Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry
http://scidac.psc.edu/

SciDAC: Computational Chemistry
(DOE Office of Science, BES: Chemical Sciences, Program Manager: R. Hilderbrandt)
Work-in-Progress Report – *Period from 04/01/04 to 03/31/05*

List of Principal Investigators

• Hong G. Im (University of Michigan, UMI, *hgim@umich.edu*)
• Arnaud Trouvé (University of Maryland, UMD, *atrouve@eng.umd.edu*)
• Christopher J. Rutland (University of Wisconsin, UWI, *rutland@engr.wisc.edu*)
• Jacqueline Chen (Sandia National Laboratories, SNL, *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 vehicle towards description of sub-models needed in device-level simulations. The new S3D software is enhanced with new numerical algorithms and physical models to provide predictive capabilities for spray dynamics, combustion, and pollutant formation processes.

Program Scope

The primary goal of the SciDAC TSTC project for FY04-07 is to extend the S3D code with new physical and algorithmic modules. The ultimate demonstration of the task will be simulations of partially premixed turbulent flames with liquid spray description, thereby achieving the full potential of the state-of-the-art DNS capability as a companion of detailed experimental studies. The specific objectives of this project include:

- To develop and complete the high-fidelity numerical algorithms under the component-based and parallel computing platform. This includes high-order, implicit/explicit (IMEX) stiff time integrators based on additive Runge-Kutta, and the immersed boundary method (IBM) for solid body representation associated with high-order interpolation schemes.

- To expand and upgrade the physical submodels to describe the underlying mechanisms with great details. The existing modules of radiation, soot, and spray evaporation model will be further enhanced to allow direct comparisons against experimental studies. In particular, detailed soot formation model using the method of moments will be developed and improved spray models will be added to represent direct injection and droplet distortion effects.

- To demonstrate the capability of the terascale DNS code in investigating fundamental science issues by several pilot simulations of canonical flames observed in turbulent combustion. The pilot configurations proposed for TSTC Phase II include partially-premixed turbulent counterflow and jet flames, and turbulent spray jet evaporation and ignition problems. The S3D DNS code will further allow access to various post-processing functionalities for effective data-mining and visualization that are being developed under BES Chemical Sciences core program.

Recent Progress

We present here a summary of progress made during the past 12 months work period of this project extending from 04/01/04 to 03/31/05.

Software design developments:

- As a completion to the collaboration with Pittsburgh Supercomputing Center under TSTC Phase I, S3D has been modified to fit into GrACE (grid adaptive computational engine) and componentized into the CCA (common component architecture) framework (PSC/ Raghurama Reddy).
- S3D has been ported to the CrayX1 architecture and optimized by rewriting key modules, i.e. chemistry and thermodynamics, to facilitate vectorization (SNL).
- Performed test simulations of S3D to identify optimal physical and numerical parameters for INCITE goal (SNL).
- As part of 2005 Joule Software Effectiveness Study, benchmark test simulations were performed to identify the code efficiencies with radiation/soot models (UMI/UMD) and spray vaporization models (UWI) on two supercomputing facilities at NERSC and ORNL CCS.

Numerical developments:

- New improved characteristic boundary conditions have been formulated to properly account for multi-dimensional flow effects in nonreflecting inflow and outflow conditions. Applications to various counterflow configurations demonstrate accurate and robust solutions over a wide range of flow and scalar variables, allowing high fidelity in detailed numerical studies of turbulent counterflow flames. This work has been submitted for publication in *Combustion Theory and Modelling* (UMI/UMD).

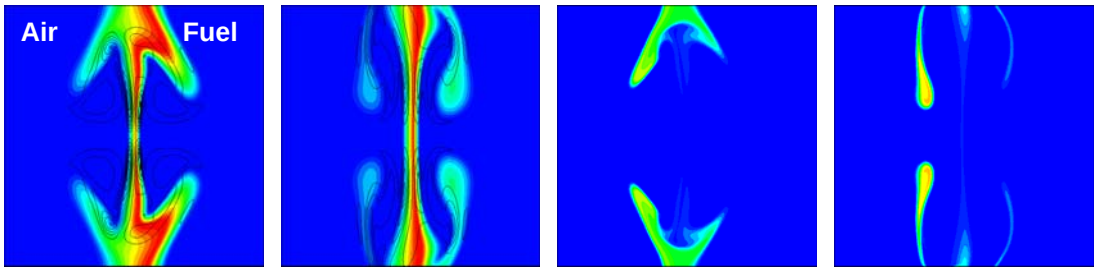
Physical model developments:

- Two alternative radiative heat transfer models, discrete ordinate method (DOM) and discrete transfer method (DTM) have been established and validated. Their overall performance was tested under the Joule Software Effectiveness Study (UMI/UMD).
- The spray module has been improved to efficiently handle a large number of fuel droplets. The code effectiveness has been tested under the Joule Software Effectiveness Study (UWI).

