

Register of Research HPC Clusters at UCL

For the purpose of this register, a research computing cluster is defined as having a minimum of 4 nodes, a job scheduling service, and shared storage.

Cluster	Grace HPC	Myriad HTC	Kathleen HPC	Thomas	Michael	Economics	Bioscience	Physics HEP	Physics Lemon	Computer Science	Sainsbury Wellcome Centre
Service Owner & Contact	Owain Kenway	Owain Kenway	Owain Kenway	Owain Kenway	Owain Kenway / David Scanlon	Owain Kenway / Lars Nesheim	Owain Kenway / Richard Mott	Ben Waugh	Ben Waugh	Denis Timm / Tristan Clark	John Pelan
Hosted by	ISD RITS	ISD RITS	ISD RITS	ISD RITS	ISD RITS	ISD RITS	ISD RITS	Physics and Astronomy	Physics and Astronomy	CS	Sainsbury Wellcome Centre (SWC)
Eligibility	All UCL Researchers	All UCL Researchers	All UCL Researchers	Materials & Molecular Modelling	EV battery research	Economics	Genetics, Evolution & Environment	High-Energy Physics research group	Biological Physics research group	Computer Science	All SWC Researchers
Purpose	Large multi-node parallel jobs. Jobs that require less than 32 cores are subject to a priority penalty.	High-I/O, high-throughput cluster. It contains different types of nodes, including GPUs. It runs jobs that will run within a single node rather than multi-node parallel jobs.	Large multi-node parallel jobs. Jobs that require less than 80 cores are subject to a priority penalty.	UK National Tier 2 High Performance Computing Hub in Materials and Molecular Modelling	Research into new models for EV battery systems and next-generation, solid-state batteries	High-I/O, high-throughput cluster. It contains different types of nodes, including GPUs. It runs jobs that will run within a single node rather than multi-node parallel jobs.	High-I/O, high-throughput cluster. It contains different types of nodes, including GPUs. It runs jobs that will run within a single node rather than multi-node parallel job.	Analysis of HEP experimental data and Monte-Carlo simulation of high-energy particle collisions.	Biophysics calculations.	General Purpose cluster to cater for a wide range of users. Lots of ancillary services plugged in.VM's, visualisation,many node types, GPUS. Parts designed to run specific job types. Tightly integrated storage.	General purpose heterogenous cluster to cater for theoretical & experimental neuroscience and machine learning.
How to get access	Free for any research staff at UCL. Non-permanent UCL researchers require approval from Supervisor	Free for any research staff at UCL. Non-permanent UCL researchers require approval from Supervisor	Free for any research staff at UCL. Non-permanent UCL researchers require approval from Supervisor	Nominated partner provides user name who must be researching materials science	Managed by David Scanlon in Chemistry	User must be a member of Myriad Economics Group and have a Myriad account.	User must be a member of Myriad Biosciences Group and have a Myriad account.	Accounts created for all HEP group members	By arrangement with the Biophysics group academics.	Researcher Funded. Access on request at our discretion. Large spread of UCL researchers and beyond. Multi Insitution projects	All SWC researchers are granted access automatically.
Scheduler	Son of GridEngine	Son of GridEngine	Son of GridEngine	Son of GridEngine	Son of GridEngine	Son of GridEngine	Son of GridEngine	Torque / Maui	Torque / Maui	Son of SGE	SLURM
Connection to UCL storage services	Nothing planned	Mounting RDSS planned for 2020	Nothing planned	No	No	Nothing planned	Nothing planned	no	no	Planned 2018-2020	Nothing planned
Listed in Service Catalogue?	UCL Computing Service – not listed individually	UCL Computing Service – not listed individually	UCL Computing Service – not listed individually	UCL Computing Service – not listed individually	UCL Computing Service – not listed individually	UCL Computing Service – not listed individually	UCL Computing Service – not listed individually	no	no	no	no
# of servers	680	150	192	712	320 + 208	(26)	(5)	28	6	~1100	~60
CPU Architecture <i>Incl # of cores</i>	Intel Xeon E5-2630v3 64GB processors (10,880 Cores)	Intel Xeon Gold 6140/6240 processors with 192GB and 1.5TB. (5,400 Cores)	Intel Cascade Lake 40 core nodes, 192GB of RAM (8,320 Cores)	Intel Broadwell 24 core nodes, 128GB of RAM (17,088 Cores)	Intel Broadwell 24 core nodes, 128GB of RAM (7,632 Cores) Intel Cascade Lake 40 core nodes, 192GB of RAM (8,320 Cores)	Intel Xeon Gold 6240 processors with 192GB. (936 cores (in Myriad total))	Intel Xeon Gold 6140 processors with 192GB and 1.5TB. (180 cores (in Myriad total))	X86, 656 cores	x86, 120 cores	X86 Various Nehalem through to Skykake 16GB – 3TB RAM (~ 9000 cpu cores + 300,000 GPU Cores)	Mixed x86 (~700 cores) with at least 8GB per core.
