• Premier UK University and research institution ranked #2= (with Cambridge) in QS World University rankings (MIT #1)
• #9 in worldwide Universities (THES) and #3 in Europe
• 15,000 students, 6,200 of them postgrad
• 7,200 staff (2,600 of which dedicated to research)
• Science based – engineering/technology/medicine
• Lots of industrial research collaboration
• £350M per year research income
Main Campus South Kensington London

- Located on the site of the 1851 Great Exhibition in London (pic wikipedia Dickinsons)
HPC Service

- University wide service
- £2M annual budget for hardware and software
- Additional income directly from research groups
- 5 dedicated HPC staff
- Largest UK University HPC system (HPC-SIG)
3 HPC systems

- cx1 – low end cluster mostly ethernet
- cx2 – high end parallel MPI cluster (SGI ICE-X)
- ax3/4 – large shared memory dedicated to genomics (UV)
• Large memory SMP
• Two SGI UV
  - 160 processors 4 TB memory
  - 1024 processors 16 TB memory
• Main user is Bioscience – Next Generation Gene Sequencing
• PBS topology aware scheduling, cpuset
High end MPP commissioned Autumn 09, upgraded several times, system refresh Winter 2015, supporting large highly parallel jobs

• SGI Altix ICE 8400 EX + ICE-X 12288 cores
• Dedicated to large MPI parallel jobs
• PBS topology aware scheduling – simple config
• Focus on capability, running jobs on thousands of cores
• Low end cluster
• Mostly gigabit ethernet, some infiniband islands
• Upgrading all the time, parts of the system owned by particular research groups
• 23026 cores, 1352 nodes, 12 distinct hardware types plus GPUs
• Serial and small parallel workload many shapes and sizes
• Tricky to schedule! 3 million jobs per year …
• Focus on low cost/throughput
Why cx1 and cx2?

• Cost
• Flexibility
• Users able to contribute funds/hardware to cx1
10 years of Service

- Celebrating 10 years of successful service this summer
- Where to next?
More of the same

• For sure – users like what they get!
• They want more
• We have rolling replacement programmes
• Finance and space constraints
  • Users’ grants may last for 5 years, which is a bit long in the tooth for a server, but they have no more funds in the 5 year period to refresh
  • Central funds are fixed and can’t replace older hardware to a 3 year lifespan
• Space
  • Computer room is full and limits expansion
• Demand is there for expansion, more resources for current users plus newer areas, like bioscience and social science are growing fast
• Additional demand for higher fidelity simulations from traditional computational science – larger molecules, more degrees of freedom, smaller timesteps, higher Reynolds number, more complex algorithms etc
• National resources constrained
• Good cases for expansion and likely funding – but how?
Possible Options?

- New computer room
  - Where, how big
  - Running costs (actually could be quite reasonable)
- Co-Lo’s
  - Not really well suited for HPC hardware
  - Prices not fixed – market driven?
  - Readily available at the moment
- Cloud
  - For some work cloud gives good results, for large scale parallel simulations it doesn’t
  - Can be pricey and costs are variable – hard to fund
- Stay tuned ....
Software Challenges

- It's not just hardware though, should we invest in software?
- New processors have more and more cores/threads running more slowly
- These processors need carefully optimised code to reach their rated FLOP rates
  - 3 levels of optimisation needed
    - At the thread level (vectorisation)
    - At the socket level (on chip communications, e.g., OpenMP)
    - Between nodes (via the interconnect, e.g., MP)
- Memory access times becoming more problematic
  - More NUMA levels:
    - Registers/vector registers/cache
    - On socket cache
    - Off socket cache and user controlled buffers
    - Main memory
• Although some of this optimisation can be automated, most needs careful programming
• There is a real shortage of computational scientists who can do this work
• It’s not fashionable to be a computational scientist in a research group
• Programming skills not being taught at lower levels
• Computing skills not regarded as worthwhile (not taught) in mainstream science and engineering degrees
• Skills shortage is a huge issue
• More training and recognition of programming and computation skills is badly needed across the board – the next generation of HPC won’t succeed without it.
HPC is fragile!

- HPC is
  - Disruptive
  - Challenging
  - Expensive
  - Changeable
- It needs a nurturing ecosystem in order to succeed
- Universities need to take care not to break it
  - Long term sustainability needed
  - Computer room infrastructure (15-30 year)
  - It is not IT, it is not commodity, HPC is special and needs a special place of its own in the organisation. Essentially it’s a research instrument
- Industrial collaboration and exchange is vital
  - Working with the real world focusses on real challenges and issues.
  - HPC could help in more areas than now by providing a safe place to conduct digital experiments, cheaply and effectively. It needs to be driven!
- Specialist Programming skills need to be fostered, encouraged and rewarded.
Questions?

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