

SMP Computing Workshop



*Dr. Michael Bromley – School of Maths/Physics
O-week Semester 2 - 2018*

Cluster Example

- Use windows Remote Desktop Protocol to log in
- Run command

```
srun --cpus-per-task=1 --time=0-2:00 --mem=12G  
--x11 --pty mathematica
```

Overview

- UQ ITS/SMP Desktop Systems and Support
- National Facilities
- UQ / QCIF / RCC systems
- SMP core computing facility
<http://research.smp.uq.edu.au/computing/> for howto

About Me – Senior Lecturer

- BSc – Physics, Computer Science, Maths (N.T.U.) - 1995
- NT Govt – traineeship in Unix Software/Database (Sun/Mosaic/Sybase/perl)
- Graduate traineeship - Local/Wide Area Cisco Networking
- Ph.D. in computational/theoretical physics (N.T.U.)
Large scale (sparse) eigenproblems on DEC Workstations
- Postdoc - MPI calcs at SAPAC (#106 at time)
- Faculty at San Diego State University (USA)
-> NSF grant to setup rack cluster there
- Future Fellowship on Atomic Physics via HPC → non-linear PDEs / eigenproblems
- Teach PHYS3071 / PHYS4070 / COSC3500



ITS – Centralised Support

- Rose Radloff – Relationship Manager (Faculty of Science)
 - Karl Blakeney - IT Service Delivery Manager (west team)
 - ITS local technical/computer support is
 - Physics - Sam Zammit, Frank Audsley, Room 6-306
 - Maths - Nalini Gowda, Room 67-340
 - → consultation times Tue/Thu between 2pm-3pm
 - Phone 07 336 56000 → ITS helpdesk: to log urgent job,
 - <https://its.uq.edu.au/> → ITS helpdesk: login to log job
- OR email help@its.uq.edu.au include in the email:
with “Attention Sam @ Physics” or “Nalini @ Maths”

ITS – Research Infrastructure

- former Faculty of Science IT Staff
- Dr. Leslie Elliott
Infrastructure Support Specialist, Research Infrastructure
- Ian Mortimer
Systems Administrator, Research Infrastructure

ITS notices...

- Office 365 Mail - <https://its.uq.edu.au/projects/office-365>
Cloud Migration for Outlook/email. (Office 2016 desktop)
- SMP almost complete; public folders still to be transferred
- 1 TB One drive was enabled for each staff member when their email account was migrated to the cloud. Guides <https://its.uq.edu.au/services-and-guides/software-and-online-tools/software/microsoft-software/onedrive-personal-file-storage/onedrive-online>
- Mirroring360 works - <https://its.uq.edu.au/mirroring360>
- ZOOM - <https://its.uq.edu.au/zoom>
- In UniFi eMarket <https://its.uq.edu.au/purchasing>

Desktop systems and support

- ITS prefers Windows PCs for homogenised support.
- SMP prefers Windows PCs to keep costs down but tries to support the provision of MacOS/linux OS desktops.
- PhD/MPhil get a desktop (MSc/Honours/B.Adv.Sci maybe)
- SMP operates a pool of laptops/laser pointers etc for borrowing: see Physics or Maths admin for more info.
- Extra software Windows, look for “Software Center”
Extra software macOS, look for “Self Service”
- Other applications can be added to the above software portals (licensing allowable) with a request to ITS...
SMP Mathematica/Origin/Minitab/Maple/Labview/ComSol
- [BYO Laptop – Log a ITS job for advice- minimal support]

Printers/Scanners - SMP

- Send to (also photocopying and scan-to-email)

`\\uq-print01.soe.uq.edu.au\smp-ricoh`

(colour printers - ~\$1 per 10 pages)

- Username as UQ\username e.g UQ\s7654321
- Log a job ITS - to get allocated to printer group
- other physics printers are

