

# ASPIRE2A

## General QuickStart Guide

### Table of Contents

1. Introduction	2
2. User Policy	2
3. ASPIRE2A Overview	3
3.1 Compute Node Specification	3
4. Stakeholders Access to ASPIRE2A	4
5. Non-stakeholders Access to ASPIRE2A	5
6. Software Environment	7
6.1 GNU Environment	7
6.2 Intel Environment	7
7. Submitting Your First Job	8
7.1 How to Submit Serial Jobs?	9
7.2 How to Submit Array Jobs?	9
7.3 How to Submit Parallel Jobs?	9
8. Need Help?	10
9. Got Feedback?	10
10 <b>Frequently Asked Questions (FAQs)</b>	11
1. How do I submit a Serial Job?	11
2. How do I submit Array Jobs?	11
3. How do I submit Parallel Jobs?	11
4. What are the queues available in ASPIRE2A?	11
5. What is the maximum memory that can be used?	11
6. Can I transfer my own data from ASPIRE1 to ASPIRE2A?	11
7. What is my disk quota ( <code>/scratch</code> & <code>/home</code> ) on ASPIRE2A?	11
8. How do I check my user and project quota on ASPIRE2A?	12
9. How long will ASPIRE1 remain available?	12
10. Are there other options besides installing the Duo 2FA mobile app?	12
11. Is it possible to use VPN clients such as OpenVPN or Tunnelblick?	12
12. Who should I contact if the Duo 2FA does not work?	12

# 1. Introduction

This guide contains information on how to access and submit jobs on ASPIRE 2A.

With respect to this special Call for Early Use of ASPIRE 2A, please take note of the following:

**The system is made available to the research community for early access AS-IS AND WITHOUT WARRANTIES, including without limitation and 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, miscalculation or loss of data as part of the Call for Early Use of ASPIRE 2A.**

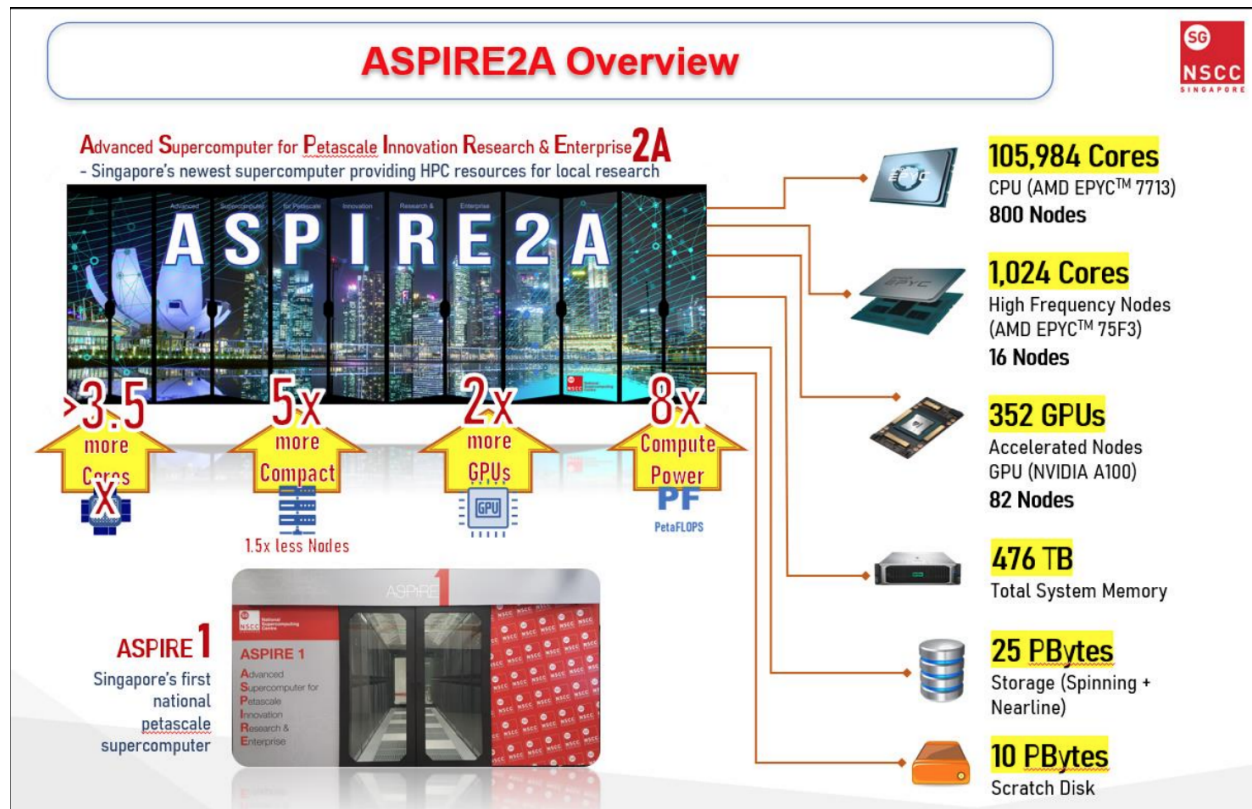
Please note that there may be limited support (eg. training and documentation) from the contracted system Managed Services Team during this early use call. However, NSCC will endeavour to address your needs and challenges as best we can during this pilot use of the new system.

