The WTCHG Research Computing Core

Talk 1: What is the ResComp Core?

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A series of introductory talks…

A set of six talks of about 45 minutes each (plus questions)

- Talk 1: What is the ResComp Core?
  (Mon 23/1 10:00 Room B; Robert Esnouf)
- Talk 2: A basic introduction to Linux
  (Wed 25/1 10:00 Room B; Robert Esnouf)
- Talk 3: Submitting jobs to the cluster
  (Thu 26/1 10:00 Room B; Robert Esnouf)
- Talk 4: Monitoring and troubleshooting
  (Mon 30/1 11:00 Room B; Robert Esnouf)
- Talk 5: ResComp centrally-managed applications
  (Wed 1/2 10:00 Room B; Jon Diprose)
- Talk 6: Doing your own thing (compiling and customizing)
  (Thu 2/2 10:00 Room B; Jon Diprose)

Overview of this talk…

- Why is there a ResComp Core?
- The IT and ResComp Cores
- High-performance, normal and "archive" storage
- Networks
- Clusters and project servers
- Topology of the ResComp hardware
- System administration within ResComp
- How big is the ResComp Core?
- Getting access to the ResComp facilities

Computing in the WTCHG

The Human Genetics department was founded in 1994

- WTCHG opens 1999, STRUBI founded
- Core funding renewed for 5 years from Dec 2016

- Relatively little computing – mostly in STRUBI
- In 1999 STRUBI had 360GB disk space in total!
- Steady growth of genetics computing until 2007…

What happened in 2007 …

NGS

… and then in 2014 …

CRYO-EM

Oxford Particle Imaging Centre (OPIC)

- An EM facility unique in Europe
  - Biosafety containment suite (ACDP3/DEFRA4)
  - FEI Tecnai Polara EM with Gatan K2 detector
  - Can be accessed by UK researchers (25% eBIC)
- Second EM in normal containment
- 400fps movies "flattened" to images (>1 TB/day)
- At least 2.2Å resolution

… and beginning in 2016 …

LONG READ SEQUENCING

Long-read sequencing technologies

- ONT MinION

Minion

MinION

- ONT PromethION

- Other systems (PacBio)

… and new for 2017 …

Why is there a ResComp Core?

We now support specialist computing for genomics, statistical genetics and electron microscopy

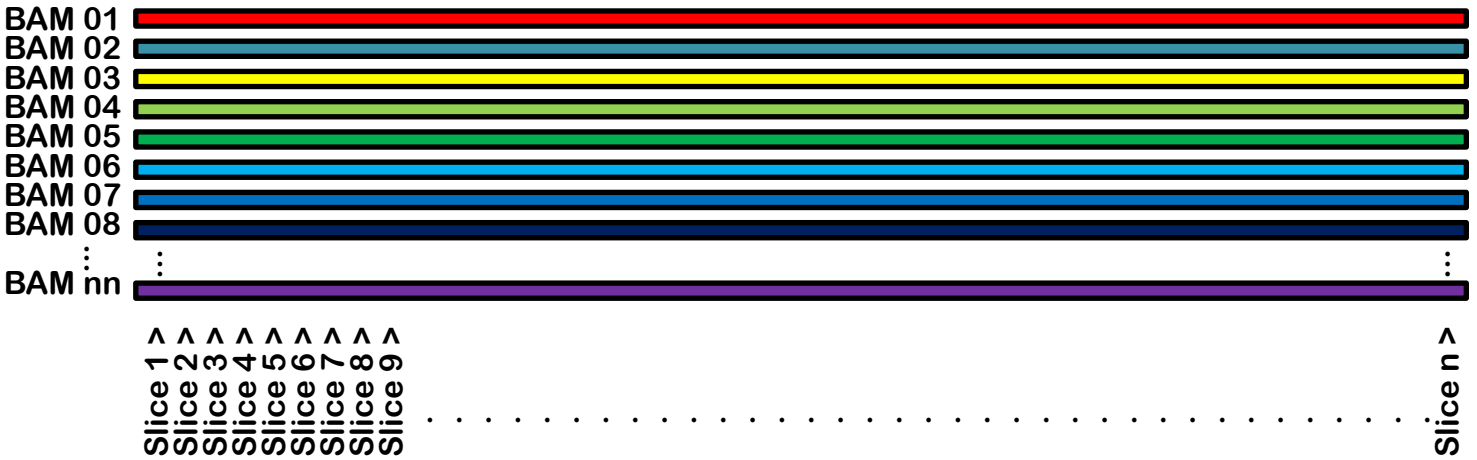
We cope with large volumes of unstructured data (e.g. 1000 30x genomes at 30GB each = 30TB in a single data set)

