# OOKAMI PROJECT APPLICATION

**Date: 12/02/2021**

**Project Title: Porting VASP for A64FX**

**Usage:**

☒ Testbed

☐ Production

**Principal Investigator:Henrique Miranda**

University/Company/Institute: VASP Software GmbH

Mailing address including country: Sensengasse 8/12, A-1090, Vienna, Austria

Phone number: +43-1-4277-51402

Email: miranda.henrique@gmail.com

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

- Henrique Miranda, miranda.henrique@vasp.at

**Usage Description:**
Porting and tuning VASP for A64FX
The Vienna Ab initio Simulation Package (VASP) is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.

VASP computes an approximate solution to the many-body Schrödinger equation, either within density functional theory (DFT), solving the Kohn-Sham equations, or within the Hartree-Fock (HF) approximation, solving the Roothaan equations. Hybrid functionals that mix the Hartree-Fock approach with density functional theory are implemented as well. Furthermore, Green's functions methods (GW quasiparticles, and ACFDT-RPA) and many-body perturbation theory (2nd-order Møller-Plesset) are available in VASP.

**Computational Resources:**

Total node hours per year: < 15,000

Size (nodes) and duration (hours) for a typical batch job: 1 node 24 hours

Disk space (home, project, scratch): 30GB, 1TB, 1TB

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

**Required software:**

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

Agency:

Grant number(s):

---

**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