



Hartree Centre

Science & Technology Facilities Council

Cliff Brereton

Director, Hartree Centre

Being 'Essential'



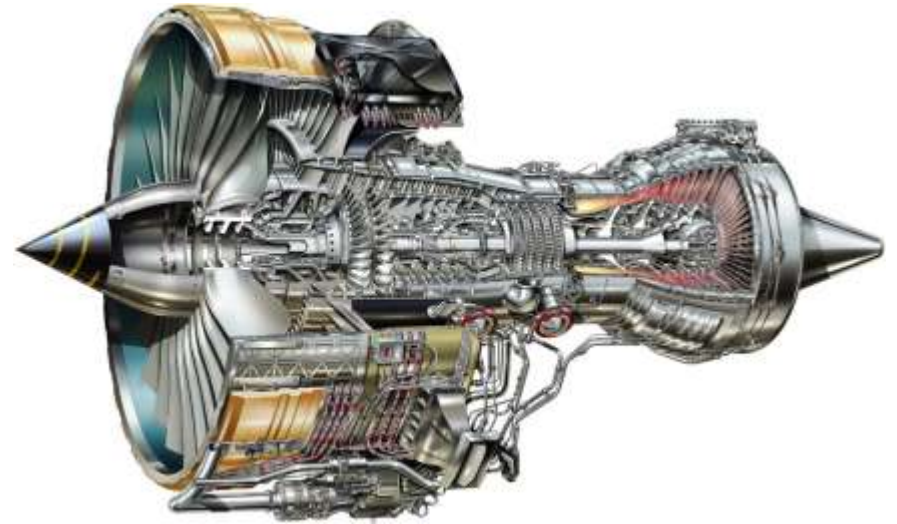
E-Infrastructure

- 2011 Tildesley Report
- £160M Investment from BIS
- Economic Impact through Software & Modelling

