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LDRD HPC4Energy Wrapup Report - LDRD 12-ERD-074

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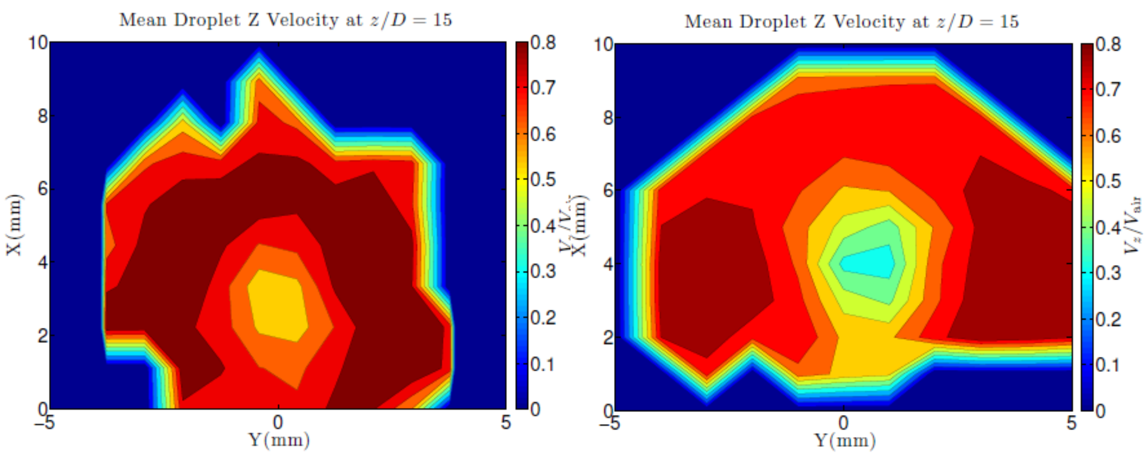
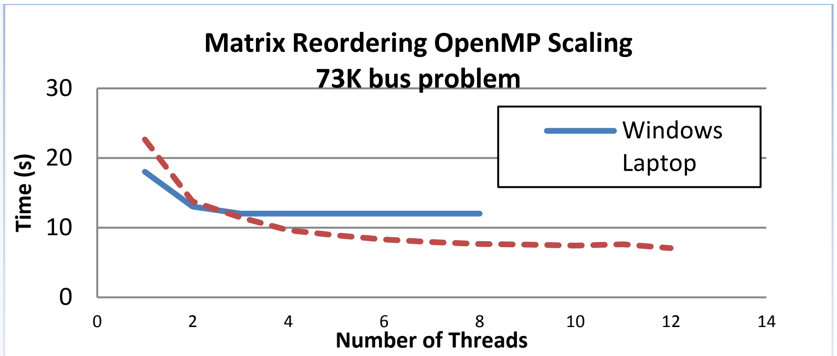
Image 

Caption: Panel Discussion with Industry Technical Leads and facilitated by John Grosh, and Dimitri Kusnezov, NNSA chief scientist delivering keynote at the Hpc4nergy Incubator Workshop November 5, 2012.

Image

Image 

Caption: Comparison of drop velocities from JIC numerical simulations with experimental data. Encouraging match with experimental data from GE Global Research. Simulation needs more time averaging to smooth out statistical error

Image 

Caption: LLNL assisted GE Energy to significantly improve the matrix reordering algorithm solution times through optimization and threading with speedup of 9.6 times on Windows and 7.2 times on Linux.

Project Description:

High-performance computing and simulation has the potential to optimize production, distribution, and conversion of energy. Although a number of concepts have been discussed, a comprehensive research project to establish and quantify the effectiveness of computing and simulation at scale to core energy problems has not been conducted. We propose to perform the basic research to adapt existing high-performance computing tools and simulation approaches to two selected classes of problems common across the energy sector. The first, applying uncertainty quantification and contingency analysis techniques to energy optimization, allows us to assess the effectiveness of LLNL core competencies to problems such as grid optimization and building-system efficiency. The second, applying adaptive meshing and numerical analysis techniques to physical problems at fine scale, could allow immediate impacts in key areas such as efficient combustion and fracture and spallation. By creating an integrated project team with the necessary expertise, we can efficiently address these issues, delivering both near-term results as well as quantifying developments needed to address future energy challenges.

