

WORKSHOP: How to use HPC & Cloud Clusters to enhance your research outcomes

Paul Coddington, Deputy Director eRSA 9 March 2016



Workshop Schedule

9:30 – 10:40 Introduction to eRSA and Introduction to

High Performance Computing

10:40 – 11:00 Break and refreshments

11:10 - 12:30 Using Tizard

12:30 – 1:30 Lunch break

1:30 – 3:00 Hands-on session

Unix tutorial

Running jobs on Tizard

3:00 – 4:00 Help with running your own applications on Tizard



Introduction to eRSA

- What is eResearch?
- eResearch services
- National eResearch initiatives
- Introduction to eRSA
- eRSA services



What is eRSA?

- An incorporated joint venture of the three South Australian universities.
- The point of focus in S.A. for eResearch infrastructure and support.
- The South Australian partner in national eResearch initiatives.
- A mechanism for attracting funding for shared eResearch infrastructure to SA, e.g. through ARC LIEF grants and federal eResearch infrastructure programs









The mission of eRSA is to enable discovery, innovation and collaboration by providing eResearch facilities, services, training and expertise for South Australian researchers.



eRSA

- 20 staff, 15 technical staff
- Expertise in high-performance computing, data storage, data management, cloud, software development, sysadmin, user support
- Director reports to Board of 3 uni DVCRs and independent chair
- Offices at Uni of Adelaide Thebarton campus
- Facilities in data centres at Uni of Adelaide North Terrace campus and UniSA City West



What is eResearch?

- The application of advanced Information and Communication Technologies (ICT) to research
- Usually in the context of accessing external resources (compute, data, web services, etc)
 - i.e. not being restricted by what can be done on a standalone personal computer
- Often called e-Science (e.g. in the UK)
 - but also used for the humanities, so the Australian government uses the term eResearch
- Has grown out of a number of advances in distributed computing, digital data repositories, web applications, grid/cloud computing, high-speed networks, etc



Why eResearch?

- We are in the digital information age
 - computers are changing almost all aspects of society, including how research is done
- New electronics technologies and digitization of information have led to a "data deluge"
 - many instruments can now generate TBytes/day
- Research is increasingly collaborative, across disciplines and geographic locations
 - increasing need for remote communication and data sharing, enabled by high-speed networks, the Internet and the web
- Computational science and simulation
 - third paradigm augmenting theory and experiment



eResearch Services

- Research collaboration tools
- Videocollaboration
- Data storage
- Data management and sharing
- High-performance computing
- Cloud computing
- Web applications
- Visualization



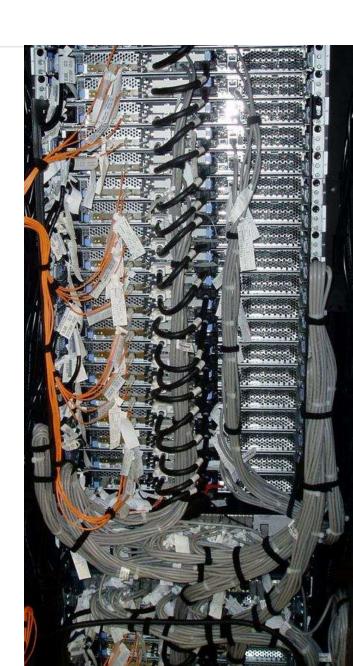
Data Management and Sharing

- Management and sharing of research data is currently often rather ad-hoc
 - Data stored on researchers' PCs, CDs, DVDs
 - Sharing via email, DVD, hard disk, etc
- This works up to a point, but is not scalable
- Can't guarantee data will be accessible or understandable longterm, e.g. if researchers or students leave
- Want sustainable data repositories
 - data online, easily discoverable and accessible, backed-up, with associated metadata
- International and national moves to require that data from publicly-funded research be made publicly available



High-Performance Computing

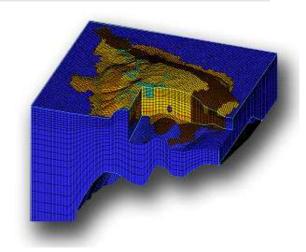
- Supercomputers provide hundreds or thousands of times more compute power and memory than a PC
- HPC enables much faster data processing, analysis, simulation and modelling
- Also enables researchers to tackle larger, more complex problems than could otherwise be done
- Has been used for many years in physics, chemistry, engineering
- Recently much broader usage, e.g. molecular biology, analysis of large data sets in many fields

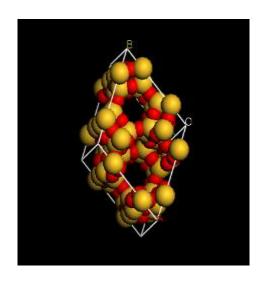




Visualization

- It is often difficult for humans to extract information from large data sets without having some visual representation of the data
- Visualization tools can help a researcher (or a group of researchers) understand their data, and explain their results to others in a convincing and engaging way
- Stereoscopic visualizations of 3D objects can help understand them, e.g. molecular structure and function of proteins, building design







