Science & Technology Facilities Council

The Scientific Computing Department Today

A high level overview of SCD. **David Corney**

SCARF a local HPC cluster supporting STFC scientists, collaborators and users from SCD, ISIS, CLF, RAL Space and Diamond. **Derek Ross**

Data analysis and data interpretation through modelling and simulation. **Barbara Montanari**

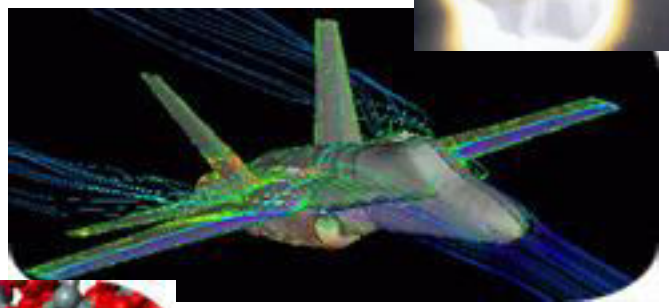
ATLAS@50 13 Nov 2014

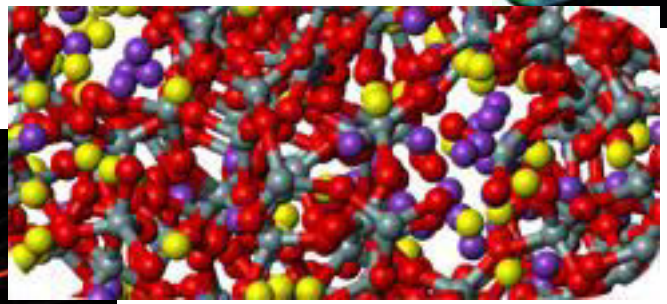
Science & Technology Facilities Council

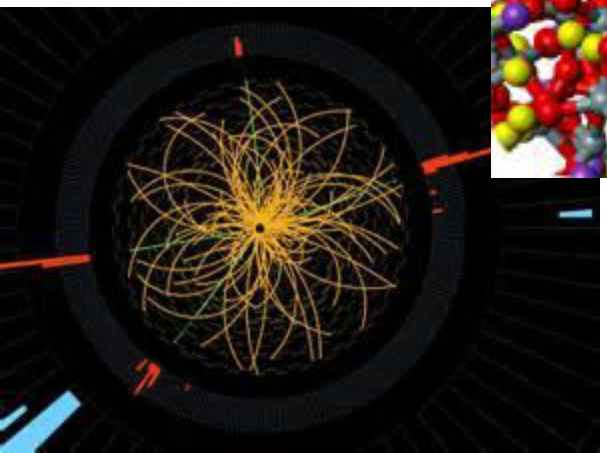
Scientific Computing Department

Established 1st April 2014

- 180 staff supporting over 7500 users
- Applications development and support
- Compute and data facilities and services
- Research: over100 publications pa
- Deliver over 3500 training days pa
- Systems administration, data services, high-performance computing, numerical analysis & software engineering.







World leading computational expertise to support Science and UK Industry

Science & Technology Facilities Council

www.stfc.ac.uk

Scientific Computing Department

Acting Director

David Corney

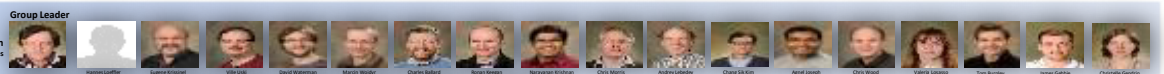
APPLICATIONS

Division Head

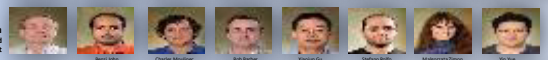
Paul Sherwood
Applications

Group Leader

Martyn Winn
Biology and Life Sciences

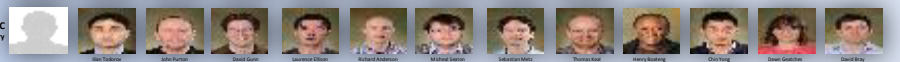


Dave Emerson
Engineering and Environment



Barbara Montanari
Theoretical and Computational Physics

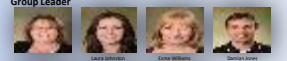
TBC
Computational Chemistry



CORE ACTIVITIES

Group Leader

Shirley Miller
DL Administration



RAL Administration

Finance

CECAM

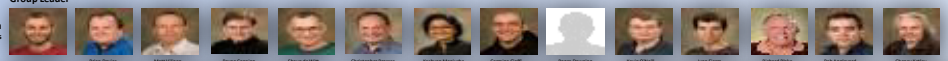
DATA

Division Head

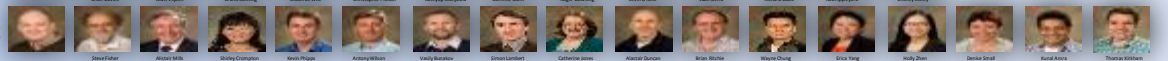
Juan Bicarregui
Data

Group Leader

Jens Jensen
Data Services

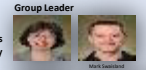


Brian Matthews
Research Data



Chadwick and RAL Libraries

Group Leader



Debbie Franks
Daresbury Laboratory

Rutherford Appleton Laboratory

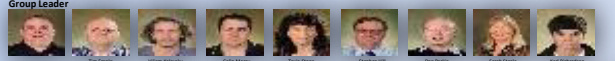
SYSTEMS

Acting Division Head

Andrew Sansum
Systems

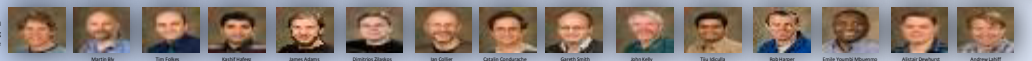
Group Leader

Dave Cable
High Performance Systems



Nick Hill
Research Infrastructure

Andrew Sansum
Peta Scale Computing and Storage



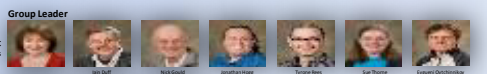
TECHNOLOGY

Division Head

Peter Oliver
Technology

Group Leader

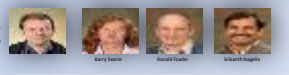
Jennifer Scott
Numerical Analysis



Chris Greenough
Software Engineering

Mike Ashworth
Application Performance Engineering

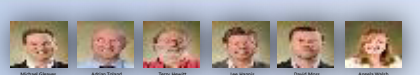
Martin Turner
Visualisation



HARTREE CENTRE

Division Head

Cliff Brereton
Hartree Centre



GRADUATES

HONORARY SCIENTISTS

Bill Smith
Dzidka Szotek
Valerie Burke
Paul Kummer
Bob McMeeking
John Reid
Paul Strange

