NCI AUSTRALIA

Convergence of HPC, AI, and Quantum for Research Scientists: Unleashing the Power of Advanced Computing

Australasia Leadership Supercomputing Symposium 14-16 June 2023 debrief

We acknowledge and celebrate the First Australians on whose traditional lands we meet and pay our respect to the Elders past and present.

Artist: Lynnice Letty Church – Tribes: Ngunnawal, Wiradjuri & Kamilaroi (ACT and NSW)
Gadi - "to search for" in Ngunnawal language - January 2020 for NCI Gadi Supercomputer

What is NCI?

A world-class, high-end supercomputer and data science hub

- NCI is the premier facility in Australia providing:
  - High-performance computing (supercomputing)
  - Cloud computing
  - Data storage and services
- We support over 5500 Australian researchers.
- We enable transformative research that informs policy
- We deliver outcomes with national benefits

Invited Plenary Speakers

Prof Rick Stevens	Argonne NATIONAL LABORATORY
Dr Seiji Tsutsumi	JAXA
Prof Lisa Kewley	CENTER FOR ASTROPHYSICS HARVARD & SMITHSONIAN
Prof David Thomas	Garvan Institute of Medical Research
Prof Lloyd C.L. Hollenberg	THE UNIVERSITY OF MELBOURNE
Dr Adele Morrison	Australian National University
Asst Prof Simon Scheidegger	UNIL | Université de Lausan
Prof Karin Verspoor	RMIT UNIVERSITY
Dr Emily Kahl	THE UNIVERSITY OF QUEENSLAND AUSTRALIA
A/Prof Tan Tin Wee	National Supercomputing Centre SINGAPORE
A/Prof Alice Gabriel	UC San Diego | SCRIPPS INSTITUTION OF OCEANOGRAPHY

WELCOME TO ALCS 2023!

ALCS 23
AUSTRALASIAN LEADERSHIP COMPUTING SYMPOSIUM

14-16 JUNE 2023
THE SHINE DOME, CANBERRA

NCI AUSTRALIA | pawsey | NeSI

Use the hashtag
#ALCS2023
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Scientific Committee

Prof Richard Sandberg	The University of Melbourne
Prof Debra Bernhardt Prof Megan O'Mara	The University Of Queensland Australia
Prof Andy Hogg	ACCESS Australian Earth System Simulator
Prof Dietmar Müller	The University of Sydney
Prof Christian Jakob	Monash University
Prof Matthew Bailes	Swinburne University of Technology
A/Prof Fatemeh Vafaee	UNSW Sydney
Prof Fedor Iskhakov	Australian National University
Dr Chris Scott	NeSI New Zealand eScience Infrastructure
Dr Sam Yates	pawsey
Dr Ben Evans Dr Jingbo Wang	NCI Australia

