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Powering Success
Pweru Llwyddiant

HPC Wales User Group Meeting

Multi-Site Video Conference

14th May: 14.00 pm – 16.00 pm



Ewrop & Chymru:
Buddsoddi yn eich dyfodol
Cronfa Datblygu Rhanbarthol Ewrop

Europe & Wales:
Investing in your future
European Regional Development Fund



Agenda

| Time | Item | Speaker |
|-------|------------------------------|---|
| 14.00 | General HPC Wales Update | Martyn Guest |
| | User Concerns & Solutions | |
| 14.25 | HPC Wales Fair Use Policy | Ade Fewings |
| 14.35 | Progress on Gateways | Charlie Godfrey |
| 14.45 | Thematic User Groups | |
| 14.55 | Near Term Technology Roadmap | Glenn Fitzgerald (Fujitsu) |
| 15.15 | SME Case study | Ben Barton (Knowtra) |
| 15.25 | Studentship Video | Farzana Rahman (UoSW) and James Pack |
| 15.35 | Forum Discussion | Group Discussions & Feedback |
| 15.55 | Q&A and Close | Martyn Guest |



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General HPC Wales Update

Usage of the HPC Wales Systems

May 2013 – April 2014



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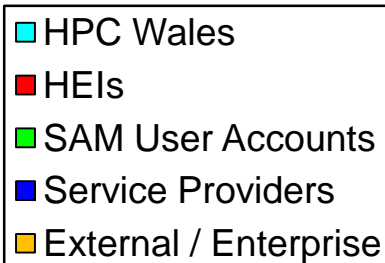
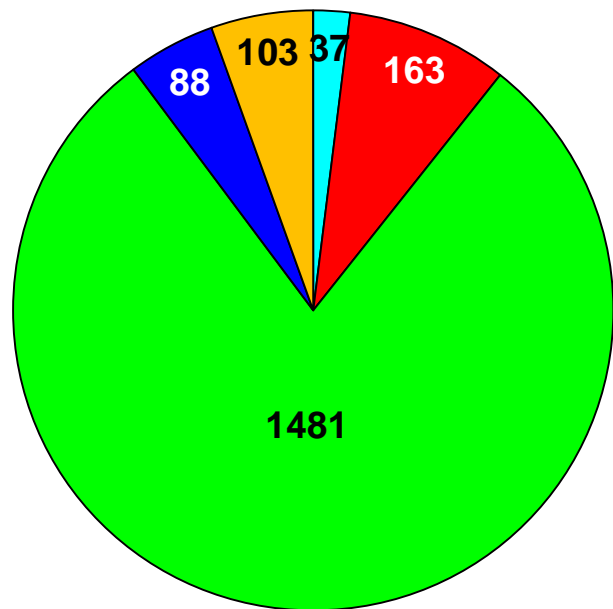



