

## **Guideline for Application Form – Call for Early Use of ASPIRE 2A**

### 1. Introduction

This call aims to open the ASPIRE 2A supercomputer to all interested applicants for the early use of the system in preparation for the official launch of the system. This will allow them to be better prepared to effectively use the system.

More information can be found at <https://help.nscg.sg/call-for-early-use-of-aspire-2a/>.

Application period: 1 October 2022 to 31 May 2023 (subject to change)

Resource Allocation Period: Q4-2022 to 30 June 2023 (subject to change)

Successful applicants will be informed as soon as the system is ready for use.

**DISCLAIMER: The system is made available to the research community for early access AS-IS AND WITHOUT WARRANTIES, including without limitation any express or implied warranty as to fitness for purpose, reliability, accuracy, validity or otherwise of the system. In particular, NSCC does not warrant the system to be free from design, implementation, and operational issues, or from flaws which may result in system failure, mis-calculation or loss of data.**

## 2. Application Form

### 2.1. Basic Information

#### **Existing Project ID**

If you have an existing ongoing project on ASPIRE 1, please provide your 8-digit project ID. Please note that eventually all projects will be migrated from ASPIRE 1 to ASPIRE 2A.

If you do not have a project or if you do not wish to migrate your existing project to ASPIRE 2A, please indicate "0".

#### **NSCC User ID**

Please provide your NSCC user ID from ASPIRE 1. If you do not have a user ID yet, please create one via the Self-Service Portal: <https://user.nsc.sg/saml/>.

If your organisation is not part of the Self-Service Portal, please contact [projects-admin@nsc.sg](mailto:projects-admin@nsc.sg) for assistance.

#### **Project Details**

Please provide a summary that accurately describes your project, including the following information:

- project objectives;
- scientific rationale;
- innovation potential;
- expected outcomes and scientific advances.

If you are supported by a grant from a funding agency, please use the exact form of your project abstract in your research grant proposal.

### 2.2. Resource Request

Please refer to the [ASPIRE 2A Architecture and Specifications](#) for more information on ASPIRE 2A.

#### **ASPIRE 2A CPU (CPU core hours)**

This refers to the Cray EX CPU Nodes (128 physical cores per node).

Provide the calculation of the CPU core hours required.

*Example:*

*Resources required for molecular dynamics software, e.g., GROMACS, LAMMPS, etc.*

*(X1 cores) x (Y1 hours) x (Z1 runs) = A core hours*

*For quantum chemistry software, e.g., Quantum ESPRESSO, BerkeleyGW, etc.*

*(X2 cores) x (Y2 hours) x (Z2 runs) = B core hours*

*Total: A + B = C core hours*

## **ASPIRE 2A GPU (GPU card hours)**

This refers to the Cray EX 4-GPU Nodes (4 A100 GPUs per node).

Provide the calculation of the GPU card hours required.

*Example:*

*Resources required for molecular dynamics software, e.g., GROMACS, LAMMPS, etc.*

$$(X \text{ cards}) \times (Y \text{ hours}) \times (Z \text{ runs}) = \underline{A \text{ card hours}}$$

## **ASPIRE 2A AI System (card hours)**

This refers to the Apollo 4/8-GPU Nodes. These GPU nodes come with local storage. In general, AI applications will benefit from local storage but not traditional HPC applications.

Provide the calculation of the AI System card hours required.

*Example:*

*Resources required for AI model,*

$$(X \text{ cards}) \times (Y \text{ hours}) \times (Z \text{ runs}) = \underline{A \text{ card hours}}$$

## **High Performance Storage (GB)**

This is for the estimation of the local high performance storage space that is needed. You may use the scratch disk for the storing of temporary data.

*Example:*

*Resources required for molecular dynamics software, e.g., GROMACS, LAMMPS, etc.*

$$(X1 \text{ GB per run}) \times (Y1 \text{ runs}) = A \text{ GB}$$

*For quantum chemistry software, e.g., Quantum ESPRESSO, BerkeleyGW, etc.*

$$(X2 \text{ GB per run}) \times (Y2 \text{ runs}) = B \text{ GB}$$

$$\underline{\text{Total: } A \text{ GB} + B \text{ GB} = C \text{ GB}}$$

## **Size of Job**

### **Number of cores per job**

For reference: A compute node on ASPIRE 2A has 128 compute cores. A compute node on ASPIRE 1 has 24 cores.

Note that this is referring to the maximum cores used per job and not the core hours.

### **Estimate memory size per job**

For reference: A compute node on ASPIRE 2A has 512 GB of RAM. A compute node on ASPIRE 1 has 128 GB.

### **Estimated input and output file size (GB)**

This refers to the size of the data to be read and the size of the data to be generated.

## **Applications**

Please provide the applications and their versions. You may refer to the [ASPIRE 2A Software List](#) for the list of software on ASPIRE 2A.

Example:

abyss/2.3.2  
bazel/4.2.2  
cuda/11.6.2  
gcc/8.5.0-nsc

## **Resource Utilisation Plan**

Please provide the utilisation plan over the months.

Example:

1<sup>st</sup> – 3<sup>rd</sup> month: Production run, 20 cases, x core hours and/or y card hours

4<sup>th</sup> – 6<sup>th</sup> month: Post simulation analysis, 15 cases, x core hours and/or y card hours

7<sup>th</sup> – 9<sup>th</sup> month: Consolidation of results and rerun for post-processing, 10 cases, x core hours and/or y card hours