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ALCS 2023 AT A GLANCE

200+ REGISTERED PARTICIPANTS

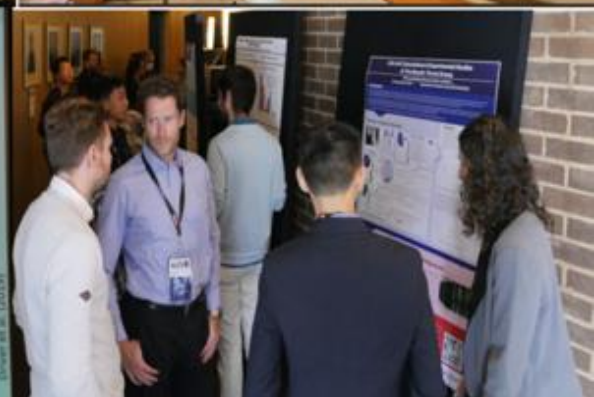
40 MORE THAN 40 ORGANIZATIONS

6 COUNTRIES REPRESENTED

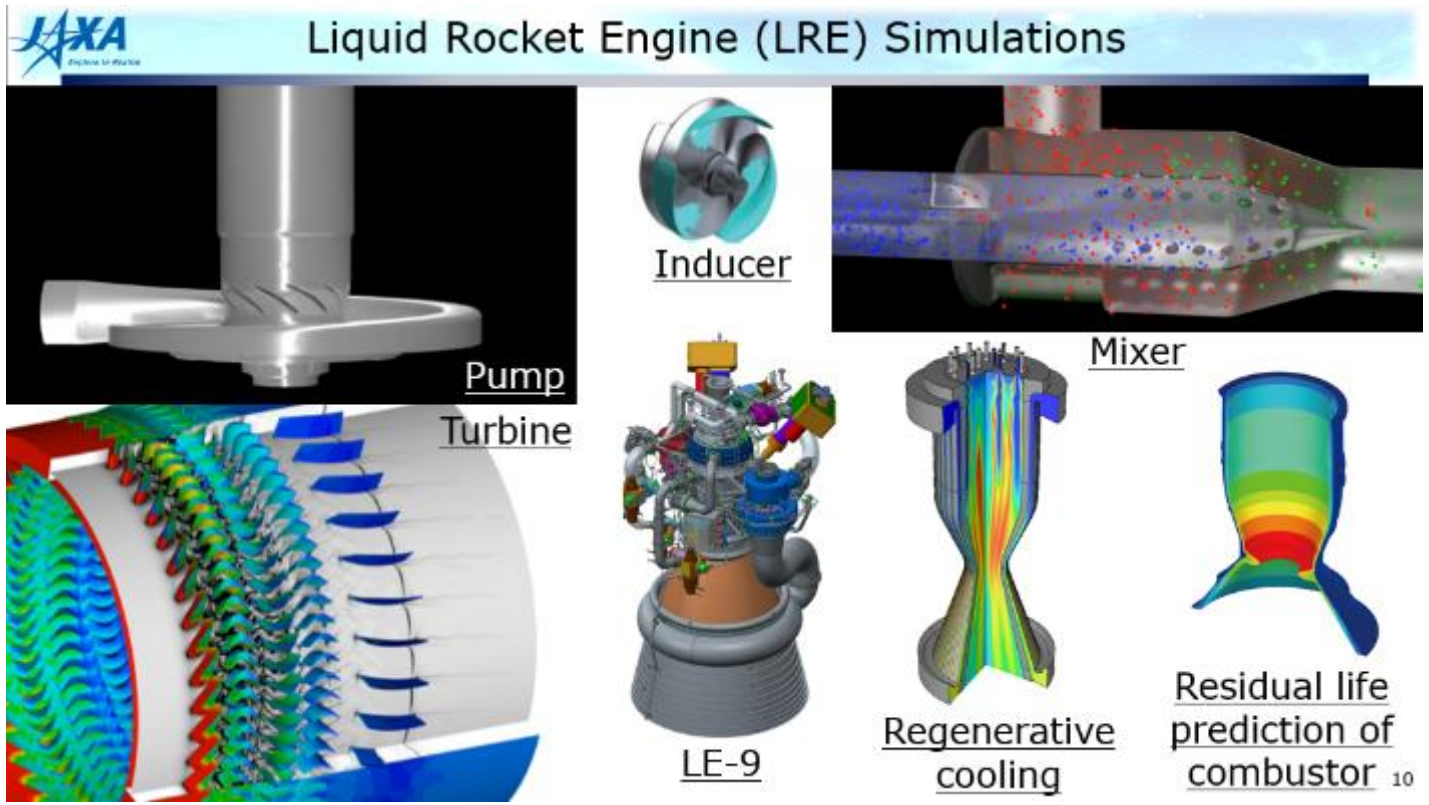
10 PLENARY TALKS

5 SCIENTIFIC STREAM BREAK OUT SESSIONS

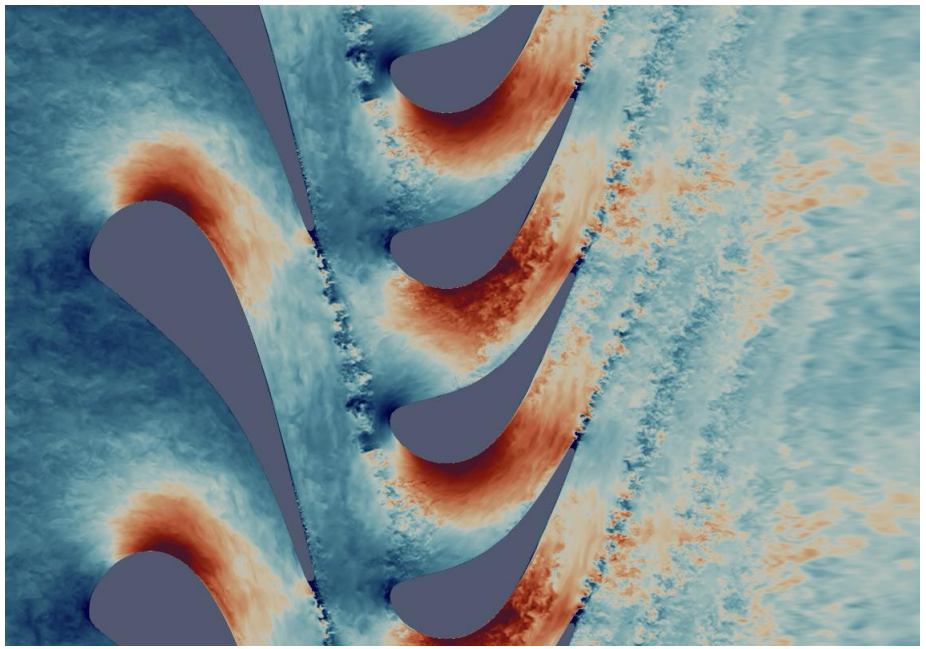
40 MORE THAN 40 PLUS POSTER SESSIONS AND LIGHTENING TALKS



Summary of CFD Session



- Develop pooled software development capabilities
- Remove barriers to experimentation/adoption of open-source codes
- More storage
- Mesh generation – a huge bottleneck
- Quantum – expect inhomogeneous platforms but not yet clear where the first ‘positive gain’ applications will be



