Case Study
Intel® Software Development Tools
Intel® Compilers, Intel® VTune™ Amplifier XE, Intel® MPI Library (Intel® MPI), Intel® Math Kernel Library (Intel® MKL), Intel® Parallel Studio XE Cluster Edition, Intel® Xeon Phi™ coprocessor

Software

Walker Molecular Dynamics Laboratory Optimizes Biomedical Software

Intel® Software Development tools increase application performance and productivity

"Intel® Math Kernel Library and Intel® MPI Library implementations provide very large speed increases with minimal effort on the part of the developer, and are well worth the investment from an end-user perspective."

– Professor Ross Walker
Associate Professor
Walker Molecular Dynamics Lab
SDSC, UCSD

Overview

The Walker Molecular Dynamics Laboratory at the San Diego Supercomputer Center (SDSC) focuses on advanced classical Molecular Mechanics (MM) and hybrid Quantum/Molecular Mechanical (QM/MM) simulation research. Up to 20,000 scientific researchers in academia and industry use Walker's Amber* molecular dynamics software. It enables simulation of biomolecular systems for research, including drug discovery, biocatalysis, enzyme engineering, and advanced biomaterial development. The Walker Laboratory applies many of its research and development results to Amber software—providing users with the most advanced techniques for molecular dynamics simulations.

The broader research focus of the Walker Laboratory encompasses the fields of computational chemistry, molecular biology, and high performance computing. The lab is particularly interested in the development of efficient algorithms for parallel and accelerated computation of classical MM and hybrid QM/MM techniques. The research also focuses on the use of MM and QM/MM Molecular Dynamics algorithms for the determination of physical and chemical properties of enzymes.

Amber provides researchers with:

1. A set of molecular mechanical force fields for the simulation of biomolecules. These are in the public domain, and are used in a variety of simulation programs.
2. A package of molecular simulation programs, including source code and demos.

The software and force fields are used for the simulation of enzymes, lipid membranes, advanced bio-materials, and catalysts. This impacts drug discovery—providing the ability to predict drug-binding affinity and accurately determine drug permeability in cells, as well as interaction with lipid-bound proteins.

The Challenge

Walker Laboratory sought to improve the vectorization of a mixed precision model within Amber's highly optimized molecular dynamics engine (PMEMD) in order to achieve higher performance on Intel® architectures. It wanted to boost parallel scalability and build a solid foundation for support of Intel® Xeon Phi™ coprocessor offload acceleration. In addition, it sought to accommodate the use of Intel® Many Integrated Core Architecture (Intel® MIC Architecture) in Amber to meet customer and user requirements.

"Intel® VTune™ Amplifier XE is an invaluable tool for identifying hotspots when optimizing code. Its user interface is easy to use and informative, quickening the pace of development. Without access to Intel VTune's line-by-line performance counters, we would never have been able to identify the reasons why our mixed-precision code was running slower than our original double-precision code."

– Dr. Perri Needham
Postdoctoral Researcher
Walker Molecular Dynamics Lab
SDSC, UCSD

Based on previous experience, Walker Laboratory began making changes to Amber to enable the software to execute on the latest Intel® processors. But, this resulted in poorer performance than expected and it was difficult to determine how to make performance improvements. Initial assumptions regarding the way single- to double-precision casting would work within the code proved to be incorrect, and engineers were at a loss to explain why they were not achieving the anticipated performance improvements.

Amber is a computationally intensive application. As such, users demand that the software run on the most advanced HPC computer architectures available. Walker Laboratory approached Intel and, through Intel® Parallel Computing Centers, began a project to enable Amber to run on the Intel Xeon Phi coprocessor, and then to optimize performance on both Intel® Xeon® and Xeon Phi processor architecture.

The Solution

Working closely with Intel application engineer Ashraf Bhuiyan, the Walker Laboratory team was introduced to Intel® VTune™ Amplifier, as well as the latest features in Intel® MPI Library (Intel® MPI) and Intel® Math Kernel Library (Intel® MKL). Introducing support for Intel MPI provided an immediate improvement in parallel performance of between 10 and 20%, depending on MPI process count. Making use of Intel's optimized FFT routines within Intel MKL also provided a performance boost over the modified version of pubFFT that Walker Laboratory originally used.

In addition, the use of Intel VTune Amplifier XE allowed the Walker Laboratory team to dig deeply into the code and identify a number of performance bottlenecks. In particular, it allowed them to identify where excessive casting of double- to single-precision was occurring in the code, thus preventing its hybrid precision model from delivering the expected speed improvements. With Intel VTune Amplifier XE, Walker Laboratory was able to locate the specific lines in the code where this was occurring and then escalate this to Intel® compiler engineers to determine why the compiler was unnecessarily casting. Without Intel VTune Amplifier XE's ability to provide a line-by-line breakdown of timings, it would not have been possible to identify the location of this performance hotspot.