- 10's of genomes can be analysed on a workstation
- 100's of genomes can be analysed on a server
- 1000's of genomes need a cluster and specialist hardware

Bioinformaticists and structural biologists are not specially trained in high-performance computing (HPC) – they just want to get jobs done!

A common genetics workflow…

- Embarrassingly parallel serial computing (*e.g.* 1000s of jobs sliced up by chromosome position)
- Need large memory to hold computation (≥8GB/core)
- Need to read data sets repeatedly – large, fast storage
- Very little parallel computing, e.g. MPI work (except electron microscopy!)



Genetics is high-performance computing

Researchers always want to run on bigger data sets, but...

- Applications often do not scale well
- Repeatedly read the same data
- Hold all files open all the time or storm of open/close operations
- Memory requirements explode
- Read data in tiny chunks
- Written inefficiently using ageing methods and libraries

Many genetics jobs scale up to be truly HPC challenges stretching the limits of:

- Hard disk drives (typically per drive: 8TB, 120MB/s, 50 IOPS)
- Ethernet networking (1Gb/s = 10TB/day)
- Workstation memory (~32GB, *i.e.* just one compressed 30x genome)
- System stability for long-running jobs

Explosive growth in need for compute…

Late 2008: First cluster (CLUSTER1; 1152 cores; 36TB storage)

Early 2009: sequencing cluster (CLUSTER2; 120 cores; 96TB)

Dec 2009: ResComp Core created

Nov 2010: First centralized storage (Ibrix; 540TB)

Nov 2011: General access cluster (CLUSTER3; 672 cores)

Apr 2012: CLUSTER3 expanded to 912 cores

Jan 2013: Ibrix replaced with GPFS1 (1200TB)

July 2013: Jon Diprose joins ResComp

Dec 2013: GPFS1 expanded (1770TB)

Apr 2014: Current ResComp cluster, C nodes (1440 cores)

Jun 2014: Colin Freeman joins ResComp (20% full-time)

Sep 2014: Extra C nodes for EM work (now 1728 cores)

Feb 2015: First archive storage added (228TB – now 1824TB)

Sep 2015: GPFS2 installed (2460TB)

Jun 2016: Sequencing cluster replaced by D nodes (768 cores)

Then and now…

The IT and the ResComp Cores

WTCHG IT Core (support@well.ox.ac.uk)

- Tim Bardsley, Mark Gibbons and Ruth Porter
- Desktops, laptops, tablets, smartphones and other devices
- Diverse networking (LAN and WiFi) with many security challenges
- Basic services including email, calendaring, booking...

STRUBI IT Support (support@strubi.ox.ac.uk)

- Jun Dong and Callum Smith
- All the above for STRUBI: everything on STRUBI LAN
- Low throughput, high diversity

ResComp Core (rescomp@well.ox.ac.uk)

- Robert Esnouf, Jon Diprose and Colin Freeman
- Project servers and clusters: things in the cluster room!
- High-capacity and high-performance storage
- High throughput, low diversity

Types of storage in ResComp

Genetics is a "big data" science: lots of unstructured data

- The ResComp Core manages more data than most of the rest of the University combined (>1800 data disks, >8.2PB storage)

High-performance storage (GPFS)

- /gpfs0 (6.7 usable TB "RAID10"): /users, /apps, /mgmt
- /gpfs1 (1291 TB "RAID60") & /gpfs2 (1784TB "RAID60"): /well
- /well is charged at £35 per usable TB per 6 months

Normal project server & sequencing storage

- Sequencing machine storage pools (7x 37.3 TB RAID6)
- Project server local storage (e.g. 37.3 TB or 55.9TB RAID6)