Summary of Molecular Simulations and Bioinformatics Session

Cohorts used in case:control studies

Study	Discovery cases	Replication cases	Discovery controls	Replication controls
International Sarcoma Kindred Study (ISKS)	1474			
Genetic Cancer Risk in the Young Study (RisC)	105			
The French Exome project (FREX)*			364*	
The Cancer Genome Atlas (TCGA-SARC)		253		
Norwegian Sarcoma Consortium (NoSarC)		310		
Hartwig Foundation (sarcoma only)		276		
Spontaneous coronary artery dissection (SCAD)				88
Total	**1644**	**839**	**3611**	**4299**

Total data storage @NCI for these germline studies >825Tb

Total compute for these analyses: 4.175M core hours

(Credit: David Thomas)

- quantum mechanical calculations
- molecular dynamics simulations of both materials and biomolecular systems
- bioinformatics methods for large scale genome, proteome, or metabolome analysis.

quantum mechanical energy/force calculations scale as >=N^4
molecular dynamics simulations, scaling ranges from NlogN to N^2

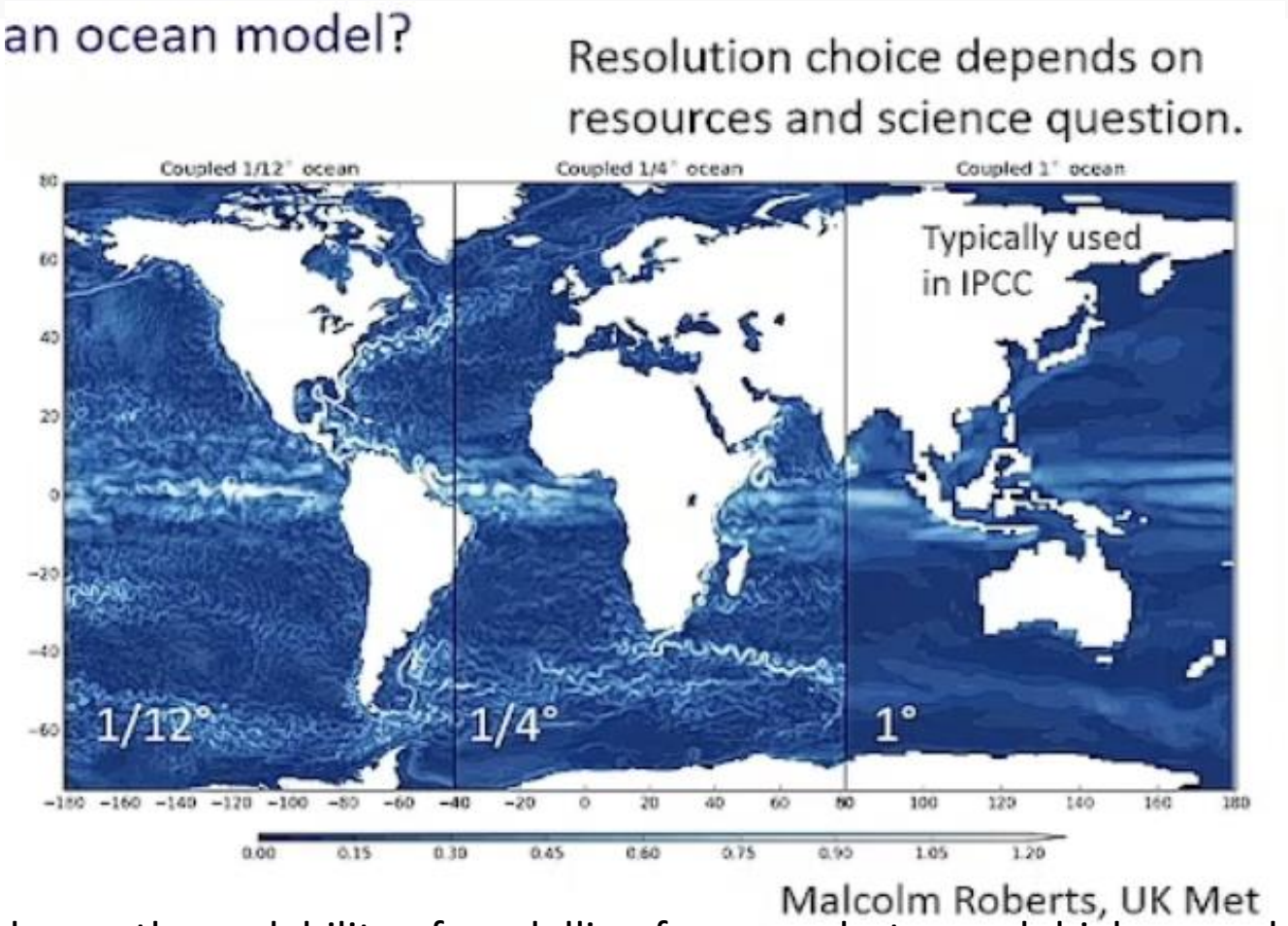
Molecular dynamics simulations are well-suited to GPUs and there has been significant re-optimisation of existing code and development of new code to take advantage of highly parallel architecture.

diversity of system sizes, compute and memory

Summary of Climate and Weather Session

1. Training ML models on processes occurring in high-resolution models to tune parameterisation schemes for lower resolution simulations;
2. Use of AI/ML to diagnose model dynamics, or to train on model output to dynamically interpolate sparse observations
3. To provide short-term forecasts of weather, waves, ocean state, and so on.