Llywodraeth Cymru
Welsh Government

HPC Wales User Accounts

1st May 2014

/home/hpcw.tech/user_lists

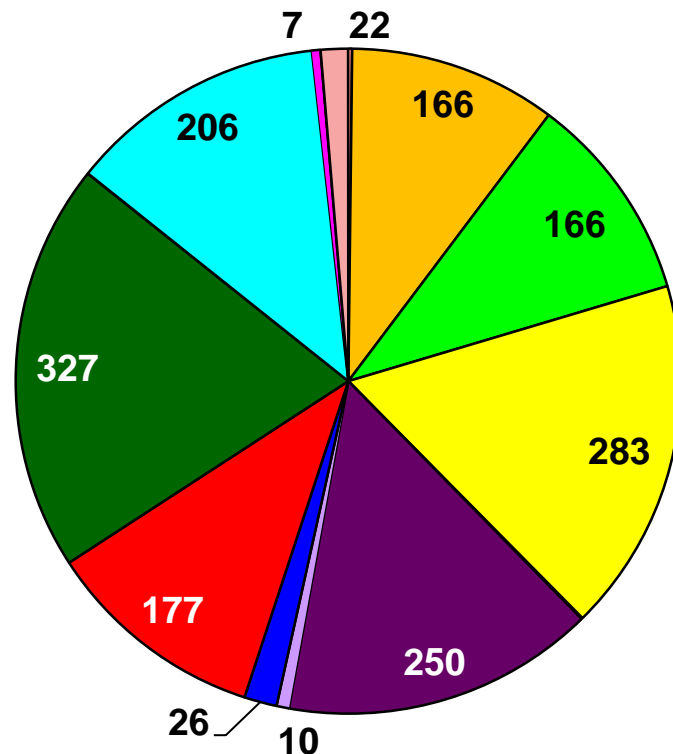


*Total of 1644 User Accounts **[+31]***

HEIs + SAMs

*Total of 1872 User Accounts **[+23]***

Figures in **[]** indicate change in past month



Upcoming Events

- Supercharging Pembrokeshire – Official Launch of Tier 2Bs (23rd May 2014)
- HPC Wales Summer School, Bangor (June 2014)
 - Introduction to HPC, C++ and MPI
- Digital 2014, Cardiff (9th – 10th June 2014)
- Eurovis 2014, Swansea (9th – 13th June 2014)
- ISC'14, Leipzig, Germany (22nd – 26th June)
- StartUp Weekend 2014, Swansea (21st – 23rd November 2014)

