SUPER Engagement: *Activities and Impacts*

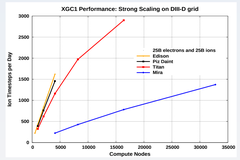
SUPER
INSTITUTE FOR SUSTAINED PERFORMANCE, ENERGY, AND RESILIENCE

U.S. DEPARTMENT OF ENERGY | Office of Science

EPSi

FES/ASCR Center for Edge Physics Simulation (EPSi)

- Contributed to port of computational kernel to GPU, then optimized MPI and load balancing, achieving 4X improvement for full system XGC1 run on Cray XK7 (Titan).
- Ported XGC1 and (partially) optimized performance on Cray XC30 (Edison and Piz Daint) and IBM BG/Q (Mira), evaluating potential compared to Titan.

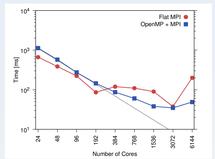


- Enhanced threading in new collision operator, improving performance by 1.7X for full system XGC1 production run on Titan (a FASTMATH collaboration).

Multiscale Climate

BER/ASCR Multiscale Methods for Accurate, Efficient, and Scale-Aware Models of the Earth System

- Contributed to OpenMP parallelization of MPAS-Ocean code, leveraging new TAU OpenMP capability.

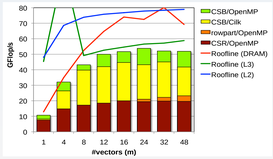


- Replaced native profile timers, improving model performance by 1.3X.
- Investigating alternative domain decomposition strategies, to improve load balance (>15% improvement in model so far); a FASTMATH collaboration.
- Investigating communication aggregation, more efficient communication scheduling, and elimination of overhead of indirect addressing (>10% improvement in model so far).
- See also the poster “SUPER performance auto-tuning and MPAS-Ocean optimization”.

NUCLEI

NP/ASCR Nuclear Computational Low-Energy Initiative (NUCLEI)

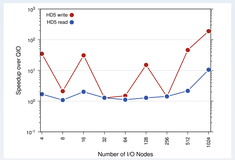
- Investigating performance of replacing Lanczos with a block eigensolver, requiring efficient implementation of a Sparse Matrix-Dense Matrix Multiplication (SpMM) operator and a transposed variant (a FASTMATH collaboration).
- Initial work improved performance of combined SpMM and its transpose by 3X. Ongoing work guided by Roofline performance model.



CalLat

NP/ASCR A Multi-Scale Approach to Nuclear Structure and Reactions (CalLAT)

- Added support for parallel-HDF5 file I/O, replacing QIO. Initial results are noisy, but HDF5 performance is always superior.



- Advantage of HDF5 is more than just raw performance: it provides a compact standard scientific data storage format, improving data portability; it is built for large and complex hierarchically organized data, which fits Lattice QCD data types; it is a high-performance I/O model and supports massively parallel systems. Further, metadata in HDF5 uses XML format, which is also used by QDP++.

Awards of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357, and of the Oak Ridge Leadership Computing Facility located in the Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract DE-AC05-00OR22725.

Introduction

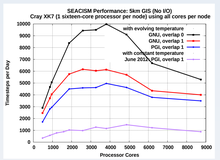
Engagement with SciDAC-3 Science Application Partnership (SAP) projects is at the core of SUPER, providing motivation, research directions, example code and problems, and opportunities for verification of approaches and near-term impacts. As of July 2014, SUPER has funded collaborations with 14 application projects.

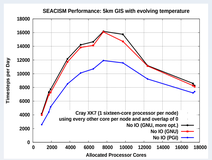
SUPER contributes to the SAPs by promoting best practices, by providing technology and architecture expertise, and by collaborating directly on performance engineering tasks. Some example activities and quantifiable impacts are described here.