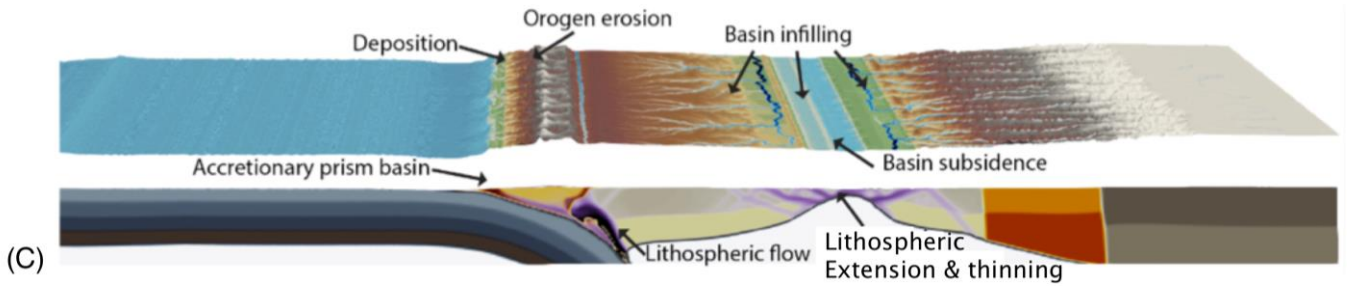
we are moving towards a climate system that is outside the bounds of the observed record! It follows that training (particularly for forecasting) may be compromised in many situations and motivates the need to continue working with traditional forward models.