## 2. User Policy

- All computational jobs must be submitted and run via the workload manager/scheduler.
- No computational jobs are allowed on the login nodes.
- Use project-directory assigned (**/home/project/<Project ID>/**) for sharing and storing data (dataset, database, results, input-output, etc.) and for installing controlled/licensed or unique-to-the-project applications.
- Users are welcome to install applications/software under their own `$HOME` or project-directory.
- Directory is ACL controlled. Please seek permission if you are unable to access the directory.
- Project members can access project directory based on project group permission (each project directory will be assigned to a group with the same name as the project ID). Project owners are given full access and will be able to adjust group permission within the project folder.
- Users are responsible for management and control of their own data. NSCC accepts no liability for any data loss or unauthorised data access.
- All terms of use are subject to the prevailing **NSCC Acceptable Use Policy** <https://help.nscg.sg/aup/>

### 3. ASPIRE 2A Overview

ASPIRE 2A is an AMD-Based Cray EX supercomputer with 10 PB of Lustre FS storage and Slingshot interconnect. The following diagram shows the summary infrastructure of ASPIRE 2A.



#### 3.1 Compute Node Specification

Full list of HPC cluster node types and specification:

Server	CPU Model	Cores per socket	Socket per server	Total Physical cores per server	Available RAM (DDR4)	GPUs
Standard Compute Node (768 nodes)	Dual-CPU AMD EPYC 7713	64	2	128	512 GB	No GPU
GPU compute node (64 nodes)	Single-CPU AMD EPYC 7713	64	1	64	512 GB	4x Nvidia A100 40GB
GPU AI Node (12 nodes)	Single-CPU AMD EPYC 7713	64	1	64	512 GB	4x Nvidia A100 40GB (11TB nvme)
GPU AI Node (6 nodes)	Dual-CPU AMD EPYC 7713	64	2	128	1 TB	8x Nvidia A100 40GB (14TB nvme)
Large memory node (12 nodes)	Dual-CPU AMD EPYC 7713	64	2	128	2 TB	No GPU
Large memory node (4 nodes)	Dual-CPU AMD EPYC 7713	64	2	128	4 TB	No GPU
High frequency node (16 nodes)	Dual-CPU AMD EPYC 75F3	32	2	64	512 GB	No GPU

## 4. Stakeholders Access to ASPIRE 2A

All pilot users from stakeholders are recommended to connect via high speed access link to access the system. Users can access via high speed links to ASPIRE 2A as shown in Diagram 1 below (Blue colour path) using respective FQDN as listed below:-