VISITING SCIENTISTS

Coralia Cartis
Jack Dongarra
Kirk Jordan
Stanko Tmoic

VISITORS

Liam Jones OCF
Jeremy Appleyard NVIDIA

September 2014

Science & Technology Facilities Council

Emerald

NSCCS

NSCCS (National Service Computational Chemistry Software)

Providing National and International Compute, Training and support

EPSRC Mid-Range Service

- SGI Altix UV SMP system, 512 CPUs, 4TB shared memory
- Supports over 100 active users
- ~70 peer reviewed papers per year
- Over 40 applications installed

Portal to submit jobs

- to allow access to less computationally aware chemists

EPSRC
Pioneering research and skills

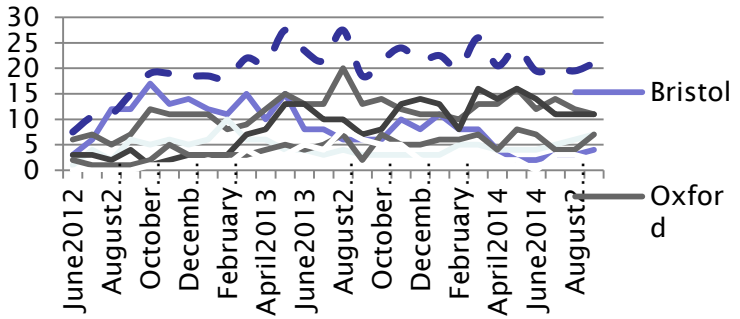
Imperial College London

372 Nvidia M2090 GPU cluster purchased in 2012

Run for a consortium of universities – Bristol, Oxford, Southampton and UCL and a small number of external users from academia and industry

- Wide range of scientific usage from drug discovery to climate modelling: http://www.cfi.ses.ac.uk/show-cases/

Two functions – large scale GPU resource and also supporting porting codes to GPU



- Data Archive for BBSRC
- Data Support Service for MRC

JASMIN/CEMS Hardware

Science & Technology Facilities Council

NERC SCIENCE OF THE ENVIRONMENT

The JASMIN "super-data-cluster"

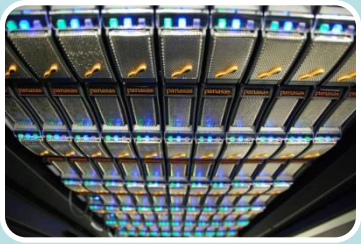
- Bringing the compute to the data for all NERC sciences.
  - Data : Measured and Simulation
- Facilitating further comparison and eval. of models with data
- Initially UK and Worldwide climate and weather modelling community.
  - CEMS (Climate and Environmental Monitoring from Space) with UKSA and Industry
  - CMIP5 / IPCC (Climate Change) Data Analysis (~1PB)
  - MetOffice, ECMWF etc
- Now all of NERC environmental sciences since JASMIN2
  - Eg Genomics, Hydrology, Oceanography, Oil & Gas…
- Supports 10,000 UK and World users via ~2PB CEDA archive (Centre for Environmental Data Archive).
  - http,ftp,scp, etc + helpdesk services
- Supports ~500 UK and World direct login users
- Supporting 'long tail' users via Cloud SaaS and PaaS Cloud technologies. Eg "Environmental Workbench".
- High speed dedicated network links to :
MetOffice, ARCHER, Leeds Uni., KNMI Holland, ESGF (Australia and USA)

National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL

National Centre for Earth Observation
NATURAL ENVIRONMENT RESEARCH COUNCIL

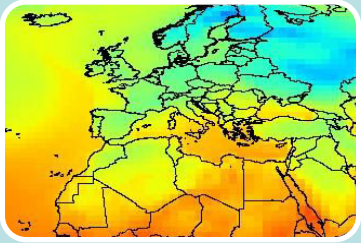
Science & Technology Facilities Council

JASMIN's Purpose



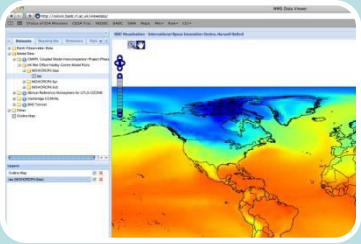
CEDA data storage & services

- Curated data archive
- Archive management services
- Archive access services (HTTP, FTP, Helpdesk, ...)



Data intensive scientific computing

- Global / regional datasets & models
- High spatial, temporal resolution
- Private cloud