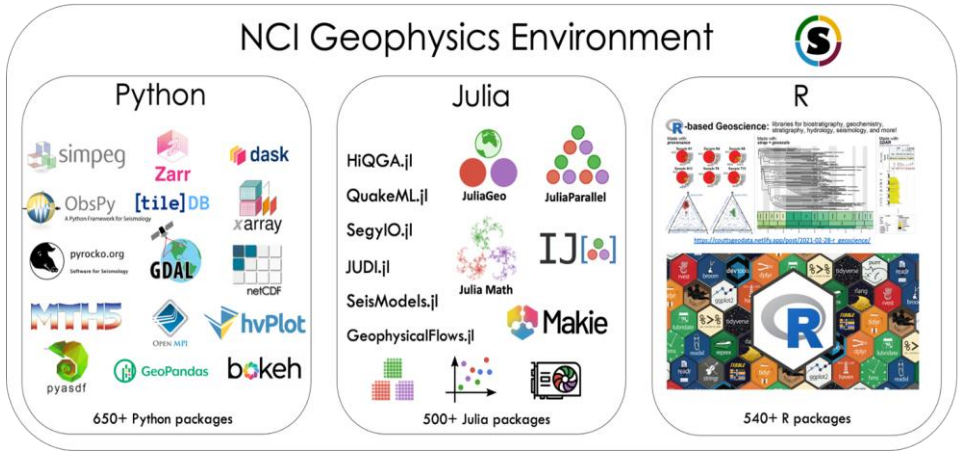


enhance the scalability of modelling frameworks to reach higher resolution

Summary of Geophysics Session

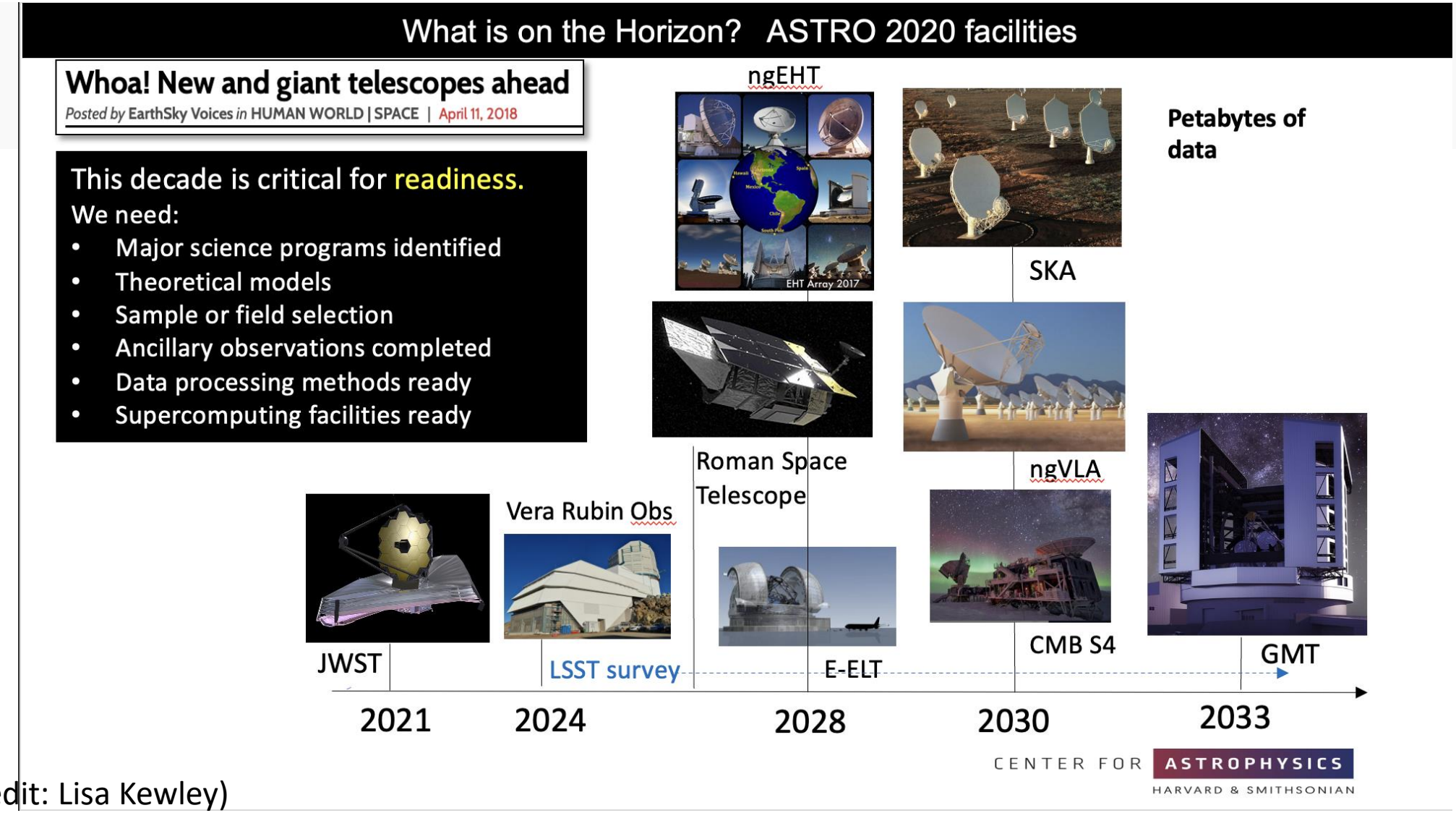
- Computational and Data intensive multi-physics activities being attempted across Australia
- Assembling both high-end new codes around major collaborations
- Rescuing, assembling and reprocessing data to new standards





- Co-location of HPC and data and mix of environments in one place makes things much easier
- Increase in research productivity using platform for sharing – even when individual activities can be siloed.

Summary of astronomy Session



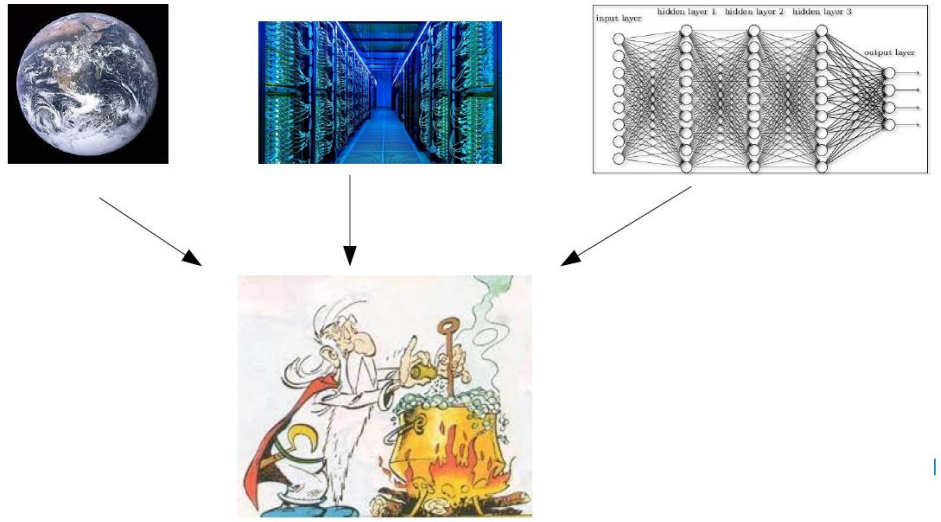
(Credit: Lisa Kewley)

Summary of Social Sciences Session – Computational economics

Our Modeling Wish List

- Rich specified integrated assessment models (IAMs).
- Include state-of-the-art climate science (to the extent possible).
- Time-to-solution on human time-scales (minutes to hours on a laptop), not 100k node hours on a HPC system.

→ Interdisciplinary endeavor encompassing climate science, applied math., comp. science, economics.



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UNIL | Université de Lausanne
HEC Lausanne

(credit: Simon Scheidegger)

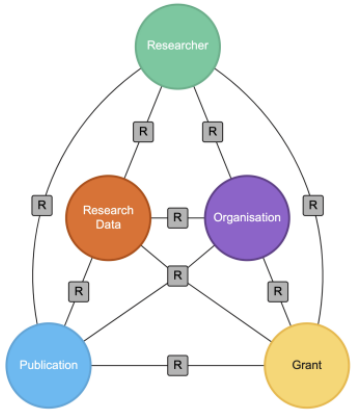
Summary of Social Sciences Session – Knowledge graph empowered by LLM

