

# Future Proofing Australia's Research Infrastructure



# Conference Theme

In keeping with the theme of the conference....

HPC Futures - Hyperscalers, Exa, AI, Quantum and Beyond

Will these be part of the the future?

In short the answer is **YES** – *HPC Futures* will be built on *Hyperscale* technology, it will need *EXA* scale compute and data resources, it will require *AI* to run and develop new scientific insights. It will need to take advantage of *Quantum* computing through continually adapting and integrating new technologies and push *Beyond* the boundaries of the current fields using HPC.

How do we know what the future will be?

How do we develop and deploy the infrastructure we need?

How to we prepare and develop our staff and researchers?

In order to understand the future you need a firm grounding on what exists so that you can build on it..



# The National Computational Infrastructure today



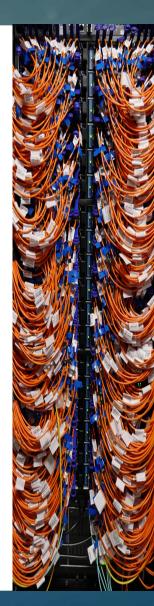
#### Mission

Provide world-class, high-performance computing and data services for Australian research and innovation

**Defining Focus: National and Strategic Capabilities** 

#### **Operational Values:**

- Make world class tier 1 compute and data capabilities easy, transparent and accessible for Australia's scientists
- Be research outcome driven
- Enable high-impact research which advances knowledge, science, technology, and informs policy
- Strategically focus on collaborations that lead to transformative outcomes with national benefits





# The NCI ...

Operates the nation's fastest supercomputer, highest-performance research cloud, fastest filesystems and largest repository of managed, high-performance research data.

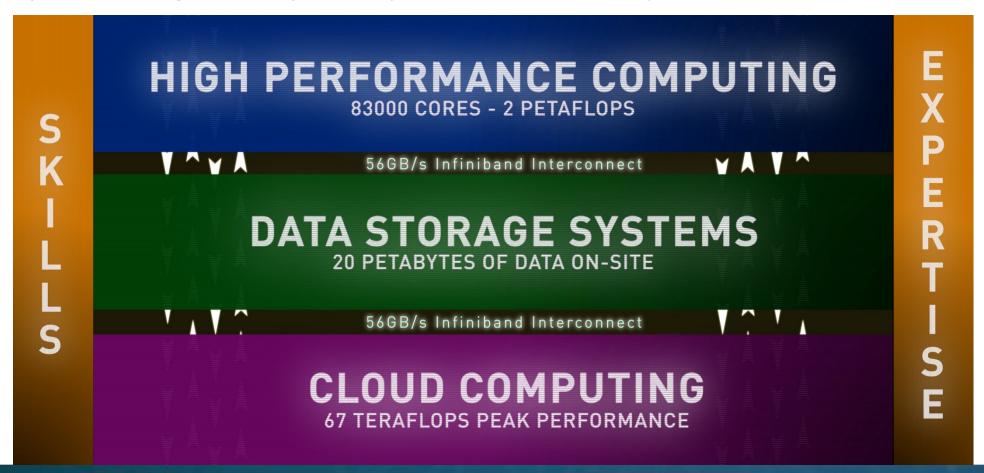
Manages this infrastructure and delivers the extensive services built on top of it with a team of ~60 staff: a unique national critical mass of expertise known internationally for their expertise.



# NCI today: Services and Technologies

NCI is Australia's most highly-integrated, high-performance compute and data e-infrastructure for research, supported by world-leading expertise.

New mode of data sharing and analysis: compute, datasets and analysis all co-located.





# NCI today: Research Engagement and Initiatives

NCI provides frictionless high-performance data services to users, enabling rapid and easy access to data analysis and visualisation solutions.