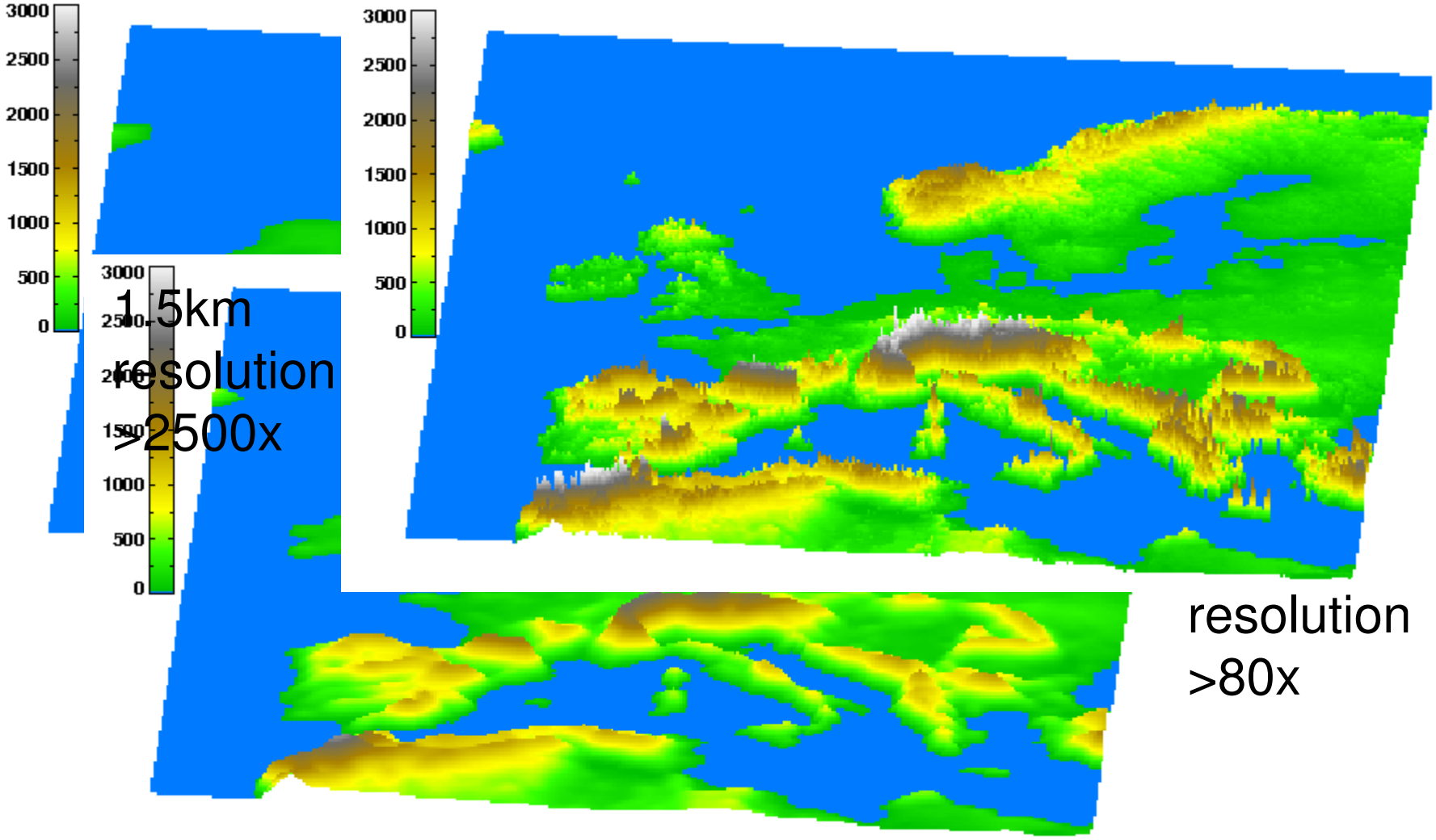


Flexible access to high-volume & complex data for climate & earth observation communities

- Online workspaces
- Services for sharing & collaboration

Value of model resolution – orographic height

Slide by permission of
Pier Luigi Vidale, NCAS (UoR)
Malcolm Roberts and
Matthew Mizielinski , UK Met Office



Tropical cyclone track density (transits per month)

Slide by permission of
Pier Luigi Vidale, NCAS (UoR)
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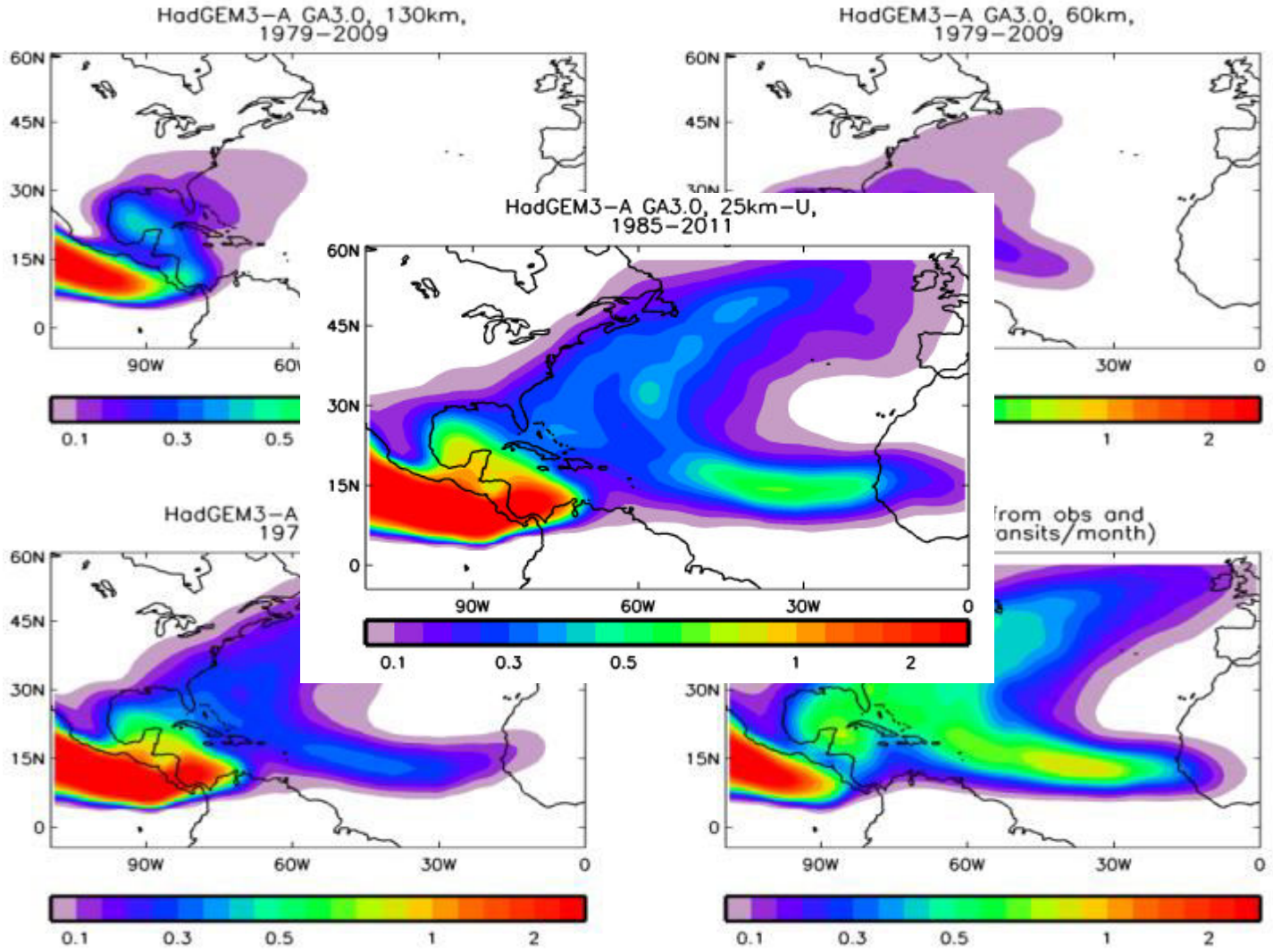


