Driving Innovation at the Hartree Centre with the OpenPOWER Architecture

Dr Mike Ashworth et al
STFC Hartree Centre

Revolutionizing the Datacenter
STFC Hartree Centre

- Provide **market led research** and innovation and development services for **competitive advantage** and wider **economic impact** by accelerating the application of High Performance Computing, Data Science, and Cognitive techniques
STFC Hartree Centre

2012 Creation of Hartree Centre as an industrial driver in HPC

- 2011 Tildesley Report recommendation
- Investment from UK Government (BIS)
- Economic impact through Software & Modelling
- Focus on industrial engagement

2013 Follow-On Investment

- Energy Efficient Computing
- Data Analytics

2015 Major Investment in Collaborative Research

- Data Centric & Cognitive Computing
- Embedded IBM Research Centre
- Extended industrial & scientific reach
Hartree Centre Case Studies

Smaller, affordable particle accelerators for healthcare and security

Accelerating product design and development at Jaguar Land Rover

New processes emerging for more economical oil extraction

Building next generation materials simulation tools with NPL

Accelerating the product discovery process at Unilever

Supporting new product design at Bentley

Many more available

http://www.stfc.ac.uk/about-us/our-impacts-achievements/case-studies/hartree-centre-case-studies/

6th April 2016
Hartree Centre Offerings

Mission

• To bring the benefits of HPC & Big Data to industry & commerce

Tools

• Hardware, software & skills

Skills

• 160 staff in Hartree Centre & Scientific Computing Department
• CFD & Engineering
• Materials
• Computational Chemistry
• Environmental Modelling
• Energy Efficient Computing

How can we help you?

- You solve the problem
  • Access to hardware
- We solve the problem
  • Consultancy & professional services
- We develop a solution
  • Software development
- We solve the problem together
  • Collaborative R&D
- We train you to solve the problem
  • Training & education

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Panther system: POWER8 + K80 GPUs

- 32 Compute Nodes
  - 2 x 8 cores @3.32GHz
  - 28 nodes with 52GB RAM
  - 4 nodes with 1TB RAM
  - 2 x nVidia K80 GPU
  - 2 x 1TB HDD

- Infiniband (FDR)

- 2 x IBM ESS GS4 storage arrays,
  - 96 x 800GB SSD

- IBM FlashStorage 900 57TB
  (Infiniband QDR attached)

- IBM FlashStorage 900 57TB
  (CAPI attached)

- Ribbons and bows courtesy of OCF
Hartree Centre PADC – Press Release

New facility helps UK business exploit high performance computing

New Centre Designed to Optimise Performance of OpenPOWER Systems for Modelling & Simulation and Big Data Analytics

22 Oct 2015 – The UK's first POWER Acceleration and Design Centre (PADC) aims to improve modelling, simulation and big data analytical capabilities on IBM’s OpenPOWER systems.

“The PADC will help industry and academia take advantage of IBM and NVIDIA’s technological leadership in supercomputing and the Hartree Centre's expertise and experience in delivering solutions to real-world problems.”

Dr Peter Allan, Director of the Hartree Centre”
Early Experience with POWER - HPCx

- First Terascale system in the UK
- UK National Service from 2002-2010 at Daresbury Lab
- Upgraded twice: 3, 6, 12 Tflop/s RMax
- Final system POWER5 with HPS switch: 160 nodes, 2560 cores
  
  [Image of server room]

  www.hpcx.ac.uk

- Daresbury Laboratory had a POWER3 system prior to HPCx
  
  [Image of server room]

  http://tardis.dl.ac.uk/computing_history/computing_history.pdf
Hartree Centre Major Applications

- Expertise across the full range of length and time scales from sub-atomic processes to environmental modelling at global scales
Early Result: DL_MESO Lattice Boltzmann

- POWER8 evaluation system
- single node, 24 cores, six cores per socket
- DL_MESO mesoscale code has DPD and LBE variants
- Scales well to 24 cores
- SMT gives additional performance to 96 virtual cores (SMT=4)
Summary

- The STFC Hartree Centre has invested in a significant system: IBM OpenPOWER + NVIDIA GPUs
- The Hartree Centre is open for business as the first PADC in the UK
- We are porting and optimizing a wide range of codes for clients across industry and academia
- Large-scale simulation, data analytics and cognitive computing are all high priority
- Look for us at future OpenPOWER events for more information

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