**DATA SERVICES HPC AND DATA** AND VIRTUAL INNOVATION **ENVIRONMENTS DATA VISUALISATION MANAGEMENT** 



# Supporting the gamut of scientific/technological research









#### fundamental

### strategic

## applied

## industry

- Physics
- Chemistry
- Mathematics
- Astronomy
- ARC and NHMRC Centres of Excellence

- Environmental science
- Medical research
- Geoscience
- Agriculture
- Materials science

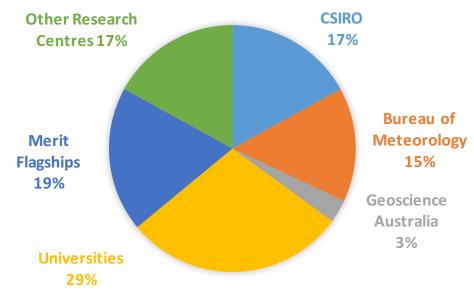
- Weather forecasting
- Extreme weather
- Disaster management/mitigation
- Victor Chang Cardiac Research Institute
- DHI: hydrological modelling

Excellence, Impact and National Benefits

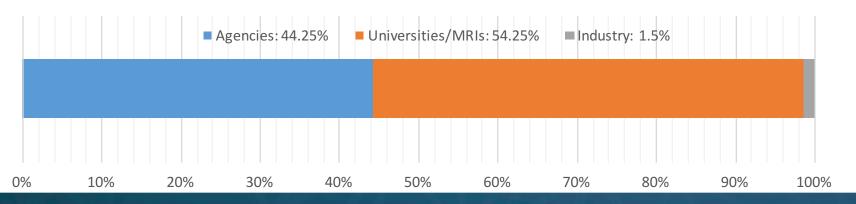


# HPC resource usage at NCI

#### Distribution by Research Organisation









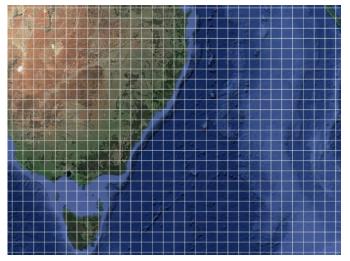


## How do we know what the future is?

## We **DON'T** but we can be prepared...







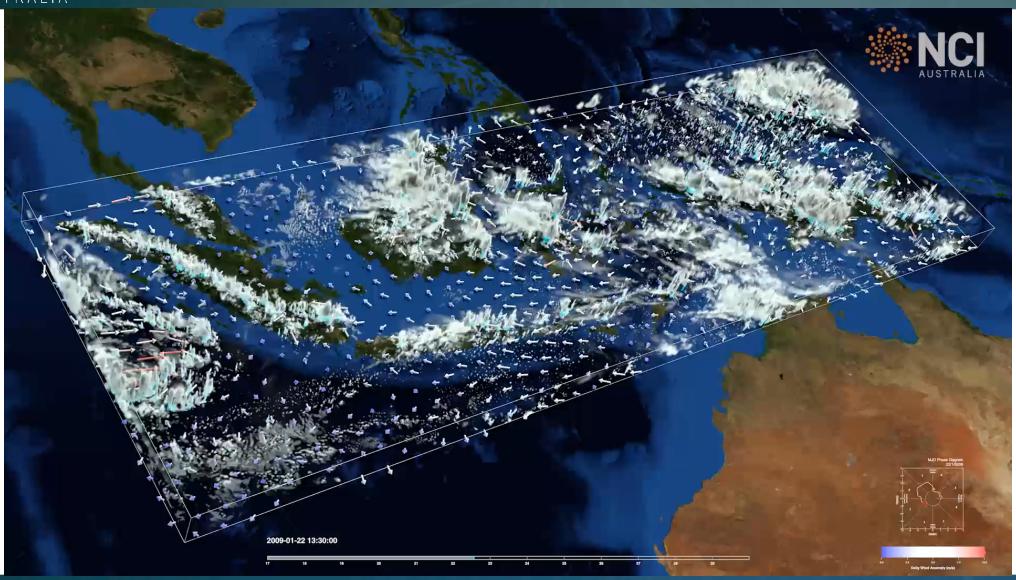


NCI is research driven and therefore needs to be:

- Adaptable
- Innovative
- Collaborative
- Support and foster expertise



# Weather patterns of the Maritime Continent





# Needs to support the data deluge with well-organized national research collections

High Performance Data (HPD): data that is carefully prepared, standardised and structured so that it can be used in Data-Intensive Science on HPC." Evans et al, ISESS, 2015.