Archive grade storage

- Currently three machines (arc1, arc2 & arc3)
- /arc[1-3][a-f] (894 TB RAID6); /arc3g (523TB RAID6)
- Archive space charged at £14.16 per usable TB per 6 months

High-performance GPFS storage

/gpfs0: DDN EF3015

- 24x 600GB disks in RAID10 at about 400MB/s
- /users/<*project*>: restricted by fileset quotas
- /apps, /mgmt: no user write permission

/gpfs1: DDN SFA12K-20

- 590x 3TB SATA HDDs in 10-disk RAID6 sets
- 10x 800GB SSDs in RAID1 sets (copies=2) for meta-data
- About 8.5GB/s in fully fault-tolerant configuration

/gpfs2: DDN SFA12KXE-20

- 410x 6TB SAS HDDs in 10-disk RAID6 sets (space for 830x disks)
- 10x 1.6TB SSDs in RAID1 sets (copies=2) for meta-data
- About 12GB/s in fully fault-tolerant configuration

/well/<*project*>: on either /gpfs1 or /gpfs2

- Restricted by fileset quotas

GPFS0, GPFS1 & GPFS2 (/well) storage

Visibility of GPFS storage

The GPFS systems are the primary storage for ResComp

It is mounted as a local file system on all cluster nodes

- Daemon on each node (mmfsd) manages metadata as required
- Local cache (called the Pagepool) improves performance
- Lots of token checking to manage multiple writes to a file/directory

It is exported to named servers across the Centre

- Uses a pair of clustered NFS servers (cnfs1 and cnfs2)
- Exports "root-squash" to specific managed servers only

It is not exported to Windows or Macs

- We do not export to machines where the user has root access
- We do not export via CIFS/SAMBA
- Can be browsed, if necessary, using sshfs

Checking your group's quota

- e.g. df –BG /well/tomlinson

Archive-grade storage

Bought to allow "expensive" GPFS space to be freed up

- arc1 & arc2: each 72x 4TB SATA HDD
- arc3: 72x 8TB + 84x 8TB "shingled/SMR" SATA HDD
- Cheap storage but hopefully reliable
- Good way of using up grant money!

Archive storage has restricted use

- Copies to archive storage done only by ResComp people
- Available read-only to relevant servers
- Not visible to cluster nodes

ResComp backups…

NO STORAGE IN RESCOMP IS BACKED UP!

- We look after storage carefully
- We'll get an email within 10 minutes if a disk fails
- Everything is checked at least daily
- We have shelf spare disks waiting to go
- We'll come in at night to replace failed disks
- …but there is no backup of anything!

You need to keep a copy of essential raw data and final results

- Keep stuff on archive as well
- Deposit in other repositories

ResComp networking

Three main networks in the cluster room

- Centre LAN (129.67.44.0/22; managed by the IT Core)
  - 1 Gbit/s end connections, 10Gb/s trunk routes
  - Network used by users to get to login nodes and project servers
- Management/IPMI network (192.168.0.0/16)
  - 1 Gbit/s Ethernet
  - Imaging machines, monitoring machines, distributing jobs, controlling access, rebooting machines
- Storage network (10.0.0.0/16)
  - FDR InfiniBand (Mellanox)
  - Optimized for large data transfers to/from storage and for short low-latency messages (MPI)
- Local Ethernet connectivity
  - 10 Gbit/s Ethernet

