Faculty of Engineering

Changes to High Performance Computing

John Zaitseff
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UNSW – A world leader in Research Quality

UNSW will be among the leading research-intensive universities worldwide, known for innovative, pioneering research that has a global impact. Our collegiate and entrepreneurial ethos, high-quality infrastructure and flexible whole-of-career Fellowship Program will make us a magnet for the most talented researchers and research students worldwide and for partnerships with industry, international organisations, governments and other leading universities around the world.

— UNSW 2025 Strategy
HPC – A Research Quality enabler

- “High Performance Computing is a critical component in modern engineering research worldwide…”

  — Associate Professor Evatt Hawkes, ARC Future Fellow, School of Mechanical and Manufacturing Engineering and School of Photovoltaic and Renewable Energy Engineering

- “In the coming decade, theory and modelling will harness massive advances in high performance computing to enable an unprecedented acceleration in discovery and development of new materials for the energy, environment, health and IT sectors… Speed is of the essence in delivering a competitive edge…”

  — Professor Sean Smith, Director, Integrated Materials Design Centre, School of Chemical Engineering
HPC – A Research Quality enabler

Key question for you:

How can I perform my research
faster, better, smarter?
Faster, better, smarter research

Aspiration:

that UNSW will be the best university in Australia in which to carry out computationally intensive research

How?

- Modern world-class cutting-edge HPC facilities
- Access to national-scale facilities
- Dedicated local specialist HPC support including “value-add” services
- HPC training courses, clinics and drop-in sessions
Current state: Leonardi cluster

- 2944 × AMD Opteron 6174 2.2GHz and Opteron 6276 2.3GHz processors
- 8448 GB of main memory
- 917 TB of storage (5.1 TB for home, 88 TB for scratch, 800 TB for shared storage)
- 2×10Gb Ethernet network interconnect
- Provides 25.4M SU (Service Units)
- Commissioned **September 2010** to **November 2012**
Current state: Trentino cluster

- School of Mechanical and Manufacturing Engineering
- 1024 × AMD Opteron 6272 2.1GHz processors
- 2048 GB of main memory
- 30 TB of storage
- 4×1Gb Ethernet network interconnect
- Provides 8.8M SU (1 SU = 1 CPU core for one hour)
- Commissioned July 2012 to November 2012
Current state of HPC in Engineering

- **Leonardi** has been one of the key research enablers for the Faculty over its life
- Grew from a handful of users to over 300 researchers as at September 2017
- Helped produce 369 HERDC outputs to 2015 (*HPC NextGen Business Case*): three books, six book chapters, 153 peer-reviewed journal articles, 207 conference papers
- Top twenty users produced successful research outcomes involving more than $15M of external funding in 2015 alone

Key problems:

- Aging infrastructure: Leonardi, Trentino and other clusters are at end of life
- Limited physical on-premise space for a “step change” in HPC
Engineering HPC Future Committee

- Established mid-2014
- Academic representatives from each School
- Visits to other HPC facilities
- Survey of all users (June 2015)
  - 85 questions
  - 149 submissions (68%)
  - 147 pages of analytics
Engineering HPC Business Case and RFI

- Comprehensive *HPC NextGen Business Case* in September 2015
  - Total of 770 pages (68 pages including the main appendices)
  - Recommended expenditure of $6.14M to $9.29M over five years
  - On-premise solution of between 25.7M SU and 48.9M SU per year

- Thorough *Request for Information* (RFI) from November 2015 to March 2016
  - 31-page RFI sent to 21 vendors
  - Responses received from 12 vendors
  - Over 1290 pages of responses (excluding appendices)
A UNSW-wide approach

Division of Research – Research Infrastructure

- Viability paper in July 2016
- Pilot from Q4 2016 to Q3 2017
  - 21M SU procured from NCI
  - Over 110% utilisation
- Business case in July 2017
  - $23.5M over five years
  - $46.3M to 2025
  - Approved August 2017
UNSW Research Computing

- Create a new Research Computing team of 8.0 FTE
- Create a shared UNSW-wide scheme for HPC resources, mostly “as a service”
- Provide a total of at least 800M SU over five years (160M SU per year)
- Source about 550M SU (69%) from external providers including NCI
- Replace end-of-life Leonardi cluster with 35M SU capacity
- Provide 24M SU to Faculty of Science in lieu of their Katana cluster
- Transition Katana to a shared UNSW-wide on-premise facility
- Create cloud allocation schemes to leverage new platform capabilities
- Create a co-funding model for specialist shoulder systems
UNSW Research Computing team

- **Professor Grainne Moran**, Pro Vice-Chancellor, Research Infrastructure
- **Luc Betbeder-Matibet**, Director, Research Technology Services
- **Dr Joachim Mai**, HPCD Manager
- One Faculty of Engineering staff member: **John Zaitseff**
- Two Faculty of Science staff members
- One Central IT staff member (research data and cloud compute)
- **New**: Academic Level B computing role to provide additional consultation capability
- **New**: Full-time and casual HPC support roles
UNSW-wide shared scheme