HPC – turning compute into IO-bound problems

HPD – exploiting HPC for data analysis opportunities

#### **HPC and HPD Analysis requires**

- On-demand direct access to large curated data with fast-and-flexible data access
- Balance between processing power and ability to access data (data scaling)

#### **User Applications**

local or remote, serial or parallel, file formats

#### High-level I/O Library

**GDAL**: Geospatial Data Abstraction Library converting among many formats like GeoTIFF, NetCDF **NetCDF4**: Network Common Data Form

Simplified data abstraction, self-describing **HDF5:** Hierarchical Data Formats chunking, compression

#### I/O Middleware

MPIIO: higher level of data abstraction MPI hints

**POSIX I/O:** full and low-level control of serial I/O transfer regions of bytes

#### **Parallel File System**

Lustre: Parallel access to multiple OSTs



# How do we deploy and develop the infrastructure we need?

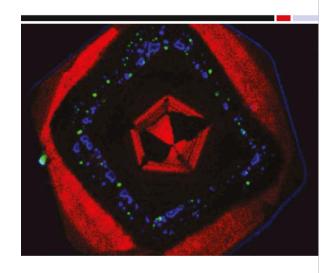




# Long term funding



2016 NATIONAL RESEARCH INFRASTRUCTURE ROADMAP



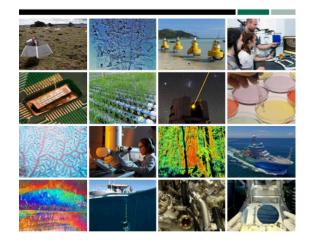
#### 2016 – Urgent case for refunding HPC

- Recommends long term funding for infrastructure
- Need for skill development
- Greater integration of service
- National HPC strategy



#### FACILITIES FOR THE FUTURE UNDERPINNING AUSTRALIA'S RESEARCH AND INNOVATION

Government Response to the 2016 National Research Infrastructure Roadmap Research Infrastructure Investment Plan





#### 2018 Capital Investment

- Long term investment \$1.9b /12yr
- 5 year contracts
- Review roadmap every 2 years

#### In the next 5 years...

- \$70M NCI renewal of HPC
- \$70M Pawsey renewal HPC
- \$72M research platforms (cloud & storage)



# Collaboration for Sustainability

Over two thirds of our funding comes from partners, who co-invest for a share of resources in return.

• The majority of our partners are publicly-funded research organisations, supporting staff and their collaborators who have requirements that can't be met by the market. We also have a few industry users, accessing resources on a fee-for-service basis.



















































# Collaboration for National Services







#### AUSTRALIAN ACCESS FEDERATION



Australian Research Data Commons



and global collaborative research. "

"The underpinning Australian eResearch infrastructure should include cloud computing, HPC, networks, access, authentication and trusted data repositories."



# International Collaboration and Development

Shared science, model evaluation and technical development:

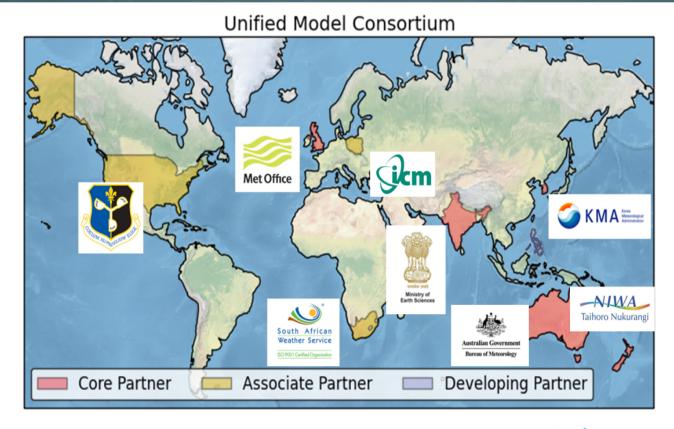
- Joint process evaluation groups
- Technical infrastructure teams
- User workshops & tutorials

A foundation for relationships with other organisations:

- Science & model development
- Weather & climate services
- Jointly growing with businesses

Operational users complemented by:

- research partners in national / international universities & organisations
- capacity building consultancy projects with other partners











# How to we prepare and develop our staff and researchers?

# Emphasis on Expertise, Skills and Education To develop a national computational sciences capability

- Aligned with peak facilities NCI and Pawsey
- Supporting national research priorities though reengineering codes
- Consultancy capability for industries and science agencies
- Supporting industry-focussed on-ramps
- Support for National Centres of Excellence
- Leadership for a vibrant undergraduate and graduate education program to skill a future workforce
- Participation in international HPC collaborations



# Conference Theme

**HPC Futures** will be built on **Hyperscale** technology, it will need **EXA**scale compute and data resources, it will require **AI** to run and develop new scientific insights. It will need to take advantage of **Quantum** computing through continually adapting and integrating new technologies and push **Beyond** the boundaries of the current fields using HPC.

