APPLICATION BRIEF

Researchers Achieve Breakthrough In Situ CFD Scalability with VisIt/Libsim on AVF-LESLIE Combustion Simulation Code Using NERSC's Cray Supercomputer

Organizations

Intelligent Light
Rutherford, N.J.
www.ilight.com

Lawrence Berkeley National Laboratory
Berkeley, Calif.
www.lbl.gov

Georgia Tech
Atlanta, Ga.
www.gatech.edu

National Energy Research Scientific Computing Center
Oakland, Calif.
www.nersc.gov

About VisIt/Libsim

VisIt/Libsim is a scalable, open source visualization application created by the US Department of Energy. Intelligent Light instrumented the AVF-LESLIE combustion simulation code with VisIt/Libsim to allow surface extracts to be created in situ, still resident in memory and without writing out solution files. VisIt/Libsim has been tuned to achieve good in situ scaling through 64,000 cores.

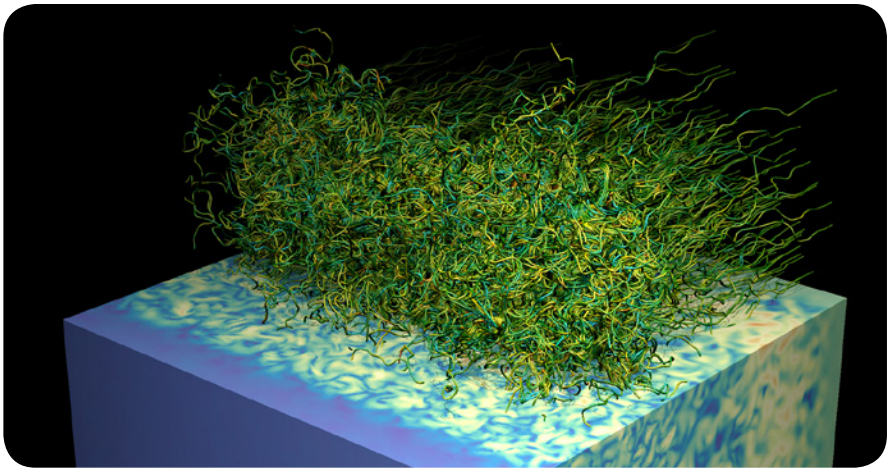
About Intelligent Light

Intelligent Light leads computational fluid dynamics (CFD) with products and services delivered by globally respected CFD and visualization practitioners. With a mission to expand the capabilities of CFD and deliver on the promise of HPC for CFD users, Intelligent Light is pioneering the use of in situ processing and XDB extract generation for CFD as an essential element of ultra-scale computing workflows. The company's established partnership with Cray has already led to breakthrough productivity with large-scale CFD data and is now bringing in situ capability to deliver HPC benefits through the entire CFD workflow.

About Cray

Cray provides advanced systems for the most difficult computing, storage and data analytics challenges. The company's portfolio includes cluster systems, supercomputers, storage solutions and data analytics and discovery platforms. Founded in 1972, Cray has been developing, building and supporting supercomputing technologies for over 40 years.

Cray Inc.
901 Fifth Avenue, Suite 1000
Seattle, WA 98164
Tel: 206.701.2000
Fax: 206.701.2500
www.cray.com



Challenge

Today, high performance computing (HPC) is a requirement for high-fidelity, time-accurate simulations of sophisticated physics. Petascale-sized supercomputers make it possible to run these simulations and deliver results in reasonable timeframes. But when it comes to running simulations using tens or hundreds of thousands of cores, the time needed to write, re-read and post-process the resulting files using traditional volume-based post-processing can be impractical or impossible. The result is wasted human and computing resources as well as lost science.

In situ processing is performed as solutions are generated and still resident in system memory, making it possible and practical to post-process at the speed at which results are computed and without writing solution or post-processing files to disk. In situ processing may also be used to create and deliver XDB extracts for further interrogation or archives. XDB files are numerically accurate, though only a fraction of the size of the simulation results data. This approach eliminates the writing of large solution files to disk and their transfer to other systems. Because the time to write to disk is typically far slower than the rate at which solutions can be generated, HPC power becomes engineering productivity when in situ methods are used.

But therein lies the challenge. Production-quality software tools for integrating solvers with in situ methods at extreme scale must coordinate across tens to hundreds of thousands of processor cores to produce useful scientific results.

With the in situ processing capability to support ultrascale CFD, Cray and Intelligent Light are working together with Georgia Tech on the AVF-LESLIE combustion code to address this challenge of large-scale CFD data generation and improve scaling performance — aiming to improve efficient code scalability from 5,000 to 64,000 cores and beyond.

Solution and Results

The team has achieved milestones in scalability on the AVF-LESLIE code using petascale Cray supercomputers at the National Energy Research Scientific Computing Center (NERSC). Working under a DOE grant from the Advanced Scientific Computing Research program, they instrumented the code with VisIt/Libsim to enable in situ extraction of surfaces of interest and output them to compact XDB files for secondary processing using FieldView, Intelligent Light's post-processing tool.

In situ XDB generation and CFD data management is delivering results for today's large-scale CFD users. Architectural bottlenecks in the workflow are eliminated, so useful information is generated at a rate that allows users to keep up with the fast pace of data generation possible with HPC systems.

The project plan carries testing and development to even higher core counts once running on NERSC's next-generation system, "Cori." Scheduled for unveiling in the fall of 2015, Cori will feature approximately 1,400 compute nodes (44,800 cores).

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research under Award Number DE-SC0012449. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.