Science & Technology Facilities Council

The Hartree Centre
A Research Collaboration in Association with IBM

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Outline

- What's so good about HPC?
- STFC
- SCD
- Hartree Centre
  - What we do
  - Facilities and Resources
  - Capabilities
  - 2 Examples

IDC said ….

- Software leadership will become the New Battleground
  - Only 1% of HPC codes can exploit 10,000 or more cores
  - There May Be More Emphasis on Software … Finally
- Big Data Methods Will Start to Transform the HPC Market, Including Storage
  - HPC and commercial Big Data are starting to collide
- Petascale Performance on Big Systems Will Create New Business Opportunities
- The HPC Staffing Shortage Will Grow More Acute

Return on investment

- UK tax revenues exceed 35% of GDP
  - Forecast tax revenue for 2016 is >£700,000M
  - Forecast GDP for 2016 is >£2,000,000M
- A 0.1% increase in GDP leads to additional annual £700M in tax revenues (net taxes & NI contributions)
  - IDC & others forecast a much greater increase in GDP than this
- So a £145M investment shows a pretty decent return on investment; even a 0.01% increase in GDP pays for itself after 2 years
- And, by the way, we paid £6.3M in VAT for our HPC systems!

What is HPC used for?

- Some examples

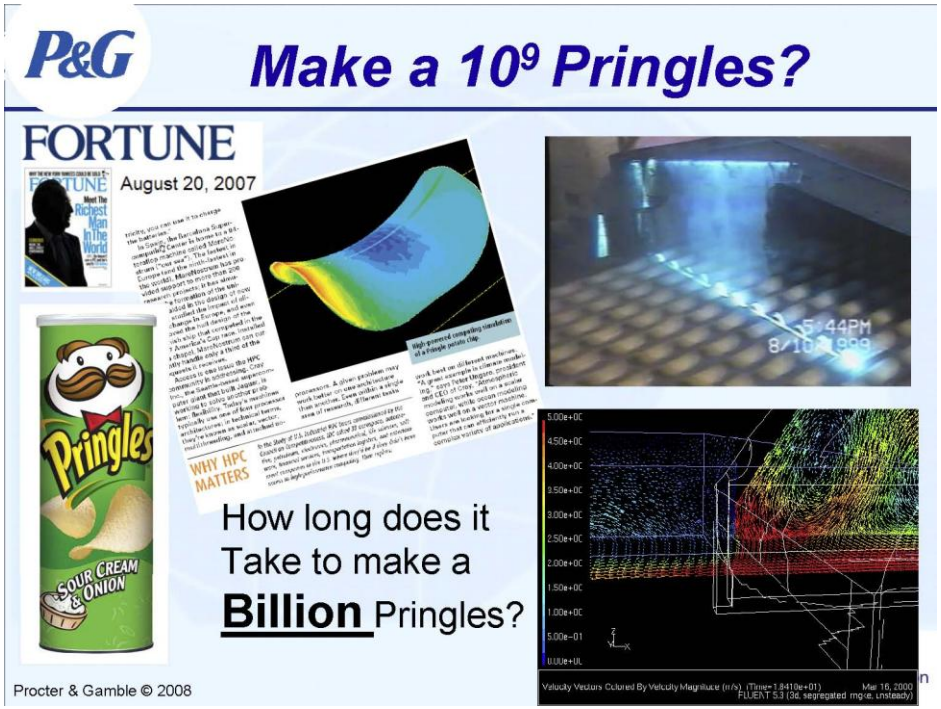
- Product design and performance
- Design and test of new medicines and drugs
- Understanding the origins of the universe
- Designing safer and more efficient vehicles
- Understanding climate change
- Predicting tomorrows weather, floods, …
- Finance, insurance, investments

HPC in Procter & Gamble

Competitive Advantage

- How long to make 10^9 pringles?
  - Aerodynamics
  - How long does it take for the oil to drain away?