New combustion science:

- The S3D solver has been applied to study the interaction of turbulent ethylene-air jet diffusion flame and a solid wall. The simulations feature flame extinction events resulting from excessive wall cooling, and convective heat transfer up to 100 kW/m^2. The structure of the simulated wall flames is studied in terms of a classical fuel-air-based mixture fraction and an excess enthalpy variable. Preliminary results have been submitted for publication in *Combustion and Flame* (UMD).
- Various cases of fuel spray ignition with different initial droplet sizes and velocities were simulated to investigate the impact on turbulent mixing, auto-ignition and initial combustion of n-heptane fuel spray using detailed chemistry (UWI).

- Using the developed radiation and soot models, the interaction of counter-rotating vortices and laminar nonpremixed flame and their impact on the soot formation characteristics have been studied (UMI/UMD).



(a) temperature and vorticity (b) soot volume fraction, f_v

Figure 1. Temporal variations of (a) temperature (flood) and vorticity (black lines), and (b) soot volume fraction, f_v, during the interaction of an ethylene nonpremixed flame and counter-rotating vortices, exhibiting highly transient nature of the soot formation process during flame extinction.

Future Plans

- Develop new method for turbulence injection for wall-bounded flows to improve the accuracy and realism of turbulent fluctuations that are equilibrated with the mean flow, and to reduce the length of the turbulence development section in spatially-evolving flows (SNL)
- Immersed boundary method for solid body representation (UMD).
- Advanced soot models based on the method of moments (UMI)
- Continuation of studies on the radiation/soot interaction in counterflow (UMD/UMI)
- Three dimensional simulations of n-heptane fuel spray injections to investigate autoignition of fuel spray in realistic turbulent flow and mixing fields (UWI).

Publications

Journals

[1] Wang, Y. and Trouvé, A. (2004), "Artificial acoustic stiffness reduction in fully compressible, direct numerical simulation of combustion," *Combust. Theory Modelling*, **8**:633-660.

[2] Wang, Y. and Rutland, C. J. (2004), "Effects of temperature and equivalence ratio on the ignition of n-heptane fuel droplets in turbulent flow," *Proc. Combust. Inst.*, **30**:893-900.

[3] Yoo, C. S. and Im, H. G. (2004), "Transient dynamics of edge flames in a laminar nonpremixed hydrogen-air counterflow," *Proc. Combust. Inst.*, **30**:349-356.

[4] Sankaran, R., Im, H. G., Hawkes, E. R. and Chen, J. H. (2004), "The effects of nonuniform temperature distribution on the ignition of a lean homogeneous hydrogen-air mixture," *Proc. Combust. Inst.*, **30**:875-882.

[5] Chen, J. H., Hawkes, E. Sankaran, R., Mason, S. D., and Im, H. G. (2005), "Direct numerical simulation of ignition front propagation in a constant volume with temperature inhomogeneities, Part I: Fundamental analysis and diagnostics," *Combustion and Flame*, submitted.

[6] Hawkes, E., Sankaran, R., Pébay, P. P., and Chen, J. H. (2005), "Direct numerical simulation of ignition front propagation in a constant volume with temperature inhomogeneities, Part II: Parametric Study," *Combustion and Flame*, submitted.

[7] Yoo, C. S., Wang, Y., Trouvé A. and Im, H. G. (2005), "Characteristic boundary conditions for direct simulations of turbulent counterflow flames", *Combust. Theory Modelling*, submitted.

[8] Wang, Y. and Trouvé A. (2005), "Direct numerical simulation of non-premixed flame-wall interactions", *Combustion and Flame*, submitted.

Communications

[1] Trouvé, A., (2002), "Artificial removal of the acoustic penalty in fully compressible, direct numerical simulations of combustion," *9th SIAM Intl. Conf. on Numerical Combustion*, Sorrento, Italy.

