The Hartree Centre helps businesses unlock the potential of HPC

Fostering collaboration and innovation across UK industry with help from IBM

Overview

The need
The Hartree Centre needs leading-edge computing resources and expertise to hand in order to fulfill its mission to enhance accessibility and software development for high-performance computing (HPC).

The solution
In an ongoing collaboration, the Hartree Centre works closely with IBM and OCF to tailor HPC services to help users get the maximum benefit and develop and refine its supercomputing platforms.

The benefit
By lowering the cost and complexity surrounding HPC, the center is able to remove the barriers to entry for businesses, fostering innovation and maximizing the impact of investments.

Founded in 2012 with a 37.5 million GBP investment from the UK government, the Hartree Centre was created by the UK's Science and Technology Facilities Council (STFC) to develop, deploy and demonstrate high-performance computing (HPC) solutions. Part of a center of expertise in computational science and engineering, the Hartree Centre is a research collaboratory in association with IBM, with facilities at the Sci-Tech Daresbury and Harwell Oxford national science and innovation campuses.

Untapped potential
Using parallel processing to deliver unprecedented computing speeds, HPC can be used to tackle new frontiers of problem-solving, prediction and data analysis. As advanced modeling and simulation combined with Big Data capabilities continue to change the face of science and engineering, its potential for other industries is only just beginning to be revealed.

The Hartree Centre's mission is to bring down the barriers to entry for businesses that may not have even considered using HPC services before. With a recent report estimating that European leadership in HPC could add as much as between two and three percent to Europe's GDP by 2020[1], investments in the field of supercomputing potentially offer high returns with relatively low risk.

Cliff Brereton, Director of the Hartree Centre explains: "Through its investment in the Hartree Centre, the UK government aims to capitalize on the UK's reputation for world-leading design and innovation by applying modeling and simulation techniques to cut down on design cycles and accelerate time to value."
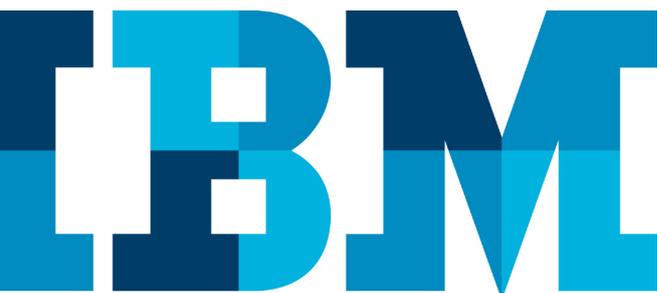
Solution components

Hardware
- IBM® Blue Gene®/Q
- IBM System Storage® TS3500 tape library with TS1140 Enterprise tape drives
- IBM System x® iDataPlex® dx360 M4
- DataDirect Networks SFA 10K-X disk systems

Software
- IBM General Parallel File System (GPFS™)
- Red Hat Enterprise Linux

Services
- IBM Systems and Technology Group Services for HPC
- IBM Laboratory Services
- IBM Business Development

IBM Business Partner
- OCF plc

Recognizing the challenges

To make HPC a cost-effective proposition for users, the Hartree Centre needs to ensure maximum efficiency while delivering massive computing power. Moreover, ensuring that services are accessible to non-specialist users requires user-friendly interfaces and tailored support.

Michael Gleaves, Head of Business Development at the Hartree Centre, says: "It is up to STFC [the Science and Technology Facilities Council] and IBM to maximize return on investments in the Hartree Centre and broaden its offering beyond the traditional users of modeling, simulation and data exploration. To reach new users, our services need to be cost-effective and easy to use."

Building a solution

Using IBM technology, the Hartree Centre, IBM and IBM Business Partner OCF have built two supercomputers, named Blue Joule and Blue Wonder. The Hartree Centre can call upon the expertise of 170 staff within the Scientific Computing Department to continue to work with leading-industry experts from IBM to develop software for the platforms.

Blue Joule is built on IBM® Blue Gene®/Q technology, a system comprising seven full rack units of Power A2 processors, with a total of more than 114,000 processor cores and 7 TB RAM.

The second supercomputer, named Blue Wonder, is an IBM System x® iDataPlex® dx360 M4 cluster, composed of 512 computing nodes, each with dual eight-core Intel Xeon E5-2670 processors with a minimum of 32 GB of memory. The systems are connected by IBM General Parallel File System (GPFS™) software to 5.7 PB of high-performance DDN SFA10K disk storage and a 15 PB IBM System Storage® TS3500 tape library.