Ashraf helped with the Intel VTune Amplifier XE environment setup to identify hotspots in Amber, as well as with the tuning of Intel MPI for optimal performance. He developed the current working version for the offload code; joint development is still ongoing. Amber v14 now supports Intel MPI, which is configured using a flag when building. In addition, Ashraf assisted in ensuring the correct paths and environment for Intel MPI support and coordinated provision for Intel Xeon Phi coprocessor development hardware and associated software at SDSC.

Results

Performance Gains

Based on the tuning work done with Intel VTune Amplifier XE and the provision for using Intel MPI and Intel MKL, the Walker Laboratory was able to deliver early performance improvements, for explicit solvent particle mesh ewald (PME) simulations of approximately 20% for parallel scaling and 10 to 15% (depending on simulation specifics) serial improvement and for implicit solvent Generalized Born simulations speedups of between 2.7 and 4.0x, from use of Intel MPI, the Intel compilers and Intel MKL. The following table shows detail performance improvements for sample data sets. Provisional offload support for Intel Xeon Phi coprocessor adds about a 10% performance improvement for explicit solvent simulations of > 400,000 atoms, and work is ongoing, aided by Intel VTune Amplifier XE, to obtain longer term performance gains from the Intel Xeon Phi coprocessor architecture.

AMBER			MPI/COMPILER		
			GNU - RED HAT 4.4.7-3 / MPICH2 V1.5	INTEL (2013/ IMPI 4.1.1.036)	
MODEL	SYSTEM	SYSTEM SIZE (ATOMS)	SIMULATIONS COMPLETED NANO-SECONDS/ DAY	SIMULATIONS COMPLETED NANO-SECONDS/ DAY	SPEED-UP (INTEL/GNU)
GNERALIZED BORN	TRPCAGE	304	63.57	176.12	2.77x
	MYOGLOBIN	2,492	1.17	4.43	3.79x
	NUCLEOSOME	25,095	0.01	0.04	4.00x
PARTICLE MESH EWALD-NVE ENSEMBLE	JAC - 4fs	23,558	13.09	15.36	1.17x
	JAC -2fs	23,558	6.88	8.01	1.16x

Productivity

Intel VTune Amplifier XE enabled hotspots in the code to be identified, reducing development time. Specifically, it identified regions in the hybrid single/double precision model where unnecessary casting was occurring, thus reducing performance. Intel VTune Amplifier XE allowed Walker Laboratory to experiment with different code layouts to investigate why the compiler was optimizing the way it was. It also highlighted the key hotspots in the code as a function of different input settings, such as different cutoff sizes and different FFT grid sizes.

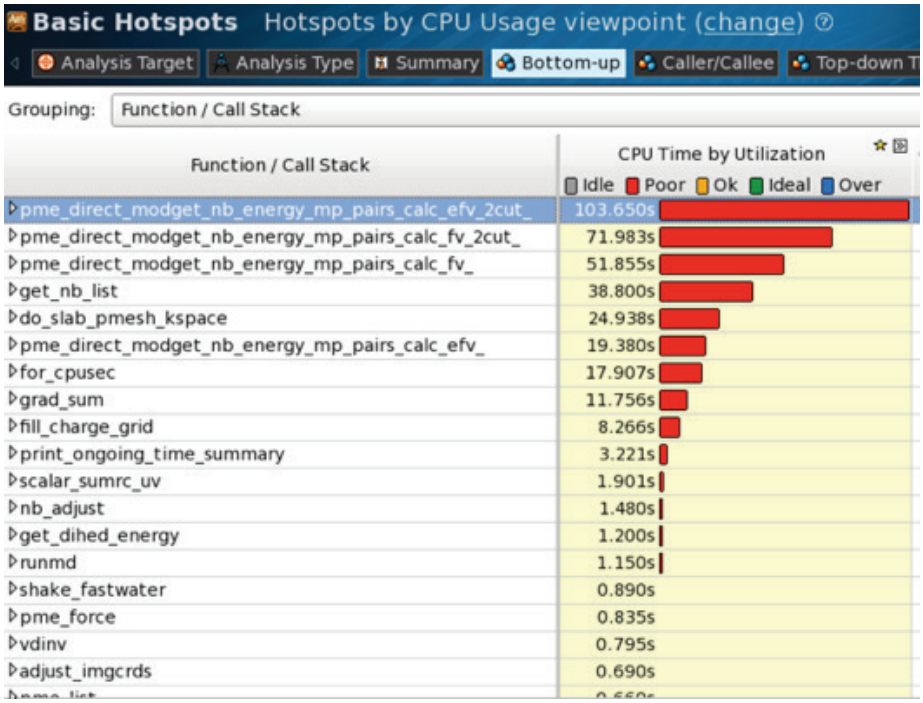

Figure 1. The identification of specific code hotspots.

