

High Speed Combustion and Detonation (HSCD)

ALCF-2 Early Science Program Technical Report

Argonne Leadership Computing Facility

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ALCF ESP Technical Report

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High-level description of science

The goal of the project is to carry out first-principles three-dimensional direct numerical simulations for understanding and predicting high-speed combustion and deflagration-to-detonation transition (DDT) in hydrogen-oxygen gaseous mixtures. DDT and the resulting detonation waves in hydrogen may have especially catastrophic consequences in a variety of industrial and energy producing settings, including the production, transportation and use of hydrogen fuel, and safety on nuclear reactors where hydrogen can be accumulated in cooling pipe systems due to radiolysis of water. We want to use first-principles simulations for fundamental understanding of the physics of the strong, non-linear, multi-scale coupling of the constituent combustion processes leading to DDT, and eventually for predicting the onset of detonation in DDT experiments and engineering devices.

To date, we carried out a series of first-principles reactive compressible Navier-Stokes fluid dynamic simulations of reflected shock bifurcation in $2H_2 + O_2$ and in CO_2 in square tubes and simulations of weak and strong ignition and detonation behind reflected shocks using 8-species reaction kinetics network including H , H_2 , O , O_2 , OH , H_2O , HO_2 , and H_2O_2 , multi-species mass diffusion, heat conduction, viscosity, and equation of state relevant to DDT in hydrogen-oxygen mixtures. The theoretical explanation of weak ignition has been an outstanding problem of combustion theory for decades. Three-dimensional first-principle simulations of the process have not been previously performed. They provided new insights into the bifurcation process and the successful simulation of weak ignition is a major accomplishment of the project. The simulations reproduced the two main characteristics of weak ignition - a change in the location of auto-igniting hot spots and the decrease of ignition time compared to one-dimensional predictions. Ignition time delays obtained in our simulations are consistent with experimental data for $2H_2 + O_2$ in both strong and weak ignition regimes.

Code description and numerical methods

First-principles high-speed combustion and detonation (HSCD) problems, DDT in particular, are described by compressible, reactive flow Navier-Stokes (NS) equations of fluid dynamics and must include treatment of shocks. The HSCD code is a distributed memory parallel adaptive mesh refinement (AMR) reactive flow NS code augmented with the equation of state (EOS), microscopic transport, and chemical kinetics suitable for hydrogen combustion. Euler fluxes are calculated using a second-order accurate, Godunov-type, conservative scheme with a Riemann solver. Viscous, mass diffusion, and heat fluxes are calculated using second-order central differencing.

A distinct feature of the code is a dynamic cell-by-cell AMR based on a parallel fully threaded tree (FTT) structure. In ordinary trees pointers are directed from parents to children. In FTT, the pointers are inverted and directed from groups of children to parents and parent's siblings. This arrangement eliminates expensive tree searches which are notoriously difficult to parallelize and it allows all operations, including mesh refinement and de-refinement, to be performed in parallel.

Architecturally, the code consists of three separate layers: (1) the FTT library which provides general services related to all parallel aspects of the code's execution; (2) the reactive Navier-Stokes AMR code, ALLA, which rides on top of FTT and is responsible for numerical integration and AMR; (3) problem-specific algorithms such as material properties routines (equation of state, kinetics, microscopic transport) and problem initialization routines called from ALLA.

The FTT library contains a parallel implementation of a multi-level adaptive computational mesh. To a user, FTT provides a shared view of the mesh with added global services such as I/O, automatic and on-demand load balance, data synchronization across MPI processors, functions for mesh refinement, and iterators for global parallel operations of the mesh. A space-filling curve approach is used in FTT for domain decomposition.

Computations in ALLA are organized as a set of global computational steps, with each step followed by communication work which synchronizes data across the domain decomposition boundaries. Application algorithms are programmed in terms of work-functions which are passed to and executed by the global parallel iterator. The code is parallelized using a hybrid OpenMP/MPI strategy. On each MPI rank the iterator parses the mesh and passes small chunks of cells to a work-function until the entire mesh is processed. The loop over the cells in a chunk is performed inside the work-functions themselves. These loops are parallelized using OpenMP.