This can only be achieved through **Adaptability, Innovation, Expertise, Collaboration, Collaboration, Collaboration** that is driven by **research outcomes.** 





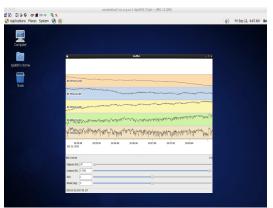




# Integrated HPC compute and data-intensive science capability

#### **Compute Intensive: batch & Interactive**





#### **Virtual Laboratories**



67970/VTOL\_VR/

**Portal** views



underwater-milwaukee-harbor-map

Machine Connected



**Data Platform** 

Fast/Deep **Data Access** 

Data **Services**  Server-side **functions** 



**Program** access



# Where are we going?

- From little things big things grow: supercomputing is no longer solely about huge monolithic calculations, but equally about Impact, Integration and (peta; exa)-scale of both the data and the compute.
- Collaborative data projects of institutional, national and global significance: making it work from the simple essentials to the complex bleeding edge.
- Enabling expertise at the interface between science, industry and large scale computing is more than ever in demand. NCI will be pivotal in providing this critical service for university, government and industry sectors as Australia's bridge to HPC/HPD.
- Win-win scenarios for collaboration between national facilties and commercial cloud. This will be all about seamless workload sharing coupled with flexible business models.



Thank You.



Questions?

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# National Research Priorities: Advanced Manufacturing

#### **Industrial catalysis using nanoparticles**

NCI facilities help research how different kinds of nanoparticles play a role in catalysing chemical reactions. This is incredibly important for industrial uses where catalysts are used in many different processes. Finding ways to produce healthy and safe catalysts is important for developing future industries.

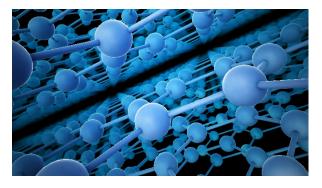
Professor Tiffany Walsh,
Deakin University

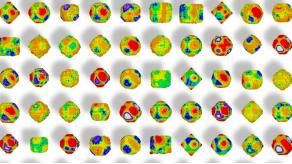


Raijin is being used to model diamond nanoparticle structures, carbon nanotubes, nanowire, and nano-textured surfaces. This has led to the development of a brain tumour treatment new optoelectronic devices, and new night-vision detectors.

Dr. Amanda Barnard, CSIRO

Professor Chennupati Jagadish, The Australian National University Dr Bjorn Sturmberg, ARC CoE for Ultrahigh-bandwidth Devices for Optical Systems