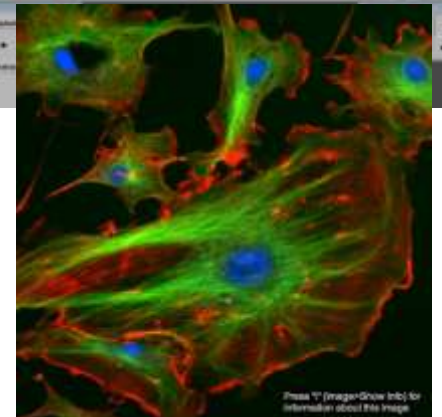
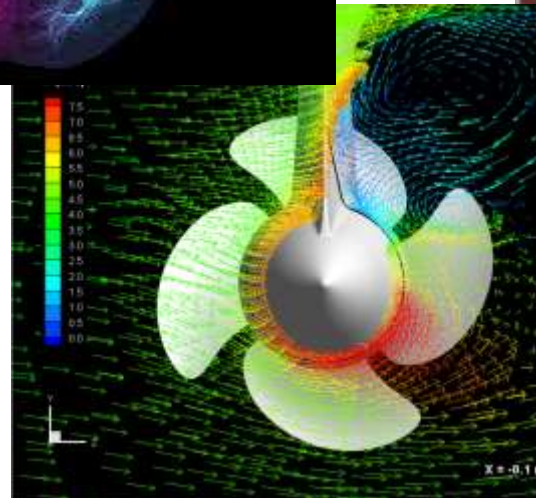
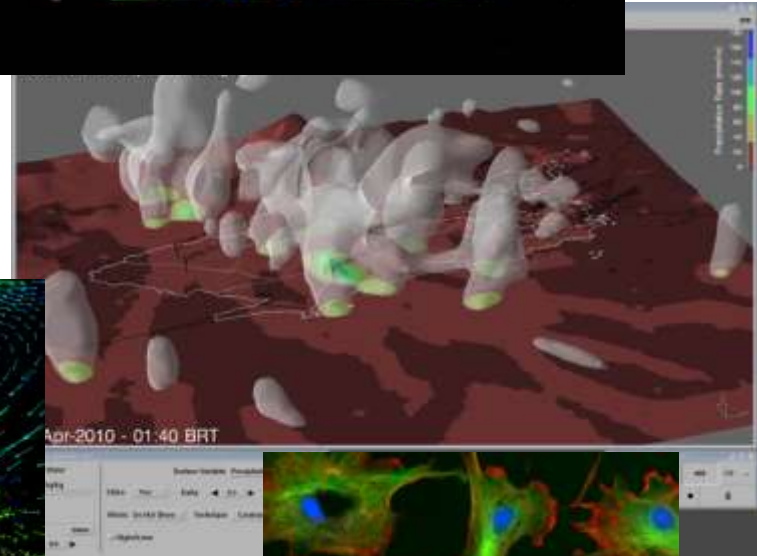
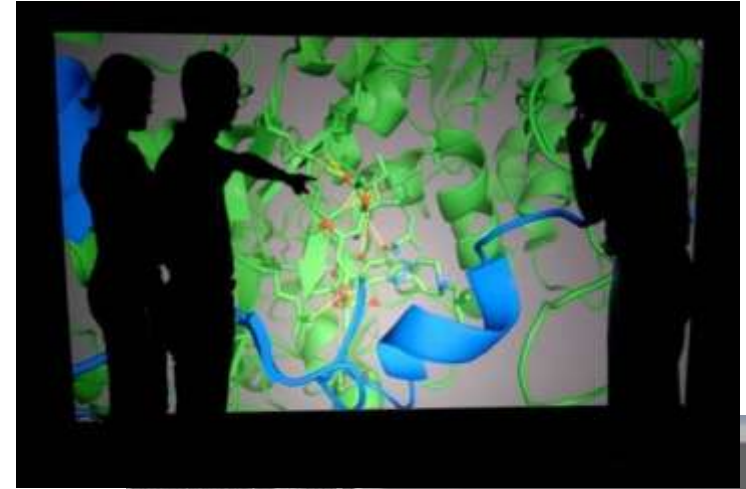
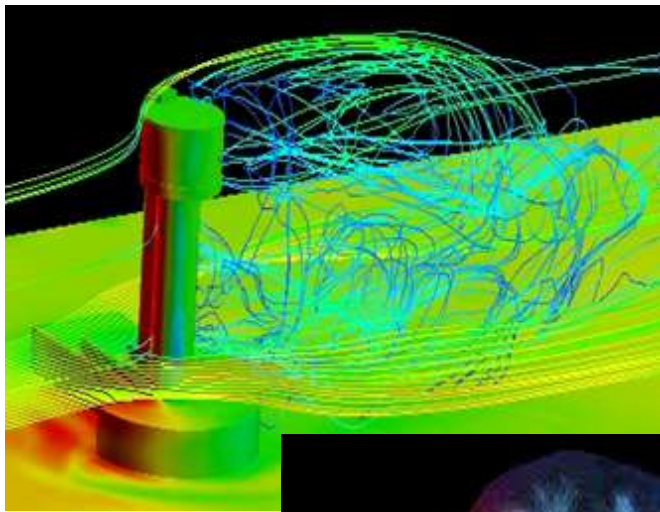
“To out compute is to out compete”



By Design



ARM, BAE, Bentley, Glaxo Smithkline, Unilever, JLR,



‘Value’

"It costs £500,000 to do each physical test of a car crash, and it's not repeatable. It costs £12 to run a virtual simulation of a car crash, and it's fully repeatable"
Andy Searle, Head of Computer Aided Engineering,
Jaguar Land Rover.