The ResComp InfiniBand fabric

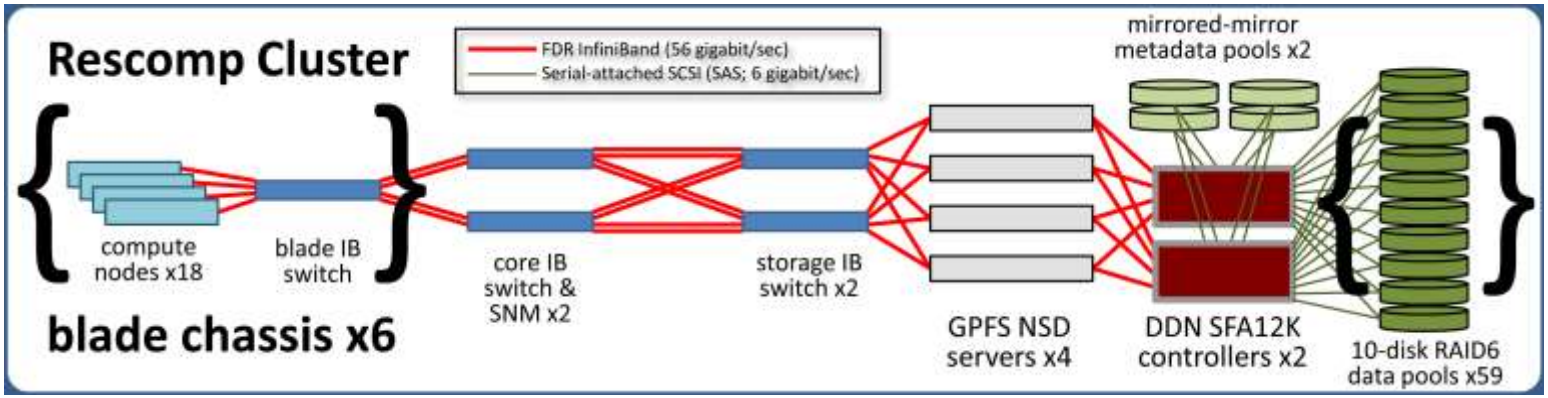
Main storage network is FDR InfiniBand (Mellanox)

- Fast, short-range networking
- 56 Gb/s, 64 data bits + 2 checksum bits – 6.8GB/s per link
- Multiple links aggregate performance and/or provide redundancy
- Main storage-to-cluster trunk is 8x 56 Gb/s, *i.e.* 448 Gb/s!

We run multiple protocols over the InfiniBand data link

- Verbs (RDMA), IPoIB (IP; 10.0.0.0/16 subnet), SRP ("iSCSI"), PSM (short messages)

Good for transferring large amounts of data, ideal for MPI



ResComp computing environment…

We try to provide a standard, stable, well defined environment for computation:

- CentOS 6.6 (kernel 2.6.32) – CentOS 7.x coming
- Fast, parallel access to large storage
- SGE job scheduler (6.2u5p3)
- Preinstalled applications in /apps/well and /apps/strubi
- Multiple versions of key packages such as R and python
- Monitoring of load to prevent crashes and allow users to share nodes transparently

We try to make it simple for everyone to get onto the system

- All quotas, shares *etc.* are handled at the group/project level
- No users have individual quotas or shares
- Reduces administration overhead and makes charging simpler
- Charge by quota/share not by use, so no unexpected bills!

Project servers and other special nodes

Cluster head nodes (head1 and head2)

- Manage the ResComp machines including SGE and imaging
- Not for general users!

Login nodes (rescomp1 and rescomp2)

- For general user use
- For testing and submission of jobs to the cluster
- For monitoring jobs

Project servers

- Currently: jaga, liono, jarrah, coolibah, belmont, humbug, elder, nephron
- Same as rescomp nodes, but group-restricted login and queues
- Owned by specific groups and have local storage

Other servers (storage-bsg, pootle, suzaku, wensleydale, rowan, banyan, cycloid, mobius, eucalyptus, ukb-data1, jenner1)

- Similar environment to rescomp nodes, not fully integrated

ResComp cluster nodes

Login nodes rescomp1 and rescomp2

- 2x dual 8-core Intel IvyBridge 2.6GHz, 256GB 1866MHz memory

"A" nodes (compA[000-023])

- 24x dual 6-core AMD Magny Cours 2.8GHz, 32GB 1333MHz memory
- 288 cores at 2.66GB per core

"B" nodes (compB[000-039] & compB[040-047])

- 40x dual 6-core Intel Westmere 3.06GHz, 96GB 1333MHz memory
- 8x dual 10-core Intel Ivy Bridge 2.2GHz, 160GB 1833MHz memory
- 640 cores at 8GB per core

"C" nodes (compC[000-107])

- 108x dual 8-core Intel IvyBridge 2.6GHz, 256GB 1866MHz memory
- 1728 cores at 16GB per core

"D" nodes (compD[000-031])

- 32x dual 12-core Intel Haswell 2.4GHz, 384GB 2133MHz memory
- 768 cores at 16GB per core

"H" nodes (compH[000-002])

