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Holmes, Violeta

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Original Citation

Holmes, Violeta (2013) High Performance Computing: Enabling Businesses and Researchers Access To World-Class, Secure Technology. In: Research Information Management: The Challenges and Opportunities of Open Access, 24th January 2013, London, UK.

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High-Performance Computing: Enabling Businesses and Researchers Access To World-Class, Secure Technology

University of HUDDERSFIELD

Dr Violeta Holmes

HPC Research Group Leader at the
University of Huddersfield

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Outline

- Promoting links between High-Performance Computer (HPC) users, developers and researchers across the University, throughout the UK and internationally:
  - HPC Research Group
  - HPC Resources
- Removing the technical burden from researchers
  - HPC Resource Centre
  - HPC Resources: Local and National
- Quicker and more insightful research outcomes
  - Examples
- Facilitating access to HPC research and resources for industry
  - 3M Buckley Business and Innovation Centre
- Research Data Management at the University of Huddersfield

Promoting links between High-Performance Computer (HPC) users, developers and researchers across the University, throughout the UK and internationally
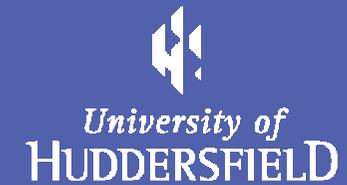
- Researchers at the University of Huddersfield currently have direct access to more computing power than ever before.
- Facilities are closely tailored to the needs of users - an important factor in attracting high-calibre researchers to the University.
- Calculations that would have taken weeks or 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.

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HPC Research Group

- HPC Research Group was formed in 2010 as a culmination of 3 years of research, with representatives from various schools and departments.
- Its goal was to:
  - Unify departmental HPC resources and provide a university-wide approach to high-performance computing
  - Foster mutually-supportive environments for research active staff involved in HPC
  - Provide an external reference point for communications with the wider community on HPC matters

HPC systems users

- In 2010 there was a handful of HPC researchers using modest departmental HPC resource
- In 2013 there are 120 active users from:
  - Engineering 23%
  - Chemistry 25%
  - Physics 20%
  - Informatics 12%
  - Biology 5%, and others
- This dramatic increase of HPC users is due to the university's investment in the resources and support for research

HPC Resources

- The University of Huddersfield Queensgate grid enables access to resources spread around 3 counties in the North West of England.
- 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
- 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
- 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

- 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

Local Resource: Sol Cluster

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- **Name:** Sol
- **Type:** Cluster
- **Cores:** 260
- **Memory:** 600GB
- **Interconnect: 4x**GigE

- **R-max:** 2457.6 GFlops
- **R-peak:** 1004.8 GFlops
- **R-av:** 749.53 GFlops

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External resources – STFC: eNcore Cluster
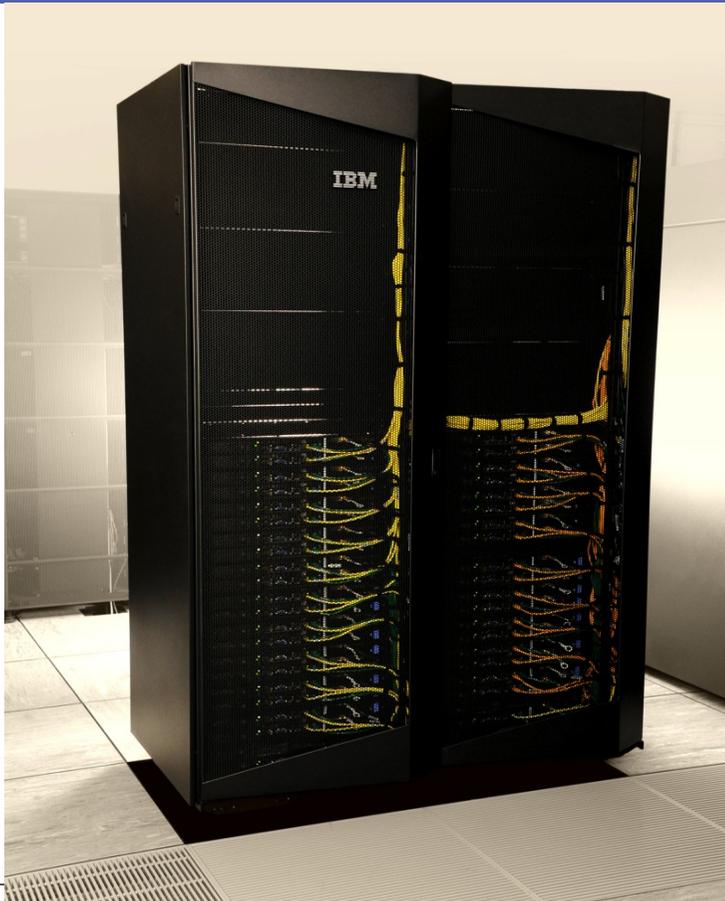
- **Name:** SID
- **Type:** IBM iDataplex
- **Cores:** 216 Cores @ 50,000 hrs/m
- **Memory:** 432GB
- **Interconnect:** Infiniband

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

- HPC with DOCABS (The Huddersfield Department of Chemistry and Biological Science) help 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