[2] Wang, Y. and Rutland, C. J. (2003), "On the combustion of normal heptane fuel droplets in isotropic turbulence with DNS," *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[3] Wang, Y. and Trouvé, A. (2003), "Artificial acoustic stiffness reduction in fully compressible, direct numerical simulation of combustion", *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[4] Yoo, C. and Im, H. G. (2003), "A computational study on the dynamics of counterflow hydrogen-air edge flames," *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[5] Chen, J. H., Mason, S. D., and Hewson, J. C. (2003), "The effect of temperature inhomogeneity on low-temperature autoignition of fuel-lean premixed hydrogen/air mixtures", *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[6] Hawkes, E. R. and Chen, J. H. (2003) "Turbulent stretch effects on hydrogen enriched lean premixed methane-air flames," *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[7] Liu, S. and Chen, J. H. (2003), "The effect of product gas enrichment on the chemical response of premixed diluted methane/air flames," *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[8] Sutherland, J. C., Smith, P. J., and Chen, J. H. (2003), "DNS of a nonpremixed CO-H_2 jet using detailed chemistry – toward improved LES models," *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[9] Wang, Y. and Rutland, C. J. (2003), "Direct numerical simulation of turbulent droplets flow with evaporation," *The 41st AIAA Aerospace Sciences Meeting and Exhibit*, AIAA Paper 2003-1281, 6-9 January 2003, Reno, Nevada, USA.

[10] Trouvé A., Wang Y., Im H. G., Yoo C. S., Rutland C. J., Wang Y., Chen J. H., Sutherland J. C., and Mason S. D. (2004), "Direct numerical simulation of turbulent combustion using a fully compressible flow formulation," *Tenth SIAM International Conference on Numerical Combustion*, May 9-12, Sedona, AZ.

[11] Yoo, C. S., Im, H. G. Trouvé, A., and Wang, Y. (2004), "Direct numerical simulation of turbulent nonpremixed counterflow ethylene-air flame with soot and radiation models," *Tenth SIAM International Conference on Numerical Combustion*, May 9-12, Sedona, AZ.

[12] Yoo, C. S. and Im, H. G. (2004), "Soft inflow boundary conditions for direct numerical simulations of compressible reacting flows," *Tenth SIAM International Conference on Numerical Combustion*, May 9-12, Sedona, AZ.

[13] Wang, Y. and Rutland, C. J., "Effects of droplet velocity and size on the ignition of n-heptane fuel spray in turbulent flow using DNS." *Tenth SIAM International Conference on Numerical Combustion*, May 9-12, Sedona, AZ.

[14] Yoo, C. S. and Im, H. G. (2004), "Transient dynamics of edge flames in a laminar nonpremixed hydrogen-air counterflow," *30th International Symposium on Combustion*, July 25-30, Chicago, IL.

[15] Wang, Y. and Rutland, C. J. (2004), "Effects of temperature and equivalence ratio on the ignition of n-heptane fuel droplets in turbulent flow," *30th International Symposium on Combustion*, July 25-30, Chicago, IL.

[16] Sankaran, R., Im, H. G., Hawkes, E. R. and Chen, J. H. (2004), "The effects of nonuniform temperature distribution on the ignition of a lean homogeneous hydrogen-air mixture," *30th International Symposium on Combustion*, July 25-30, Chicago, IL.

[17] Wang, Y. and Rutland, C. J. (2004), "DNS study of the ignition of n-heptane fuel spray under HCCI condition," the 57th APS Annual Meeting of the Division of Fluid Dynamics, Seattle, WA, November.

[18] Yoo, C. S., Wang, Y., Trouvé A. and Im, H. G. (2005) "Characteristic boundary conditions for direct simulations of turbulent counterflow flames", *Joint Meeting US Sections of Combustion Institute*, March 20-23, Philadelphia, PA.

[19] Wang, Y. and Trouvé, A. (2005) "Direct numerical simulation of non-premixed flame-wall interactions", *Joint Meeting US Sections of Combustion Institute*, March 20-23, Philadelphia, PA.

[20] Yoo, C. S., Im, H. G., Wang, Y. and Trouvé A. (2005) "Improved Navier-Stokes characteristic boundary conditions for direct simulations of compressible reacting flows", *3rd MIT Conf. Computational Fluid and Solid Mech.*, Cambridge, MA.