- Free surface flow on & through compressible partially saturated porous material
- Braun Shaver – drop it on floor
- Peeling of Yogurt cartons
- Virtual Filling
- Bottles on a production line



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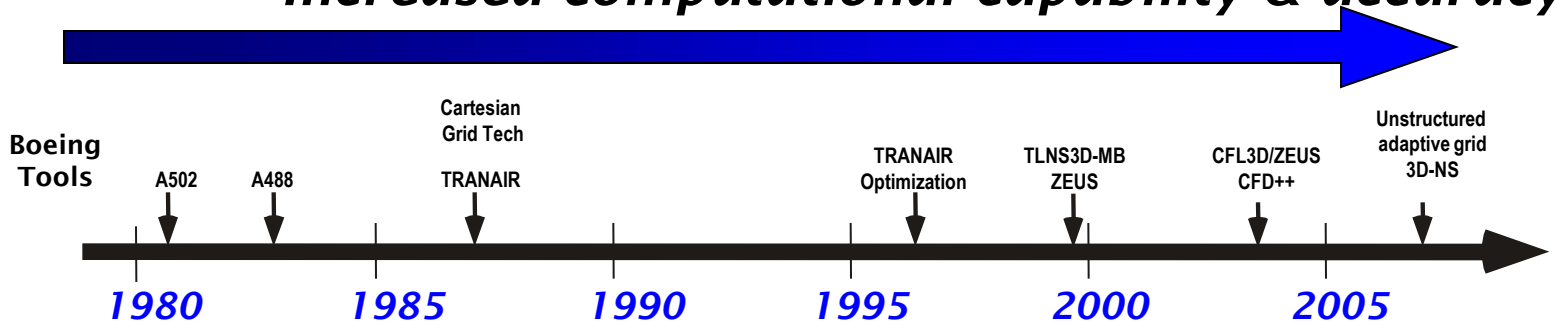
CFD Has Significantly Improved the Wing Development Process

Increased computational capability & accuracy

CFD Tools



Boeing Products

767 757 737-300

777 737NG

787

1980 state of the art

Modern close coupled nacelle installation, 0.02 Mach faster than 737-200

21 %thicker faster wing than 757, 767 technology

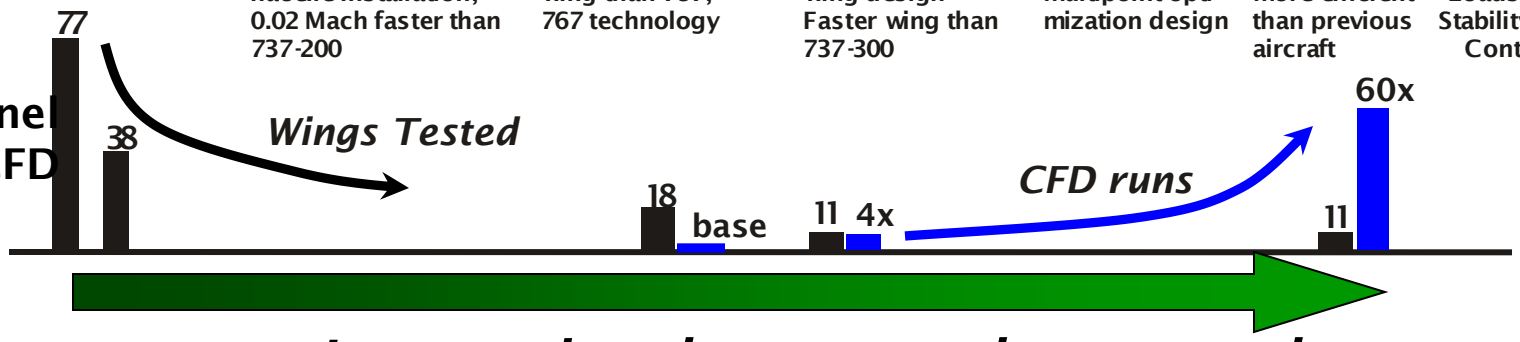
Highly constrained wing design Faster wing than 737-300