- 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
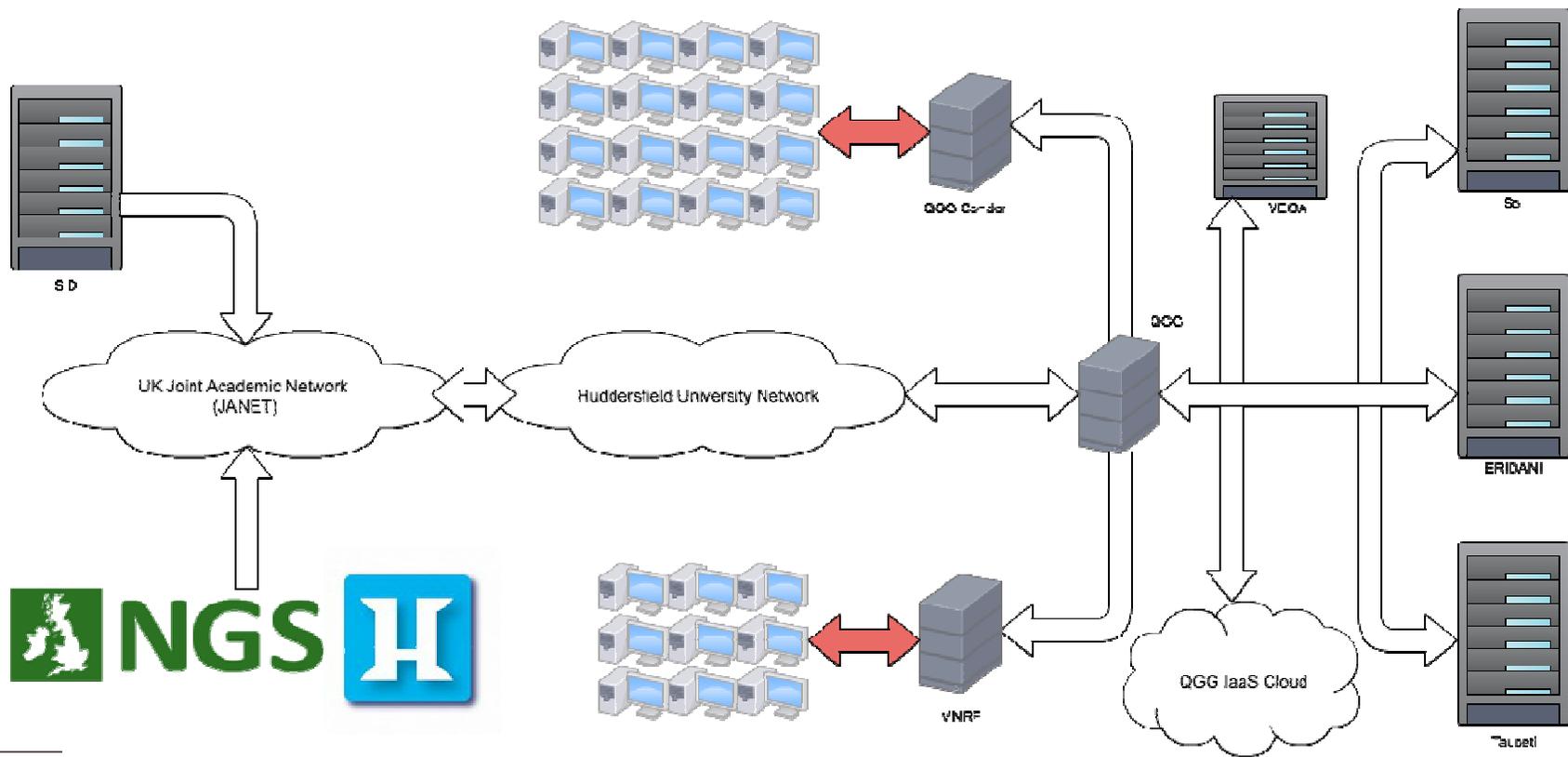
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Quicker and more insightful research outcomes - example

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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%.

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International Science Programmes supported by HPC – examples

- 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

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

- 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 one of the companies planning to use HPC for the static, dynamic, and thermal modelling and simulation of machine tools and their processes

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Research Information Management at the University of Huddersfield

- Research at Huddersfield University generates large volumes of data.
- Currently, storage of data is not centralised at the university level and often it is not easily accessible.
- The University of Huddersfield recognises that research data access should not be restricted unless there are clear legal, ethical or commercial constraints.
- From 1 May 2012 to 30 April 2015 the University will embed best practice in the management of research data (as defined by the Digital Curation Centre)
- University's Central Computer Services are investigating the requirements for research data storage with a view to invest into a new systems for storage and curation of research data.
- Our research into large data management, using Semantic Technologies, will facilitate faster access and retrieval of large data from the centralised safe storage.

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University of Huddersfield Policy for Management of Research data

- Commitment to research excellence (University strategy 2011-202) – data will be managed through the research data cycle
- Responsibility for RDM lies with Principle Investigators
- New research proposals must include RDM plans
- Training, support and advice to for RDM plans will be provided
- Mechanisms and services for storage, backup, registration, deposit and retention of data will be provide
- Data retained elsewhere will be registered with the University

University of Huddersfield Policy for Management of Research data (continued)

- RDM plan will ensure that research data will be available for access in a timely manner
- The legitimate interests of the subject of research data must be protected
- Research data of future historical interest will be offered and assess for deposit and retention in an appropriate national, international, domain repository or University repository
- Exclusive rights to reuse or publish research data should not be handed over to commercial publishers or agents
- Published results should include information on how to access research data
- All research data should be discoverable for re-use by others, therefore sufficient metadata should be recorded

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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.stfc.ac.uk/Hartree/default.aspx

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