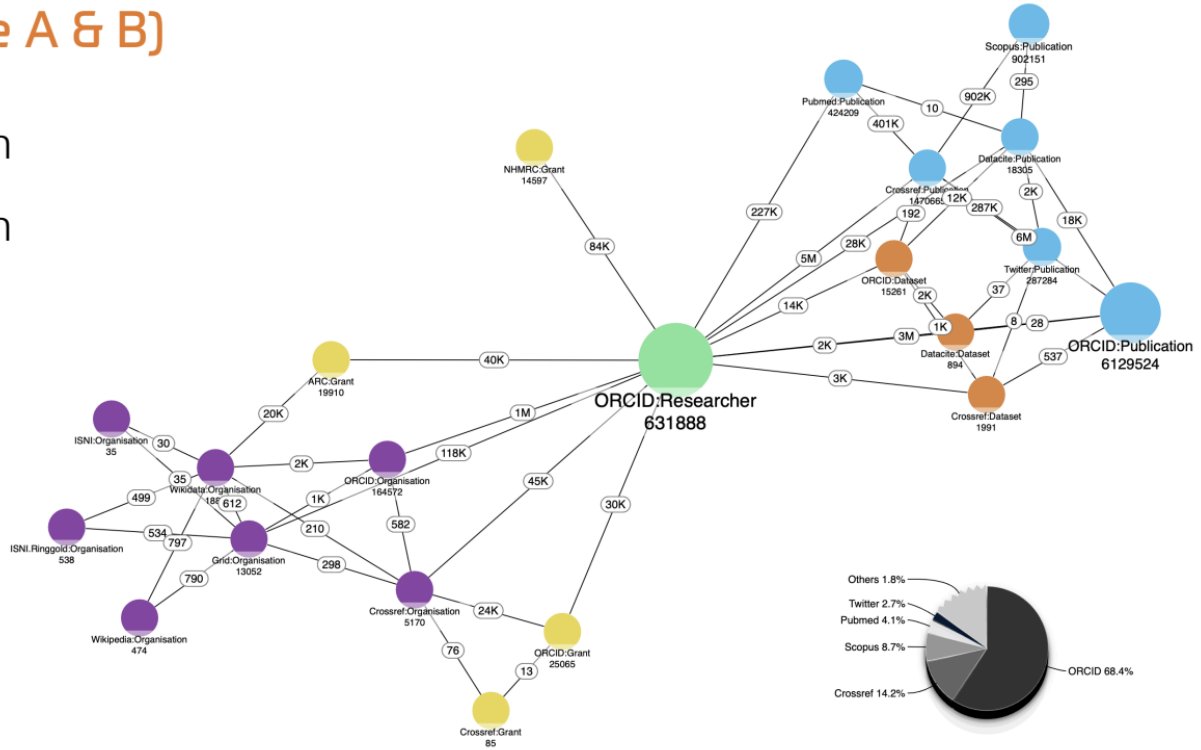
PID Graph (Type A & B)

Nodes: 11 million

Relations: 18 million

Last updated: 11 Sept 2023





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(credit: Amir Arayni)

Key message: HPC will be essential to QC, and there are many interaction pathways emerging

Summary of Quantum

1. Hybrid approaches: QC and HPC working in tandem
2. QC benchmarking and simulation requires HPC
3. HPC data processing in quantum error correction
4. Machine Learning techniques for quantum applications
5. Large-scale simulations for QC devices/hardware