Our customers tell us ‘Value’
is defined as:

- More Sales, More Customers
- Products developed Better,
Faster, Cheaper
- = Competitive Advantage



Client Projects include

- Engineering & Manufacturing
 - Vehicle Design & Testing
 - Consumer Electronics Design
 - Consumer Packaged Goods Design
- Environment
 - Weather modelling
- Life Sciences
 - Genomics for better crop yields
- Energy
 - Advanced Battery Cell Design
 - Efficient Well Head Oil extraction
- Financial Services
 - Risk Management
 - Service Modelling



The collage features several project posters with the following titles and descriptions:

- Accelerating the product discovery process at Unilever:** Unilever is taking advantage of the STFC Hartree Centre's expertise in high-performance computing (HPC) to model key ingredients of Equaliser and personal care products, compare to their own existing recipe.
- Accelerating product design and development at Jaguar Land Rover:** Innovative expertise and an on-site computing facilities for product design, testing, simulation, and development.
- Smaller, affordable particle accelerators for healthcare and life sciences:** Nuffield Foundation has awarded the highest ever computing grant to STFC Hartree Centre to develop a new generation of compact particle accelerators for research and education.
- Building next generation materials simulation tools with NPL:** The UK's National Physical Laboratory (NPL) is developing new research computing capabilities for materials simulation.
- New gas for more:** STFC Hartree Centre is currently simulating the flow of complex fluids to improve oil extraction.
- Supporting new product design at:** Following the development of a virtual reality simulation tool, STFC Hartree Centre is supporting the design of a new product.
- Newspapers at Lancaster University:** STFC Hartree Centre is currently simulating the flow of complex fluids to improve oil extraction.

Unilever



Hartree Centre
Science & Technology Facilities Council





Hartree Compute assets

- Blue Joule 98,000 Cores (1.2 Pflops)
- Blue Wonder 20,000 Cores
- 9PB of Disk Storage
- 15 PB of Tape Storage
- 3 Visualisation Walls
- Big Data Analytics Cluster (288TB)
 - At Rest
 - Streaming
- ‘Novel’ server technologies
- STFC / e-Infrastructure South
 - Nvidia Tesla GPU Cluster



Our People

- Engineers
- Chemists
- Life Scientists
- Mathematicians
- Software Developers
- Data Scientists



Hartree Service Offerings

- **Collaborative R&D**
 - Outcome focused projects
 - “Help me make a better.....”
 - Primary cost element is staff
- **Software & Algorithms**
 - New software applications for HPC or Big Data
 - New Algorithms
 - Optimisation of existing codes for new platforms / architectures
- **Training & Skills**
 - Logical course curriculum to broaden and deepen adoption and application of Modeling & Simulation
- **Platform as a Service**
 - Timeshare use of Hartree assets
 - Predominantly self service
 - Primary cost element is machine asset time
 - May or may not include Hartree owned software assets
 - May include some separately costed Hartree staff effort



Hartree Centre and LLNL HPC Innovation Centre



- Agreement signed August, 2013
- Sponsorship from respective Governments.
 - To share & grow ‘know how’ and competitive advantage
 - Industry Focus
 - Technical - Software
 - Emerging technologies – Big Data, Energy Efficient compute, etc
 - To support ‘Anglo-American’ Commercial Client Engagements
- Commitment from a shared industry partner - IBM



Workflow within our Partnership

- Industry Days
- Collaborative workshops
- Joint client projects
 - Engineering
 - Life Sciences
- Client Engagement support
 - Scale and skills
- Technology Exploration



Summing Up

- E-Infrastructure provides better products, faster and cheaper.
 - Competitive advantage and ROI
- Accessing these assets is easy
- Partnerships provide:
 - Access to clients
 - Skills
 - Know how
 - Technologies
 - 1+1=5



Thank you



**Science & Technology
Facilities Council**

Cliff Brereton

Director of the Hartree Centre

Science and Technology Facilities Council

Sci-Tech Daresbury, Keckwick Lane, Warrington, Cheshire

WA4 4AD, United Kingdom

Tel: +44 (0)1925 603236

Mobile: +44 (0)7557 633386

Email: cliff.brereton@stfc.ac.uk

Web: www.stfc.ac.uk

Twitter: @c11ffb