The mesh can be refined around shocks, discontinuities and in regions containing large gradients of physical variables such as chemical variables, temperature, vorticity, and so on. AMR is performed every fourth time step after which the cells are rebalanced across the processors using a heuristic to estimate the amount of work required by the cells and to maintain data locality.

The FTT library automatically synchronizes the data in ghost cells after global operations. ALLA algorithms may use cells located at different levels of refinement, and may carry interpolations of physical variables and mesh refinement error indicators between the levels. If parent cells and their children are located on different MPI ranks, the interpolations would require frequent synchronization of ghost cells, and thus additional frequent communication between the MPI ranks. To minimize the amount of communication, the load-balancing heuristic guarantees that after load balancing, children and their parents between the minimum and maximum levels of refinement will be located on the same MPI ranks.

Size/scale of problem possible before Mira, and actually run on Mira

Using an INCITE allocation on BG/P, we were able to simulate and reproduce a process of weak ignition behind a reflected shock in $2H_2 - O_2$ in a 5×5 cm cross-section and 1.6 meter long pipe - something that has not been possible in the past. This work advances us a step closer towards our ultimate goal of understanding and first-principles prediction of DDT. DDT simulations with the same physics in a $5 \times 5 \times 160$ cm tube geometry are being carried out using the current, third-year INCITE allocation and the ESP resources on a new Mira BG/Q supercomputer.

HSCD code has been successfully run on up to 131K cores of BG/P in the OpenMP/MPI mode. Production runs on Intrepid were using up to 64K cores in OpenMP/MPI mode and current production run job sizes on Mira are using 16 racks (1/3 of the full machine).

Modifications in preparation for Mira

The code uses now MPI, OpenMP, VisIt and Silo libraries. In 2012, ALCF staff rewrote the rebalance algorithm to reduce inefficiencies that appear at large scale. The staff also helped port and tune the code on Blue Gene/Q improving the OpenMP implementation and optimized library

use. Algorithmic improvements during the period of the INCITE project running contemporarily to the ESP project include: speedup of the I/O by a factor more than 100 (from costing 100 computational steps to less than one time step), optimization and speedup of the FTT AMR library, and implementation of Silo output for VisIt which solved problems with surface rendering in 3D.

Performance on Mira

There is no thoughtful performance analysis on Mira hitherto other than the comparison of results from time counters and other variables available directly from the code output. However, from these preliminary performance results on the BG/Q Vesta system we know that calculations on BG/Q are $\simeq 2.5$ times faster per core and $\simeq 9$ times faster per node than on BG/P. Figure 1 summarizes strong scaling of the code. The left panel compares code performance on BG/P Intrepid and BG/Q Vesta using a reflected shock tube problem. On both machines, the calculations are dominated by hydrodynamics (including Euler, Navier-Stokes, and chemical reaction terms).

