

OOKAMI PROJECT APPLICATION

Date: 09/14/2021

Project Title: UDel, NCI, DOE collaboration

Usage:

- Testbed: Primarily porting applications to A64FX processor and benchmarking their performance.

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Usage Description:

Porting NCI(National Cancer Institute)-DOE applications such as [AMPL](#) and [CANDLE](#) to new systems and hardware. These applications leverage deep learning for tasks such as drug discovery and cancer surveillance. The main purpose of this project is to port these applications to the A64FX processor learn the challenges of making such applications run on exascale systems.

Computational Resources:

- Total node hours per year: 1000-1500
- Size (nodes) and duration (hours) for a typical batch job: 2-4 nodes for a duration of 5 hours for a typical job
- Disk space (home, project, scratch): (50 GB, 10GB, 1 TB)

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

Required software:

- Python (3.7-3.8)
 - Anaconda (2020)
 - Containerization(Singularity, etc) (Not Required)

If your research is supported by US federal agencies:

- Agency: Leidos Biomedical Research/National Cancer Institute, National Institutes of Health, Frederick, MD
 - Grant number(s): 75N91019D00024/HHSN261201500003I
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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

<https://docs.google.com/presentation/d/12EIz2Kw9uISrZgmXRCqCzXum5mzO9VR8bwatxakQlwA/edit>