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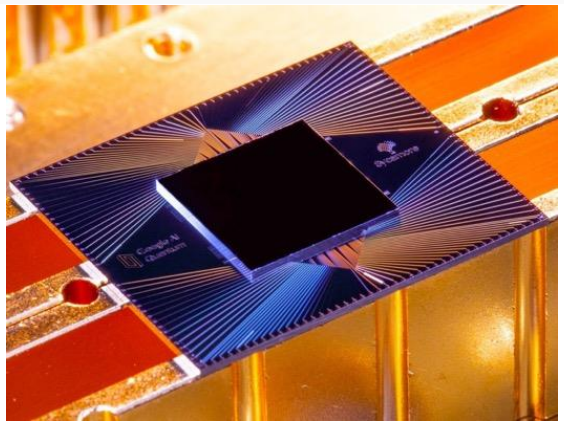
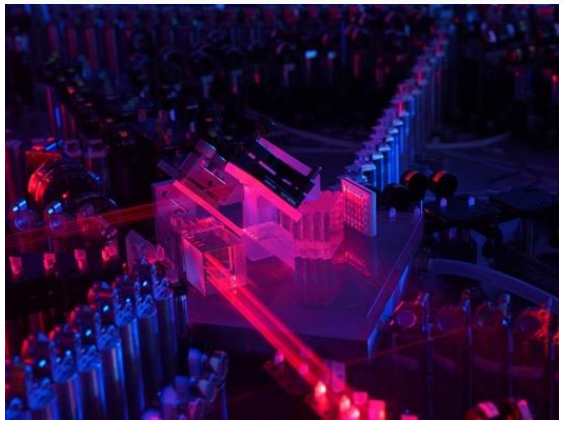
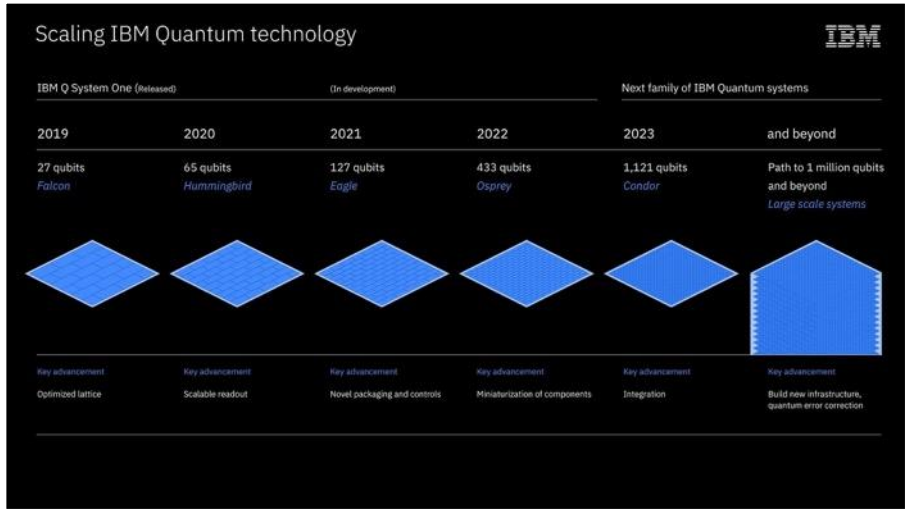
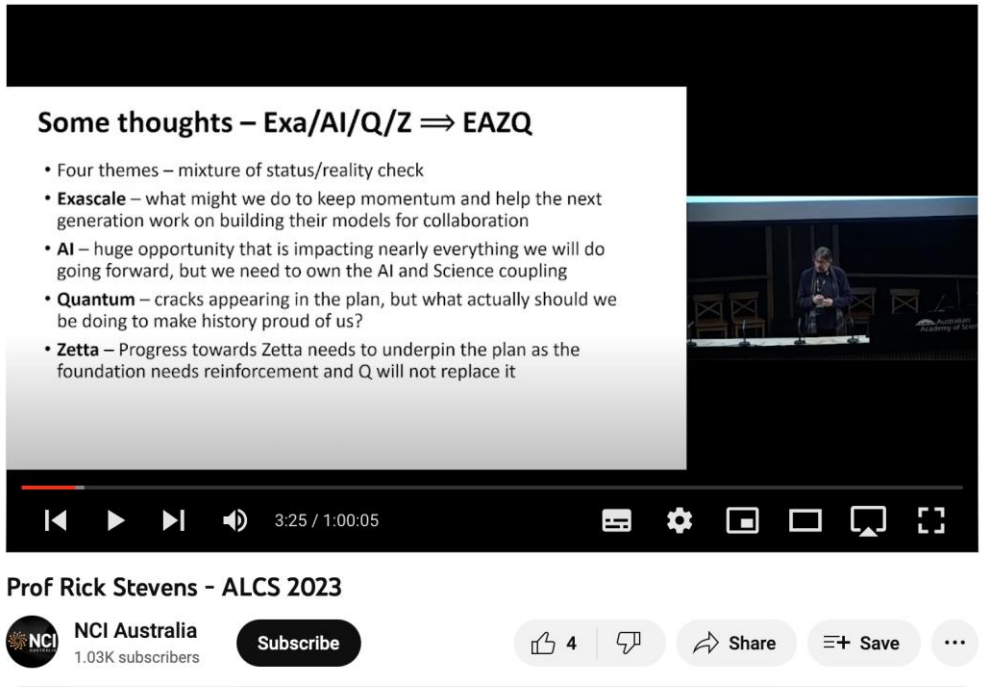


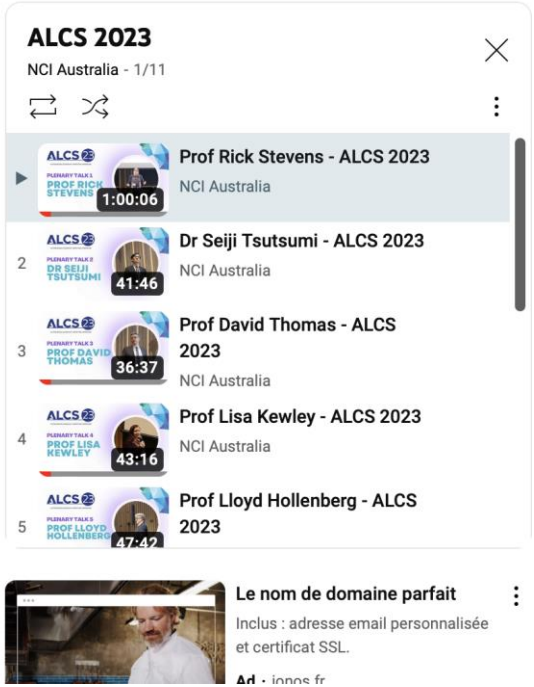




(Credit: Lloyd Hollenberg)

