

OOKAMI PROJECT APPLICATION

Date: 7/2/2021

Project Title: High precision configuration interaction calculations on A64FX

Usage:

- Testbed

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Usage Description:

Our team has developed a high precision atomic structure code package capable of predicting properties of complex atomic systems. The codes produce high quality atomic data, which are indispensable for experiments involving studies of fundamental interactions, astrophysics, atomic clocks, plasma science, and others. The programs developed here, along with the produced data, will be released as part of a larger project developing an online portal for high precision atomic data and computation. Our goal here is to compile and test our codes on Ookami, making sure they run and perform well on ARM systems. We also plan to optimize our code's performance and to run scalability tests.

Computational Resources:

- Total node hours per year: 5000
- Size (nodes) and duration (hours) for a typical batch job: Our test case will be relatively small for porting and benchmarking, around 1-5 nodes for less than 1 hour. Then we would like to occupy 5-10+ nodes for less than 1 hour at a time for scalability tests.
- Disk space (home, project, scratch): 2 TB or less.

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

None anticipated.

Required software:

CMake, Fortran compilers and MPI libraries.

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