

# OOKAMI PROJECT APPLICATION

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**Date:** 8/2/2022

**Project Title:** Porting and tuning amber for A64FX

**Usage:**

Testbed

Production

**Principal Investigator:** Carlos Simmerling

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

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**Usage Description:**

The goal of this project is to port and tune Amber (Amber is a suite of biomolecular simulation programs) for A64FX.

**Computational Resources:**

Total node hours per year: <15k

Size (nodes) and duration (hours) for a typical batch job:

Disk space (home, project, scratch):

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

**Required software:** -

**If your research is supported by US federal agencies:**

NIH RM1 GM135136

NIH R01 GM107104

NSF CTMC-1665159