panasas

- Technology:
  - 12PB Parallel Storage Panasas at STFC (Largest in the world)
    - Fast Parallel IO to Compute servers
    - Largest capacity Panasas installation in the world
    - Arguably one of top ten IO systems in the world (~250GByte/sec)
    - "Game Changing" 100x throughput capabilities
    - Plans to expand to 30PB by 2020
  - 7PB On Tape (StorageD, CASToR)
    - Growing to >30-80PB by 2020 (Demand for 300PB by 2020)
  - Virtualised and Physical Compute (~3,5000 cores)
    - Physical Batch HPC compute: "LOTUS"
      - Mostly HTC. Some but not heavy parallel HPC/MPI.
    - User + Admin provisioned Cloud of virtual machines
      - Currently VMware/vCloud. Likely OpenStack at next renewal
  - Complex low latency , zero contention L3 ECMP Networking
    - >1200 x 10GbE ports. Few at this performance/scale.
  - Multiple Data xfer private network links to UK and World sites

IBM Platform LSF

NetApp

SUPERMICRO

DELL

vmware

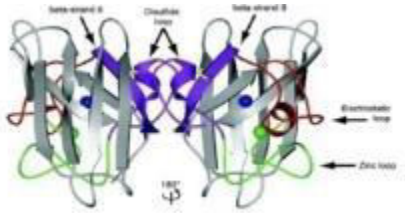
Mellanox TECHNOLOGIES

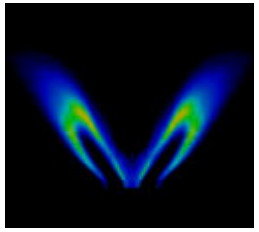
janet

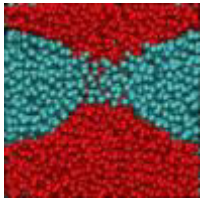
Science & Technology Facilities Council

Applications Division

- Four groups developing and applying computational science software packages to solve problems in the physical and biological sciences.
  - Computational Biology (Martyn Winn)
    - including structural biology, molecular simulation and bioinformatics
  - Theoretical and Computational Physics (Barbara Montanari),
    - electronic structure of the solid state and surfaces, atomic and molecular physics
  - Computational Engineering (David Emerson)
    - HPC solutions in fluid flow modelling, with particular strength in turbulence and microfluidics
  - Computational Chemistry (Ilian Todorov)
    - molecular dynamics, quantum chemistry and QM/MM techniques, and mesoscale methods







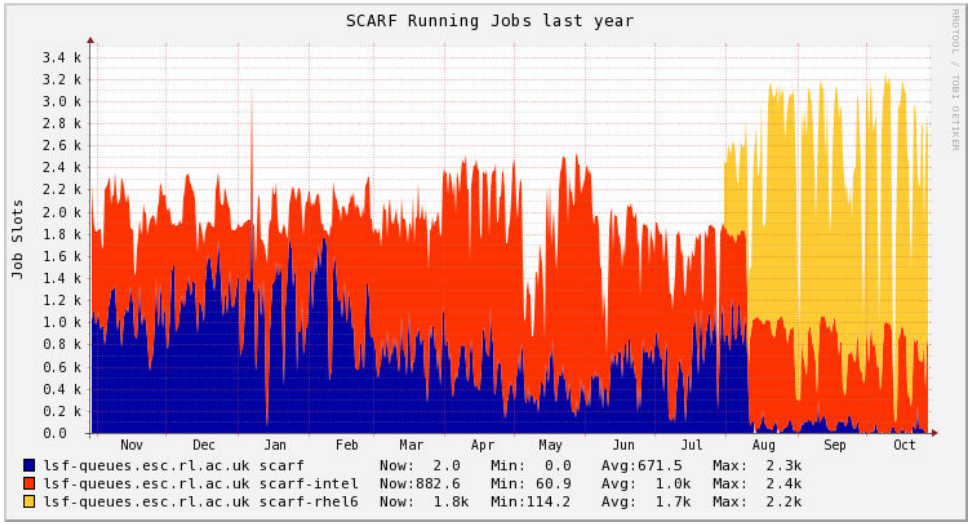
Collaborative Computational Projects

CCP4	Prof David Brown	Macromolecular Crystallography
CCP5	Prof Stephen Parker	The Computer Simulation of Condensed Phases
CCP9	Prof Mike Payne	Computational Electronic Structure of Condensed Matter
CCP12	Prof Stewart Cant	High Performance Computing in Engineering
CCP-ASEArch	Prof Mike Giles	Algorithms and Software for Emerging Architectures
CCP-BioSim	Prof Adrian Mulholland	Biomolecular Simulation at the Life Sciences Interface
CCP-EM	Dr Martyn Winn	Electron Cryo-Microscopy
CCPi	Prof Phillip Withers	Tomographic Imaging
CCPN	Prof Geerten Vuister	NMR
CCP-NC	Dr Jonathan Yates	NMR Crystallography
CCPP	Dr Tony Arber	Computational Plasma Physics
CCPQ *	Prof Tania Monteiro	Quantum Dynamics in Atomic, Molecular and Optical Physics
CCP-SAS	Prof Steve Perkins	Analysis of Structural Data in Chemical Biology and Soft Condensed Matter
CCPForge	Prof Chris Greenough	Collaborative Software Development Environment Tool