Active Enterprise User Accounts

1st May 2014

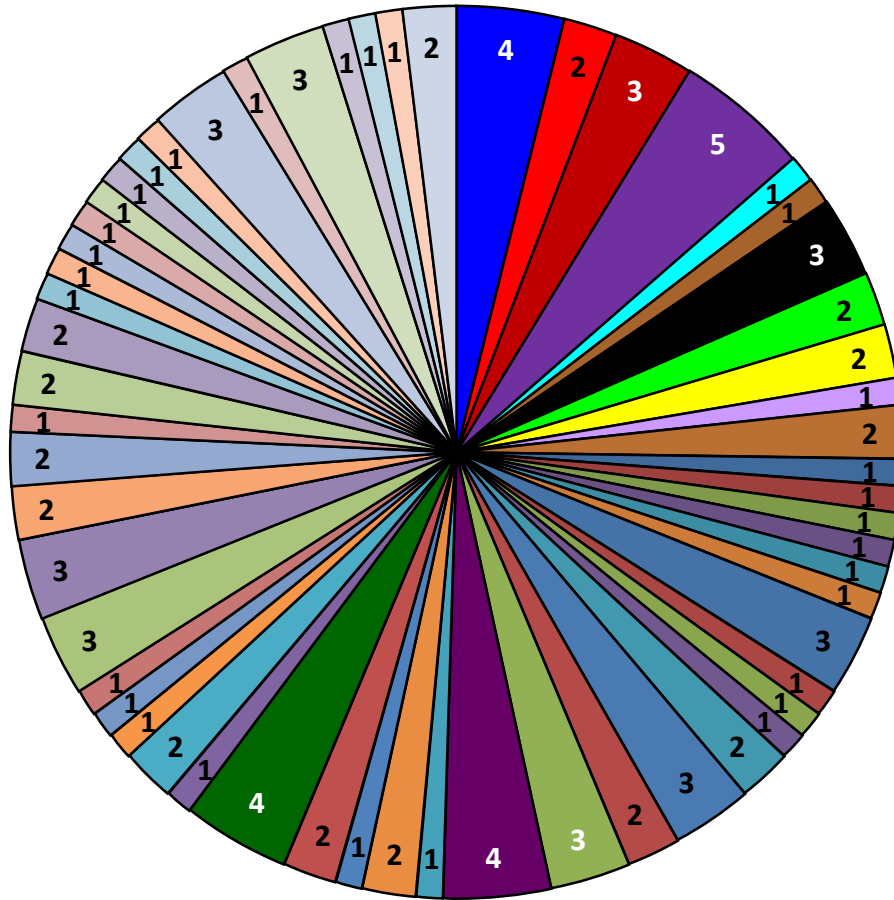


Figure in [] indicate change in past month

| | |
|-----------------------------|-----------------------------|
| ■ Accelero Digital | ■ Atticus |
| ■ Br. Ornithology Trust | ■ Calon Cardio |
| ■ Calsonic | ■ Canolfan Bedwyr |
| ■ Chaos Trend | ■ Habitat Info |
| ■ Knowtra | ■ MJR Solutions Ltd |
| ■ Nat. Botanic Garden Wales | ■ PICMO |
| ■ Qioptic | ■ TWI NDT Centre |
| ■ View Holographics | ■ Vizworx |
| ■ Zeeko | ■ ICON |
| ■ Planetary Resources | ■ Solray Works |
| ■ Koenigsegg | ■ BSM Bench Ltd |
| ■ Bloodhound Programme Ltd | ■ iCreate3D |
| ■ Thinkplay TV | ■ BapttDesigns |
| ■ Gluco Technology | ■ Ultranyx |
| ■ Vibe TV | ■ Penlon Cottage Trading |
| ■ Red Dragon Softworks Ltd | ■ Astra Games |
| ■ Dojo Arcade | ■ Syndica |
| ■ Llaisdy | ■ Neem Biotech |
| ■ Simulity | ■ Acuitas Medical |
| ■ Company85 | ■ Make and See |
| ■ Silverwing | ■ Zodiac Seats |
| ■ Altair | ■ Farmaceutical Innovations |
| ■ Partington Marine Ltd | ■ Rockfield Software |
| ■ Bait Studio | ■ Tidal Lagoon |
| ■ Rolls Royce | ■ BMT WBM |
| ■ Newmill Asset Management | ■ Stills |
| ■ Zenotech | ■ Fujitsu Japan |
| ■ Bomper Studio | ■ Butterfly |
| ■ Dischromatics | ■ Concurrent Thinking ✓ |
| ■ Cultech Ltd ✓ | ■ Torquing Group ✓ |

External / Commercial Organisations –
103 user accounts [+5]

1481 user accounts **[+30]**

| | | |
|---------|---------|---------|
| SAM0002 | SAM0003 | SAM0004 |
| SAM0009 | SAM0010 | SAM0011 |
| SAM0012 | SAM0014 | SAM0023 |
| SAM0035 | SAM0036 | SAM0041 |
| SAM0043 | SAM0059 | SAM0062 |
| SAM0076 | SAM0084 | SAM0102 |
| SAM0103 | SAM0104 | SAM0106 |
| SAM0107 | SAM0111 | SAM0112 |
| SAM0119 | SAM0130 | SAM0131 |
| SAM0132 | SAM0133 | SAM0135 |
| SAM0136 | SAM0141 | SAM0142 |
| SAM0157 | SAM0165 | SAM0168 |
| SAM0169 | SAM0173 | SAM0175 |
| SAM0182 | SAM0183 | SAM0186 |
| SAM0187 | SAM0188 | SAM0189 |
| SAM0191 | SAM0194 | SAM0196 |
| SAM0197 | SAM0199 | |