`\\uq-print02.soe.uq.edu.au\smp-06-320-p1`

`\\uq-print02.soe.uq.edu.au\smp-06-320-p2`

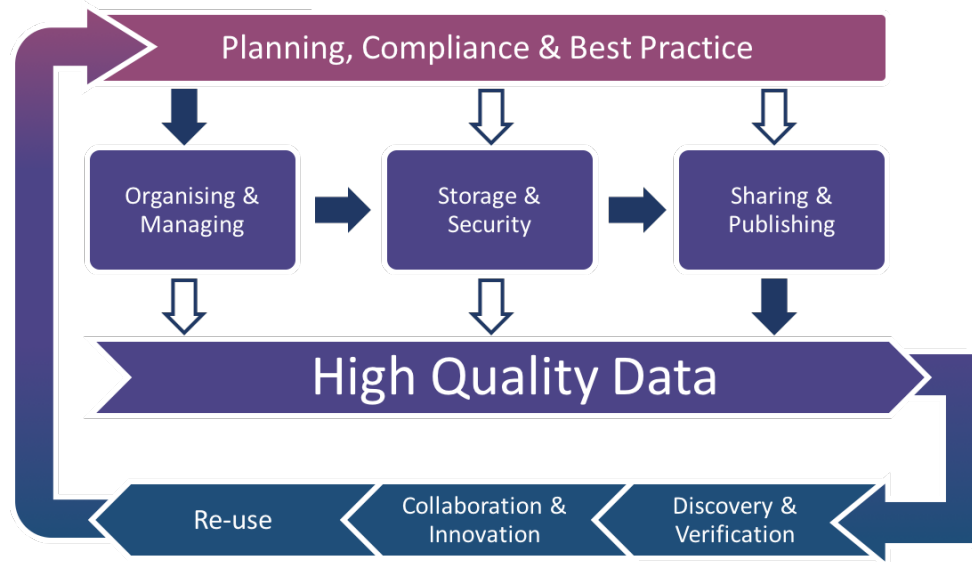
`\\uq-print02.soe.uq.edu.au\smp-06-404-p1`

UQ and SMP Data Storage

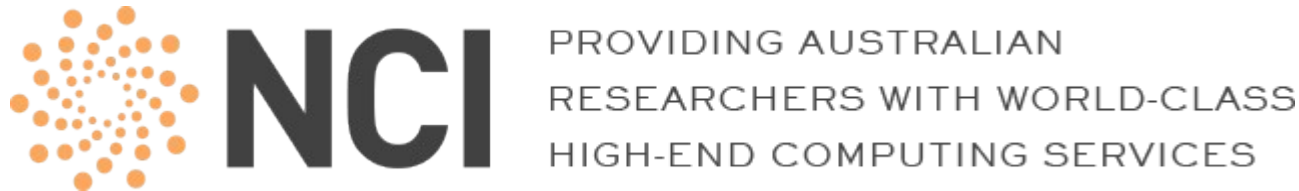
- Data storage and security is important!
- `nas02.storage.uq.edu.au` used for windows (10GB staff)
H: drive for homes, S: Operations SCI\SMP, Y:\ SCI
- `nas05.storage.uq.edu.au` has `smp-comp0x /home` dirs mounted, SMP's linux desktops, also I:\ drive
- SMP has 2 NAS (Network Attached storage) systems:
- `smp-data01.smp.uq.edu.au` (11TB+) which is used for projects and also `/scratch` storage for `smp-comp0x` (talk to supervisor for access)
- `smp-data02.smp.uq.edu.au` which is also on `smp-comp0x`
- Have warranty on SMP systems – 2019+
- Use <https://cloudstor.aarnet.edu.au/> ... 100GB quota

Data – coming soon

- SMP has bought 50TB for new ‘getafix’ cluster
- RCC has MeDiCI <https://rcc.uq.edu.au/data-storage>
- UQ Research Data Manager is coming to SMP
<https://guides.library.uq.edu.au/research-data-management>
- Uses nextcloud system for sharing



National Facilities



- ARC funded collaboration between ANU/CSIRO/BOM
- <http://nci.org.au/>
- National Computational Infrastructure: various systems:
- large-scale peak system, Raijin (a Fujitsu Primergy cluster, entered production in June 2013)
- small specialised system, Fujin (a Fujitsu PrimeHPC FX10 system, commissioned in March 2013).
- And quite a few other systems (has special software)
- SMP staff successful grants/time (eg. ask Ben Powell)

UQ / QCIF / RCC

- UQ Research Computing Centre under DVCR
- <http://www.rcc.uq.edu.au/>
- Operates various systems including for QCIF - The Queensland Cyber Infrastructure Foundation
- QRIScloud - The Queensland Node of NeCTAR / RDSI
- FlashLite - 68 nodes @ 512GB + 56Gbps and ScaleMP
- Tinaroo – 244 nodes @ 128GB (6000 cores, 5 racks!)
- Awoonga – 40 nodes @ 256GB (1032 cores)
- NEW GPU cluster 'wiener' - 40 x NVIDIA Tesla V100 (Ian McCulloch has bought 3 nodes)



<https://rcc.uq.edu.au/article/2018/02/call-gpu-accelerated-imaging-researchers-use-hpc-wiener>

smp-comp0x machines

- smp-comp01 / smp-comp02 / smp-comp03 / eg. smp-comp04.smp.uq.edu.au compute (blade) servers...
2 x Intel X5690 6-core 3.47 GHz (2011) 96 GB RAM
Runs CentOS6/CentOS6/Ubuntu14.04.2LTS/windows
well out of warranty
- smp-comp05 (CentOS6) / smp-comp06 (Ubuntu 14.04.2)
2 x Intel E5-2667 6-core 2.90 GHz (2012) 256GB RAM
are just **out of warranty** but to be added to new cluster
- smp-ts01.smp.uq.edu.au - Windows Remote Desktop
- Also there is a dedicate server for virtual machines, eg. smp-teaching.smp.uq.edu.au for PHYS3071/PHYS4070