Science & Technology Facilities Council

SCARF

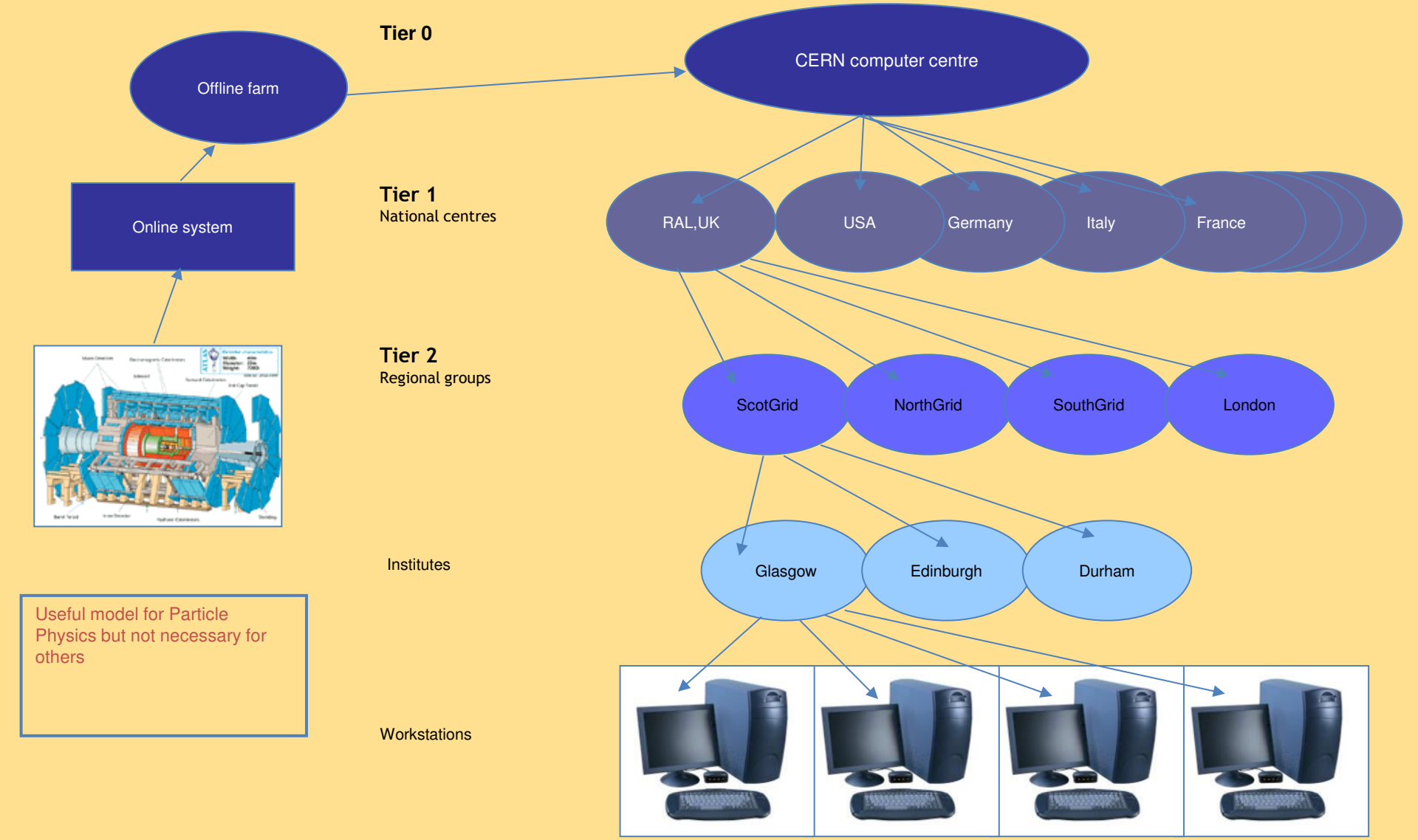
- STFC local HPC cluster supporting STFC scientists, collaborators and facility users
  - Users from SC, ISIS, CLF and others including RAL Space and Diamond
- 4400 cores, new equipment purchased yearly, decommissioned after 5-6 years
  - 3500 generally available, remainder are for particular user communities (CLF Plasma Physics, ISIS IBIS)
  - Recent years have seen additional capital investment from ISIS and CLF, each typically matching SC input
- 350 registered users



The LHC Tier 1 @ RAL

Context: WLCG architecture

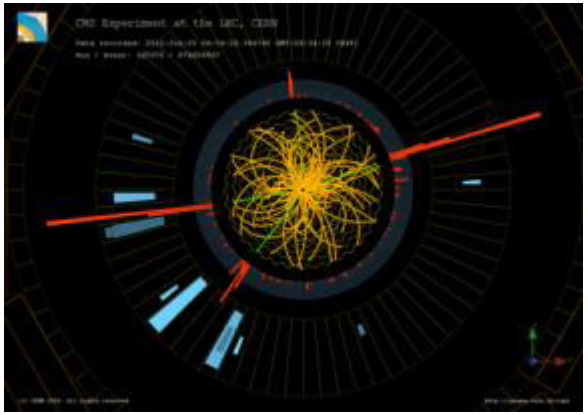
Useful model for Particle Physics but not necessary for others



The GRIDPP Tier-1 for the LHC

GridPP
UK Computing for Particle Physics

- High capacity service for hunting Higgs Particle
- Remote job submission (Grid)
- Low cost commodity hardware
- Open source middleware
- Delivered 99.2% availability in 2013 (70 hours lost all causes)
- Moves 50 petabytes/year globally (wide area transfers)
- Moves 300 petabytes/year internally (data processing)
- Preparing for Run 2 (data rates and volumes double)



- 13.6 PB disk
- 16 PB tape
- 10,000 CPU cores
- 2000 servers
- 40Gb network
- 10Gb/s direct optical link to CERN