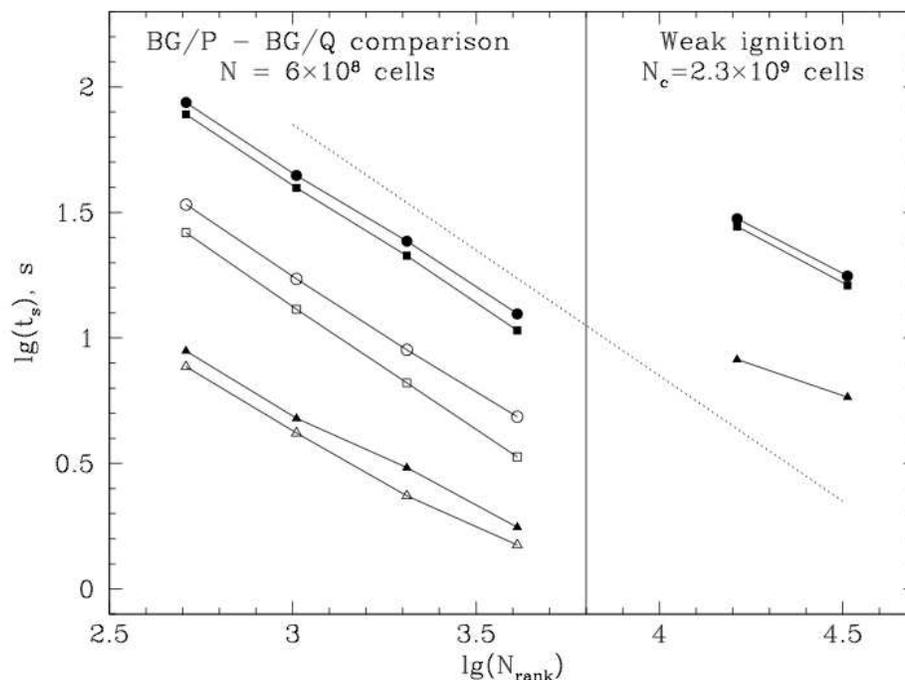


Figure 1: Strong scalability of HSCD code on BG/P Intrepid in MPI/OpenMP mode with 4 threads per rank (black symbols) and on BG/Q Vesta in MPI/OpenMP mode with 16 threads per rank and 4 ranks per node (open symbols). Squares - physics, triangles - AMR and load balance, circles - total. Time t_s is a wall-clock time of one time step. N_{rank} - number of MPI ranks. Left BG/P - BG/Q comparison. Data was averaged over 20 steps when the mesh reached $\simeq 6 \times 10^8$ computational cells in size. Right - data for a weak ignition case for the last hundred time steps of the simulation. Dashed line indicates ideal scaling.

Measurement and performance evaluation

Darshan was used in previous years to acquire data about I/O performance, however, tools like Tuning and Analysis Utilities (TAU), Rice HPCToolkit, IBM HPCT library or even gprof or mpiP

have not been used, at least, in recent versions of the code and on the BG/Q Mira system. Nevertheless, last comparisons of the cost of I/O on Mira at production run sizes (e.g. 16 racks on Mira) show an increase from 1% to 20% of the computational cost of I/O and a set of actions are in progress to get more performance data of the HSCD code. Some of these initiatives are:

- **I/O initiative:** optimize I/O using BG/Q personality and pSet info in order to take advantage of the compute to I/O node ratio (128:1 on Mira/Cetus). Work done in collaboration with Venkatram Vishwanath (MCS/ALCF staff, Performance Team).
- **MPI vs PAMI of one-sided communication section:** the use of PAMI calls instead of MPI for the section of the code that uses one-sided communications is under review. Work done in collaboration with Jeff Hammond (ALCF staff, Performance Team).
- **Visualization improvement:** the visualization subroutines and process will be reviewed by one member of the Visualization Team to tune them. The installation on Tukey of the software needed to visualize HSCD data (VisIt and Silo) have been requested. At the time of this report, we are aware of Silo installation on Tukey and VisIt should be available when Mira goes into production (on April 9th, 2013). Work done in collaboration with Joseph Insley (ALCF staff, Visualization Team).
- **Memory data:** add information about memory consumption on the code output. For commodity systems: mallinfo (C function); for BG/Q: usage of Kernel_GetMemory_Size. Work done in collaboration with Marta García (ALCF staff, Catalyst Team).

Earliest Technical Stories

This ESP project was selected as one of the public relations (PR) stories to go out in ALCF website (and ALCF Newsbytes — March 2013) about what goes on at ALCF. The full article '*High-Speed Combustion and Detonation Project Scaling Up for Mira*' can be found at:

<http://www.alcf.anl.gov/articles/high-speed-combustion-and-detonation-project-scaling-mira>



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