- 3x quad 12-core Intel IvyBridge 3.0GHz, 2048GB 1600MHz memory
- 144 cores at 42.66GB per core

GPU and KNL compute nodes

GPUs are add-in cards for games PCs, xboxes, playstations *etc.*

- SIMD architecture (single instruction, multiple data)
- Need to write special code (CUDA, OpenCL)
- Single-precision calculations much faster than double precision ones

compG000 (like a C node but with quad Tesla K80)

- 8x 2496 GPU cores each with12GB DDR5 memory

compG001 (NVidia GeForce GTX680)

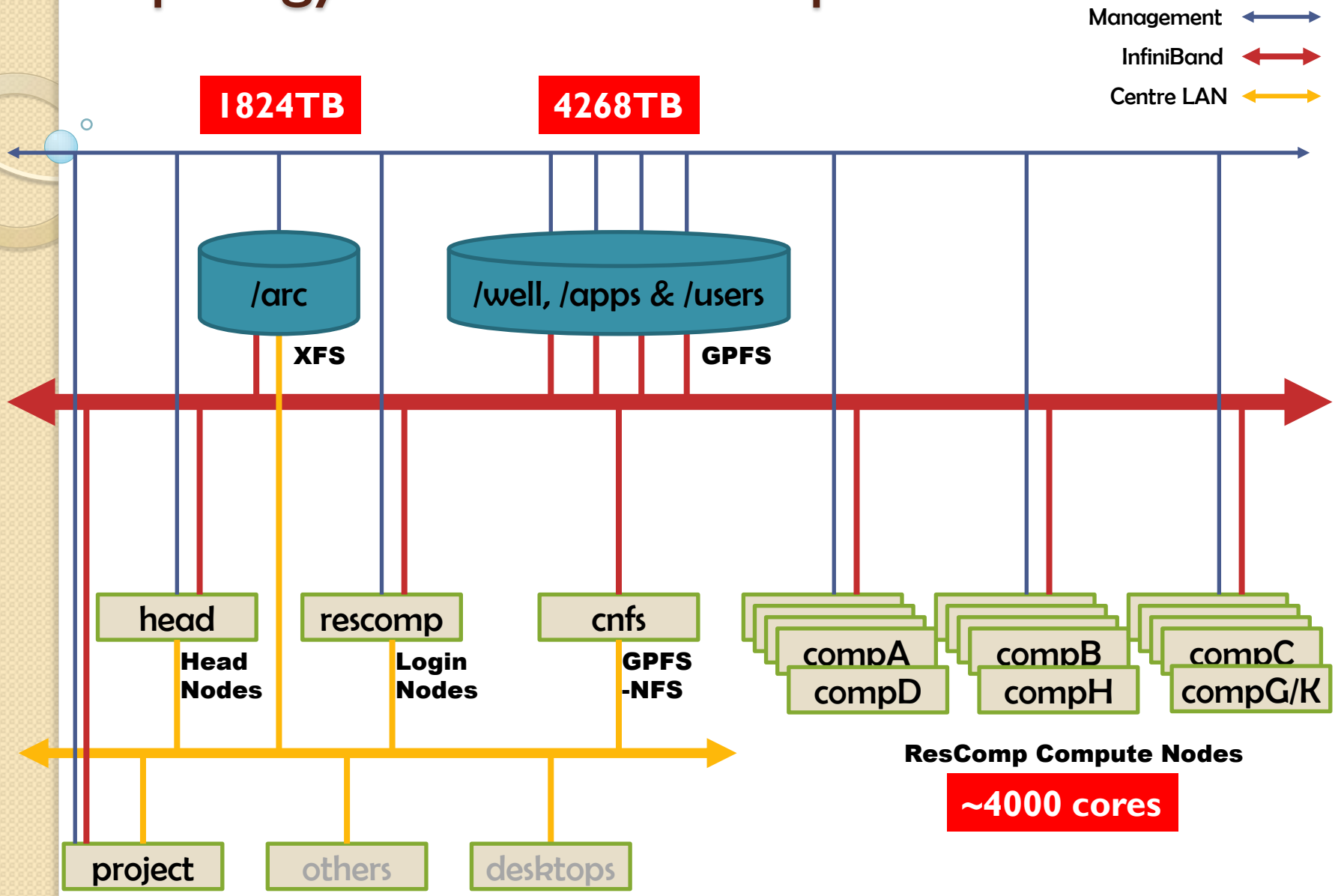
- 1536 GPU cores, 4GB DDR5 memory
- Being replaced with Titan X Pascal 2016
- 3584 cores, 12GB GDDR5X memory

compK000 is a Knights Landing machine

- Novel cross between a CPU and a GPU
- 64 cores, 16GB fast DDR5 cache
- 192GB 2133MHz memory