Accelerators	None	Nvidia P100, V100	None	None	None	Nvidia V100	None	no	no	200 x Various GPUs GTX/P100/V100	Nvidia GPU (Pascal / Tesla / Turing)
Storage Home	Backed up nightly via TSM	Backed up nightly via TSM	Backed up nightly via TSM	Backed up nightly via TSM	Backed up nightly via TSM	Backed up nightly via TSM	Backed up nightly via TSM	1 TB	1 TB	7PB +9PB +10PB Tape Cap.. +SSD's Project stores available to cluster on request.. Backed up on request per project.	All local storage is available.
Storage Scratch	1PB.	2PB.	1PB	430TB	260TB.	N/A	N/A	Various volumes available to specific	Various volumes available to specific	7PB +9PB +10PB Tape Cap.. Project	Local SAS/SSD/NVMe

Cluster	<u>Grace</u> HPC	<u>Myriad</u> HTC	<u>Kathleen</u> HPC	<u>Thomas</u>	<u>Michael</u>	Economics	Bioscience	Physics HEP	Physics Lemon	Computer Science	<u>Sainsbury</u> <u>Wellcome</u> Centre
<i>Not backed up</i>								projects, up to 10 TB in size, totalling of order 500 TB.	projects, 20 TB in total.	stores available to cluster on request.	scratch per node plus shared, parallel scratch of a few TB.
Inter-connect	40 Gigabit Infiniband	Mellanox, 100 Gigabit Infiniband	40Gigabit Infiniband	100 Gigabit Omnipath	100 Gigabit Omnipath	Mellanox, 100 Gigabit Infiniband	Mellanox, 100 Gigabit Infiniband	1Gb ethernet	1Gb ethernet	1G/10G/40G/100G Ethernet + 100G IB	1/10G Ethernet
External access	No	No	No	Yes	Yes	No	No	Via SSH gateway	Via SSH gateway	Yes via gateways	Yes via VPN/ssh
Funded by	UCL	UCL	UCL	EPSRC	Yes	Research Capital Equipment Fund.	BBSRC.	STFC + other grants	Various grants and fellowships	Various Grants	SWC
Refresh	'Kathleen'	2021	Not planned	2020	Not planned	Not planned	Not planned	Ad-hoc, depending on funding.	Ad-hoc, depending on funding.	Ongoing	Ongoing

Cluster	IPServer	Teaching	Hartree	Turing	Meitner	XPOSS	Faraday	Xenon	Cobweb	Hypatia	Splinter	eMedLab
Service Owner & Business Contact	Frank Otto	Frank Otto	Frank Otto / Graham Worth	Frank Otto	Frank Otto / Scott Woodley	Frank Otto / Sally Price	Frank Otto	Frank Otto	John Deacon , Edd Edmondson	John Deacon , Edd Edmondson	John Deacon , Edd Edmondson	David Wong / Anthony Peacock
Eligibility	Most nodes belong to individual PIs. Equipment left behind by researchers is used by the Chemistry department as a shared resource.	Open to all in the Chemistry department	Used by Prof. Graham Worth and others he invites.	PhD/Mres/MSc students from the CDT for Molecular Modelling & Materials Science	Collaboration on projects run by Prof. Scott Woodley	Prof. Sally Price, her research group, collaborators, and Pharma partners.	Materials science researches in the Chemistry department, their students and collaborators.	Various research groups within Chemistry department (Sally Price, Dewi Lewis).	Physics and Astronomy exoplanets	RCIF funded nodes and storage are <u>open for broad use</u> ; Cosmoparticle nodes and storage are attached to specific grants and only available to specific users.	Physics and Astronomy cosmology	Crick
Hosted by	Computational Chemistry	Computational Chemistry	Computational Chemistry	Computational Chemistry	Computational Chemistry	Computational Chemistry	Computational Chemistry	Computational Chemistry	Astrophysics	Astrophysics	Astrophysics	Bioinformatics Research
