-scale 3D turbulent combustion simulations conducted at Sandia National Laboratories.

Program Scope

The primary goal of the SciDAC TSTC was to extend the S3D code with enhanced physical and algorithmic modules, and undertake several large-scale simulations to investigate important scientific issues. The specific objectives of this project include:

- To enhance the computational architecture and numerical algorithms in order to allow more robust, accurate, and efficient simulations of multi-dimensional turbulent combustion in the presence of strong turbulence and chemical stiffness. The efforts include new algorithms for characteristic boundary condition treatment and improved code architecture for various hardware platforms.
- To expand and upgrade the physical submodels to describe the underlying mechanisms in greater detail. The existing modules of radiation, soot, and spray evaporation models are being further enhanced to reproduce realistic combustion processes.

- The effort has been enhanced by the INCITE 2007 project entitled “Direct Numerical Simulation of Turbulent Flame Quenching by Fine Water Droplets,” which served as a showcase of the modeling capabilities developed under this program. The targeted science issue to be addressed is fundamental characteristics of flame suppression by the complex interaction between turbulence, chemistry, radiation, and water spray. The high quality simulation data with full consideration of multi-physics processes are currently being analyzed, allowing fundamental understanding of the key physical and chemical mechanisms in the flame quenching behavior.

Partnership

The TSTC project was originally launched in 2001 as part of the DOE Scientific Discovery through Advanced Computing (SciDAC) program in order to address the complexities and challenges associated with performing first-principles numerical simulations of turbulent combustion on massively parallel computing architectures. Recognizing these challenges, a consortium of research institutions (University of Maryland, University of Michigan, University of Wisconsin, Sandia National Laboratories, Pittsburgh Supercomputing Center) was established in TSTC Phase I (2001-04) to achieve a critical mass of interdisciplinary skills and to develop a scalable, massively parallel DNS solver for turbulent combustion. The partnership was renewed in TSTC Phase II (2004-07), albeit without Pittsburgh Supercomputing Center. During TSTC Phases I and II, the DNS solver S3D has been re-designed for effective use on terascale high-performance computing platforms, as well as enhanced with new numerical and physical modeling capabilities. In the following, major computational and scientific accomplishments during TSTC Phase II are summarized.

Accomplishments

Computational and model developments:

- Two alternative radiation models based on the spectrally-averaged gray gas approximation have been implemented: the discrete ordinate method (DOM), also referred to as the S_n approximation, has been implemented by taking the advantage of low cost and ease of integration into the finite-difference grid structure. As an alternative approach, the discrete transfer method (DTM) was also employed as a ray-tracing method in which the grid-based radiation power density is reconstructed from the ray-based decomposition using a simplified projection operator. While these models have been existent for quite some time, the TSTC developments correspond to one of the first attempts at DOM and DTM in high-order DNS applications. Both of these models are coupled with a soot formation model based on a two-variable formulation for soot mass fraction and soot number density.

- To understand the mechanism of spray combustion and its dependency on droplet evaporation, turbulence mixing and ignition, a spray module has also been developed. The module includes full coupling between gas and liquid phases for evaporating sprays. A Lagrangian method is employed to track the individual droplets, and is embedded into the Eulerian framework for the gas-phase flow in S3D. The spray model adopts the classical PICell (Particle-In-Cell) method (a method that is widely used in the field of spray/particle fluid dynamics); it also uses a fourth-order interpolation scheme to identify the local gas properties at the droplet location and a general method to distribute the source terms according to an arbitrarily defined basis function, such that the distribution of drop source terms is smooth and independent of the grid size.

- Generalized characteristic boundary conditions have been derived and developed in order to account for multi-dimensional, viscous, and reaction effects in nonreflecting and solid surface boundaries (Figure 1). More recently, the method was extended to address additional source terms associated with liquid spray evaporation near the inflow and outflow boundaries. This new development has been critical in ensuring accurate simulation of water spray quenching of a steady state laminar and turbulent flames conducted under the INCITE 2007 project.

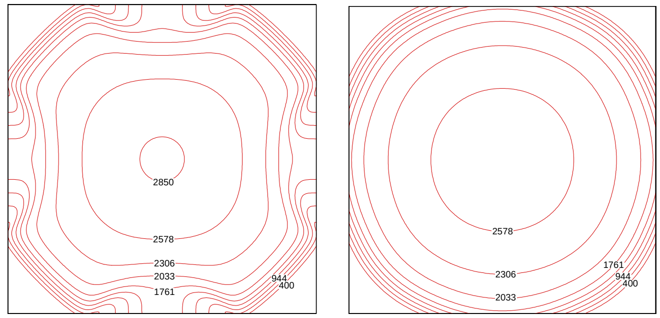

Figure 1: 2D simulation of ignition front propagation, demonstrating that the radially propagating front shape is highly distorted using the conventional boundary conditions (left), while the improved boundary condition treatment captures the correct front shape while it passes through the nonreflecting boundaries (right).

