Guidelines on Call for Projects V3.0 (18 Sep 2025)

1. Basic Information

1.1. Project Name

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

1.2. Project Description

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.

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

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

1.3. Project Significance (National or Global benchmark)

Please describe the significance of your project in terms of national or global contribution.

1.4. Primary Scientific Domain

Please specify the scientific domain of research for your project.

1.5. Organisation

Please select the organisation that you belong to.

1.6. Software Applications

Please provide the applications and their versions.

Example:

abyss/2.3.2

bazel/4.2.2

cuda/11.6.2

gcc/8.5.0-nscc

1.7. Principal Investigator (PI) / Project Supervisor

Please provide the contact information of the PI or supervisor. If your project does not have a, please provide the contact information of your supervisor (manager, director or the equivalent).

Note that the PI / project supervisor must be from the same institute as the applicant.

1.8. Project Team (Add member)

This section allows you to add users to the project using their NSCC user IDs. You may add users to the project at a later date by completing Part I of the <u>request form</u> and sending it via email to <u>projects-admin@nscc.sg</u>.

2. Project Type

2.1. Project Grant ID

This is the Grant ID given by your project funding's grant agency. Please do not use the NSCC project ID.

2.2. Project Start and End Date

Please specify the expected start and end date of your entire project that requires computational support from NSCC.

2.3. Overall Project Funding (SGD)

This question is required for us to have a high-level understanding of the scale of your project.

2.4. Status of Project Funding

Approved: Funding approved by funding agency.

Submitted: Project and funding information has been sent to the funding agency and pending for approval.

Under Review: Project and funding information under review to be submitted to the funding agency.

Under Preparation: Process of preparing project and funding information.

2.5. Is there a compute budget (out of the overall project funding) allocated?

A HPC Compute Budget refers to the funds set aside as part of the overall applied project funding for the provisioning of HPC resources which includes CPU core hours, GPU card hours and storage.

2.6. Compute Budget

All projects must include a HPC Compute Budget for the entire project cycle. Estimation of the HPC Compute Budget should bebased on commercial Cloud Service Provider (CSP) rates of the respective institutions/organisations' existing contracts.

Thisensures that PIs have sufficient HPC Compute Budget for the CSPs, should their Call for Projects application be unsuccessful.

All HPC Resources allocated are subjected to charges, as mandated by NRF. The charges will be based on NSCC Singapore's RIE-funded projects rate.

3. Project Deliverables

Please provide the expected deliverables throughout the *full duration* of your project. Please indicate the number of manpower involved in the project only and not the entire research lab/institute.

4. Resource Request

Please provide the resources you require for the entire project duration. You may request for resources that you require only and there is no need to select every type of resource.

4.1. CPU / GPU

CPU

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

Provide the calculations for the CPU core hours required.

Example (please elaborate on the job types):

Resources required for DFT calculations on a 200 atoms system:

(A) Geometry relaxation with PBE: (256 cores per job) x (24 hours) x (150 jobs) = 921,600 core hours

(B) Band structure calculation with HSE: $(1,024 \text{ cores per job}) \times (24 \text{ hours}) \times (50 \text{ jobs}) = 1,228,800 \text{ core hours}$

Total: 921,600 + 1,228,800 = 2,150,400 core hours

GPU (A100)

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

Provide the calculations for the A100 GPU card hours required.

Example (please elaborate on the job types):

Resources required for DFT calculations on a 200 atoms system:

(A) Geometry relaxation with PBE: (1 A100 card) x (24 hours) x (150 jobs) = 3,600 card hours

(B) Band structure calculation with HSE: (4 A100 cards) x (24 hours) x (50 jobs) = 4,800 card hours

Total: 3,600 + 4,800 = 8,400 card hours

GPU (H100)

This refers to Nvidia DGX H100 compute nodes (8 H100 GPUs per node).

Provide the calculations for the H100 GPU card hours required.

Example (please elaborate on the job types):

Resources required for distributed LLM training:

(A) Finetune Llama 1B with DDP at BF16: (4 H100 cards per job) x (24 hours) x (100 jobs) = 9,600 card hours

(B) Finetune Llama 8B with FSDP at BF16: (64 H100 cards per job) x (120 hours) x (10 jobs) = 76,800 card hours

Total: 9,600 + 76,800 = 86,400 card hours

4.2. Al System

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.

Please provide the justification for the AI System card hours required, including the calculations and utilisation plan.

Example:

Resources required for AI model,

(X cards) x (Y hours) x (Z runs) = A card hours

Utilisation plan over the months:

4.3. 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 GB per run) x (Y1 runs) = A GB

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

(X2 GB per run) x (Y2 runs) = B GB

Total: A GB + B GB = C GB