OOKAMI PROJECT APPLICATION

Date: **10/26/2021**

Project Title: Exploring Charm++ Applications on A64FX

Usage:

☒ Testbed

☐ Production

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Usage Description:
With the eventual goal of scaling on Fugaku, we would like to study the performance characteristics of the Charm++ parallel programming framework on A64FX. Towards this end, Ookami represents a perfect testbed for exploring our applications with A64FX, which notably span domains like cosmology (e.g., ChaNGa, ParaTreeT) and molecular dynamics (e.g., NAMD). Our applications could immensely benefit from A64FX's claimed GPU-like parallelism with the programmability of CPUs, particularly ParaTreeT – the Parallel Tree Toolkit. If able, we would like to study ParaTreeT's CPU scaling on Ookami, perhaps up to a hundred nodes; this would lend us insights into the effectiveness of Charm++'s adaptive load balancing on A64FX-based machines.

Aside from large runs, there is much to study within a node of Ookami as well. In particular, we would like to examine Charm++'s energy usage, correctness, and performance characteristics on A64FX, spanning features like: communication, scheduling, ULTs, isomalloc (global addressing through virtual memory), and others. In closing, testing Charm++ and its applications on Ookami would be a great opportunity to develop key insights into the next-generation of supercomputers.

Computational Resources:

Total node hours per year: 12,000 node hours.

Size (nodes) and duration (hours) for a typical batch job: 1-4 Nodes.

Disk space (home, project, scratch): No special requirements.

Personnel Resources (assistance in porting/tuning, or training for your users**):**
None expected.

Required software:
CMAKE. GCC/G++. UCX.

If your research is supported by US federal agencies:

Agency: NSF.

Grant number(s): 1910428, 1855096, and 1763658.

Production projects:

Production projects should provide an additional 1-2 pages of documentation about how
(a) the code has been tuned to perform well on A64FX (ideally including benchmark data comparing performance with other architectures such as x86 or GPUs)
(b) it can make effective use of the key A64FX architectural features (notably SVE, the high-bandwidth memory, and NUMA characteristics)
(c) it can accomplish the scientific objectives within the available 32 Gbyte memory per node