Sussex HPC facilities and service development

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Changes in 2012

- Tildesley report   - tinyurl.com/tildesley
- £158m BIS funding for e-infrastructure
  - ARCHER National Facility, Regional HPC centres via EPSRC, etc
- From STFC via GridPP for network infrastructure
  - £28k funding to Sussex for infiniband network expansion
- Facilitates move cluster enabling expansion, March
- Cluster consolidation + upgraded Bright and Lustre, August
  - Can deploy SL 6, use larger disks in Lustre file system, more efficient
- Informatics research grant funds 2 x 64 core nodes + 20TB Lustre storage (£20k)

Apollo Cluster - Hardware

- **QDR Infiniband interconnect.**
- **Memory generally 4GB/core, total of 3TB**
- **Compute: Total 1004 cores**
  - **ITServices   436**
  - **EPP   184**
  - **Informatics   256 (128 in legacy blades, out of maintenance)**
  - **Chemistry   128 (out of maintenance)**
- **Storage: Total 40TB NFS home and 163TB Lustre scratch file systems.**
  - **IT Services: 20TB NFS,   30TB Lustre**
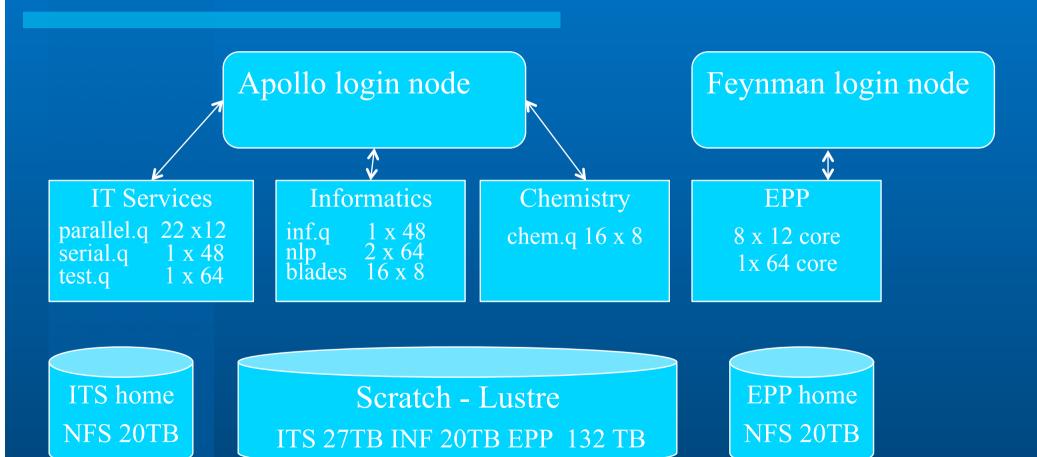 - **EPP: 20TB NFS   117TB Lustre**
  - **Informatics   18TB Lustre**
- **~80 Active users, 120+ registered.**

Apollo Cluster - Software

Compilers/tools	Libraries	Programs
ant	acml	adf
gcc	atlas	aimpro
Intel (c, c++, fortran)	blas, gotoblas	alberta
git	fftw2, fftw3	fsl
jdk 1.6_024	gmp	freesurfer
mercurial	gsl	gadget
open64	hpl	gap
python	lapack, scalapack	Gaussian 09
sbcl	MVAPICH2	hdf5
	mpfr	idl
	nag	matlab
	openMPI	mricron
		netcdf
		paraview
		stata

Basic Cluster Topology

New usage patterns

- Malcolm Heggie -> Surrey; less theoretical chemistry usage
- New users from LifeSciences
  - Drug discovery, Evolutionary Biology, Biochemistry
- More users from Maths and Engineering
- Increased use re Neuroscience and MRI imaging

Examples of Research Areas

- BSMS: fMRI analysis and DICOM archive
- Engineering and Design: Computational Fluid Dynamics
- LifeSci: Biochemistry, Bioinformatics, Theoretical Chemistry, Evolutionary Biology, Drug Discovery
- Geography: Climate Change
- Informatics: Computational Neuroscience, Text Analytics, Adaptive Systems
- Maths: Finite Element Analysis, Spatial Pattern Formation
- Physics: ATLAS, Sno+,Cosmology
- Psychology: MRI analysis

Future plans

- Research File Storage for Schools
- HPC Training workshops (ITS/EPP) this term.
- Better documentation
- HPC Wiki
- Formation of advisory group re HPC
- GridPP hardware expansion
- Another Lustre upgrade when GridPP storage purchased
- Move to SL6
- More nodes ??

Questions?

See slides at

http://www.sussex.ac.uk/its/services/research/highperformance/