Note that there are 4 variants of the pme_direct_modget_nb_energy. Intel VTune Amplifier XE gave Walker Laboratory the ability to split one routine into four function-specific routines and avoid if statements in inner loops, while still being able to track the cost of each function and prioritize further optimization.

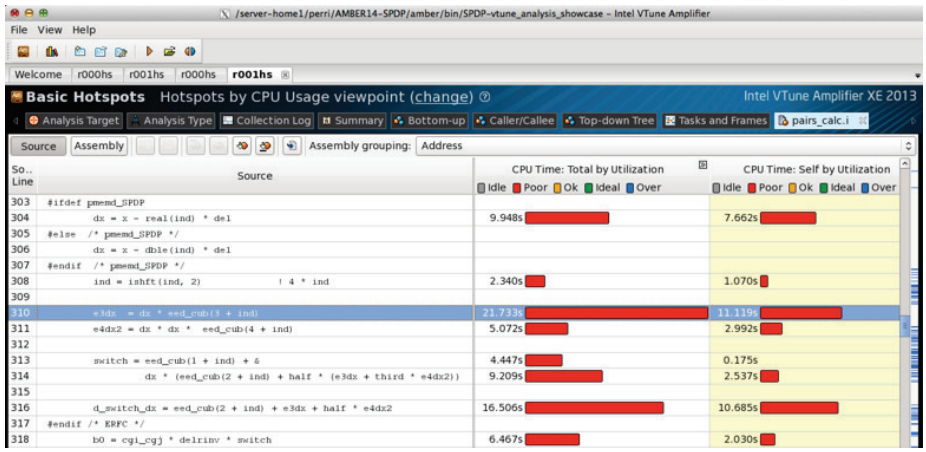

Figure 2. Locating CPU hotspots.

Intel VTune Amplifier XE was critical in locating specific lines in the code that were taking more CPU time than predicted. Walker Laboratory looked further into this by finding the compiled machine code corresponding to these lines. They identified that the compiler was casting single precision to double precision and back again without an explanation. Identification of the specific locations of these hotspots in the compiled executable allowed Walker Laboratory to escalate this to Intel compiler engineers to investigate the problem.

Improved MPI performance enables simulations in less time and, more importantly, the ability to run simulations for longer. This allows users to carry out more simulations on different systems of interest, such as a larger range of potential drugs. It also helps them to improve the convergence of individual simulations and to look for rare events and longer timescale motions. This ultimately leads to better opportunities for scientific discovery.

Conclusion

Amber currently supports GPUs and is broadening support to include Intel Xeon Phi coprocessor architecture. Walker Laboratory anticipates that the flexibility of the Intel Xeon Phi coprocessor will allow users to run either multiple simulations simultaneously via the native mode or provide comparable speed-ups to the Amber GPU engine through offload mode.

Walker Laboratory is confident that future optimization and performance results, in particular, a focus on the latest Intel Xeon Phi coprocessors, will enable substantially faster simulations. Users of Amber will benefit by being able to run longer simulations and conduct scientific research at a quicker pace. It will also open up new approaches to conducting research, such as providing the opportunity for real-time feedback from simulations allowing for interactive computation and computational experimentation on the desktop.

About

The research focus of the Walker Molecular Dynamics Laboratory—based at the San Diego Supercomputer Center at the University of California San Diego—encompasses the fields of computational chemistry, molecular biology, and high performance computing. The lab is particularly interested in the development of efficient algorithms, parallel- and GPU-accelerated computation of Quantum Mechanical and hybrid Quantum/Molecular Mechanical (QM/MM) techniques, as well as improvements in the computational efficiency and accuracy of classical MM dynamics simulations. The research also focuses on the use of MM and QM/MM Molecular Dynamics algorithms for the determination of physical and chemical properties of protein-based systems.

The Walker Laboratory is funded through a combination of grants from the National Science Foundation (NSF); National Institutes of Health (NIH); the University of California; Intel; NVIDIA, Microsoft; and the UK Foreign and Commonwealth Office; and the Department for Business, Innovation & Skills. Practical applications of the techniques developed in the lab include the development of next-generation viral inhibitors, improvements in bioethanol production, drug discovery, and advanced algorithms for high performance of scientific application on supercomputers.

Learn more: http://www.wmd-lab.org/

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Intel has been providing standards-driven tools for developers in the high performance computing industry for more than 25 years. Its industry-leading software tools include Intel® Parallel Studio XE Composer, Professional, and Cluster Editions.

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