OOKAMI PROJECT APPLICATION

Date: Oct 24, '23

Project Title: Controlled ice-nucleation using cellulosic hydrogels

Usage:

☒ Testbed

☐ Production

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Usage Description: In this ambitious project, our focus is on understaning how ice-nucleation kinetics could be modified with cellulosic hydrogels, shown by our experimental collaborators to impede ice-formation. Our goal is to develop a multiscale understanding of these processes at the ice-celluose interface from the atomic scale to the mesoscale. Using *ab initio* density functional theory (DFT) calculations, and classical molecular dynamics (MD) simulations, we will be developing an in-house parallel code to model the ice-formation at the mesoscale using the lattice boltzmann approach.

Computational Resources:

Total node hours per year: 15,000

Size (nodes) and duration (hours) for a typical batch job: 4-8 nodes, 24 hours

Disk space (home, project, scratch): 2 TB, 8 TB, unlimited

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

Required software: Quantum Espresso, VASP (license of Prof. Rajput), LAMMPS, OpenLB, PALABOS

If your research is supported by US federal agencies:

Agency: US Army
Grant number(s): W912HZ2020054

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