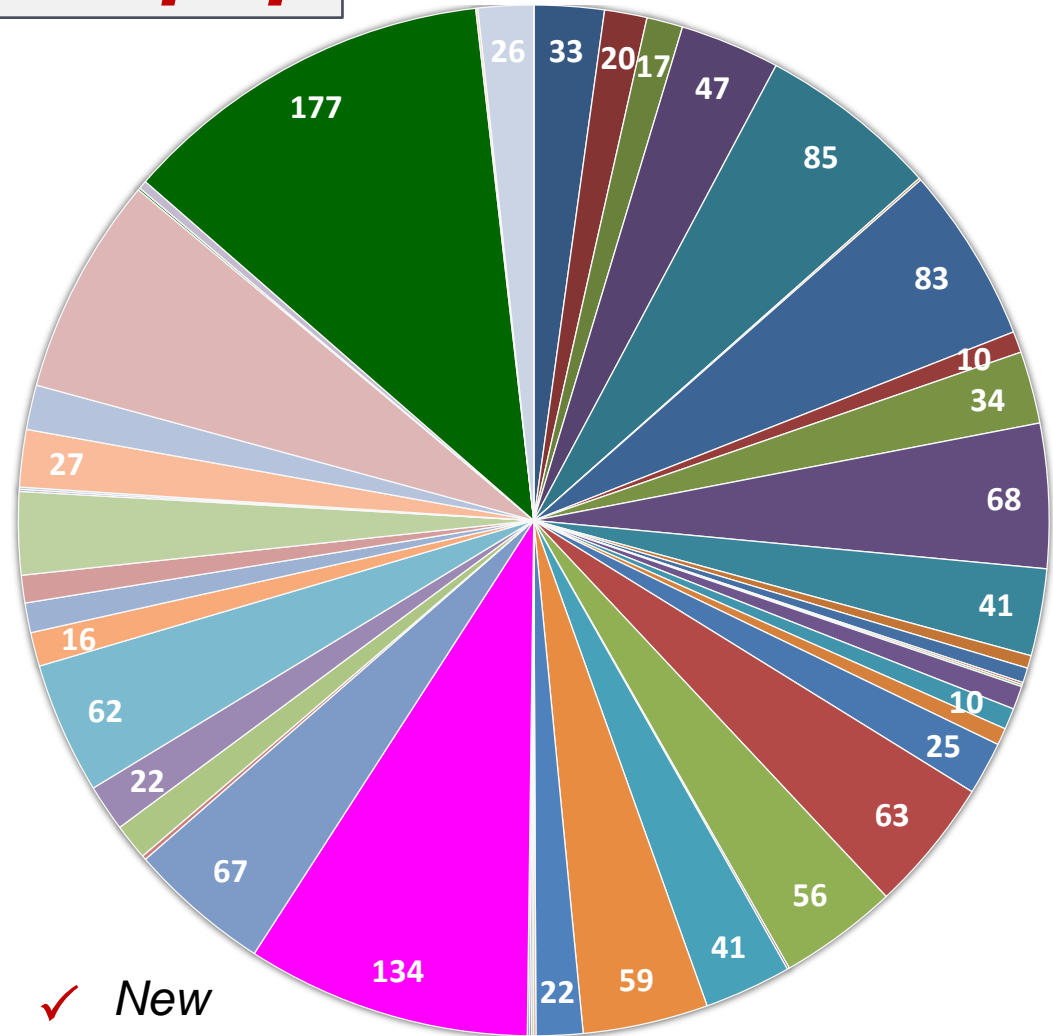
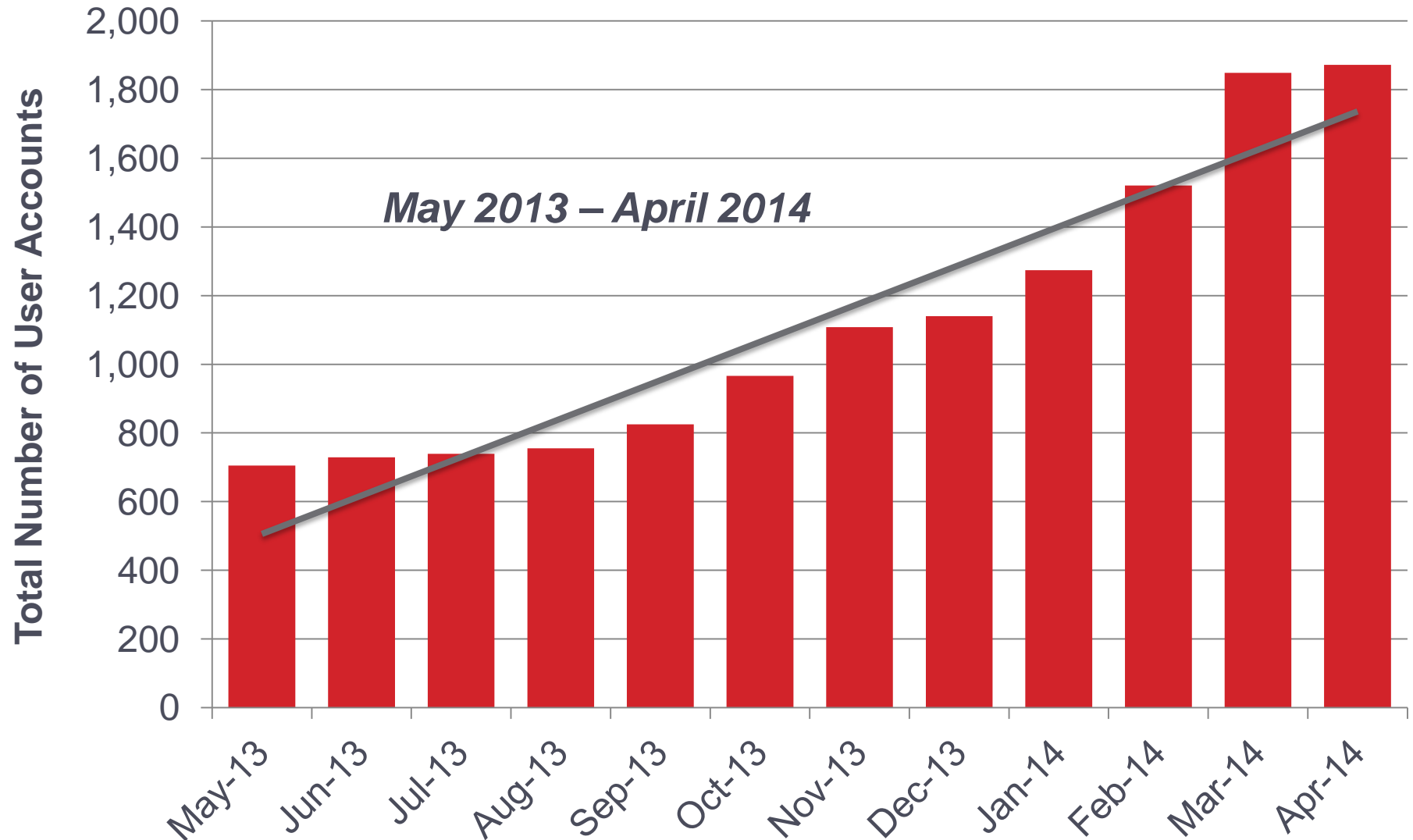