Expected Results

We expect to provide fundamental progress in the basic scientific challenges of applying high-performance computing and simulation to energy issues. Partnering with the private sector, we have identified representative near-term research topics and goals. Specifically, we intend to demonstrate application of uncertainty quantification and contingency analysis to the solution of large energy-grid problems such as electricity production and distribution. We will also provide computer simulations related to improved engine combustion and efficient fracture and spallation for oil and gas drilling. In addition, we will assess the capabilities that must be developed to make longer-term progress in applying computing and simulation to energy issues. **High-profile publications as well as significant intellectual property are expected as a result of this research.**

Mission Relevance:

Applying LLNL's competency in high-performance computing and simulation expertise to energy production, distribution, and use directly supports the Laboratory’s strategic mission focus in energy security and could allow the Laboratory to optimize a potential expansion of its efforts in these areas.

Proposed Work (must address each point)

In FY12 we will address five key deliverables. Specifically, we will (1) demonstrate that high-fidelity simulation of combustion can increase energy efficiency in advanced concepts of combustion engines, (2) adapt existing simulation code and optimize it for fracture and spallation issues in energy-related drilling, (3) quantify the increase in solution convergence in energy distribution grids of over 150,000 buses, (4) optimize existing uncertainty quantification techniques to large energy-grid problems with input variables spanning broad time constants, and (5) optimize uncertainty quantification techniques for increasing the efficiency of energy use in buildings.

Accomplishments:

In FY12 we (1) ran scaling tests and moved data to our computational system and commenced large, very-fine-scale calculations, in collaboration with industrial partners GE Global Research and Bosch; (2) completed 7,000 simulations in two dimensions in collaboration with Potter Drilling, determining the relative importance of different factors on thermal spallation and 30 simulations in three dimensions providing valuable insight into actual mechanism for spall formation; (3) collaborated with GE Energy to scale up a computer code and performed a test case of over 4,000 contingency analyses reducing time requirements from 23.5 days estimated on a single core to 23 minutes on over 4,000 nodes; (4) demonstrated reduced time requirements in completed 400 unit commitment solutions with ISO New England from 200 hours on 1 node to 2 hours on 10 nodes in preparation to intelligently evaluate robust unit commitment for the electricity grid; and (5) collaborated with United Technologies Research Center to complete a large number of simulations to better understand which of 917 parameters affect building energy use most significantly.

2013 Proposed Work:

In FY13 a full day status-update workshop will be held to bring together the participating companies with LLNL representatives to discuss technical work and future partnerships. The results from simulations will be compared to results obtained with the conventional design and development cycle. Specifically, we will (1) determine the benefits and disadvantages of the two software codes developed in collaboration with GE Global Research in describing fuel spray in a combustion chamber as compared with experimental data, (2) compare the Robert Bosch LLC simulations of an internal combustion engine transitioning from spark ignition to homogeneous-charge compression ignition in four scenarios to experimental data and explain the observed phenomena, (3) conduct parametric and sensitivity analyses with Potter Drilling, Inc. to determine the most influential parameters in optimizing thermal spallation drilling, (4) run test cases with GE Energy using the parallelized code to demonstrate and quantify the increase in solution convergence for representations of large electricity grids up to 150,000 buses, (5) work with ISO New England to identify the appropriate levels under which the algorithm of robust unit commitment exhibits economic advantages over the current industry-accepted deterministic method for the dispatch of available electricity generation sources, and (6) work with United Technologies Research Center to use building energy models to determine the first-level parameters and second-level interaction parameters that have the greatest effect on the energy efficiency of buildings.