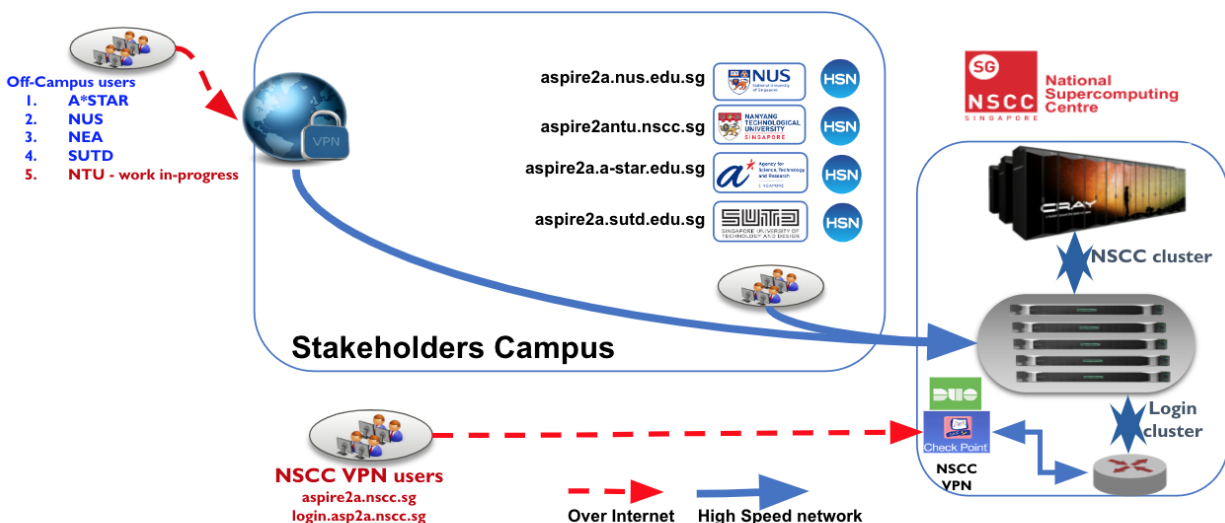
Stakeholder	FQDN for LoginNode	If connect from outside campus network
NUS (Note1)	aspire2a.nus.edu.sg	Connect to NUS VPN first
NTU (Note2)	aspire2antu.nscs.sg	Work in-progress, request for NSCC VPN enrollment if this required
A*STAR	aspire2a.a-star.edu.sg	Connect to A*STAR VPN first
SUTD	aspire2a.sutd.edu.sg	Connect to SUTD VPN first

Example, User from NUS could reach login node using ssh client via

```
"ssh <userid>@aspire2a.nus.edu.sg"
```

(Note1) NUS users originating from 172.23.0.0/16 and 172.24.0.0/16 are not able to directly access to login nodes at this moment due to technical constraints. NSCC is working with a NUS tech representative to address the issue.

(Note2) NTU users are not able to directly access to login nodes from off-campus VPN connection at this moment due to technical constraints. This is currently still work in-progress. NTU off-campus users are required to request for NSCC VPN enrollment if off-campus access to ASPIRE2A is required.



**NTU off-campus users to note:**

kindly put up a request to enroll NSCC VPN if required. All stakeholder users are not enrolled to NSCC VPN automatically

Diagram 1 : Users accessing ASPIRE 2A via High speed link and NSCC VPN

## 5. Non-stakeholders Access to ASPIRE 2A

All pilot users from non-stakeholders are required to connect via VPN to access the system. For more information on how to connect to the VPN, please follow the respective Windows, Mac or Unix VPN connection guides.

Non-stakeholders are referring to those user not belong to any stakeholders such as NTU, NUS, SUTD, A\*Star, NEA and SUTD

**Step 1:** Users are required to enrol in **DUO 2FA** before connecting to the ASPIRE 2A VPN. Users will receive an instruction email from DUO to install the DUO mobile app on their mobile phones. Once installed, users may proceed to connect to the VPN.

Please refer to the following guide for the DUO 2FA enrollment steps.

