

OOKAMI PROJECT APPLICATION

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Project Title: Siesta in OOKAMI

Usage:

- Testbed

Principal Investigator: Marivi Fernandez-Serra

- University/Company/Institute: Stony Brook University
- Mailing address including country:
- Phone number: 6318801831
- Email: maria.fernandez-serra@stonybrook.edu

Names & Email of initial project users:

Marivi Fernandez-Serra, maria.fernandez-serra@stonybrook.edu Anthony Manino:
anthony.manino@stonybrook.edu

Usage Description:

We want to compile and test our workhorse code, SIESTA. Siesta is an electronic structure code and we use it all throughout our research. Right now it has not yet been compiled in OOkami and it would be good to evaluate its performance here. We might also need to install auxiliary python codes we use for post-processing.

Computational Resources:

- Total node hours per year: For this test we do not expect a heavy usage 10000H/y
- Size (nodes) and duration (hours) for a typical batch job: 20-40 cores, 10 hours max.
- Disk space (home, project, scratch): 10-100 Gb

Personnel Resources:**Required software:**

We will install siesta. We need a compiled blas and scalapack, openmpi or mvapich.

If your research is supported by US federal agencies:

- Agency: DOE
 - Grant number(s):DE-SC0001137
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Production projects:

Production projects should provide an additional 1-2 pages of documentation about how

1. the code has been tuned to perform well on A64FX (ideally including benchmark data comparing performance with other architectures such as x86 or GPUs)
2. it can make effective use of the key A64FX architectural features (notably SVE, the high-bandwidth memory, and NUMA characteristics)
3. it can accomplish the scientific objectives within the available 32 Gbyte memory per node