Plenary talks are available on NCI YouTube Channel





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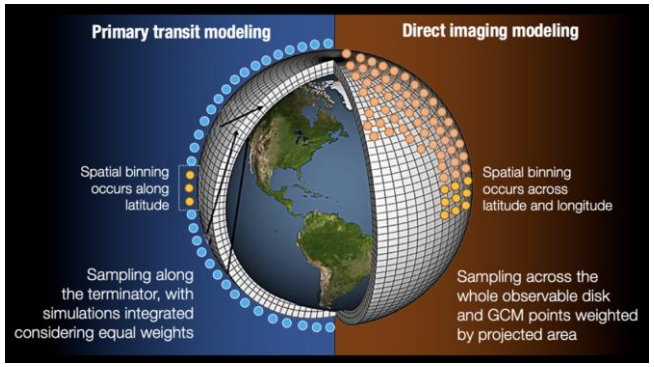
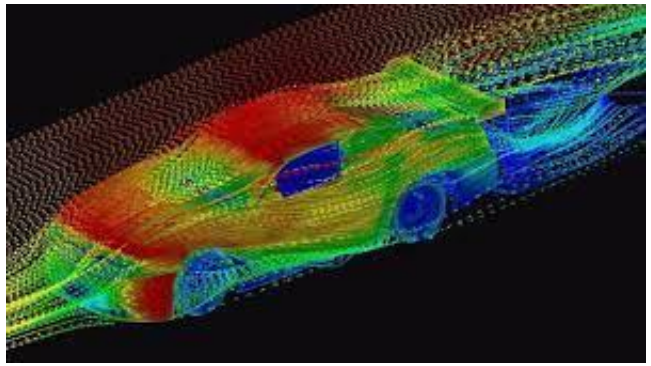
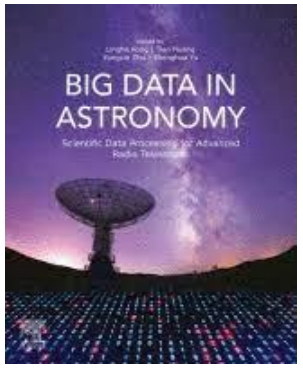
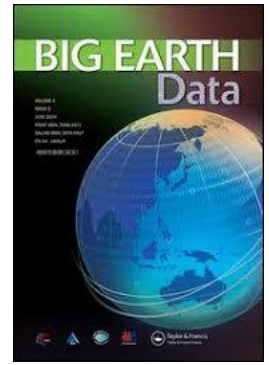
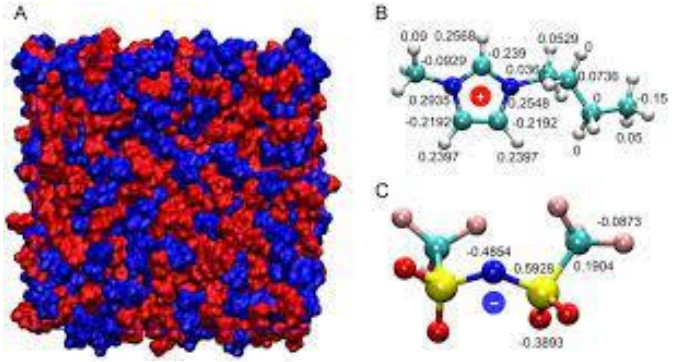
Numeric simulation, uncertain quantification to instrumental science, large scale data processing

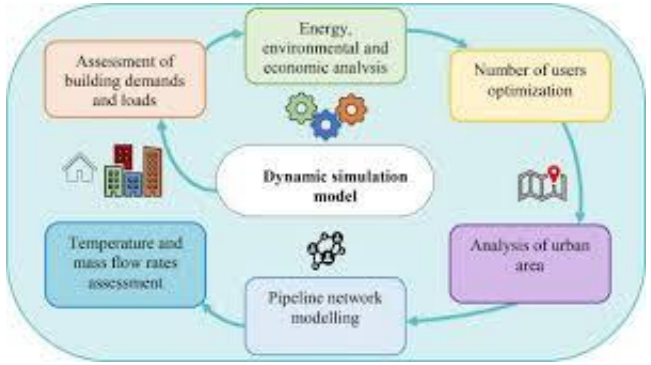


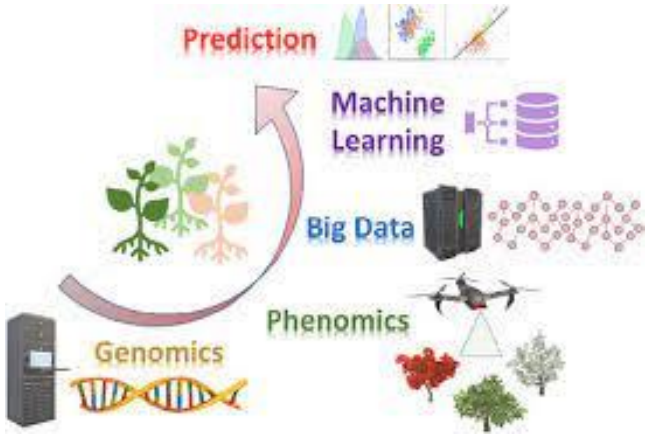










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Exascale readiness in AI, HPC and Quantum
ADAC14 Open Symposium 22 Feb 2024
International Convention Centre
Sydney, Australia
19-22 February 2024