Purpose	General HPC jobs, including multi-node jobs that need a fast interconnect. The cluster is equipped with Infiniband (40Gb/s).	Used for teaching students in CC. Outside of teaching season, used by Master students for their projects. Provides JupyterHub and WebMO as web interfaces.	General computational chemistry jobs. Standard packages (Gaussian, Turbomole, etc) as well as in-house development of the Quantics package.	Supports the CDT for Molecular Modelling and Materials Science	Computational backend for 2 projects: 1) database of chemical clusters - hive.chem.ucl.ac.uk2) database of solid crystal structures and surfaces – saint.chem.ucl.ac.u	Research work on "Control and Prediction of the Organic Solid State". Some compute nodes reserved for collaboration projects with Pharma partners	Collaboration cluster within computational Chemistry	Collaboration cluster within computational Chemistry	Exoplanet group research	Cosmoparticle research and group-wide use	Cosmology group research	To analyse human genome data and medical images, together with clinical and other physiological and social data, for the benefit of human health.
How to get access	Contact PI	Contact F. Otto	Contact Prof Worth	Contact Prof Woodley	Contact Prof Woodley	Contact Prof Price	Contact F. Otto	Contact F. Otto	Access requires grant holder permission.	RCIF available via application EE+Andrew Pontzen. Cosmoparticle by grant holder permission.	Access requires grant holder permission.	
Scheduler	SGE	SGE	SGE	SGE	SGE	SGE	SGE	SGE	Slurm	Slurm	Slurm	
Listed in Service Catalogue?	No	No	No	No	No	No	No	No	No	No	No	No
# of servers	112	35 + Extension of 10 nodes	32	14	10	19	12	5	6 + 2 GPU	RCIF = 4 nodes; Cosmoparticle = 14 in total	29 in total	
CPU Architecture <i>Incl # of cores</i>	Nodes vary in age with 8 to 24 cores	4 cores per node; Extension has 8 to 20 cores.	Nodes vary in age with 4 to 16 cores	Dual Xeon E5-2650v3 with 64GB RAM	Dual Xeon E5-2650v2 with 64GB RAM	Nodes vary in age with 8 to 28 cores	Dual Xeon E5-2650v3 with 64GB RAM	Dual Xeon E5-2650v3 with 64GB RAM	Intel Xeon with 24 cores each GPU: Xeon with 20 + 32	12x24/8x40/1x60/1x80 cores	456 cores in total	
Accelerator Architecture	None	None	None	None	None	None	None	None	1 * Nvidia K40 and 3 * V100		2 * NVIDIA K80 cards and 1 * V100	
Connection to UCL storage services	No	No	No	No	No	No	No	No	No	No		
Storage Home									1TB not backed up	10TB backed up nightly	600G not backed up	
Storage Scratch <i>Not backed up</i>	18TB. Backed up nightly inside dept.	1TB. Backed up nightly inside dept.	4.4TB. Backed up nightly inside dept.	8.8TB. Backed up nightly inside dept.	4.4TB. Backed up nightly inside dept.	3TB. Backed up nightly inside dept.	2.8TB. Backed up nightly inside dept.	7.7TB. Backed up nightly inside dept.	~100TB	~300TB	~400TB	
Inter-connect	Infiniband network	IB 10Gb/s	1Gb Ethernet	1Gb Ethernet	1Gb Ethernet	1Gb Ethernet	1Gb Ethernet	1Gb Ethernet	Intel/QLogic QDR Infiniband	Mellanox EDR Infiniband	Gigabit ethernet	
External access	Only accessible through UCL IP range.	Only accessible through UCL IP range.	Only accessible through UCL IP range.	Only accessible through UCL IP range.	Only accessible through UCL IP range.	Only accessible through UCL IP range.	Only accessible through UCL IP range.	Only accessible through UCL IP range.				