- The acoustic speed reduction (ASR) method has been implemented to allow a significant speed-up of computational time for subsonic problems by an artificial deceleration of acoustic waves. This method is an optional feature that is most effective in reacting flow simulations with relatively simple chemistry.

- As part of the 2005 Joule Software Effectiveness study, S3D have been ported to the Cray X1 and XT3 platforms at the NCCS/ORNL. Furthermore, several key modules of S3D were optimized and rewritten to improve the performance of the code on different platforms. As a result, the performance improved by 45% on the scalar architectures. The new modules were also suitable for vectorization, which enabled a terascale combustion science simulation on the Cray X1E.

- A new turbulence injection procedure has been developed, which allows time evolving turbulence from an ancillary cold non-reacting DNS to be fed in at the inflow of the main reacting DNS. This procedure was applied to recent simulations of a spatially developing flame-wall interaction problem where a realistic wall-bounded turbulence inflow was necessary for accuracy (Figure 2).

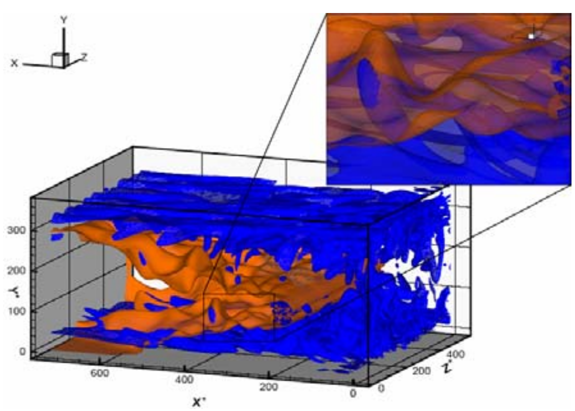

Figure 2: 3D simulation of the flame-wall interaction in a spatially developing configuration where the premixed flame is anchored at the center of the channel.

- As an effort related to the INCITE 2007 project, a modified mixture fraction variable formulation has been derived in order to account for mass addition due to spray. This new development allows us to correctly capture the flame location, and to accurately track important flame characteristics, such as fuel-air mixing, flame temperature, and water loading under spray conditions. This was employed in order to understand flame extinction dynamics due to combined aerodynamic quenching and evaporative cooling.

Scientific Accomplishments:

- Using the developed radiation and soot models, characteristics of soot formation in turbulent nonpremixed flames have been studied, in which the effects of turbulent transport on the transient soot dynamics and their impact on the overall soot production have been examined in detail (Figure 3). The study revealed the importance of detailed information of the local and transient flow-chemistry interaction in accurate prediction of the soot formation characteristics.

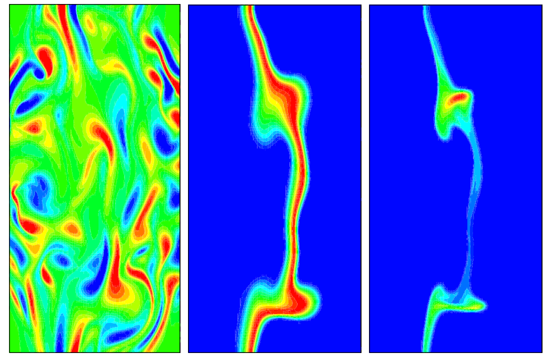

Figure 3: Simulations of turbulent nonpremixed ethylene-air flames, showing from left to right the vorticity, temperature, and soot volume fraction.

- 2D simulations have been performed on the basic interaction of a turbulent ethylene-air jet diffusion flame with cold solid wall boundaries (Figure 4). The simulations feature sooting flames and thermal radiation transport and provide fundamental insight into flame extinction events, soot leakage mechanisms, and turbulence-radiation interactions. The structure of the simulated wall flames is studied in terms of a classical fuel-air-based mixture fraction and an excess enthalpy variable. The excess enthalpy concept provides a convenient description of the deviations from adiabatic behavior, due to both convective and radiative cooling. Flame extinction is explained in terms of an extended scalar dissipation rate criterion; the extended criterion accounts for flame weakening due to convective/radiative thermal losses.

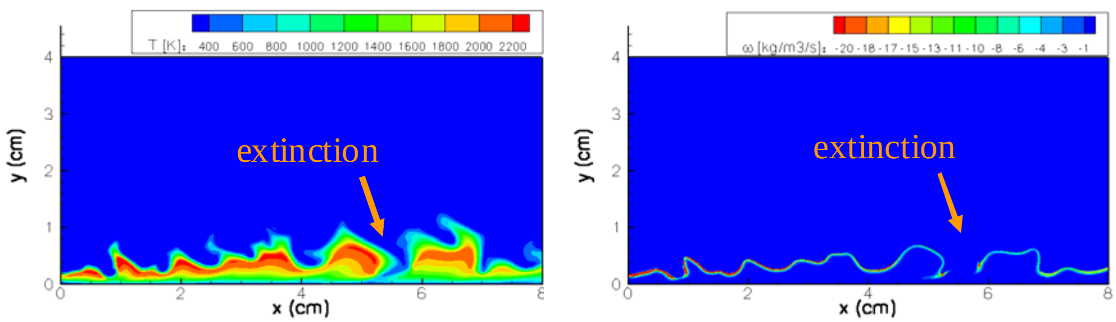

Figure 4: Two dimensional simulation of flame-wall interaction: temperature (left) and heat release rate (right) iso-contours show the local flame extinction event due to the wall heat loss.