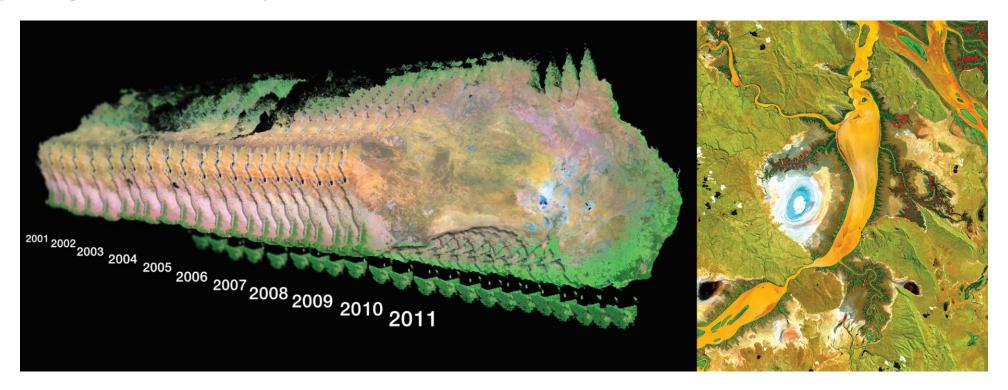






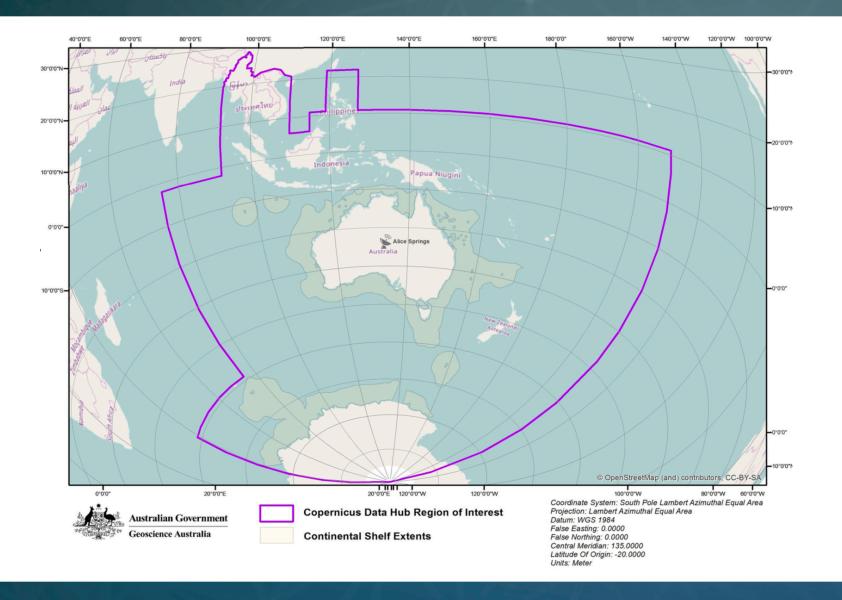
# Big Data

- Data-intensive science
  - Digital Earth Australia continental-scale earth observations from space
  - Decades of images from the US Landsat satellites
  - Daily images from EU, Japanese and US satellites are now accessible



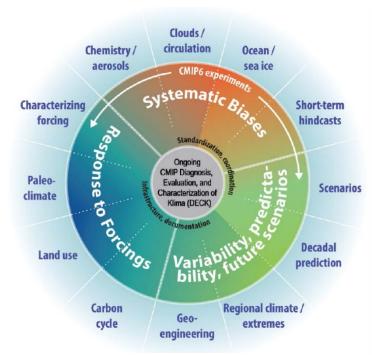


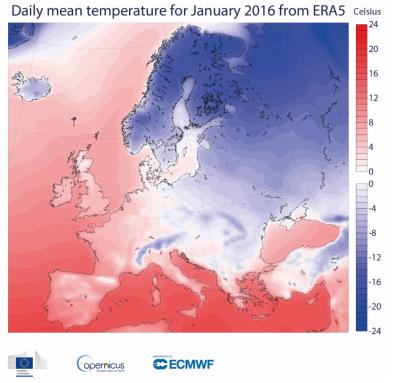
# Copernicus Hub – Region of interest





# Current large data deluges that are well-organized as national research collections







Climate & Weather model data

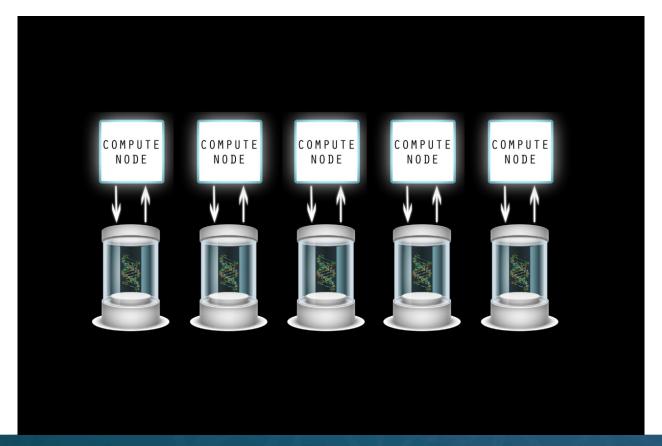
Reanalysis data

Satellite Observations



# Data-intensive science

- Genomics works with large genetic datasets that a single computer would take years to analyse
- A supercomputer can analyse many genomes simultaneously: we performed a world first alignment of 1200 human genomes overnight





# Bureau of Meteorology Re-Analysis Program:

The reanalysis over the Australian domain is provided with a resolution of approximately 12 km and extends over 70 levels up to 80 km into the atmosphere. For a small number of subdomains, the 12-km reanalysis is downscaled to a 1.5 km resolution.