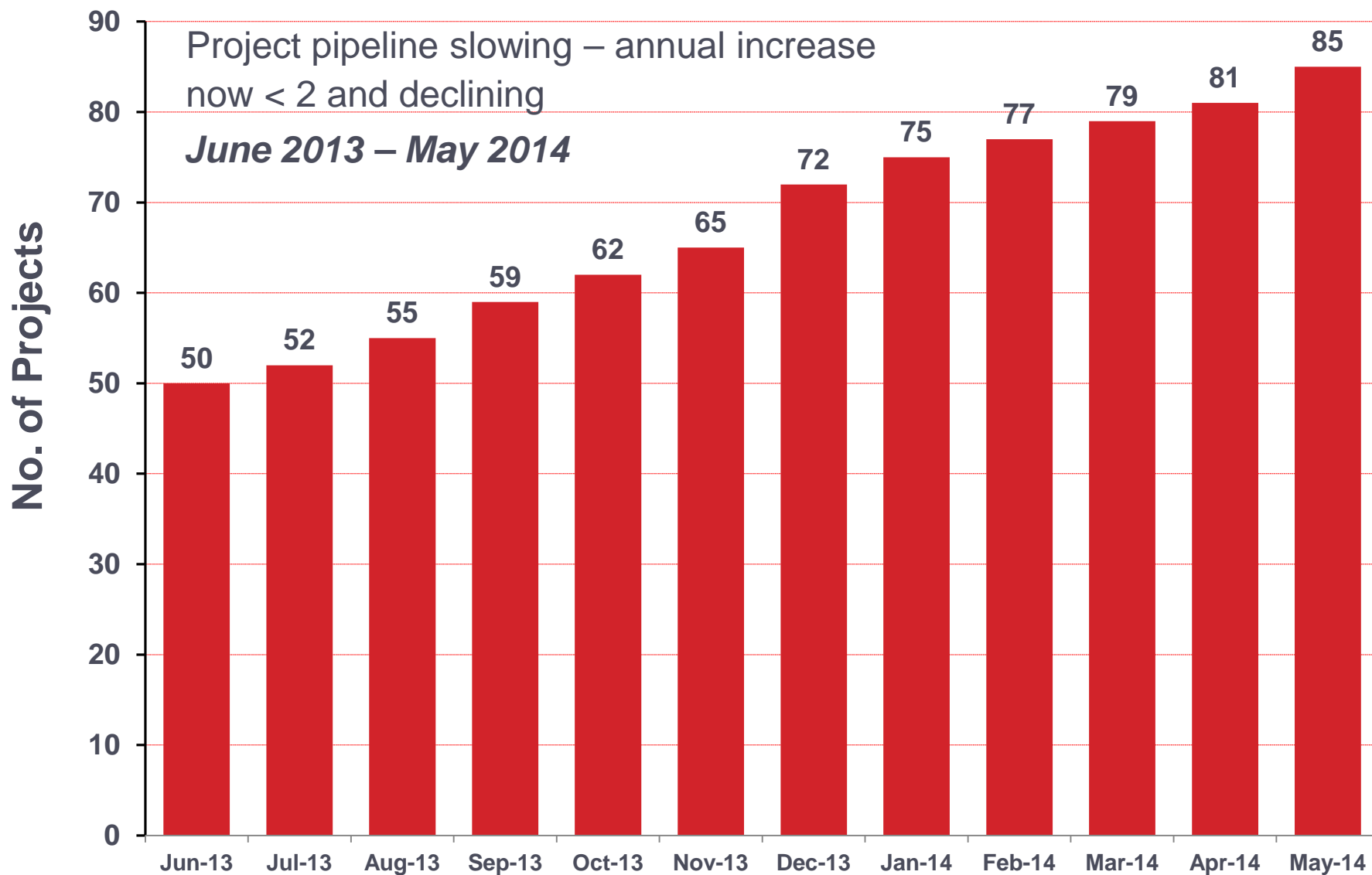