Tesla K80

Topology of the ResComp Hardware



ResComp hardware environment

Home devised but
PUE measured at 1.32

What next for the ResComp Core?

Retirement of A and B nodes in 2017

- Replace 938 cores with about 3500 high-memory ones

More high-performance storage

- Expansion of GPFS2 to 4980TB
- Planning to decommission GPFS1

Faster core networks

- HDR InfiniBand (200Gb/s) & OPA (100Gb/s)

Improved approach to archive storage

- Object stores (*e.g.* Ceph or Cleversafe)
- Multisite redundancy

Searching for off-site data centre solutions

- Integration with the Big Data Institute developments
- Long battle with the University to improve computing

System administration within ResComp

Completely independent of Centre LAN and wider networks

- Username and groups names and numbers (UIDs and GIDs) kept in sync

Services on head1 and/or head2

- All services either dual-active or failover
- xCAT management and imaging of nodes
- LDAP authentication of user accounts and group memberships
- DHCP and DNS name/IP address assignment, NTP time services
- SGE scheduler communication

Servers in the Cluster Room that use ResComp authentication

- All cluster nodes, rescomp1, rescomp2, head1 and head2
- jaga, liono, jarrah, coolibah, belmont, humbug, elder, nephron

Other servers use the Centre NIS

- Storage-bsg, pootle, suzaku, wensleydale, banyan, cycloid, eucalyptus, rowan

How big is the ResComp Core?

The ResComp Core serves just the WTCHG and has no external support

- Funds from WT for the C nodes & networking (~£0.6M)
- The rest comes by charging your project grants (~£2.5M)
- New core award will allow upgrade of compute (~£1.4M over 5 years)

In terms of compute cores…

- ARC (7000 cores), ResComp (4200 cores), GridPP (3000 cores),…

In terms of network speeds…

- ResComp (448 trunk & 56Gb/s), ARC (40Gb/s), GridPP *etc.* (10Gb/s),…

In terms of storage capacity…

- ResComp (8.2PB), GridPP (1.5PB), TDI (0.9PB), ARC (0.6PB),…

About 25% of the compute and storage capacity of the WT Sanger Institute

Who uses the ResComp Core?

Nearly every group now uses ResComp…

- This includes external collaborators across Oxford and further afield
- e.g. Dept. Statistics, UK BioBank, TDI, Oncology and groups associated with the hospitals

Audit of use from 1/1/2015 until 25/11/2015:

- ResComp has 284 registered users
- ResComp was used by 147 active users
- ResComp has delivered 48.2 billion CPU seconds
- ResComp is used at about 80% of theoretical compute capacity
- Each of 14 different users exceeded 1 billion CPU seconds
- These 14 users come from 9 different research groups

Getting access to the ResComp facilities

You must have a WTCHG account!

- This defines your shared, unique username and UID
- Contact support@well.ox.ac.uk – includes STRUBI people

Ask ResComp Core to create your account

- Which group are you, what access do you need?
- An email from your group head / main IT contact!
- Remember ResComp is managed independently, *i.e.* it is a separate account so password can be different
- Contact rescomp@well.ox.ac.uk

Cluster shares and storage quota are controlled at the group (not user!) level

- Model is like each group has its own little facility – one group cannot push another group off the system

Getting started on ResComp facilities

Use ssh to access rescomp1, rescomp2 or a ResComp-managed project server to reset your password

- You will initially be given a pre-expired password
- You have to change it before you can start working

Use ssh to access rescomp1, rescomp2 or a ResComp-managed project server with your new password

- Start submitting jobs!

Thank you for your attention… any questions?

Next talk 10am Wednesday… "Basic introduction to Linux"