

# OOKAMI PROJECT APPLICATION

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**Date:**

July 12, 2021

**Project Title:**

Performance testing for common research applications and preliminary development

**Usage:**

- Testbed

**Principal Investigator:**

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**Names & Email of initial project users:**

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**Usage Description:**

We are looking at the Arm architecture for future computing expansions here at Flatiron Institute. Our users come from a large variety of backgrounds: computational mathematics, neuroscience, biology, astrophysics, informatics, and quantum mechanics, with an appropriately huge variance in workflows. We will be testing some of the more common workflows for our users to see if there are any major issues, and get a good sense for the performance and compatibility of their codes. This involves running many custom codes, but

also common packages such as GROMACS, PyTorch, and others. There are also some prototype C++ codes that I'd like to explore performance tuning to Arm, if the results from the benchmarking and testing are positive.

### **Computational Resources:**

- Total node hours per year: 300
- Size (nodes) and duration (hours) for a typical batch job: 1-16 nodes for appx. 1-20 minutes per job.
- Disk space (home, project, scratch):
  - home: 50GB
  - project: 2TB
  - scratch: Appx. 0 [some projects unknown, but likely very small]

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

We are both experienced HPC users and developers, though we might need some assistance with both porting and tuning, depending on the assessment of some of our custom codes.

### **Required software:**

Can compile any library ourselves if needed, though these are common requirements.

- gcc [ $\geq 7$ ], Arm compiler
- BLAS/LAPACK/FFTW [usually use OpenBLAS/MKL on x86, but will be trialing whatever is available]
- python [ $\geq 3.7$ ]
- PyTorch, mpi4py, etc.
- GROMACS [ $\geq 2021$ ]