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Holmes, Violeta and Kureshi, Ibad

Creating an HE ICT Infrastructure Fit for the 21st Century

### Original Citation

Holmes, Violeta and Kureshi, Ibad (2013) Creating an HE ICT Infrastructure Fit for the 21st Century. In: Higher Education Show 2013, 25 April 2013, London, UK. (Unpublished)

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# Creating an HE ICT Infrastructure Fit for the 21<sup>st</sup> Century

Dr Violeta Holmes - HPC Research Group Leader  
Ibad Kureshi – UoH HPC System Administrator  
The University of Huddersfield

- High-Performance Computing at the University of Huddersfield
  - HPC System Users
  - HPC Resources
- Removing the technical burden from researchers
  - HPC Resource Centre
  - HPC Resources: Local and National
- Quicker and more insightful research outcomes
  - Examples
- Promoting links between High-Performance Computer (HPC) users, developers and researchers across the University, throughout the UK and internationally:
- Facilitating access to HPC research and resources for industry
  - 3M Buckley Business and Innovation Centre
- Streamlining funding mechanisms to introduce training in the use of HPC technologies



- Researchers at the University of Huddersfield currently have direct access to more computing power than ever before.
- Facilities are closely tailored to the needs of users - an important factor in attracting high-calibre researchers to the University.
- Calculations that would have taken weeks or months on a desktop machine can now be carried out in hours.
- Cutting-edge research in fields such as molecular biology, accelerator physics, engineering, fluid dynamics, computational chemistry, image rendering and informatics is reaping the benefit.

# HPC systems users



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- In 2010 there was a handful of HPC researchers using modest departmental HPC resources
- In 2013 there are 200 active users from:
  - Engineering 23%
  - Chemistry 25%
  - Physics 20%
  - Informatics 12%
  - Biology 5%, and others
- This dramatic increase of HPC systems users is due to the university's investment in the HPC resources and support for research

- The University of Huddersfield Queensgate Grid enables access to Local and External National resources.
- Local HPC resources - Campus grid Queensgate Grid (QGG) compute clusters and Condor pool
- A share in an IBM iDataPlex system as part of the STFC enCore cloud service at Daresbury Laboratories, Hartree centre – IBM Blue Gene
- Local HPC resources are integrated with:
  - The National e-Infrastructure Service and UK-NGI
  - The North West Grid

# Removing the technical burden from researchers

- To provide support for growing research community, the HPC Resource Centre (HPCRC) was formed. It provides support and services to researchers in accessing and using HPC resources.
- HPCRC manages:
  - User accounts to local systems for researchers, staff and students
  - Central repository of software
  - Central knowledge base for users
  - Training for accessing and using HPC resources
  - All HPC systems within the QGG Campus Grid and access to STFC Hartree Centre
- HPCRC liaises with administrators of remote national and international resources and acts as a local Registration Authority for the National e-Infrastructure Services (NES)

# The Queensgate Grid – Local HPC resources



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- HPC Systems - Clusters
  - Dual boot Intel based cluster - Eridani,
  - AMD/Nvidia based cluster with GPUs – Vega,
  - Large memory nodes - TauCeti,
  - SUN cluster – SOL,
- A HTC High Throughput System - 2000+ slot Condor Pool,
- Cycle Stealing Render Farm - 120 Machine Backburner Render Farm (handling Mental Ray, 3Ds Max, and Maya),
- Large File Storage
- IaaS Cloud Computing Platform (OpenStack)



