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ICHEC Getting Started Guidev2.0

First, you should register for a central ICHEC account <u>here</u>. Once your account has been approved, you can apply for two different mechanisms to access computational cycles in ICHEC HPC machines

- Apply for your own National Service Project or join an existing National HPC Service project already granted to someone else (who must approve your application to join his/her project via the web portal)
- Use the condominium access, applying for access in their corresponding institution (in this case TU Dublin's condominium access more details <u>here</u>)

The focus of this guide is applying for your own National Service Project.

National Service Project Application

To begin, you must log in to your central ICHEC account and scroll down until you see the following:

Project Applications			
National Service Project Application			
To apply for a <u>National HPC Service</u> project please review the information on the use this web form:			
Full National Service Application Form			

Click on "Full National Service Application Form" and you will see the following:

Project details					
Project title:					
			(not all uppercase)		
Scientific area:	Please choose 🗸				
Project class:	C A = Grand Challenge, B = Regular, C = Discovery				
Funding source:	Please choose		~		
Funding grant number:					
Project proposal:	Choose File No file chosen	(.doc, .docx or .pdf only)			
Project abstract:	Choose File No file chosen	(.doc, .docx or .pdf only)			
Proposed start date:	(DD-MM-YYYY)				
Proposed end date:	(DD-MM-YYYY)				
Number of researchers:	2-5 V (estimate)				
Software requirements: Software Libraries and Compilers					
Application Packages Databases Required					
Databases Required					
			(optional)		

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HPC Requirements	
Core Hrs Requested = Number Core Component) + (1 * Number Core Hrs	ed as a template to determine the total number of core hours required. Hrs on Thin Component + (3.3 * Number Core Hrs on Shared Memory Component) + (2.3 * Number Core Hrs on GPU s on KNL Component) ro component request is required in the text box below.
CPU usage:	(CPU hours)
Storage:	(GB)
Method of estimation: How have you estimated the resources required on this system?	
Do you intend to use the shared men	nory partition? Note: Use of a shared memory core is charged at 3.3 times a regular compute core on the HPC system.
Use shared memory:	⊖Yes ⊖No
If "Yes", please specify:	
	partition? Note: Use of a core with GPU access is charged at 2.3 times a regular compute core on the HPC system.
Use accelerators (NVIDIA V100 or Intel KNL):	UYes UN0
If "Yes", please specify:	
Other requirements	
Any other requirements? e.g. requests for moving large amounts of data regularly across the network.	(optional)

There are elements for Class A (High Impact) projects not shown but these are unnecessary for most student requirements. A Class C (Discovery) project is highly recommended for students starting out.

Before filling out this online form and submitting, you must complete two documents for upload:

- Project Proposal (PDF recommended)
- Project Abstract (PDF recommended)

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It is recommended to complete the Project Proposal first (template available <u>here</u>) and then copy the abstract from the Project Proposal document directly into the Project Abstract file (which can be created by the student as there is no template available). Further information can be found <u>here</u>.

One of the main issues when submitting a project is the calculation of the HPC requirements. ICHEC has provided a calculator tool for this purpose <u>here</u>:

Add Row F	Reset Rows				
Node Type	Number of Jobs	Number of Nodes	Walltime hours	in Core Hours	
Thin (1x) 🗘	0	0	0		
Estimated core hours					
Node Type	Number of Job	s Number o	f Nodes	Walltime in hours	Core Hours
Thin	0	0		0	0

The node classifications are as follows (in relation to the current Kay supercomputer):

- Thin (1x) This refers to a "cluster of 336 nodes where each node has 2x 20-core 2.4 GHz Intel Xeon Gold 6148 (Skylake) processors, 192 GiB of RAM, a 400 GiB local SSD for scratch space and a 100Gbit OmniPath network adaptor. This partition has a total of 13,440 cores and 63 TiB of distributed memory."
- **GPU** (2.3x) This refers to a "partition of 16 nodes with the same specification as above, plus 2x NVIDIA Tesla V100 16GB PCIe (Volta architecture) GPUs on each node. Each GPU has 5,120 CUDA cores and 640 Tensor Cores."
- Shared Memory (3.3x) This refers to a "a set of 6 nodes each containing 1.5 TiB of RAM, 2x 20-core 2.4 GHz Intel Xeon Gold 6148 (Skylake) processors and 1 TiB of dedicated local SSD for scratch storage."
- KNL (1x) This refers to "a partition of 16 nodes, each containing 1x self-hosted Intel Xeon Phi Processor 7210 (Knights Landing or KNL architecture) with 64 cores @ 1.3 GHz, 192 GiB RAM and a 400 GiB local SSD for scratch space."

Each student needs to make an assumption in relation to the hardware (Thin, GPU, Shared Memory or KNL) on which they will work, the number of jobs, the number of nodes and the wall time in hours (real time running). The following equation can then be used to calculate the core hours as per the online form:



 Core Hrs Requested = Number Core Hrs on Thin Component + (3.3 * Number Core Hrs on Shared Memory Component) + (2.3 * Number Core Hrs on GPU Component) + (1 * Number Core Hrs on KNL Component)

This number can then be entered in the "CPU usage box" and is also required in the Project Proposal, alongside RAM and Storage requirements. A reasonable RAM estimation could be ~32GB to handle any major workloads, and ~100 GB to handle any larger output files.

Conclusion

This guide should cover the most queried information when applying for National HPC service. The remaining information requested in the online form and Project Proposal should not cause students too much difficulty. Once everything is complete, the application can be submitted and the review process will start. After the technical evaluation, Class C applicants are notified and their respective projects are activated.

The following links should help further. For this unfamiliar with SSH and terminal-based computing, it is advisable to start with the <u>Documentation</u> link and read all the available information thoroughly. For Windows users, <u>MobaXterm</u> is highly recommended for accessing ICHEC services, with instructions and videos at the bottom of <u>this page</u>.

<u>Useful links</u>:

- <u>Access to HPC | ICHEC</u>
- <u>National Service Projects | ICHEC</u>
- Documentation | ICHEC
- Kay User Guide | ICHEC
- FAQs | ICHEC
- Tutorials | ICHEC
- Setting up SSH Keys | ICHEC
- Software | ICHEC