PISCEES

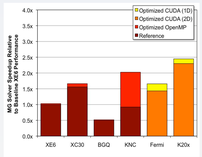
BER/ASCR Predicting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES)

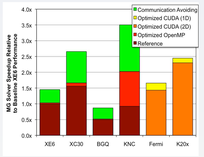
- Characterized performance of the baseline Community Ice Sheet Mode (CISM) dynamical core on the Cray XK7, as the first step in designing the performance measurement aspect of the Land Ice Verification and Validation (LIVV) test suite. Identified 4X performance improvement from a combination of algorithm and system-specific optimizations.





- Constructed and analyzed a simplified MultiGrid solver on x86 CPUs (Opterons/SNBe), IBM BG/Q, NVIDIA GPUs (Fermi/Kepler), and Intel MIC in order to quickly understand their performance/productivity challenges, in support of the BISICLES AMR-based dynamical core.



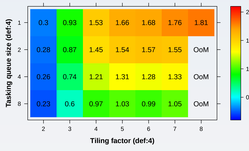


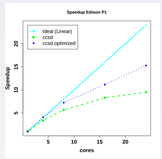
- Improved performance of the FELIX finite element-based dynamical core by 2X.

Electronic Excitations

BES/ASCR Simulating the Generation, Evolution and Fate of Electronic Excitations in Molecular and Nanoscale Materials with First Principles Methods

- Developed a NUMA-aware memory allocator and garbage collector for the libtensor kernel.
- Tuned tensor tiling factor and task queue quanta, improving on-node performance by 1.8X.



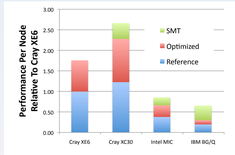


- Diagnosed bottlenecks associated with master-worker execution model.

NWCHEM

BES/ASCR Charge Transfer and Charge Transport in Photoactivated Systems (NWChem)

- Optimized performance of TEXAS Integral Package by up to 1.7X on four different node architectures. Also demonstrated that underlying tuning strategy could be used effectively on all four architectures.



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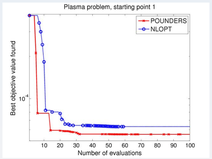
- Collaborating on development of hybrid MPI/OpenMP version, which so far maintains existing performance but uses much less memory.
- Improved performance of TCE (ccsd_t) module by 1.3X .

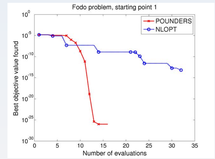
This research also used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. This work was supported by a grant from the Swiss National Supercomputing Centre (CSCS) under project ID g40.

COMPASS

HEP/ASCR Community Project for Accelerator Science and Simulation (ComPASS)

- Developing and benchmarking performance of numerical optimization algorithms. Typical problems allow for very few design evaluations given computational expense and resources needed for each particle accelerator simulation.





- New serial optimization software POUNDERS obtains better solutions and is faster than current libraries; a parallel version is under development

Others

BER/ASCR Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC)

- 1.6X improvement for long running suite of low resolution coupled climate experiments on Cray XK7; 2X improvement for high resolution ocean simulation on Cray XK7; >1.4X improvement for new MOAB-based mesh intersection kernel on IBM BG/Q (a FASTMath collaboration).

NNSA/ASCR ParaDis

- 2X improvement on 524,000 cores of IBM BG/Q from threading optimization; ongoing work with FASTMath achieved a further 11% improvement from optimization in the remote force calculation; preliminary work on improving load balancing has achieved 15% improvement.

BES/ASCR Charge Transfer and Charge Transport in Photoactivated Systems (NWChem)

- Improvement to numerical optimization algorithms enabled solution of calibration problems that had never been feasible before.

BER/ASCR Multiscale Methods for Accurate, Efficient, and Scale-Aware Models of the Earth System

- Contributed to 1.3X improvement in implicit solver for atmosphere model.

HEP/ASCR GEANT4

- See poster “Transforming Geant4 for the Future”.

Support for this work was provided through the Scientific Discovery through Advanced Computing (SciDAC) program funded by the U.S. Department of Energy Office of Advanced Scientific Computing Research