

## Adapter Allocation Scheme Recipients – Q4 2023

The NCI Adapter Allocation Scheme is a merit-based scheme to allocate supercomputing, cloud and data storage resources to meritorious researchers around Australia. The Scheme, running quarterly, provides flexible access to relatively small allocations to support new and varied workloads across the scientific disciplines.

Successful Adapter Scheme recipients for allocations in Q3 2023 are listed below. The allocated resources are measured in thousands of Service Units (KSU). One KSU on the Gadi supercomputer is equivalent to 500 core hours, 1 KSU on the Nirin Cloud is equivalent to occupancy of 0.36 virtual cores for one quarter and 1 KSU of storage is equivalent to 0.16 Terabytes of storage for one quarter.

Lead CI, Institution	Project Title	Gadi allocation (KSU)	Storage allocation (KSU)
Aaron Schindeler, University of Sydney	Screening of a curated structure library for novel senolytic compounds	250	0
Alexander Mikheyev, The Australian National University	Honey bee viruses: a model for understanding the emergence of infectious diseases	142	0
Ali Ahrari, UNSW Sydney	Developing a novel method and benchmark problems for multimodal multi-objective optimisation	55	0
Amila Madhusanka Kumara Wickramasinghe, The University of Tasmania	Enhancing Wildland Urban Interface Resilience: Physics-Based Modelling for Validation of Ember Attack on Houses During Wildfires	225	25
Amy Geddes, The University of Queensland	Modelling cross-linked, multilayer graphene-oxide flake filtration membranes for water purification	105	0
Andre Fellipe Vilanova de Araujo Aquino, UNSW Sydney	Assessment of computational flow dynamics frameworks to model airborne droplets dispersion in indoor settings.	250	0
Andrey Molotnikov, RMIT University	Integrated Computational Materials Engineering (ICME) Driven Ultra-sound Assisted Additive Manufacturing of Metallic Alloys	100	5



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Belinda Wright, University of Sydney	Investigating the role of host genetics in chlamydial disease and vaccination in koalas	100	75
Bernd Gruber, University of Canberra	Recent demographic inference from contemporary genomics under critical conservation scenarios	200	2
Chunguang Tang, Deakin University	Benchmarking of density functional approximations on stacking fault energies of high entropy alloys	135	0
David Chalmers, Monash University	Parallel Cascade Selection Molecular Dynamics (PaCS-MD) for peptide binding characterisation	195	5
David J Adams, University of Wollongong	Intracellular pH and nitrogen cation effects on guanidinium toxin inhibition of NaV1.4 channels	248	2
Declan Finn Keogh, University of Sydney	Dynamics of the Large-Scale Circulation in spatially extended cylinders	250	0
Deepak Saini, The University of Melbourne	Advancing Hydrogen Fuel Safety by Conducting Numerical Simulations	250	0
Dong Gong, UNSW Sydney	Detection and Adaptation of Data Distribution Shift for Large-Scale Foundation Models	250	0
Dr. Nicholas Gibbons, The University of Queensland	NATO Collaborative Validation of Turbulence Models for High-speed Flow Simulation	227	0



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Duncan Sutherland, UNSW Sydney	Role of near-surface wind in propagation and intensity of merging fire	220	0
Eirini Goudeli <i>,</i> The University of Melbourne	Nanoparticle self-assembly in the gas-phase by hierarchical multiscale modelling	240	2
Eric Mascot, The University of Melbourne	Topological superconductivity in magnet/superconductor hybrid systems	247	3
Hengrui Liu, UNSW Sydney	Safety in hydrogen storage – pilot study for efficiency assessment of thin water mist sheet in blocking hydrogen jet flame from leaked storage tanks	250	0
Jaime Gongora, University of Sydney	Genomic Insights into Adaptive Diversity: A Comprehensive Analysis of Platypus, Arabian Oryx, and Crocodilian Species	70	30
Jamie-Lee Thompson, Victor Chang Cardiac Research Institute	Investigating parental mosaicism as a cause of de novo mutations in patients with Congenital Heart Disease	200	0
Joanna Achinger-Kawecka, Garvan Institute of Medical Research	Targeting 3D Epigenome in Metastatic Prostate Cancer	194	44
Joe Berry, The University of Melbourne	State property modelling of cryogenic hydrogen vapor	246	4
Johanna Beckmann, Monash University	Detection and attribution study of the mass loss of the Antarctic Ice Sheet - Part A	226	4