Successful multipoint opti - mization design

Faster and more efficient than previous aircraft

CFD for Loads and Stability and Control

Wind Tunnel vs. CFD



Less testing, lower cost, better products

Business Benefits

- Reduce the following
  - Time to market of a design
  - Component costs
  - Design and certification costs
  - Number of destructive tests of components and engines
- Increase the quality of the product (via better fidelity of the simulations)
- Reduces service & maintenance costs
- Ensure the integrity of the design

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HM Government & HM TREASURY

BIS | Department for Business Innovation & Skills

RESEARCH COUNCILS UK

Arts & Humanities Research Council

BBSRC bioscience for the future

E·S·R·C ECONOMIC & SOCIAL RESEARCH COUNCIL

EPSRC Pioneering research and skills

MRC Medical Research Council

NATURAL ENVIRONMENT RESEARCH COUNCIL

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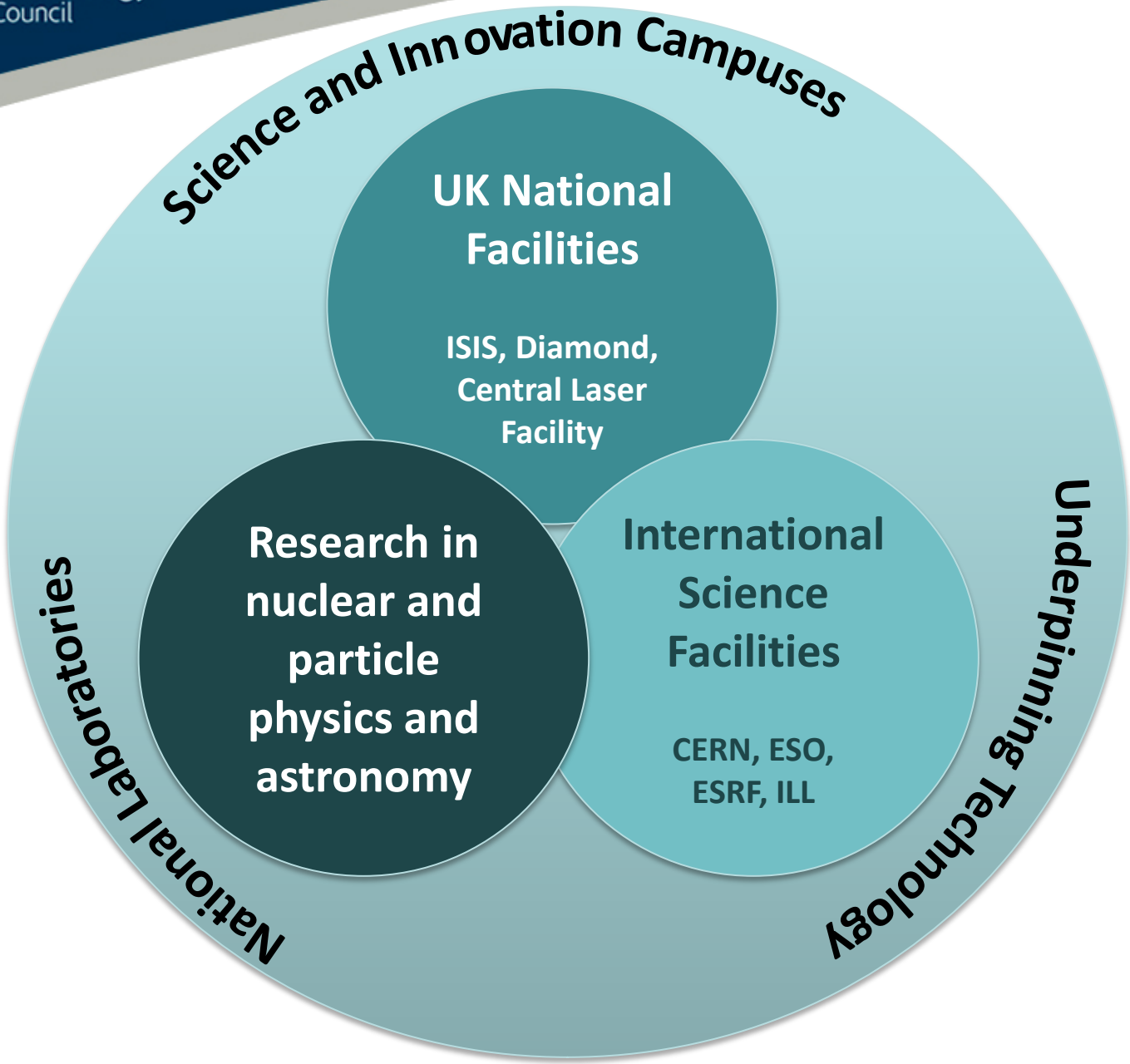
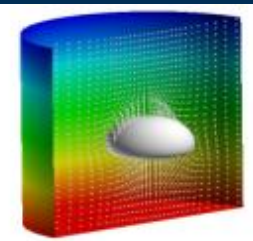
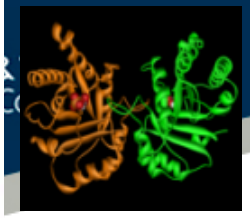
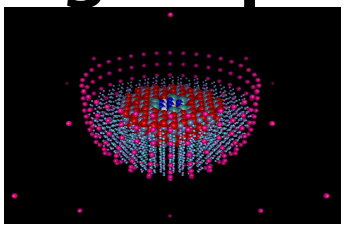
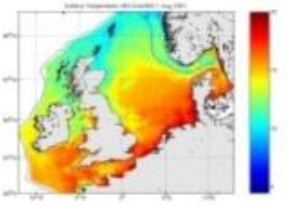