# Local Resource: Sol Cluster

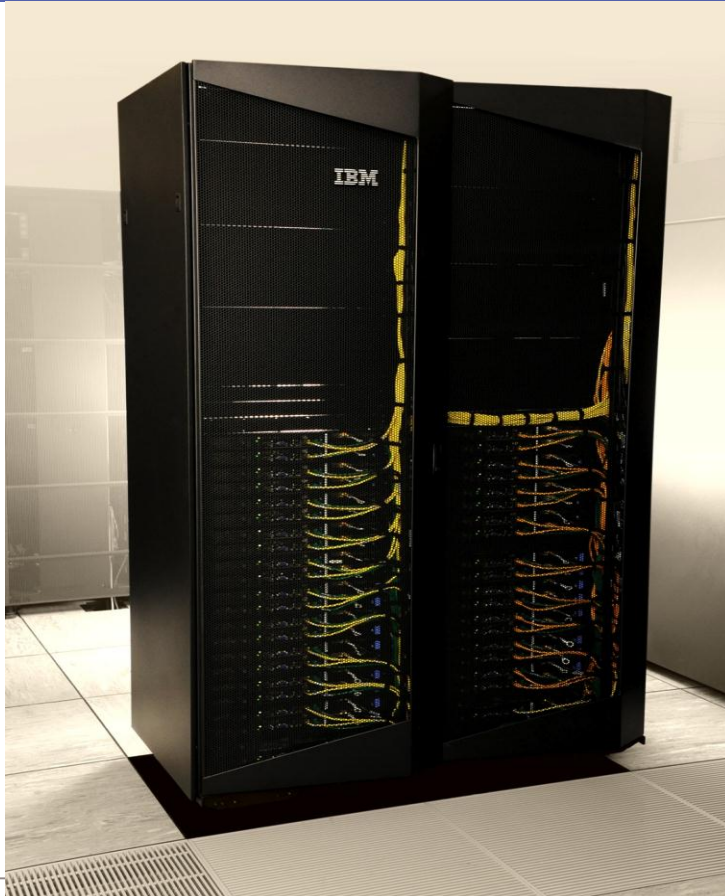


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- **Name:** Sol
- **Type:** Cluster
- **Cores:** 260
- **Memory:** 600GB
- **Interconnect:** 4xGigE
- **R-max:** 2457.6 GFlops
- **R-peak:** 1004.8 GFlops
- **R-av:** 749.53 GFlops



# External resources – STFC: eNcore Cluster



- **Name:** SID
- **Type:** IBM iDataplex
- **Cores:** 216 Cores @ 50,000 hrs/m
- **Memory:** 432GB
- **Interconnect:** Infiniband

# National resources – National e-Infrastructure Services (NES) VO Support

- HPC with DOCABS (The Huddersfield Department of Chemistry and Biological Science) helps users get credentials on the National Grid
- Local Users on Campus can connect out to NES (former NGS) resources.
- We accept incoming connections from users in the NES VO.
- The VDT (Virtual Data Toolkit) is installed to allow users to manage jobs and transfer files across all NES resources with a single sign-on or through the Globus interface.