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— Adrian Wander, Director of the Scientific Computing Department at the STFC Daresbury Laboratory and STFC Rutherford Appleton Laboratory

Blue Joule is the fastest and most energy-efficient supercomputer in the UK. It is currently the sixteenth fastest computer in the world. Blue Wonder is ranked at 158 on the list of the world's fastest supercomputers.[2]

The Hartree Centre also works with OCF to offer enCORE on-demand HPC services that can be purchased at a scale to suit the customer. This helps small businesses eliminate the requirements for capital expenditure and in-house skills development that can often be a barrier to entry, and allows customers to sample the benefits that HPC can bring for the first time.

The Hartree Centre utilizes IBM expertise to deliver optimal performance while saving on electricity costs. For example, the center and IBM are investigating the use of energy-aware task scheduling to enable similar tasks to be bundled together, which could reduce the time and energy wasted on reconfiguring resources between jobs. The center is also looking at optimizing the balance between clock speed and energy consumption, where large energy savings can be achieved with nominal impact on performance.

The IBM teams have been able to draw on past experiences to help boost user-friendliness of the Hartree Center's HPC solutions, as Adrian Wander, Director of the Scientific Computing Department at the STFC Daresbury Laboratory and STFC Rutherford Appleton Laboratory describes: "A key advantage of working with IBM is that not only are they at the leading edge of HPC, but they also have experience of bringing this technology to non-specialist users.

"For example, IBM recently worked on a project with Unilever where iPads were used as the user interface. We have been able to replicate elements of this interface for our own users – making a very complex set of assets much more accessible."

"Working with the Hartree Centre, companies such as Bentley Motors and Jaguar Land Rover are collaborating with organizations such as VEC [Virtual Engineering Centre] and Optis to explore ways to dramatically reduce development cycles."

— Michael Gleaves, Head of Business Development, the Hartree Centre

Working with Big Data

Both Blue Joule and Blue Wonder use IBM GPFS software to manage massive volumes of high-performance data which are growing exponentially. GPFS allows thousands of compute nodes to access data simultaneously, enabling the massive parallelization of workload crucial for complex computing tasks at the center.

The Hartree Centre is exploring the use of Apache Hadoop, an open-source software project that enables the distributed processing of large data-sets across clusters of servers, to extract meaningful insights from large amounts of unstructured data. The center is also looking into the analysis of information in motion.

Michael Gleaves says: "Getting a handle on Big Data is a key challenge for businesses around the world, making it a significant opportunity for the Hartree Centre. Big Data is still within an early adopter phase within most businesses, and so offering a place where companies can come and explore the potential to gain insight and value from their data combined with available open data sets within projects is a critical goal for Hartree."

Seeing it in action

One of the first major projects to benefit from the Hartree Centre's services is "Gung-Ho": a project to design and build a next-generation weather forecasting model for the UK; a collaboration between the Met Office, the Natural Environment Research Council (NERC) and STFC.

Adrian Wander comments: "Severe winter weather experienced in the UK over the last couple of years is expected to have reduced the UK's GDP by 0.5 percent, with the disruption to travel costing the economy up to £280 million per day.[3] As a result, more accurate weather forecasting can have a huge impact. By using sophisticated models that study and simulate how air moves, we can help the Met Office and NERC gain a more detailed and precise understanding of weather conditions."

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Encouraging collaboration

Fostering collaboration and innovation is at the heart of the Hartree Centre's ethos, and its participants are already seeing the positive consequences.

One example is the automotive industry, as Michael Gleaves explains: "Automotive companies are a great example of the difference HPC can make. Building a physical wind tunnel to test the aerodynamics of your design costs millions, while running virtual tests with us can yield accurate results at a tiny fraction of the cost and time. Working with the Hartree Centre, companies such as Bentley Motors and Jaguar Land Rover are collaborating with organizations such as VEC [Virtual Engineering Centre] and Optis to explore ways to dramatically reduce development cycles."

The Hartree Centre is also working with laboratories and research organizations around the world. Adrian Wander concludes: "Collaboration and knowledge-sharing are part of the Hartree Centre's DNA. By joining up with similar organizations we can identify skills and assets that complement our own, and deliver even more value to UK businesses."

For more information

Contact your IBM sales representative or IBM Business Partner, or visit us at: **ibm.com**/technicalcomputing

1. Source: A Strategic Agenda for European Leadership in Supercomputing: HPC 2020 — IDC Final Report of the HPC Study for the DG Information Society of the European Commission (www.hpcuserforum.com/EU/downloads/SR03S10.15.2010.pdf)

2. Source: Top500 List - November 2012 (www.top500.org/list/2012/11)

3. Source: The next step on the road to more accurate weather forecasts (www.stfc.ac.uk/Hartree/resources/PDF/GungHoArticle.pdf)