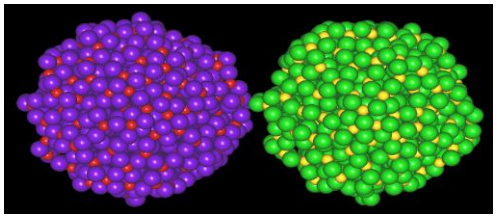


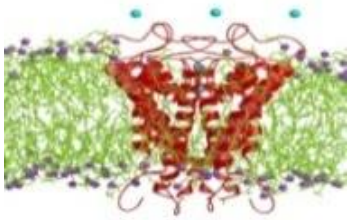
Scientific Computing Department

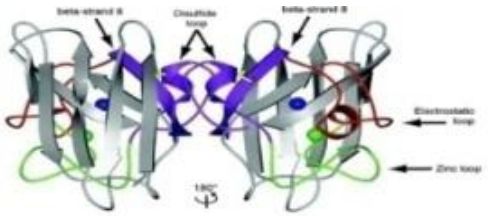


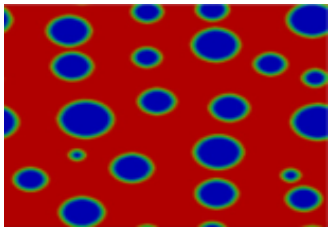


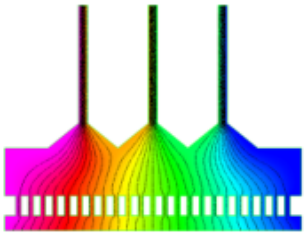
- 160 staff supporting over 7500 users
- Applications development and support
- Compute and data facilities and services
- Research: > 100 publications pa
- Deliver >3500 training days pa
- Systems administration, data services, high-performance computing, numerical analysis & software engineering.