- Provide a total of at least 800M SU over five years (160M SU per year)
- Shared “HPC as a service” pool of compute time, starting at 20M SU in 2018, growing to at least 60M SU in 2021, excluding other pools
- Each project (Lead Investigator plus other HPC users) requests HPC resources by submitting a short proposal
- Resources allocated by a UNSW-wide Allocation Committee
- Mid-term reallocations may be possible
- In addition to any time granted by the National Computational Merit Allocation Scheme (NCMAS) and any Engineering allocations
- ANU has a similar scheme in place for 107.7M SU (see anumas.nci.org.au)
Engineering HPC allocation

- Leonardi has reached its end of life, to be decommissioned by **December 2017**
- R1 Data Centre to be decommissioned in **January 2018**
- 35M SU to be provided to Engineering as a replacement:
  - 25M SU to replace Leonardi, 10M SU to replace Trentino and Newton
  - No reduction in research capacity
  - Internal Engineering HPC Allocations Committee
  - Flexible: does not need to be NCI!
- Migration from Leonardi to start **1st October 2017** (no new accounts from this date)
- **Recommended:** migrate to the Raijin cluster at NCI
The NCI Raijin cluster

- 84,656 Intel Xeon Sandy Bridge 2.6GHz, Broadwell 2.6GHz processor cores
- 120 NVIDIA Tesla K80 and 8 Tesla P100 GPU coprocessors
- 32 Intel Xeon Phi processors
- 309 TB of main memory
- 12.5 PB of storage
- 56Gb and 100Gb Infiniband network interconnect
Current Katana cluster

- 2160 Intel Xeon processors (various)
- 16,522 GB of main memory
- 10Gb and 1Gb Ethernet network interconnect
- Currently uses a “buy-in” scheme: ~$9k per node (16 cores, 128GB memory)
- “Trial queue” (with no buy-in) allows jobs of up to 48 cores for <12 hours
- Standard queues of <12 hours, 12–48 hours, 48–100 hours, 100–200 hours
- <100 hours on your own nodes + small pool of core nodes; <200 hours on your nodes
- To become the shared UNSW-wide on-premise facility
- Watch this space: the shared facility may end up with different rules
Rationale for UNSW-wide HPC as a service

- Quickly and effectively fulfil HPC demand
  - No lead time while a new facility is built
- Leverage peak national infrastructure and Federal Government funding
- Flexibly select multiple providers with minimal lock-in
  - Currently Raijin at NCI
  - Possibly Pawsey Supercomputing Centre, Intersect, Amazon AWS and/or other providers
- Researchers have access to current-generation HPC
  - No multi-year lock-in due to fixed hardware
## Challenges for migration

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Leonardi</th>
<th>Raijin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processor cores</td>
<td>2944</td>
<td>84,656</td>
</tr>
<tr>
<td>Number of users</td>
<td>305</td>
<td>9067</td>
</tr>
<tr>
<td>Queuing system</td>
<td>SLURM</td>
<td>Altair PBS Pro</td>
</tr>
<tr>
<td>Queue length (today)</td>
<td>26 jobs, 6 queued</td>
<td>4010 jobs, 974 queued</td>
</tr>
<tr>
<td>Queue costs</td>
<td>Not charged</td>
<td>Charged at different rates</td>
</tr>
<tr>
<td>Maximum walltime</td>
<td>72 hours or unlimited</td>
<td><strong>48 hours</strong> by default</td>
</tr>
<tr>
<td>Home directory</td>
<td>25 GB</td>
<td>2 GB by default</td>
</tr>
<tr>
<td>Scratch directory</td>
<td>Up to 88 TB (no quotas)</td>
<td>72 GB by default</td>
</tr>
<tr>
<td>Storage directory</td>
<td>Up to 12×64TB</td>
<td>On application</td>
</tr>
</tbody>
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Mitigation for the challenges

We will help you migrate!

Over the next two months:

- Create project groups and accounts for Lead Investigators and users
- Grant preliminary allocations
- Transfer or archive data files, scripts and applications
- Optimise for checkpointing and multi-core use
What you can do now

• Create an account at NCI (~10 minutes) – can be done immediately

• Create a project at NCI (~1 hour)
  - Must be done by an **academic staff member** only (but you *can* help them write the application)

• Copy or remove all data, scripts and your applications from Leonardi
  - Do **not** wait until December 2017!

• Ask us for help with any of the above
Conclusion

- Total investment of $23.5M over five years, $46.3M to 2025
- Providing a total of at least 800M SU over five years
- Leonardi decommissioned December 2017
- Replacement scheme of 35M SU starting 1st October 2017
- UNSW-wide shared pool starting at 20M SU in 2018

- John Zaitseff <J.Zaitseff@unsw.edu.au>
- Luc Betbeder-Matibet <luc@unsw.edu.au>
- Joachim Mai <Joachim.Mai@unsw.edu.au>