[DUO 2FA Enrollment Guide](#)

**Note:** User **MUST** complete Step 1 before proceeding to Step 2 to successfully connect to the VPN.

### Step 2: Access via NSCC VPN and logging in to ASPIRE 2A

Please refer to the following guides for the setup and connection of the VPN to ASPIRE2A for different Operating Systems:

[ASPIRE 2A VPN for Windows](#)

[ASPIRE 2A VPN for MAC](#)

[ASPIRE 2A VPN for Linux](#)

**Note:** Please check your 2FA mobile device pop-up request for the 2FA approval while logging into the VPN using the ASPIRE 1 credentials. **VPN connection will fail without the DUO 2FA approval.**

### Step 3: SSH

**Login node FQDN:** aspire2a.nsc.sg

**Alternate FQDN:** login.asp2a.nsc.sg

```
ssh -Y <userid>@aspire2a.nsc.sg
```

OR

```
ssh -Y <userid>@login.asp2a.nsc.sg
```

Please use the current ASPIRE 1 password. Note that any password changes through the user portal (for stakeholder users) will take effect on ASPIRE2A and be reflected in ASPIRE 1 within 35 minutes. Contact [help@nsc.sg](mailto:help@nsc.sg) for further help.

Upon successful login you will be presented with a screen similar to Figure 1 displaying the current status of the system.

```
#####
#                               #
#      Welcome to NSCC ASPIRE2A System      #
# -----#
# All computational jobs must run via scheduler, including pre- and #
# post-processing jobs. #
# #
# Useful commands: #
# module avail - list available environment modules #
# module purge - purge all the loaded modules #
# . /app/apps/resetmodule - reset to default load modules #
#####
Last login: Thu Feb 9 16:01:48 2023 from 10.103.62.34
+-----+
| ASPIRE2A System Info: |
| CPU : AMD EPYC 7713 OS : RHEL 8.4 (Ootpa) |
| GPU : NVIDIA A100 |
+-----+
| 09 May 2022 |
| Please note that as of 9 May 2022 ASPIRE2A is not fully commissioned. |
| The system may require urgent maintenance which necessitates NSCC |
| taking the system offline on short notice. The system is not in its |
| final configuration and therefore, expected to see changes to the |
| software stack, queue configurations and other parameters. |
| |
| 05 Dec 2022 |
| The following changes has apply in the ASPIRE2A system: |
| 1) Python virtual environment (venv) installed in the home directory |
| may require updates to the hard coded paths in the scripts found in the |
| bin folder to reflect the new absolute path of the home directory. The |
| "/scratch/GPFS" in the hard coded paths should be removed. |
| 2) The ncpus specified in the PBS job script indicates the number of |
| physical CPU cores. The maximum ncpus for the CPU nodes is 128, and the |
| maximum for the GPU nodes is 64. |
| 3) Login to the login nodes using below FQDN's |
| Login node FQDN: aspire2a.nsc.sg |
| ssh -Y userid@aspire2a.nsc.sg |
| OR |
| Alternate FQDN: login.asp2a.nsc.sg |
| ssh -Y userid@login.asp2a.nsc.sg |
+-----+
| Notes: |
| 1) The job accounting is running on prepaid mode, SU will be fully |
| deducted for the requested resource and only refund once job completed. |
| 2) Due to point 1, the balance of the SU unit might not tally (Grant - |
| Used), as SU units might be deducted for current running jobs. |
| 3) The "Used" value for respective units display only include the |
| completed jobs and not running jobs. |
+-----+
Last login: Wed Feb 15 09:28:27 +0800 2023 from 10.103.62.98
```

Figure 1: Successful login to ASPIRE2A login node



## 6. Software Environment

Figure 2 represents the software environment of ASPIRE 2A.

ASPIRE 2A uses the Red Hat Enterprise Linux 8 (RHEL) as its operating system (OS). The Cray development environment will be loaded by default.

Type `module list` to see currently loaded modules.

Type `module av` to see the available modules on ASPIRE2A.