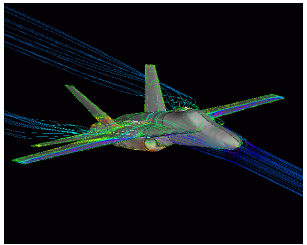


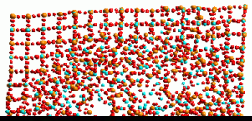


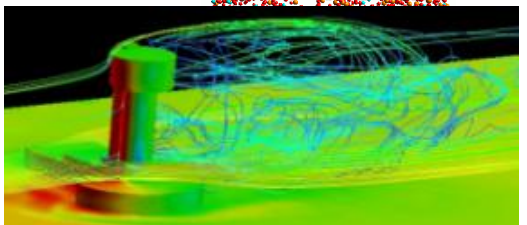




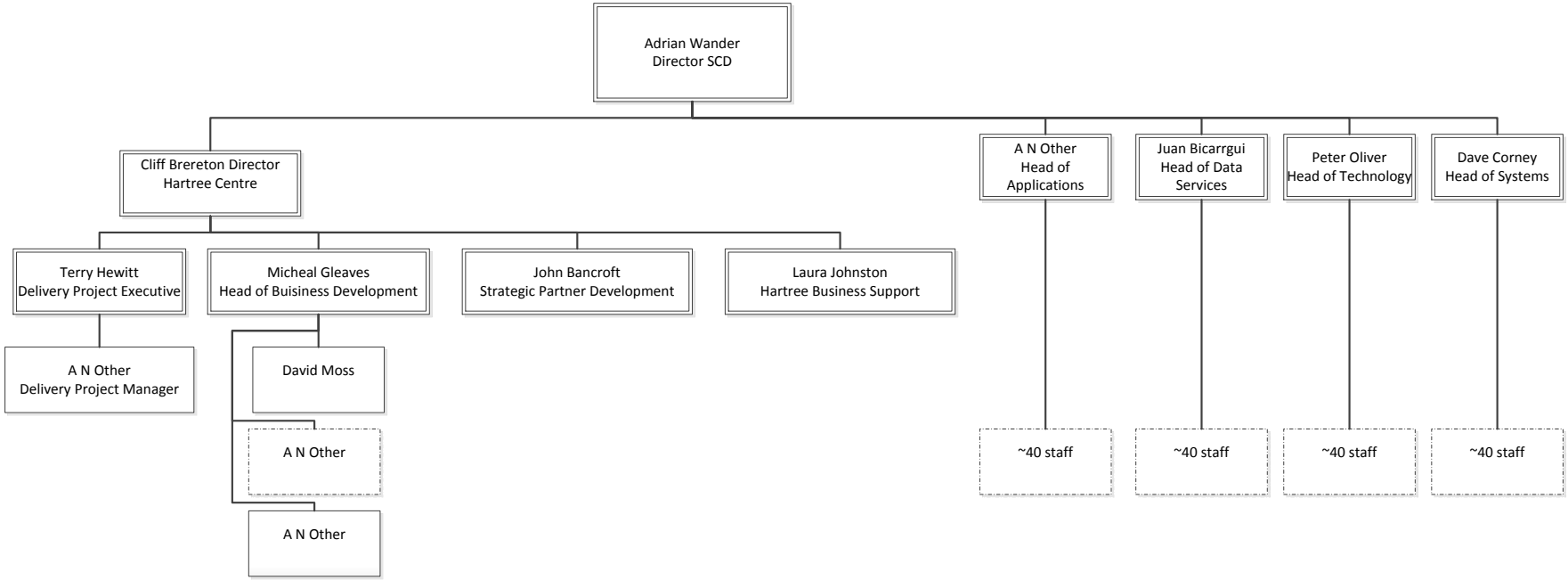








- Capital - BIS
  - £37.5M spent
  - £19M (energy efficient computing)
- Recurrent
  - STFC (£2M, £3M, …)
  - Our own efforts to gain income



Hartree Centre Objectives

Deliver future-proof software capable of exploiting the most powerful hardware platforms

To make using HPC as easy as using a laptop

Build capacity

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Douglas Rayner Hartree

- Hartree – Fock
- Appleton – Hartree Equation

- Differential Analyser
- Numerical Analysis

- Father of Computational Science

Douglas Hartree with Phyllis Nicolson at the Hartree Digital Analyser at Manchester University

- He said in 1946
  - *It may well be that the high-speed digital computer will have as great an influence on civilization as the advent of nuclear power.*