- 2D simulations of a fuel spray jet were performed to investigate the ignition and propagation of the flame front. Figure 5 shows the heat release contours in an evolving fuel spray jet, where the white line denotes the stoichiometric line. Ignition occurred downstream of the spray exit, but upstream of the spray tip. After ignition, the combustion region propagated upstream via spontaneous ignition regions. However, downstream the combustion regions propagate as flamelets following the stoichiometric

Figure 5: Heat release contours of combustion in the evolving fuel spray jet. The liquid jet is shown at the left by droplets colored by their temperature.

line. The improved characteristic boundary conditions and enhance code efficiency with a large number of droplets have enabled successful demonstration of accurate and robust realization of fuel spray combustion.

- 2D simulations have been performed under the INCITE project in order to investigate the effects of turbulence and water spray on counterflow ethylene flames. A turbulence-with-spray case was compared to a turbulence-only case in order to observe how spray affects the evolution of extinction/reignition events. The results revealed that spray evaporation takes away enthalpy from the reaction zone, leading to an additional weakening in the aerodynamically strained flame segments. One of the main goals of this study is to define a unified flame extinction criterion that combines the flame weakening effect resulting from turbulence straining, oxygen displacement, and evaporative cooling. A flame weakness factor based on the excess enthalpy variable has been defined as a means to provide a rational extinction criterion.

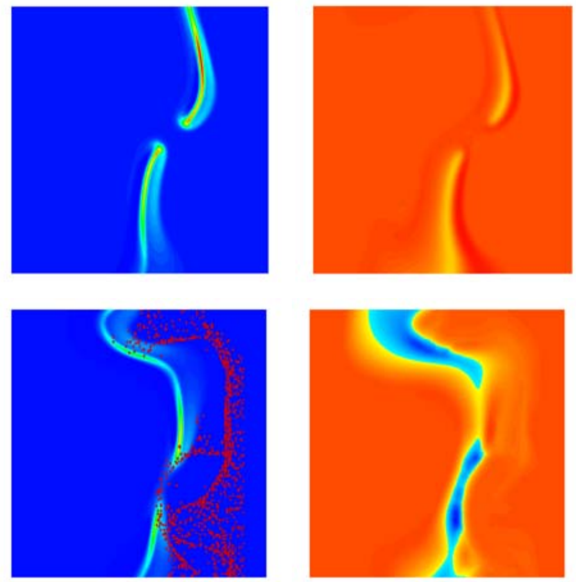

Figure 6: Comparison of turbulent flame extinction without (top row) and with (bottom row) water spray. Left column shows the heat release iso-contour with red points indicating water droplets, and right column shows the excess enthalpy variable, for which blue color indicates a larger level of flame weakening. The spray-induced extinction event clearly shows a higher level of flame weakening.

Proposed Research Program

The TSTC Phase II has achieved significant progress in the high-fidelity direct numerical simulations of turbulent combustion with realistic description of detailed chemistry/transport. gas radiation, spray transport and evaporation, and soot models. The TSTC project not only accomplished various scientific discovery of important fundamental physics of turbulent combustion, but the developed S3D code further contributed to the successful laboratory-scale 3D turbulent flame simulations conducted at Sandia National Laboratories. Building on the successes during the past seven years, a new project team (Trouvé, Im, and Haworth) proposes to develop the next-generation petascale simulation tools with advanced soot and radiation models in order to improve our scientific understanding of flame-soot-radiation interaction, as well as to provide valuable benchmark toward high-fidelity coarse-grained combustion simulations. Details of the future research plans are described in our recent pre-proposal submitted to DOE in response to Announcement DE-PS02-08-ER08-01, “Single-Investigator and Small-Group Research in Basic Energy Sciences.”

Publications

Journals: published

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Journals: in preparation

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2. Naranayan, P., Trouvé, A., Arias, P. G., and Im, H. G. (2009), "Mixture fraction and state relationships in diffusion flames interacting with an evaporating water spray," in preparation.

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+ Twenty two additional conference presentations prior to 2005.

SciDAC Publications

1. Im, H. G., Trouvé, A., Arias, P. G., Narayanan, P., (2008), "Direct numerical simulation of turbulent nonpremixed flame extinction by water spray," *Journal of Physics: Conference Series,* **125**, 012030.
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