Getafix migrations – Stage 1

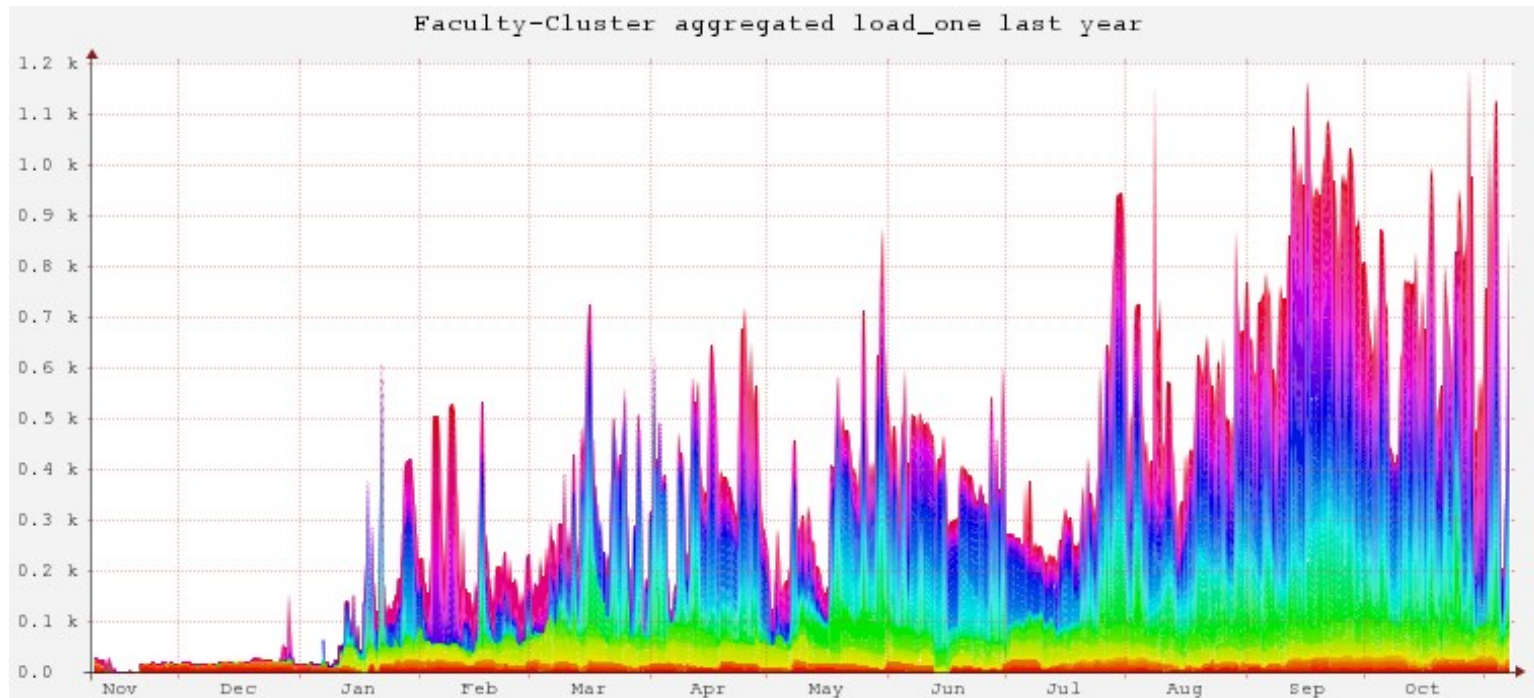
After Friday 3rd August:

- Shutdown smp-comp03, smp-comp04 compute machines
- Shutdown/relocate smp-comp05 and smp-comp06 to Prentice Data Centre
- (to act as extra login nodes for the new cluster getafix)
- Any concerns / mission critical usage please notify me

- can now apply for an account and move to getafix.smp.uq.edu.au which is running CentOS 7.

SMP Clusters – dogmatix 2017

- Main dogmatix system has over 1200 cores
- System Usage has been constantly increasing over 2017
- <http://faculty-cluster.soe.uq.edu.au/ganglia/>



SMP Clusters – dogmatix/ghost

- Holger Baumgardt's Future Fellowship GPU Clusters
- Purchase starting in 2010 \$117K ex-GST
- One whole Rack... Xenon Nitro T5 with **34 Tesla GPUs**
- 10 nodes 4U... 120 cores Intel X5650 @ 2.66GHz (2010)
- 7 nodes have 4 x Nvidia Tesla C1060
- 3 nodes have 2 x Nvidia Tesla C1060

- Moved into ITS data centre
- out of warranty but added to dogmatix queing system as:
ghost[0-9]