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Differential Analyser

Hartree Centre

- What? - Deliver 'Value'
  - More innovative products / Services – More Sales
  - Reduce time to value and associated R&D unit costs
    - **Economic Impact**
- How?
  - Creating new software and algorithms
  - Optimizing existing software for new architectures
  - Utilizing existing software models & Visualization in new use cases
    - **People, Partners**
    - **Technology, Software assets and IP**
  - Joint research projects with IBM Research
  - Support for marketing & business development from IBM
- Who for?
  - Academia, Consumer Electronics, Oil & Gas, Healthcare, Life Sciences, Automotive, Aerospace, Defence, Pharma, Electricity Generators, Banking, Government Agencies

Hartree Centre Future

- Big Data
  - Greater Insights (retrospective and real time)
    - **Volume**
    - **Velocity**
    - **Veracity**
- Exascale
  - Codes for new architectures
  - Energy Efficient computing
- Hartree@
  - Major National / International research centre collaborations
- Grand Challenges

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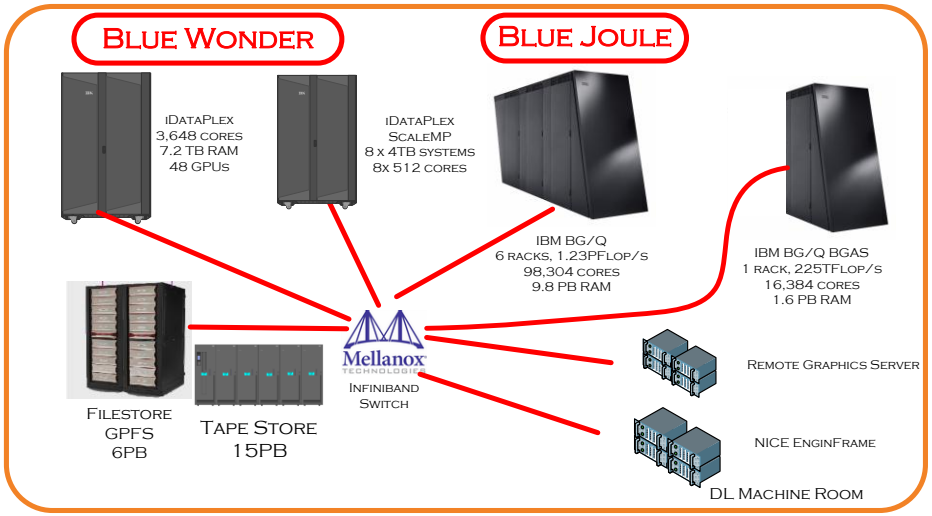
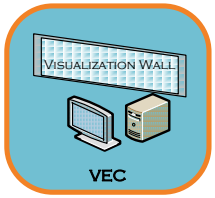
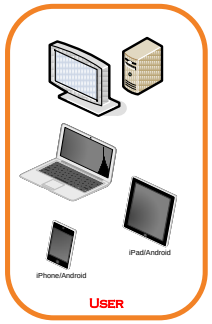
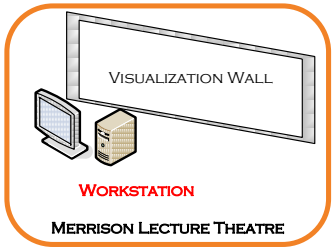
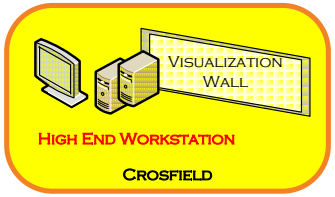
The Infrastructure