Science & Technology Facilities Council
Rutherford Appleton Laboratory

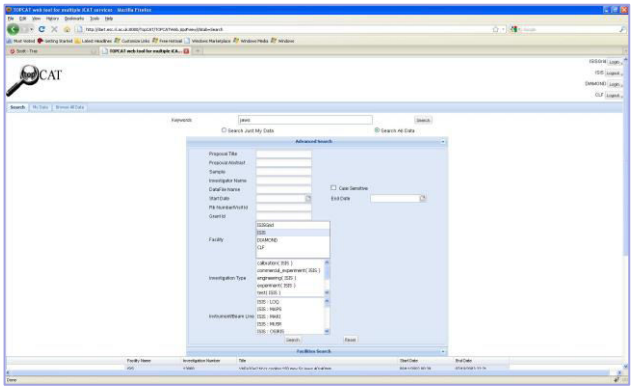
Tier-1 Facilities Infrastructure

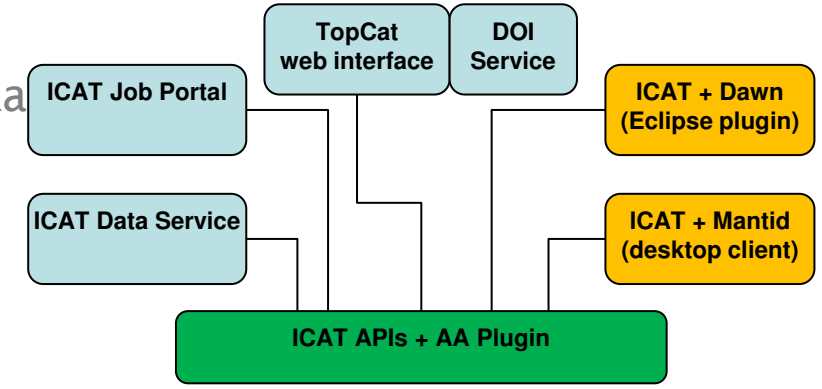
- Tier-1 Fabric team funded by facilities program to support some facilities hardware using Tier-1 infrastructure management:
  - Tier-1 virtualisation framework (HyperV)
  - Tier-1 configuration management system (Quattor)
- Tier-1 Production Team part funded to monitor and action facilities service exceptions
  - Also use Tier-1's change management process
- Facilities share funding with Tier-1 for CASTOR

- Tier-1 developing cloud access to CPU farm and large Object store (CEPH) to generalise service, giving opportunistic access to non Grid user communities (such as facilities.)

Supporting Data Management for STFC Facilities

- Integrated data management pipelines for data handling
  - From data acquisition to storage
- A Catalogue of Experimental Data
  - ICAT Tool Suite: *Metadata as Middleware*
  - Automated metadata capture
  - Integrated with the User Office system
- Providing access to the user
  - TopCat web front end
  - Integrated into Analysis frameworks
    - Mantid for Neutrons, DAWN for X-Ra
- In daily production use :
  - CLF, ISIS, DLS
- Also internationally:
  - ESRF, ILL,.SNS, …
  - PaNData Consortium





ICAT

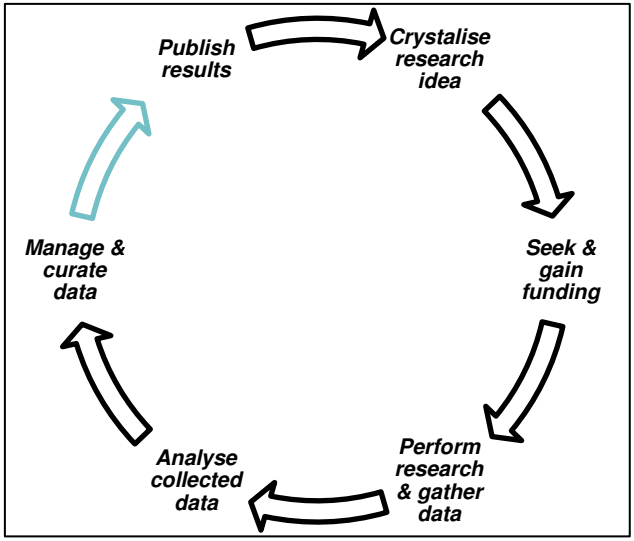
Integrating the Lifecycle

Growing opportunities to build on the data management infrastructure

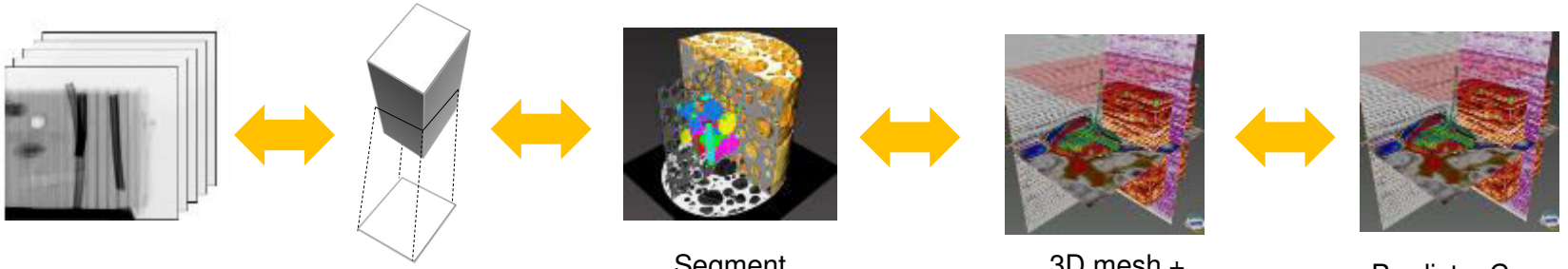
Extending the integrated data management system across the scientific lifecycle;

From Proposal to Publication

- Support post-experimental analysis
  - Image reconstruction with ISIS (IMAT) and DLS:
    - data from experiment, user access to SCARF
  - ICAT Job Portal for the LSF Octopus Facility
    - Integrated job submission
- Support Data Publication
  - DOIs issued for Data
  - Data Preservation
- Support Publications
  - STFC Epubs Repository
  - Linking data and publications to provide a record of science



Prototyping Post-experimental support



Scan | Reconstruct | Segment + Quantify | 3D mesh + Image based Modelling | Predict + Compare

Data Catalogue | Petabyte Data storage | Parallel File system | HPC **CPU+GPU** | Visualisation

Infrastructure + Software + Expertise!

