OOKAMI PROJECT APPLICATION

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Project Title: WarpX - an advanced electromagnetic Particle-

In-Cell code - on A64FX

Usage: Testbed

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Usage Description:

WarpX is a fully electromagnetic particle-in-cell code. Is is being developed by a team of the U.S. DOE Exascale Computing Project (ECP, with additional non-U.S. collaborators on part of the code) to enable the modeling of chains of tens to hundreds of plasma accelerator stages on exascale supercomputers, for future collider designs. The code is combining the latest algorithmic advances (e.g., Lorentz boosted frame and pseudo-spectral Maxwell solvers) with mesh refinement and support for the latest computing architectures.

WarpX is build on the ECP AMReX framework and thus supports a variety of compute backends: OpenMP for many- and multi-core architectures, as well as CUDA, HIP, and SYCL/DCP++ for accelerator-based machines. However, we are very interested in supporting non-ECP platforms as well. Our goal in

using Ookami is to make sure WarpX can build, run and perform well on A64FX systems. We will document the results of our developments on Ookami in our user-facing documentation. Since this work would benefit all users of WarpX, the impact in terms of enabling science cases should he high.

Computational Resources:

- Total node hours per year: 3,000
- Size (nodes) and duration (hours) for a typical batch job: small test runs for porting, benchmarking, and performance tuning, e.g. 1-4 nodes for 1-2 hours at a time. We envision scaling studies later on, but general multi-node benchmarks are regularly performed on other platforms, too.
- Disk space (home, project, scratch): 10 20TB, likely less.

Personnel Resources:

We do not anticipate a need for assistance beyond a help desk-type system where we can ask occasional questions on software and modules. A point-of-contact or workflow on how to submit Fujitsu compiler bug reports would be appreciated.

Required software:

- a C++14-capable compiler (C++17 capability preferred)
- CMake 3.15+ (latest release preferred)
- MPI 3.0+ OpenMP 3.1+ FFTW3

Optional software:

The following software is optional, yet increases our productivity:

Development	I/O	$Scripting \ / \ Analysis$
CCache 4.0+	parallel HDF5 1.10+	Python 3.7+
Ninja $1.8+$	parallel ADIOS2 $2.7.0+$	$\mathrm{Pip}\ 20+$
pkg-config		Numpy $1.15+$

If your research is supported by US federal agencies:

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