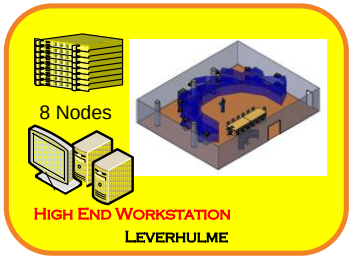










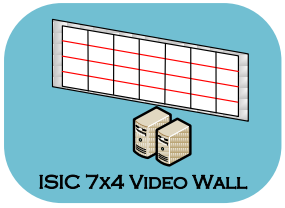


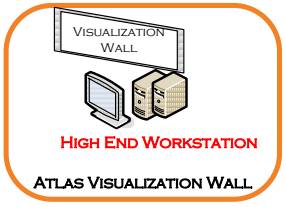
Off Campus

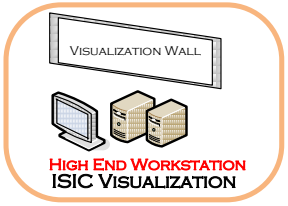
RAL

DL

Scarf
Emerald
Jasmin
NCCS







WTH Associates Ltd	
6/5/2013	Hartree Centre Architecture

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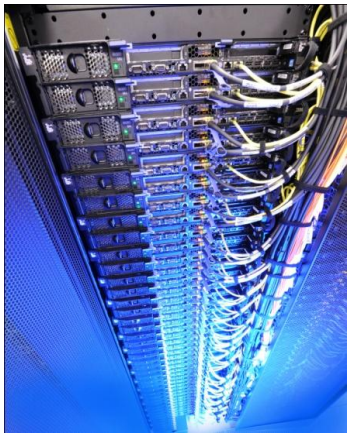
Applications and Optimisation

Software Development



HPC On-demand

Collaboration

Training and Education

EXAMPLE 1

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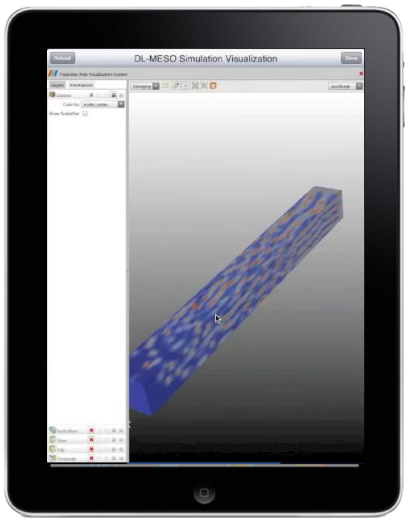
…and how to make HPC easier to use

Scenario: Chemists consult – change experimental design, run multiple simulations from mobile device in the lab to see what best choices of chemicals.

Parameters changed at bench on mobile device and results sent back to mobile device.

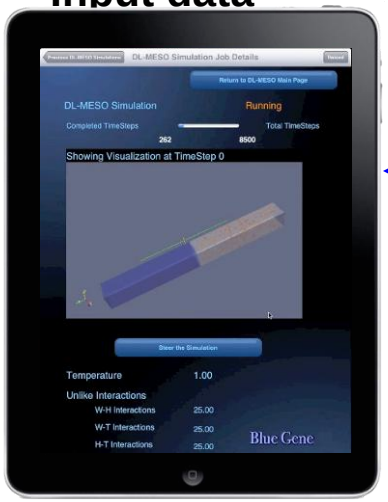
Multiple Inputs

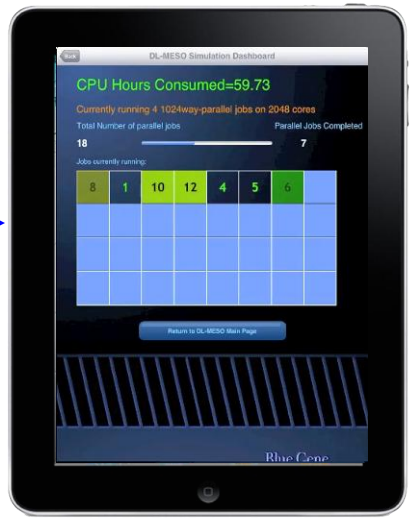
Results



Overview of Running Jobs

Input data





Unilever

EXAMPLE 2

- Over a weekend Blue Wonder, was used by the VEC on behalf of a customer
- Run in 24 hours an analysis of 100 design cases
  - takes 1 week to run on the customer's own system
- Jobs ran in 27.42 hours
  - Follow-up work on a larger problem size was also undertaken,
- In total 37,809 jobs were run,
  - using 474,762 cpu hours in 90 real-time hours.

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Track Record

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Thank you for listening

QUESTIONS