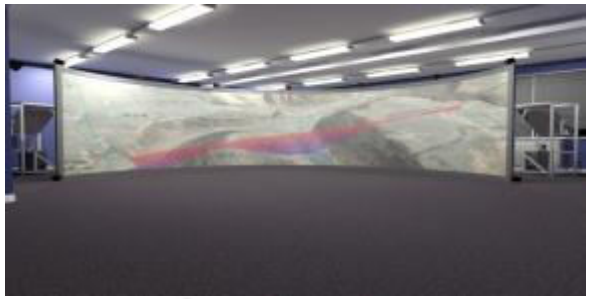
ISIS:IMAT

DLS:I12/I13

Tomography: Dealing with high data volumes – 200Gb/scan, ~5 TB/day (one experiment at DLS)

Some mage credit: Avizo, Visualization Sciences Group (VSG)

Facilities and Resources of The Hartree Centre



Projects and codes developed on state of the art systems:

BlueGene/Q – (Was) Fastest UK machine and world's largest software development platform

Over 5 PB disc and 15 PB tape stores

iDataplex cluster

Data Intensive systems

Visualisation System

Energy Efficient Computing program

Science & Technology Facilities Council

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

- SCARF a local HPC cluster supporting STFC scientists, collaborators and users from SCD, ISIS, CLF, RAL Space and Diamond. (**Derek Ross**)

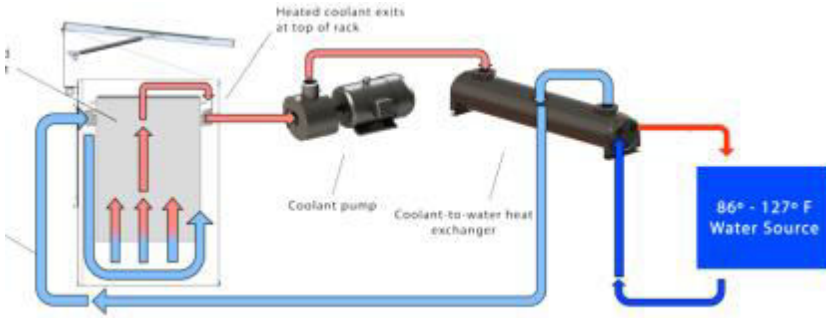
- Data analysis and data interpretation through modelling and simulation. (**Barbara Montanari**)

Science & Technology
Facilities Council

Science & Technology Facilities Council

Energy Efficient Computing

- IBM
  - NeXtScale, Idataplex, Intel Phi (£5M
    - 10,000 cores, 42 intel Phi
    - 3.2PB file store
  - BG Active Storage (£5M)
  - Low Power Processors (£0.7M)
    - NeXtScale + ARM CPUs
  - Big Data & Data Analytics (£4M)
- Insight/Clustervision
  - Novel Cooling Technology (£1M)
- Viglen/Maxeler
  - Dataflow Technology (£1M)



Science & Technology Facilities Council

EECRP topic areas

Energy Efficient Hardware: Latest semiconductor technology, Energy saving processor & memory technologies, Special hardware or accelerators.

Energy Aware Management Software: Monitor the energy consumption of the compute system and the building infrastructure, Use energy aware system software to exploit the energy saving features of the platform.

Energy Efficient Infrastructure: Reduce power loss in the power supply chain, Improve cooling technology, Reuse waste heat from systems.

Energy Aware Management Software: Develop efficient algorithms and tools, Optimise libraries, Use most efficient programming paradigm.

Science & Technology Facilities Council

HC Clients include

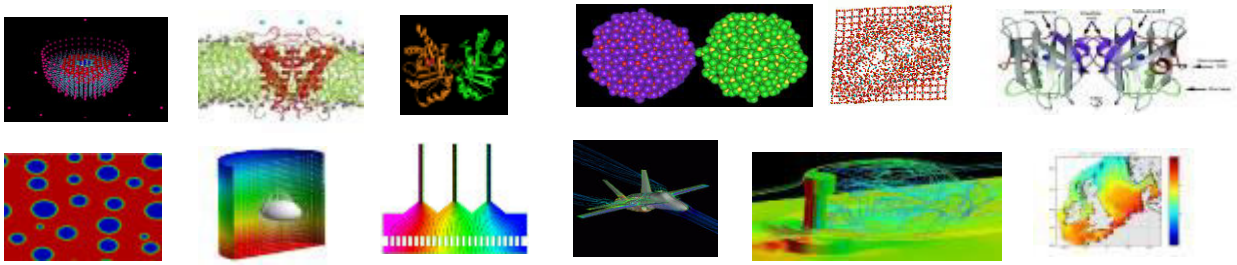
(c) 2013 Terry Hewitt

Science & Technology Facilities Council

Scientific Computing Department

- **Major funded activities**
  - 180 staff supporting over 7500 users
  - Applications development and support
  - Compute and data facilities and services
  - Research: over100 publications pa
  - Deliver over 3500 training days pa
  - Systems administration, data services, high-performance computing, numerical analysis & software engineering.

  - **Expertise across the length scales from processes occurring inside atoms to environmental modelling**



