OOKAMI PROJECT APPLICATION

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Project Title: Performance and Portability Evaluation of HPC Application Software on A64FX

Usage:

- Testbed

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Table 1: Names and email address of the initial users.

Usage Description:

We have been developing portable HPC software that aims to run across different computer architectures without losing too much performance. So far we have tested our software on Intel/AMD multicore CPUs, NVIDIA and AMD GPUs, but not much work has been done on the A64FX platform due to the lack of access. Several of us are affiliated with the RIKEN research center in Japan, and may be able to access the Fugaku supercomputer for production runs in the near future. Therefore we would like to evaluate the performance of

our current software on Ookami and assess the effort needed to optimize existing HPC software for the A64FX architecture.

One of the examples is the C++ simulation code for lattice QCD called Grid, which has been developed to target many different architectures, including Intel Xeon and Xeon Phi architectures, NVIDIA GPU, Intel GPU and AMD GPU. The design of Grid makes it easy to achieve performance portability across different architectures. However, there are some unique features of A64FX that may affect Grid's performance as is, and it would be greatly beneficial to see what changes are required to achieve optimal performance on A64FX. This would help us prepare Grid for potential future production runs on Fugaku.

Another example is the C++ toolkit for Liquid Argon Time Projection Chamber (LArTPC) detector simulations and data analysis called Wire-Cell Toolkit (WCT). As part of the High Energy Physics Center for Computational Excellence (HEP-CCE) project, we have ported a simulation module within WCT to Kokkos, which is a C++ portability abstraction that supports multiple backends. We are interested in evaluating the WCT performance on Ookami with the Kokkos OpenMP backend.

Computational Resources:

- Total node hours per year: 15,000
- Size (nodes) and duration (hours) for a typical batch job: Most of the jobs will need only one node for portability studies. We may also run some multi-node jobs to study scaling behaviors. Typical job duration will be less than 2 hours.
- Disk space (home, project, scratch): a few TBs

Personnel Resources:

N/A

Required software:

C++ compilers, MPI libraries, Eigen, HDF5, singularity if possible

If your research is supported by US federal agencies:

- Agency: Department of Energy
- Grant number(s):