SMP Clusters– dogmatix/asterix

- asterix or 'smp-gpu01', purchased 2011, \$193K ex-GST
- bought with UQ Major Equipment and Infrastructure Grant inc. \$70K matching Science/SMP funds (PIs included Anthony Roberts, Matthew Davis, etc).
- One whole Rack... Xenon Nitro T5 with **40 GPUs**
- 15 nodes .. 120 cores Intel X5650 @ 2.40GHz (2010)
- Total of 10 x Nvidia Tesla C2070 (max 2 / node)
- Total of 30 x Nvidia Tesla C2050 (max 4 / node)
- Physically located in Parnell server room
- is also now added to dogmatix queuing system as a-0-[1,3], a-1-1, a-2-[0,2-4], a-3-1

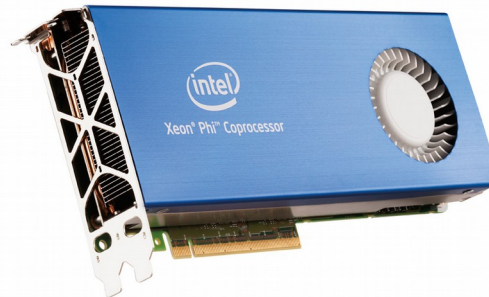
SMP Clusters – dogmatix/obelix

- Dell PowerEdge C6220 (with 35 nodes) each node 2 x Intel E5-2660 8-core 2.2GHz (2012) 196GB RAM
- Now part of dogmatix as smp-0-[0-35]
- 8 C8220X compute nodes each can fit two compute cards:
- 6 x NVIDIA Tesla K20 GPU each with 1 Kepler GK110
2496 CUDA cores - 1.17 Tflops, 5GB GDDR5 RAM
225 Watts



SMP Clusters – dogmatix/obelix

- Cluster 11 x Intel Xeon Phi coprocessor 7120P
- Intel Many Integrated Core Architecture or Intel MIC
- x86-compatible multiprocessor architecture OpenMP, OpenCL, Cilk/Cilk Plus and Intel's Fortran, C++, MKL each with 61 cores at 1.238 GHz, 16GB RAM, 300 Watts



SMP Clusters – dogmatix 2015

- With 3 more Dell C8220 servers (warranty until Oct 2018)
- 13 x Dell FC430 Blade servers (smp-9-[0-12]) (until 2020)
all with 256GB RAM
- virtualisation of the login node with redundant front-end
- Upgraded to slurm queuing system to handle GPUs/Phi's
- Used in COSC3500 High-performance computing and
PHYS4070 Advanced Computational Physics.
- frankenstein model has worked, eg. also has 2 SAFS
(School of Agriculture & Food Science) nodes with 1.5TB
of RAM that is available to SMP if not being used.

SMP Clusters – getafix 2018

- getafix.smp.uq.edu.au is coming shortly...
- disk storage (2 x 50TB) consolidate existing /data* (\$25K) slower 7.5K RPM disks than existing but RAID enabled
- 1 new FX2 Chassis (fits 8 blades)
- 2 new FC430 Blades with 512GB RAM (SMP \$32K)
- 4 new FC430 Blades with 512GB RAM (Powell/Jacko \$)
- Upgrade to Rocks7 (Rocks Cluster Distribution) ie. CentOS7 with new gcc compiler, **latest LaTeX etc**
- Disks with ZFS (enables snapshots)
- Network packets MTU=9000 to Jumbo (up from 1500)
- New front-end/hardware/disks then migrate data over
- Connect to RCC - MeDiCI (Metropolitan Data Caching)?

Getafix migrations – Stage 2

- September mid-Semester break (expect downtime):
- migration of most dogmatix nodes to new getafix
- snapshots of various home areas (and web content) to alternate storage - put in place for 60 days
- Initial copy of home data for SMP staff into new getafix file server off nas05 data server
- target to switch I:\ drive and cluster mapping to new getafix file server
- the old GPU clusters (ghost/asterix) will not be migrated to getafix but home and data areas will be adjusted
- dogmatix homes mounted read only on getafix to allow people to copy required data to new getafix home area

Other Comments - AWS

- Why not use amazon AWS? <https://aws.amazon.com/>
- Given that there is a university support programme <https://aws.amazon.com/education/awseducate/>
- 1. Cost - since dogmatix is running at >50% utilisation, the price-point of AWS is probably above what we spend (esp. dogmatix with good priced network/specs/etc)
- 2. Mostly used by our **undergrads/honours/PhD** students
- 3. issues with AWS charging post-usage – difficult to track
- 4. issues with \$\$\$ accounting back to UQ divisions
- 5. issues with cost/amount of data bandwidth to/from AWS
- Suggest people to use test accounts to see if system works for them... (**free** for 12 months per email address).