### 6.1 GNU Environment

To load the GNU environment and GNU compilers please type:

```
module swap PrgEnv-cray PrgEnv-gnu/8.3.3
```

### 6.2 Intel Environment

To load the Intel environment and Intel compilers please type:

```
module swap PrgEnv-cray PrgEnv-intel/8.3.3
```

Refer to ASPIRE2A Software List: [ASPIRE2A Software-List](#)

System	Development	Library	Profiling & Debugging	Application
<b>Workload Manager</b> Altair PBS Pro	<b>Cray Programming Environment</b> AMD AOCC GNU GCC HPE CCE Intel oneAPI NVHPC	<b>MPI Libraries</b> Cray MPICH OpenMPI <b>Scientific Libraries</b> AMD AOCL BLIS Cray LibSci FFTW GSL Intel MKL PETSc	ARM Forge Cray Stat gdb4hpc Perftools Valgrind4hpc	<b>AI</b> Tensorflow PyTorch <b>Simulation</b> BerkeleyGW GROMACS LAMMPS Mumax3 OpenFOAM Nek5000 Quantum ESPRESSO Nektar++ WRF
<b>Remote Visualization</b> Altair Access	<b>Programming</b> Nvidia CUDA Go Python Java Julia Octave R	<b>I/O Libraries</b> HDF5 NetCDF	<b>Bio Tools</b> ABySS BEAST bedtools BWA bowtie2 GATK BLAST+ SAMtools	<b>Applications and Tools</b> Anaconda3 FCM GNU Parallel FFmpeg MRtrix3 NCL RELION Nvview Tmod Velvet
<b>Container</b> Singularity *Kubernetes with Docker			<b>Workflow</b> Cyle Rose Nextflow	
<b>Parallel File System</b> GPFS Lustre				
<b>Operating System</b> Red Hat Enterprise Linux 8				

Figure 2: ASPIRE2A Software Environment

## 7. Submitting Your First Job

On the login nodes, you will be able to submit a PBS job script to the scheduler to run your HPC workload. Below is an example PBS job script for your reference.

```
#!/bin/bash
#PBS -N UM2KM
#PBS -l select=8:ncpus=128:mem=440G:mpiprocs=128:ompthreads=1
#PBS -l walltime=3:00:00
#PBS -j oe
#PBS -o out-run.txt
#PBS -P <Project ID>
#PBS -q <normal or ai>
```

```
module load anaconda3/2021.11
```

```
#PBS -P <Project ID>
```

Users are advised to always specify the **Project ID** accessible to users while submitting a job.

```
#PBS -q <normal or ai>
```

Currently only **normal** and **ai** queues are accessible to users while submitting jobs, while all other queues are execution queues, which are not directly accessible to users. However, user jobs will be routed to respective queues for execution automatically based on job configuration.

- **Normal** queue is for **CPU** and **GPU node jobs**.
- **AI** queues are for **AI workloads** where each node has been configured with high speed NVme local storage for AI/ML use cases.
  - The NVme local storage is mounted as `/raid`.

**NOTE: GPU Job** will have fixed CPU and Memory ratio enforced i.e. for every 1 GPU requested, 16 CPU and 110 GB of memory will be allocated.

The PBS directives request for 8 nodes each with 256 Hyper-Threading threads (128 physical cores) and 480 GB memory. The `ncpus=128` specified corresponds to 256 Hyper-Threading threads, which is equivalent to 128 physical cores. Each node has 512 GB of main memory, but the `mem=480G` is used considering that some of the memory will be used for the system OS.

Note that **if the job queue is not specified** in the job script the **normal queue** is automatically selected.



## 7.1 How to Submit Serial Jobs?

To submit a serial job, simply request a single chunk and single ncpus resource.

**Example:** `qsub -l select=1:ncpus=1:mem=2GB`

**Wrapping multiple serial commands in a single job script.**

**Example:**

A single PBS job script can contain script1,script2 as two serial jobs / commands. The drawback with this example is that any output from job1 or job2 will get mixed up in the batch jobs output file.

