OOKAMI PROJECT APPLICATION

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Project Title: Superconducting Hydrides Under Pressure

Usage: Testbed

Principal Investigator:

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Usage Description:

My group specializes in computational materials chemistry. We are particularly interested in the discovery of superconducting, superhard, quantum, and planetary materials, as well as those that emerge under high pressure. Towards this end, we have developed the XTALOPT evolutionary algorithm for *ab initio* crystal structure prediction. XTALOPT enables exploration of the potential energy surface of a crystal for a particular stoichiometry. It may be necessary to optimize thousands of structures to the nearest local minimum to find the global minimum, or a good approximation for it. Our first goal will be to tune XTALOPT [1, 2] on the A64FX architecture and apply it towards predicting the structure of materials primarily with VASP.

We are particularly interested in predicting warm and light element based superconducting materials that could be synthesized under pressure [3]. Once the structure of a promising compound is found via XTALOPT we need to calculate its electron phonon coupling and estimate the superconducting critical temperature. These calculations are performed with the Quantum Espresso software, and it can be extremely time-intensive to obtain converged results. Our second goal will be to test how Quantum Espresso runs on Ookami.

Computational Resources:

- Total node hours per year: less than 15,000 node hours per year
- VASP structure optimization: Size (nodes) and duration (hours) for a typical batch job: 24 hours on 1 node. For a single XTALOPT run we need ∼30 days.
- Quantum Espresso electron phonon calculations: 30 days on a single node.
- Disk space (home, project, scratch):
  Home: Default (30 GB)
  Project: 3 TB
  Scratch: 30 TB

Personnel Resources (assistance in porting/tuning, or training for your users):

Users are familier with BASH and SLURM. Installation/compilation of GULP, VASP, and Quantum Espresso are probably needed.

Required software:

VASP, Quantum Espresso, GULP; C++ compiler with C++11; git, cmake >= 3.0, Qt >= 5.2.1, Qwt >= 6.1.3, Eigen >= 3; openssh, libssh.

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References

[1] Lonie, D. C.; Zurek, E., 'XtalOpt: An open-source evolutionary algorithm for crystal structure prediction', *Comput. Phys. Commun.* **2011**, *182*, 372–387.

[2] Falls, Z.; Avery, P.; Wang, X.; Hilleke, K. P.; Zurek, E., 'The XtalOpt evolutionary algorithm for crystal structure prediction', *J. Phys. Chem. C* **2021**, *125*, 1601–1620.

[3] Zurek, E.; Bi, T., 'High-temperature superconductivity in alkaline and rare earth polyhydrides at high pressure: A theoretical perspective', *J. Chem. Phys.* **2019**, *150*, 050901 (1–13).