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Johannes Zuegg, The University of Queensland	MolXBert – optimised molecular presentation for organic and metal complex structures with antimicrobial activity	160	5
Junming Ho, UNSW Sydney	Composite Methods to Accelerate Highly Accurate Vibrational Frequency Calculations	250	0
Kasimir Phennah Gregory, The Australian National University	Decomposing cation-amino acid residue interactions with symmetry adapted perturbation theory	249	1
Lars Goerigk, The University of Melbourne	Predicting the impact of protein environments on fluorescent sensors	150	0
Leon Chan, The University of Melbourne	Effect of plastron degradation of superhydrophobic surfaces on aerodynamic drag	250	0
Li Zhao, The Australian National University	Modelling lightning ignited fire occurrence in Australia	100	35
Liang Zheng, The Australian National University	Towards building general-purpose multimodal foundation models	100	25
Mingchao Wang, The University of Queensland	Dissipative Particle Dynamics Simulation of Ion Conductivity in Diblock Copolyelectrolytes	242	0
Nadia Zatsepin, La Trobe University	Simulating serial micro-crystallography with novel compact X-ray sources	150	100



Lead CI, Institution	Project Title	Gadi allocation (KSU)	Storage allocation (KSU)
Raymond Tobler, The Australian National University	Reconstructing cultural and biological evolution in New Guinea	85	0
Sajid Ali, Monash University	A high throughput study of Semi-conducting defect-based qubits for quantum technology	210	40
Shreya Ghosh, Curtin University	Multimodal Computational Modelling of Human-Human Interaction	200	50
Simon Jiang, The Australian National University	Genomic Analysis to Identify Genetic Basis of Kidney Disease in Australian Indigenous Communities	240	10
Simon Murphy, University of Southern Queensland	Quantifying Systematic Uncertainties in delta Scuti Star Modelling for Asteroseismology	180	20
Sobin Alosious, The University of Queensland	Study of Alternating Current Electrohydrodynamics Flow	200	50
Stephan Rachel, The University of Melbourne	Numerical simulation of a fault-tolerant quantum computer	220	30
Suresh K. Bhatia, The University of Queensland	Understanding the Performance of Nanostructured Catalytic Materials	250	0
Swarit Dwivedi, Monash University	Development of a computational framework to systematically study MOF- derived nanomaterials for catalytic CO2 conversion to value-added chemicals	200	7



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Thang Quang Trinh, Griffith University	Validating a dual-U model in the DFT+U scheme for metal oxide structures.	250	0
Tim Duignan, Griffith University	Molecular simulation of aqueous systems with state-of-the-art quantum chemistry.	250	0
Tingyi Zhang, UNSW Sydney	High-fidelity numerical simulations of the wing tip vortex formation noise	250	0
Travis Mitchell, The University of Queensland	Towards zero-emission hydrogen: Decarbonising natural gas and bio-methane	250	0
Xing Zhi, The University of Melbourne	Developing fundamental pathways for ammonia electrosynthesis using liquid metal catalysts	250	0
Yendrew Yauwenas, UNSW Sydney	Flow simulation of trapezoidal cylinders in high Reynolds-number flow	200	10
Yongjun Peng, The University of Queensland	Investigating the bubble-liquid interaction and its impact on fine gangue entrainment in the Reflux Flotation Cell	238	12
Zhao Liu, Monash University	Light-matter interactions in ferromagnetic negative charge-transfer energy insulator	100	25
Zhongyan Zhang, University of Wollongong	Boosting Visual Representations with Spatial Context Information for Image Retrieval (a research of extension)	210	40



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Ziyang Lu, The Australian National University	Atomic-modified 2D iron oxide for nitrate reduction reaction	250	0