Computational Molecular Modeling – Solving Quantum Mechanics Based Calculations Concerning Molecular Properties and Structures

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Abstract

This research is in fulfilment with Blue Waters Student Internship Program (BWSIP). This project employs High Performance Computing (HPC) to solve quantum mechanics based calculations concerning molecular structures and properties. Currently studying proximal influences on FeCO bonding and vibrational dynamics in $\{FeCO\}^6$ porphyrinates.

Project Summary

The sustained-petaflop computing power and massive data resources provided by the Blue Waters system enable scientists and engineers from a wide range of disciplines to make extraordinary leaps in knowledge and discovery.

Density Functional Theory (DFT) calculations are being carried out at a variety of levels over a wide range of trans legend fields with the goal of determining the ligand field strength necessary to affect the previously reported frequency crossover the v(Fe-CO) and d(FeCO) modes.

Training

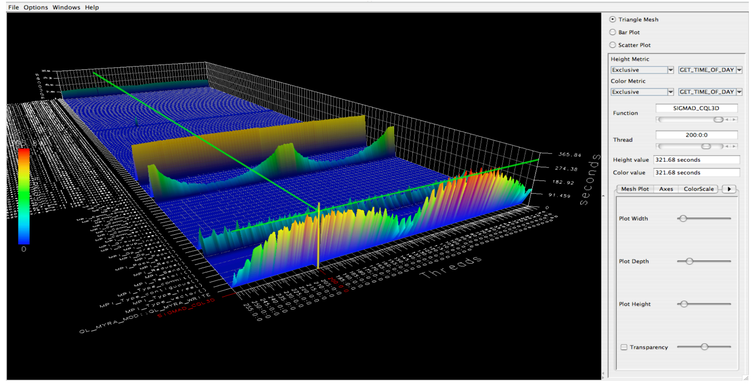
- The Blue Waters system is a Cray XE/XK hybrid machine composed of AMD 6276 “Interlagos” processors and NVIDIA GK110 (K20X) “Kepler” accelerators all connected by the Cray Gemini torus interconnect.
- Participated in two-week intensive training at Petascale Institute to learn different paradigms of parallel computing(e.g. OpenMP, MPI, OpenACC, CUDA etc.)

Blue Waters System Summary

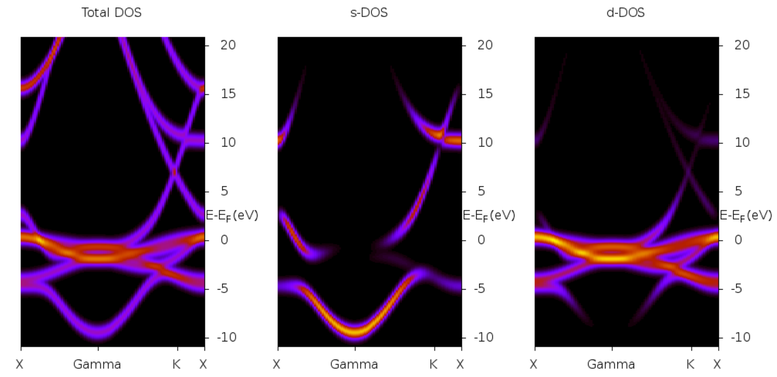
System Totals	
Total Cabinets	288
Total Peak Performance	13.34 PF
XE Peak Performance	7.1 PF
XE Bulldozer Cores*	362,240
XE Peak Performance	313.6 GF
Interconnect Architecture	3D Torus
Approved Node Hours	8000

HPC Resources

Performance Analysis / Profiling



Data / Observations



Recommendations for Future Study

- Chemistry department is synthesizing new compounds and performing elemental analysis on it, we did LCMS (Liquid chromatography-mass spectrometry) and NMR (Nuclear Magnetic Resonance Spectroscopy) to determine the physical and chemical properties.
- The current code is running on a single node, utilizing open source libraries and OpenMP and MPI iterative calls. The next step is to quantify code performance over multiple XE Nodes.
- For profiling and code performance, we’re using TAU Performance System, it is capable of gathering performance information through instrumentation of function, methods etc.

Works Cited

- "Blue Waters User Portal | System Summary." *Blue Waters User Portal | System Summary*. National Center for Supercomputing Applications, n.d. Web. 20 Sept. 2016.
- Linder, D.P. & Rodgers, K.R. J Biol Inorg Chem (2007) 12: 721. doi:10.1007/s00775-007-0223-0
- **The Diagnostic Vibrational Signature of Pentacoordination in Heme Carbonyls** Douglas P. Linder, Nathan J. Silvernail, Alexander Barabanschikov, Jiyong Zhao, E. Ercan Alp, Wolfgang Sturhahn, J. Timothy Sage, W. Robert Scheidt, and Kenton R. Rodgers *Journal of the American Chemical Society* **2014** *136* (28), 9818-982 DOI: 10.1021/ja503191