Science & Technology Facilities Council

The LHC Tier 1 @ RAL

To/from CERN:
Up to 40Gb/s

To/from SuperJanet5:
Up to 40Gb/s

- 10,000 batch cores
- ~15PB disk storage
- ~16 PB tape storage
- ~450kW power

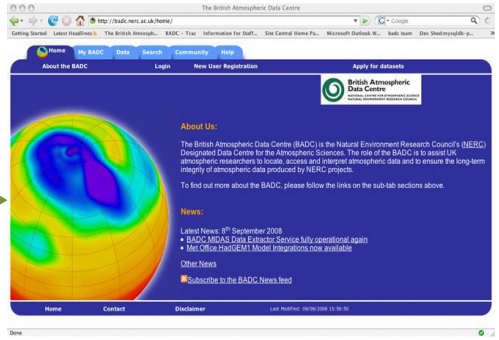
Higgs discovery

- 11 PB received by RAL
- 21 PB sent by RAL
- 60 PB processed by RAL

Common Components Architecture for Facilities Data Service

Synchrotron experiment data

CMIP5 data from CEDA



Storage-D
File
(de-) aggregator

CASTOR
HSM

XML metadata ingest

Selected experiment data

Select data for download

ICAT
Metadata
Catalogue

TopCAT web browser/**FUSE**

Catalogue query & selection

Selected experiment data

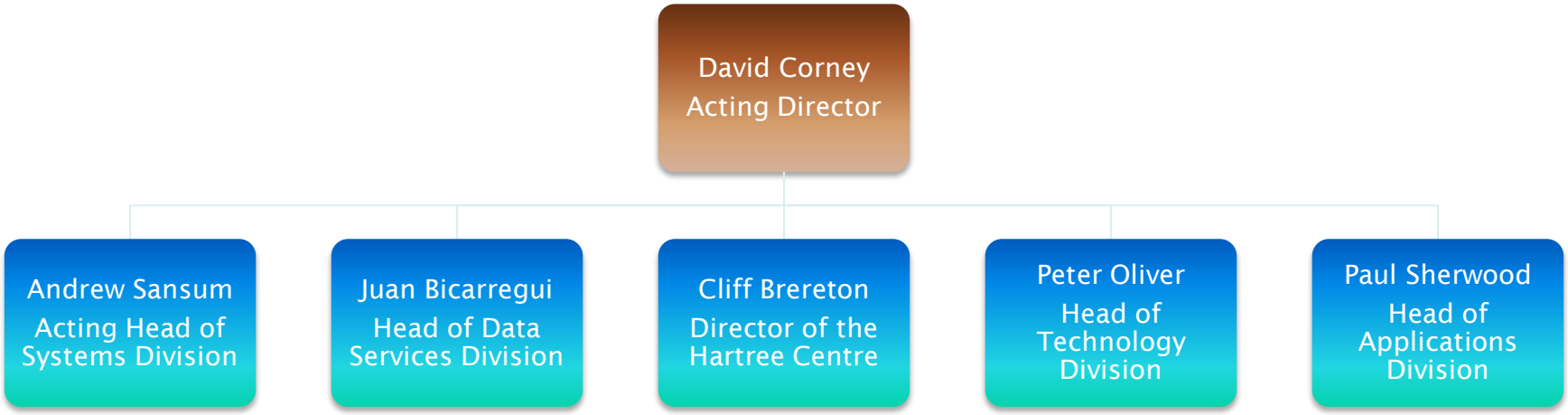
Catalogue query & selection

CEDA: 2.1 PB in 120 x10^6 files at September 2014

DLS: >2 PB in 548 x 10^6 files at September 2014

Science & Technology Facilities Council

Scientific Computing Department



Science & Technology Facilities Council

UK(1 of 2)

Imperial College London

KING'S College LONDON

Newcastle University

UNIVERSITY OF LEEDS

Aston University

Cranfield UNIVERSITY

UNIVERSITY OF BATH

Lancaster University

UCL

UNIVERSITY OF EXETER

Queen Mary University of London

Swansea University Prifysgol Abertawe

University of BRISTOL

UNIVERSITY OF CAMBRIDGE

Keele University

UNIVERSITY OF BIRMINGHAM

UNIVERSITY OF Southampton

MANCHESTER 1824 The University of Manchester

Durham University

University of Reading

University of Roehampton London

Science & Technology Facilities Council

UK (2 of 2)

THE UNIVERSITY *of* EDINBURGH
One of the world's top 20 universities

THE UNIVERSITY OF WARWICK

University of St Andrews

University of Dundee

University of HUDDERSFIELD
Inspiring tomorrow's professionals

University of Chester

US University of Sussex

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

University of Glasgow

UNIVERSITY of York

Brunel University London

UNIVERSITY OF LIVERPOOL

UNIVERSITY OF PLYMOUTH

UNIVERSITY OF WESTMINSTER

UNIVERSITY OF OXFORD

University of Strathclyde Glasgow

The University Of Sheffield.

PRIFYSGOL BANGOR UNIVERSITY

University of Leicester

UEA University of East Anglia

Brief Highlights

- We have completed 131 access projects for use of our machines
- Including use by the team of Nobel Laureate (Physics) - Prof. Konstantin Novoselov
- These projects have delivered free of charge 379 million Core / Hours
- The total value would have been £4.2M had they had to purchase these commercially
- Many attendees at Hartree Training Courses and Summer Schools
- £40K funding for PhD at Oxford/Culham

Hartree Centre
Science & Technology Facilities Council

Blue Wonder

iDataPlex
3,648 cores
7.2 TB RAM
48 GPUs

iDataPlex
ScaleMP
8 x 4TB systems
8x 512 cores

NeXtScale
8640 cores

iDataPlex
2016 cores
16 x Nvidia K20
42 x Intel Phi

Mellanox TECHNOLOGIES
Infiniband
Switch

Blue Joule

IBM BG/Q
6 racks, 1.23Pflop/s
98,304 cores
9.8 PB RAM

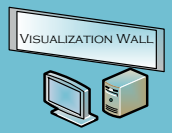
IBM BG/Q BGAS
2 rack, 450Tflop/s
32,768 cores
3.2 PB RAM
256TB Flash Memory

Filestore
GPFS
9 PB

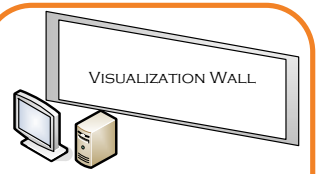
Tape Store
15PB

Remote Graphics
Server

Big Insights (912 cores, 2.6TB RAM)
Streams (128 cores, 1TB RAM)
InfoSphere Data Explorer (96 Cores, 192GB RAM)
SPSS (16 cores, 128GB RAM)
Infosphere Content Analytics (8 cores, 32GB RAM)
Cognos (24 cores, 192 GB RAM)



VEC



Workstation
Merrison Lecture Theatre

Novel Cooling
Clustervision/GRC
1920 cores, 7.6 TB RAM

NeXtScale
ARM 64 bit

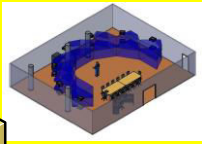
Dataflow
Maxeler
12x Cores, 128 GB RAM
40 MAIA Dataflow engines

X50
Training Stations

High End Workstation
Crosfield

DL

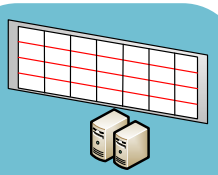
Interactive Table

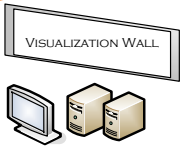

High End Workstation
Leverhulme

RAL

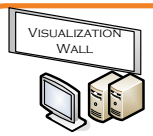
Scarf
Jasmin
Emerald
NCCS

User


ISIC 7x4 Video Wall



High End Workstation
ISIC Visualization



High End Workstation
Atlas Visualization Wall

WTH Associates Ltd
7/3/2014 | Hartree Centre Architecture