SMP Computing Workshop

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O-week  Semester 1 - 2019
Cluster Example

• Use windows Remote Desktop Protocol RDP to log into getafix.smp.uq.edu.au

• Then start a Terminal and type in 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 6-306
- → 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 – Cloud Migration  
  https://outlook.office365.com/owa/uq.edu.au

• Mirroring360 works -  https://its.uq.edu.au/mirroring360

• ZOOM -  https://its.uq.edu.au/zoom domain uqz

• 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 we try!)
• 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\smppricoh
  (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
Data Storage

- Data storage and security is important!
UQ and SMP Data Storage

- **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 (talk to supervisor for access)
  - **smp-data02.smp.uq.edu.au** – not sure...
- Have warranty on SMP systems – 2019+
- New 50TB for ‘getafix’ cluster
- Other networked storage systems on clusters
Data – remote access

• I use https://cloudstor.aarnet.edu.au/ ... 1 TB quota... install via software centre (uses Owncloud platform)
• RCC has MeDiCI https://rcc.uq.edu.au/data-storage
• UQ Research Data Manager has been rolled out https://guides.library.uq.edu.au/research-data-management
  Uses Nextcloud platform system for sharing
  Has 1TB quota for each research project... supervisor sets up and students can access
• 1 TB Microsoft One drive for each staff member: https://its.uq.edu.au/services-and-guides/software-and-online-tools/software/microsoft-software/onedrive-personal-file-storage/onedrive-online
• Not sure of Cloudstor / One drive quotas for students
National Facilities

• ARC funded collaboration between ANU/CSIRO/BOM
• 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/](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)
- GPU cluster ‘wiener’ - 40 x NVIDIA Tesla V100 (Ian McCulloch has bought 3 nodes). Upgrade in 2019

smp-comp0x machines

- smp-comp01 / smp-comp02 / smp-comp03 / eg. smp-comp04.smp.uq.edu.au compute (blade) servers… now decommissioned
- smp-comp05 (CentOS6) / smp-comp06 (Ubuntu 14.04.2) 2 x Intel E5-2667 6-core 2.90 GHz (2012) 256GB RAM are **out of warranty** but about to be added to getafix

- 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
SMP Clusters- getafix/dogmatix

- getafix/dogmatix systems have over 2000 cores
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 nodes, 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

• 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

- 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

- + 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

• getafix.smp.uq.edu.au is available
• Upgraded to Rocks7 (Rocks Cluster Distribution) ie. CentOS7 with new gcc compiler, latest LaTeX etc
• 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 $)
• Disks with ZFS (enables snapshots)
• Network packets MTU=9000 to Jumbo (up from 1500)
• New front-end/hardware/disks then migrate data over
SMP Clusters – getafix

- **getafix** had a couple of additions late 2018
- Another 50TB
- New Nodes with Extra Intel Xeon Gold class with 512GB
- And 3 nodes with 3 x Nvidia V100 GPU's on each node. Each GPU has 32GB RAM. They are on smp-8-[0-2]
- To see specs of various Nvidia do:
  
srun --cpus-per-task=1 --mem=4GB --nodelist=smp-8-0 --pty bash lspci -v

- To load gcc and cuda you need to load a module:
  
  module avail
  module load ...
  qsub -partition=gpu --constraint=V100 --gres=gpu:1 <script>
Final 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).