Funded by	Multiple sources	Second hand hardware							Multiple grants	Mixture of RCIF funding and grants.	Multiple grants	
Refresh	Old nodes replaced by new ones based on needs/funds of the individual PIs	Close to end of life, will migrate users to IB-Server	Old nodes replaced by new ones based on needs/funds.	Not planned	Not planned	Not planned	Not planned	Not planned				Facility to close in 2020.

Cluster	Hades	ND Cluster	Geography	The Bartlett	Physics CMMP	London Centre for Nanotechnology	Physics AMOPP Theory						
Service Owner & Business Contact	Hallgeir Jonvik	Dave Cash	Ajay Chauhan (for the time being)	Joe Elwood	Andrew Gormanly	Andrew Gormanly	Fabian Garza						
Eligibility	Collaborators or members of Queen Square Genomics	Collaborators or members of Neurodegenerative Diseases, Institute of Neurology	Geography staff and students	Bartlett School of Architecture students	Physics and Astronomy	London Centre for Nanotechnology	Physics and Astronomy						
Hosted by	Institute of Neurology	Institute of Neurology	Geography	IT for Bartlett	CMMP research group	London Centre for Nanotechnology	Physics and Astronomy						
Purpose	Bioinformatics. Primarily for joint standardised analyses and for diagnostic services. Restricted to users running these; not for ad hoc analyses / general HPC.	Used for simple tasks, eg 1000 simulation tasks, no high-end modelling. Mostly use Linux open source apps Use CS for a number of Dementia research centre projects.	Remote Sensing, Big Data, Geospatial analytics, water and climate modelling. Equipment is purchased for specific research and does not form part of a single cluster.	Render-farm facility Single VM as controller plus 16 physical nodes. Currently supports eight concurrent users.	High-throughput cluster used for material structure prediction and simulations of catalytic and environmental interfaces.	Dedicated departmental cluster offering distributed-memory and shared-memory queues for simulations of nanoscale systems, including electronic structure calculations and molecular dynamics.	Departmental Linux Cluster used for quantum mechanical calculations						
How to get access	Access requires sponsorship from funding PIs.	Contact D. Cash	By Request from System Admin	Bartlett students only.	Researcher Funded. Access to these groups.	Researcher Funded. Access on request for LCN and associated researchers, at our discretion.	Researcher Funded. Access granted by PI's and group leaders.						
Scheduler	Son of GridEngine		Not used		Grid Engine	Grid Engine	None						
Listed in Service Catalogue?	No	No	No	No	No	No	No						
# of servers	8 + headnode	8	~ 24 nodes, comprised of nodes of varying ages shared between research groups.	No.	180	91	16						
CPU Architecture <i>Incl # of cores</i>	Dual Intel Xeon E5-2650v4 2.2GHz, 12Core, 192 cores		Intel x86 type, Solaris and Spark Core count mostly from 4 -6	16 x 1u.	x86 various 3496 cores	x86 various 1264 cores	x86 various 234 cores						
Accelerator Architecture	No	No	2 GPUs, one is specific to a research group			2 Tesla nodes, 1 Phi node	No						
Connection to UCL storage services	No	No	Connected to local storage				No						
Storage Home		Dell Unity SAN 170TB storage (contains sensitive medical images). Backed-up offsite.	~100 TB	1TB. Rendering data is deleted ~ 30 days. Students can copy rendering data to their :N drive.	14 TB	9 TB	18 TB Mixed Home/Workspaces						
Storage Scratch <i>Not backed up</i>	580 TB		N/K	None	1 Gb Ethernet	1 Gb Ethernet 40 Gb IB	~ 65Tb						
Inter-connect	10GbE	10 Gbit	10Gbit, mixture due to age of equipment	1GB ethernet	No	No	1 Gb Ethernet						
External access	No.		Access via Gateway server	No	Various grants and fellowships	Various grants and fellowships	Access via gateway server. Used by a number of external users.						