# Supported Applications

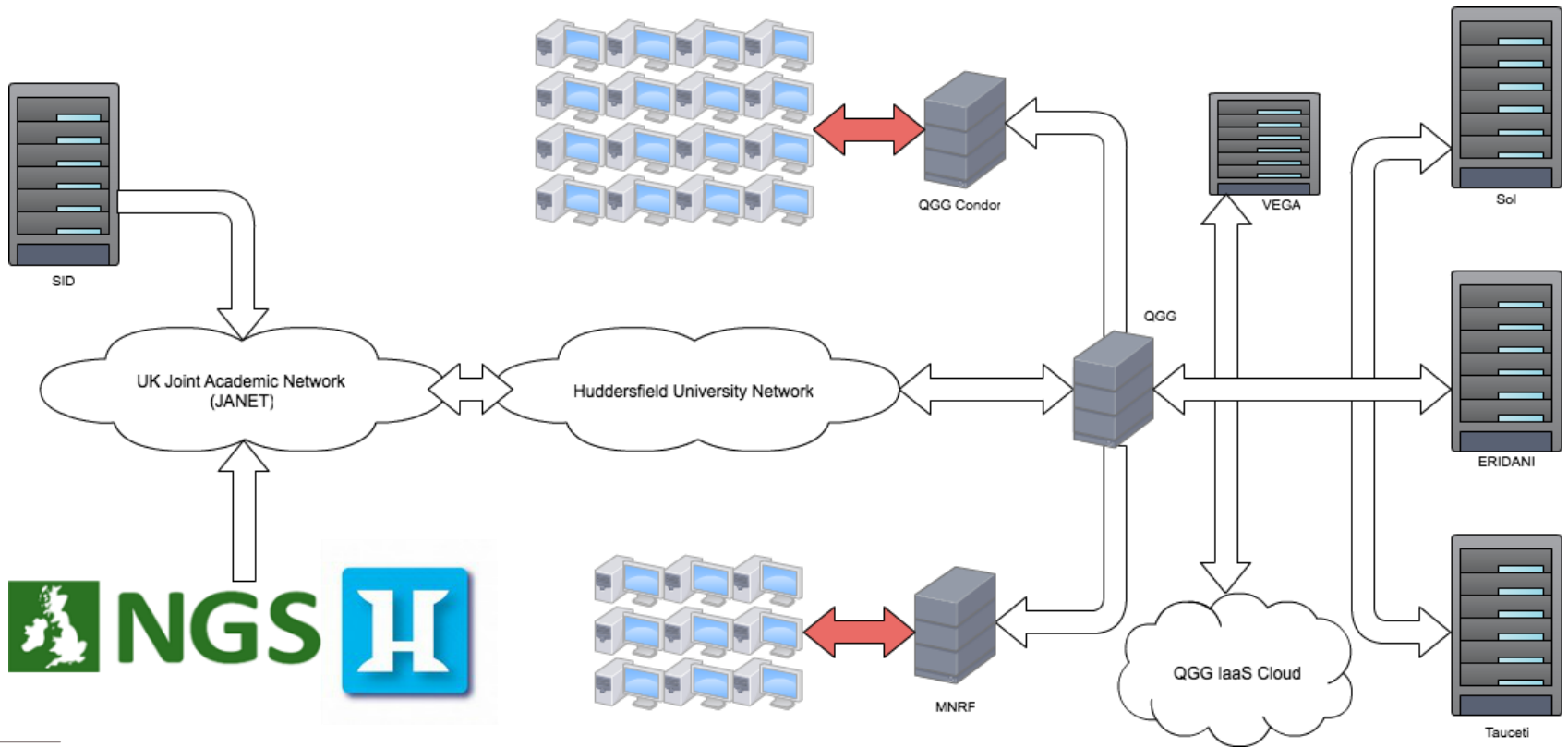


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- 3d Studio Max
- Abaqus
- Amber
- Blender
- Castep
- Comsol
- DL\_POLY
- Fluent
- GAMESS-UK
- Gulp
- HMMER
- LAMMPS
- Metadise
- NWChem
- OpenFoam
- Opera 3D
- Matlab
- Mental Ray
- Octave



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# Quicker and more insightful research outcomes - examples



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- University's HPC system was used in designing a component for truck trailers to reduce drag using Computational Fluid Dynamics.
- On a single work station each simulation required 28.5 days to complete.
- It took just under 5000 simulations over 2 years to find the best working model for the product.
- This was only possible because of HPC was used to run simulations. Every simulation took between 12-18 hours to complete and about 10-15 simulations could run at the same time.
- HPC was able to do 97.5 years of computing in 2 years.
- The end product, when prototyped and tested under controlled conditions at the Mira test track, resulted in an improved fuel efficiency of 3%.

Promoting links between High-Performance Computer (HPC) users, developers and researchers across the University throughout the UK and internationally



- Researchers at the International Institute for accelerator Applications use HPC resources for research in thorium.
- Local GPU cluster is used for visualisation of data from Microscope and Ion Accelerators for Materials Investigation (MIAMI) used for research in optimising the performance of materials to be used in the construction of new generations of nuclear reactors in the USA.
- EPSRC Centre for Innovative Manufacturing in Advanced Metrology - precision engineering, and metrology research and development. The research data from X-ray tomography instruments are visualised using HPC
- The Institute of Railway Research (IRR) is carrying out research into the interaction between railway vehicles and the track, and is using HPC for modelling

# Facilitating access to HPC research and resources for industry - 3M Buckley Business and Innovation Centre



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- Research at the University of Huddersfield has been traditionally linked with industry and applied to industry needs.
- The 3M Buckley Business and Innovation Centre (3M BIC), funded partly from the EU and the University of Huddersfield, will act as a catalyst to promote Business-to-Business and Business-to-Higher Education collaborations.
- The 3M BIC will house HPC equipment and resources for use in short to medium term collaborative and applied research and development projects involving researchers and wider support from the University.
- PTG Holroyd is a company planning to use HPC for the static, dynamic, and thermal modelling and simulation of machine tools and their processes



# HPC research and resources for industry – 3M Buckley Business and Innovation Centre



- 3M BIC HPC system – Iceotope solution <http://www.iceotope.com/>
- The Iceotope solution overcomes standard IT challenges:
  - lack of space,
  - need for more computing power
  - cooling problems,
  - energy challenges
- It uses 3M Novec liquid cooling
- It integrates compute and cooling systems
- It uses less energy to power and cool the system than others use to power

# Streamlining funding to introduce training in the use of HPC technologies

- Recent government investments in HPC infrastructure (Tier 1 and 2) are substantial - £145K in 2011-12 (Hartree Center).
- The STFC Hartree Centre offers world class HPC resources to HPC users.
- However, further investment is needed in Tier 3 HPC in HE institutions, to provide education and training of current and future users and developers of HPC systems
- HE courses should be developed to provide HPC system architects, administrators, researchers and software developers

# Streamlining funding mechanisms to introduce training in the use of HPC technologies



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To provide HPC trained staff for HPC and e-science, HE institutions should:

- Actively recruit postgraduate students working on HPC related projects
- Offer in-house training and workshops for HPC users/researchers
- Deliver undergraduate and postgraduate HPC courses

We hope for funding opportunities to further develop our existing courses and to provide much-needed training and expertise for the ICT fit for the 21<sup>st</sup> century

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# Thank you



Links:

<http://hpc.hud.ac.uk/>

<http://www.hud.ac.uk/news/researchnews/safernuclearpowerstations.php>

<http://www.3mbic.com/>

[www.ngs.ac.uk](http://www.ngs.ac.uk)

<http://www.stfc.ac.uk/Hartree/default.aspx>

<http://www.nw-grid.ac.uk/enCore>

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