National eResearch Initiatives

- Australian National Data Service (ANDS)
 - Processes and tools for managing data, especially the creation of searchable metadata
- Research Data Storage Infrastructure (RDSI) and Research Data Services (RDS)
 - Storage and services for research data
- National eResearch Collaboration Tools and Resources (NeCTAR)
 - Research cloud infrastructure and tools
- National Computational Infrastructure (NCI)
 - National supercomputing facilities



eRSA and National Initiatives

- eRSA is involved in these national initiatives, usually as the SA partner
- SA member of AeRO (Australian eResearch Organisations)
- Involved in several ANDS projects
- SA node of RDSI
 - Multi-Pbyte storage facility
- SA node of NeCTAR Australian Research Cloud
 - 3000 core node of 30,000 core national cloud



eRSA Services

- Large-scale data storage facilities
- Data sharing and data repositories
- High-performance computing facilities
- Hosting of dedicated compute facilities
- Cloud computing and virtual machines
- eResearch expertise and consulting
- Helpdesk, user support and training
- Software development
- Development and/or hosting of web applications
- Visualization services



How much does it cost?

Nothing!*

★ Some conditions apply ...



Funding

- Main funding for eRSA comes from:
 - The three S.A. universities
 - S.A. Government
 - National eResearch funding schemes (RDSI, RDS, NeCTAR, ANDS, etc)
 - ARC Linkage Infrastructure, Equipment and Facilities (LIEF) grants for facilities
- eRSA also does contract work, e.g. development of software and services, consultancies, etc for university researchers and external organizations



Fees

- This funding enables eRSA to provide most of its basic services at no cost to researchers from the 3 SA universities or their collaborators
- Services that are not free are usually at low cost for uni researchers. This includes:
 - Dedicated compute nodes or facilities
 - Software or database development
 - Significant ongoing dedicated support effort



Data Storage and Management

- eRSA services allow researchers to:
 - store your data using reliable, professionally-maintained storage systems
 - access the data easily from the desktop or the web
 - back-up large amounts of data
 - integrate your data with related national or international data repositories
 - publish your data so it can be easily discovered and accessed
 - enable data sharing across distributed locations
 - simplify the data archiving process



Data Storage and Management

- Recently significant increased eRSA storage and backup capacity through RDSI project
 - 3 Petabytes disk storage
 - 1.5 Petabytes Tape silo
 - Extensible as needed
 - Accessible from HPC systems
 - Internet access for sharing
- Standard mechanisms for data access from PC
 - sftp, scp, rsync, http
 - Other mechanisms for simpler access in train





Cloud computing

- Cloud provides on-demand virtual machines
- Faster and easier to provision and manage than your own physical server
- Nectar Australian Research Cloud provides cloud infrastructure for research
 - Similar to Amazon, Microsoft, Google, etc clouds
 - 3000 cores in SA, almost 30,000 nationally
- Virtual servers to run web sites, applications, databases, compute jobs, etc.
- Large, on-demand, elastic compute resource



HPC Facilities at eRSA

- Great success in procuring world-class HPC for SA
 - 1999 Perseus largest cluster in Australia
 - 2000 Orion #1 in Australia
 - 2003 Hydra #2 in Australia
 - 2004 Aquila large shared memory
 - 2007 Corvus #2 in Australia
 - 2012 Tizard
- Supported several hundred users in the past 10 years
- Over 100 active users every quarter





HPC Users and Applications

- Computational physics
- Computational chemistry, e.g. molecular structure
- Life sciences, e.g. genomics, proteomics, phylogenetics
- Computational Fluid Dynamics
- Geology and Geophysics, e.g. seismic analysis
- Materials science
- Petroleum engineering
- Electrical and mechanical engineering
- Optimization problems
- Computer science, e.g. parallel algorithm development
- Economics
- And many others…





Software development

- eRSA has a software development team
- Specialise in developing custom eResearch services or service integration, web application development, web databases
- Provide an existing, experienced team for research software development



Getting Started

- Talk to us about your eResearch requirements and how we can help you.
- Check the information on our website www.ersa.edu.au
- Contact our service desk <u>servicedesk@ersa.edu.au</u> and the appropriate person will contact you to discuss your requirements
- Talk to the Deputy Director, Paul Coddington paul.Coddington@ersa.edu.au
- Fill in a account request form on our website





Upcoming workshops

How to use HPC and Cloud Clusters to enhance your research outcomes

9 March, University of Adelaide

R-Studio in the Cloud

15 April, University of Adelaide

Talk to us after the workshop to register