Accomplishments:

In FY13 we:

1. Held a full day status-update workshop on November 5, 2012 with Industry and Laboratory presentations, working meetings, media outbriefs, and panel discussions. Newsline article in 11/07/2012 addition
2. We modified our goals for the GE Global research project to determine the benefits and disadvantages of a software code in describing fuel spray in a combustion chamber as compared with experimental data because the second code was ported at the end of the project time period so we had no time for comparisons. The key accomplishments for FY13 and overall were
    - Simulations capture physics consistently with experiment
    - Richer physics with better models and denser mesh
    - Perspective of industry applications involving spray breakup, and what is the current state-of-the-art.
    - Access to source algorithm allows us to “pull apart” and learn about these state-of-the-art numerical techniques, and continuing collaboration with academia
    - Codes are ported to HPC machines, configured for +10K core runs, now available for LLNL work through TASC (***tasc.llnl.gov***)
3. The key accomplishments for FY13 and overall for the Robert Bosch LLC part of the LDRD Project were
    - LES of transition feasible in timeframe relevant to make impact
    - 70% reduction in time/cycle
    - High fidelity critical to aid development of physics-based controller
    - CAIO Combustion Code Run for SI to HCCI transition
        - 4 days/engine cycle on 2000 cores
        - Ran several different multi-cycle simulations, order 10^7 CPU-hours utilized
    - Evaluated CAIO code at higher resolution than previously possible
        - “Conditions under investigation”
4. The key accomplishments for FY13 and overall for the Potter Drilling part of the LDRD Project were
    - Finished Stage 1 & 2 simulations
        - 2D: Completed over 7000 simulations
          200K CPU-hrs; 72 processors per simulation
        - 3D: Completed 50 simulations
          500K CPU-hrs; 1020 processors per simulation

- Five sets of 2D parametric runs have been completed and analysed
    - Examined: borehole conditions, microstructural properties, thermal and mechanical properties.
    - Determined factors most crucial to damage extent and spall size.
    - Results used to constrain 3D parameter space and reduce number of runs.

5. The key accomplishments for FY13 and overall for the GE Energy part of the LDRD Project were
    - Parallel execution of contingencies enables larger more complete studies
        - Reduced runtime from 23.5 days to 23 minutes
    - Large number of contingencies (4,217); current norm is 100's
    - Significantly improved matrix reordering algorithm solution times through optimization and threading
        - Reordering speedup of 9.6 times on Windows and 7.2 times on Linux
    - Technical experience and knowledge
        - Application used by California utilities
        - Looking into a power system modeling application
        - Porting Windows applications to HPC
        - Running thousands of instances of an application
    - New domain for applying LLNL developed solvers
6. The key accomplishments for FY13 and overall for the ISO-NE part of the LDRD Project were
    - Generate random samples for simulations
        - Number of historical data is small
        - Use the "cluster method" to create clusters of samples
    - Solve robust UC problems
        - Multiple robust problems can be solved at the same time.
            - 1000 ED runs for each robust UC
            - 1 robust UC and 1000 ED runs per core
            - 4800 cores used for 4800 robust UC and 4.8 million ED runs
        - Time to solve 7200 UC and 7.2 million ED problems decreased from 600 days to 9.5 hours
    - HPC can efficiently run millions of simulations, which is impossible to be achieved by the computing capability of ISO NE.
    - Simulations yield more statistically significant results.
7. The key accomplishments for FY13 and overall for the UTRC part of the LDRD Project were
    - With the Building Energy Simulation, UTRC
        - Identified the most impactful parameters
        - Found that only 50 of 917 parameters impacted the simulation
        - Speed up the process by a factor of 60
    - UTRC ran over 10,000 runs on Sierra using 1,000 cores
    - Model calibration: error reduced to 5%

- Established expertise in the Building Simulation domain

ADC/DUSA: Energy Sciences

Metrics:

Publications: