HPCBYTES

RESEARCH COMPUTING NEWSLETTER

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In This Edition

2 Pages

- Accessing HPC Clusters and the RCAM portal
- Nimbus 2.0 overview and release notes
- Introduction of the Research Computing team for new researchers

As we enter into a new academic year the Research Computing team would like to provide a refresher for how to access our HPC clusters, in particular Nimbus and the Research Computing Account Management (RCAM) portal.

Nimbus is the University of Bath's cloud based supercomputer, and is available to all academic staff and doctoral students. Nimbus is scalable to meet all computational needs with a choice from a large diversity of processors to meet specific research needs.

Nimbus is a paid system and requires some funding to use, though there is a choice of cost models guaranteed Pay-As-You-Go compute service or a significantly cheaper Spot services which carries the risk of being terminated.

All HPC finances are managed through the RCAM portal which has a hierarchical model. The top level are the RCAM accounts which is where grant funding is directly linked to the portal and managed by the grant owner. Branched from an account are the Resource Allocations, where budget from an account is allocated to specific projects and users to be used on Nimbus as jobs are submitted through Slurm. Finances can be monitored in My Transactions.

If you have grant funding to use on Nimbus, you must first <u>allocate this funding to HPC through Agresso</u>, then you must log into the RCAM portal (using the University's VPN) and create an RCAM account on the portal using that Agresso code. Once the account

Introduction to Accessing HPC and the RCAM Portal

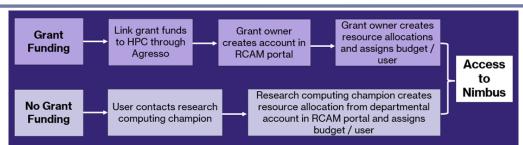


Figure 1: Overview of the pathways for access to Nimbus

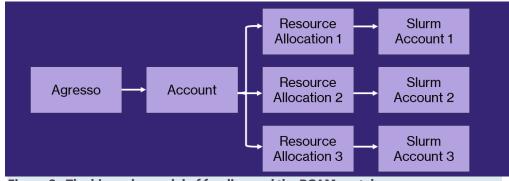


Figure 2: The hierarchy model of funding and the RCAM portal.

has been initialised you will be able to create resource allocations linked to that RCAM account. Within that resource allocation you can assign funding to yourself or other researchers. For more information on RCAM accounts and resource allocations visit the RCAM training material.

If you do not have grant funding available to use Nimbus, you must reach out to your <u>departmental champion</u> who will discuss your needs and assign you some funding from the departmental research computing budget, and arrange access through a resource allocation linked to the de-

partmental RCAM account.
Once you are assigned to a resource allocation within the RCAM portal, your Bath credentials will be authorised to allow you to log in and use Nimbus.

Within Research Computing you can access two other HPC systems Issam-bard3 which will be available for use later this year and Anatra HTC cluster which is available to researchers using software applications that can't move to the cloud, such as Gaussian and GaussView. Please get in touch with the Research Computing Team if you would like access to either of these systems.

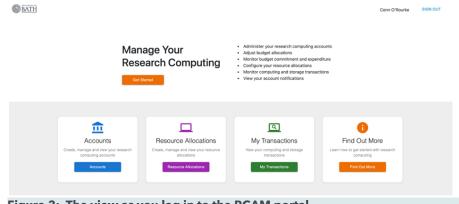


Figure 3: The view as you log in to the RCAM portal

Nimbus v2.0 has been deployed

The scheduled maintenance on our HPC cluster, Nimbus, was successfully completed at the end of July. All updates and improvements were implemented as planned, and we have been able to report a significant decrease in related issues.

Release Notes

Expanded the HPC cluster capacity by adding 140 nodes, increasing overall capacity by 20%

Fixed the problem of jobs getting stuck in the scheduled state on the RCAM portal

Resolved the issue of job node failures. It was an issue related to job post-processing

Rebuilt the entire cluster to address memory-related issues in long running HPC machine (Performance improvement)

Account managing software (Governor) was taking more time to compute the cost details of the job in each iteration, improved the performance to fetch the DB details for instance cost and job durations

Included an automated process for CI/CD

Restructured internal source code in a single repo for easy maintenance (Internal changes) and quick deployments

Renewed necessary certificates in Azure environments, specifically cost estimator tools and DevOps tools

Migrated the database system from MariaDB to MySQL for enhanced reliability (Internal)

Instance types	Previous Num of Nodes	Current Num of Nodes
Paygo-Fsv2-1	16	32
Paygo-Fsv2-2	16	32
Paygo-Fsv2-4	16	32
Paygo-Fsv2-8	16	22
Paygo-Fsv2-16	16	50
Paygo-Fsv2-24	16	20
spot-Fsv2-16	20	50
spot-hc-44	16	32
spot-hbv2-120	16	32
spot-hbv3-120	16	32

Meet the Research Computing Team

This year, in Research Computing, we have said goodbye to Roger Jardine (Director of Research Computing) and Deepak Aggarwal (Research Infrastructure Engineer) and welcomed Gavin Edwards (Chief Data and Technology Officer) as the new lead of the team. To introduce the current Research Computing Team to new researchers:



Gavin Edwards

Chief Data and Technology Officer



Brem Anand Jagannathan Krishnan

Principle Engineer (HPC)



Georgie Wellock

Research Software Engineer

The Research Computing Team are supported by the external Red Oak Consulting Team:

Roberto Scipioni - Senior HPC Support Specialist / Muneeb Khan - HPC Support Specialist / Khaled Mahjoubi - HPC Support Specialist

Acknowledgements

The Research Computing team would like to thank all contributors for the current issue of **HPCBytes**.

- We are looking for case studies! If you would like to contribute an article to be featured in *HPCBytes*, please get in touch with the Research Computing team.
- If you would like to hear more, please subscribe to the Research Computing mailing list here: https://forms.office.com/e/rF8rLWbakA

Contact us

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