**The script would look like:**

```
#!/bin/bash
#PBS -l walltime=1:00:00
#PBS -l select=1:ncpus=2
cd $PBS_O_WORKDIR
# Use '&' to start the first job in the background
./script1 &
./script2
# Use 'wait' as a barrier to collect both executables when they are
done. If not, the PBS job will finish when the script2 program
finishes and kill script1 if it is still running.
wait
```

## 7.2 How to Submit Array Jobs?

Job arrays are a great way to organise the execution of multiple short jobs with similar properties or if they are using similar data with different algorithms or if they are using serial input file numbering system eg., file01, file02, file03

**Example:** Submit 10 jobs with consecutive index numbers.

```
#!/bin/sh Examples Using a Job Script
#PBS -N Simn1010Jobs
#PBS -J 1-10
echo "Main script: index " $PBS_ARRAY_INDEX
/opt/AppA -input /home/user01/runcasel/scriptlet_${PBS_ARRAY_INDEX}
```

## 7.3 How to Submit Parallel Jobs?

**For an MPI job, select= and ncpus= can be one or more, with np= >1.**

```
#!/bin/bash
#PBS -N testrun01
#PBS -l select=6:ncpus=32:mem=128gb
#PBS -o /home/user01/my_o_files
#PBS -e /home/user01/my_e_files
#PBS -m be
mpirun -np $MPI_NPROCS -machinefile $PBS_NODEFILE ./my_scripts
```

## 8. Need Help?

If you encounter any issues, please contact us at [help@nscg.sg](mailto:help@nscg.sg) during this transition period and until further notice. For enquiries regarding **ASPIRE 2A**, please indicate the following in your email subject heading - “**ASPIRE 2A: [issue]**”

## 9. Got Feedback?

As this early use period is being used by NSCC for uncovering any implementation or other issues, we value your feedback and input about any problems you may have experienced as well as your suggestions for improvement. Please email to [support@nscg.sg](mailto:support@nscg.sg) with the email subject heading - “**ASPIRE2A: [feedback]**”

# Frequently Asked Questions (FAQs)

## 1. How do I submit a Serial Job?

To submit a serial job, ensure you request one CPU resource only, (i.e., `-l select=1:ncpus=1`). Refer to **Section 6.1** for example.

## 2. How do I submit Array Jobs?

Refer to **Section 6.2** for example.

## 3. How do I submit Parallel Jobs?

To submit a parallel job, you can request 1 or more `ncpus` resources per chunk. Refer to **Section 6.3** for example.

## 4. What are the queues available in ASPIRE2A?

The queues available for job submission are:

- normal
- ai

## 5. What is the maximum memory that can be used?

There are 3 types of nodes in the cluster based on their memory, which are 502GB, 2TB and 4TB. A job can request multiple chunks of memory with a maximum of 4TB per chunk. (For example: `-l select=2:ncpus=128:mem=4TB` is a job that is requesting 8TB memory in total and will run on 2 nodes). However, “**ai**” queues will have fixed CPU and Memory ratio enforced i.e. for every 1 GPU requested, 16 CPU and 128GB of memory will be allocated.

## 6. Can I transfer my own data from ASPIRE1 to ASPIRE2A?

Please contact us at [help@nsc.sg](mailto:help@nsc.sg) during this transition period and until further notice. For enquiries regarding **ASPIRE 2A**, please indicate the following in your email subject heading - “**ASPIRE 2A: [issue]**”

## 7. What is my disk quota ( /scratch & /home ) on ASPIRE2A?

Scratch quota remains the same as ASPIRE1.

`/home` Home Directory - 50 GB (Total inodes - 400000000)

`/scratch` Scratch Directory - 100TB (Total inodes - 200000000)

**8. How do I check my user and project quota on ASPIRE2A?**

Users may use `myusage` to check resources usage, `myprojects` to check project balance and `myquota` to check storage usage.

**9. How long will ASPIRE1 remain available?**

NSCC will keep users informed when we have further details. Meanwhile, we recommend users to move to ASPIRE2A as soon as possible.

**10. Are there other options besides installing the Duo 2FA mobile app?**

Only the mobile app is supported currently. NSCC will continue to explore other alternatives at a later stage.

**11. Is it possible to use VPN clients such as OpenVPN or Tunnelblick?**

Only Checkpoint VPN clients are supported.

**12. Who should I contact if the Duo 2FA does not work?**

Please contact us at [help@nscg.sg](mailto:help@nscg.sg) during this transition period and until further notice. For enquiries regarding **ASPIRE 2A**, please indicate the following in your email subject heading - **“ASPIRE 2A: [issue]”**