Figure in [] indicate change in past month

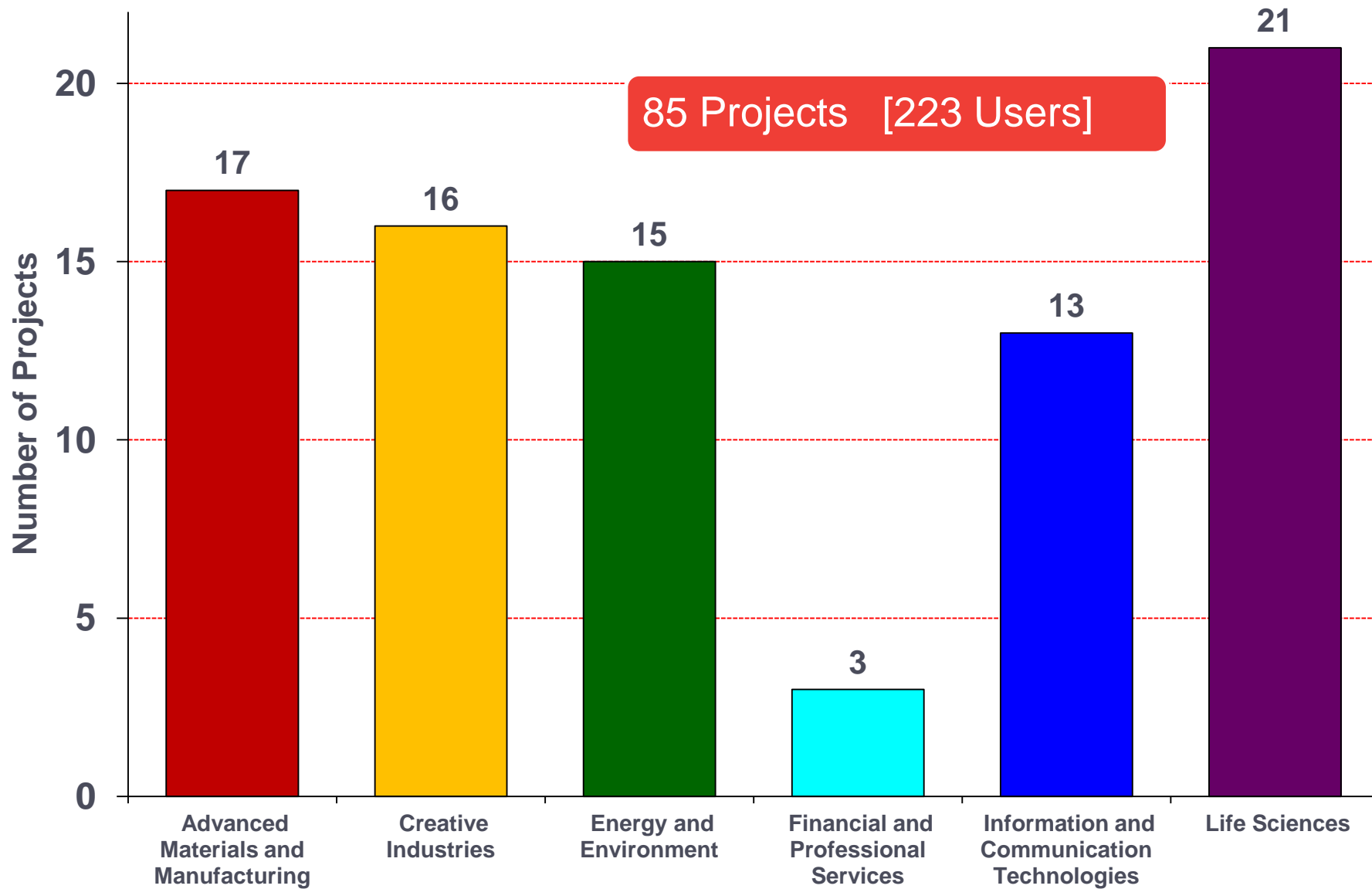
Timeline of the HPC Wales User Accounts



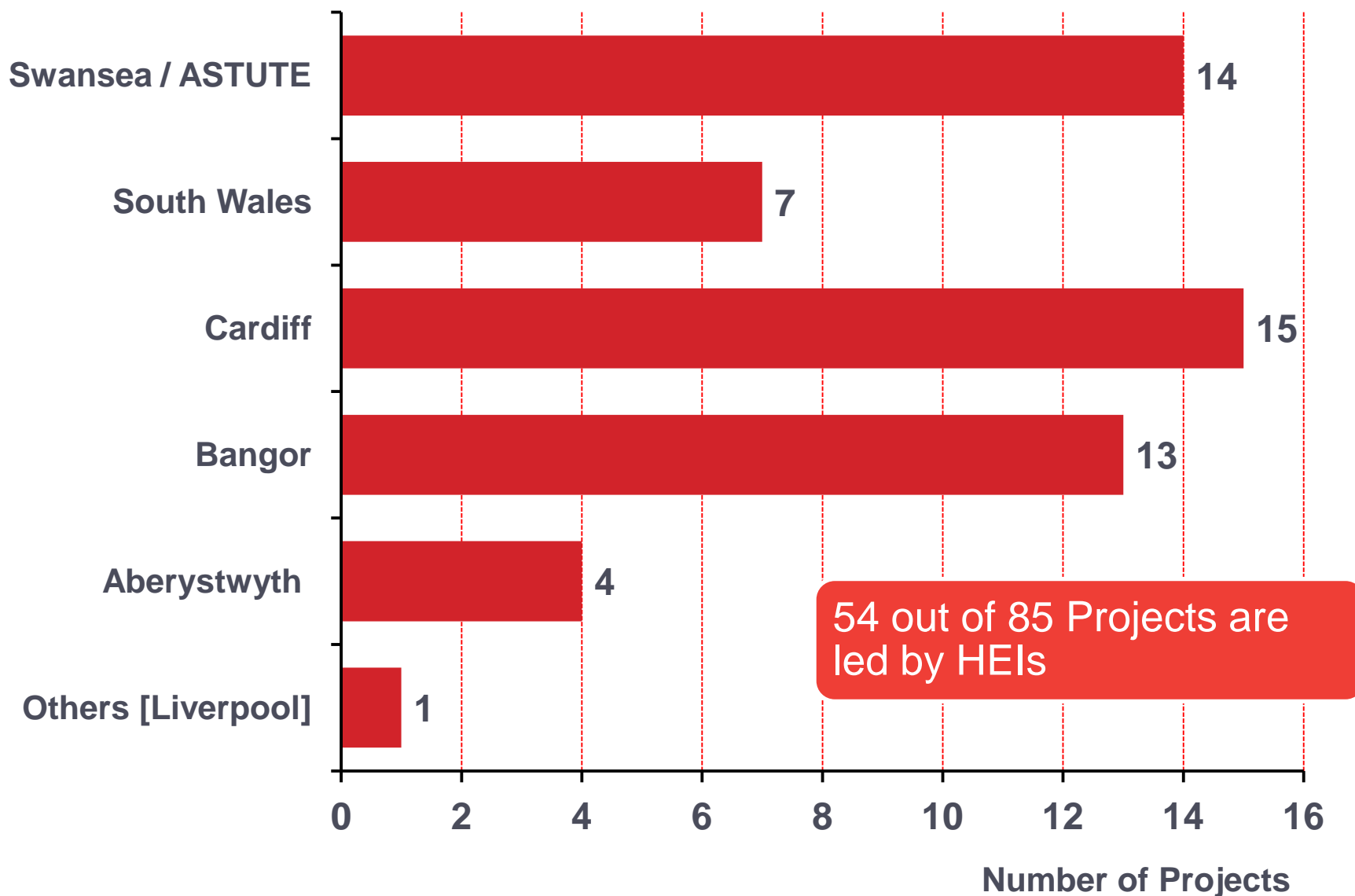
Increase in Number of HPC Wales Projects



HPC Wales Projects – By Sector



HPC Wales Projects – By HEI





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Usage of the HPC Wales Cardiff HTC System

May 2013 – April 2014



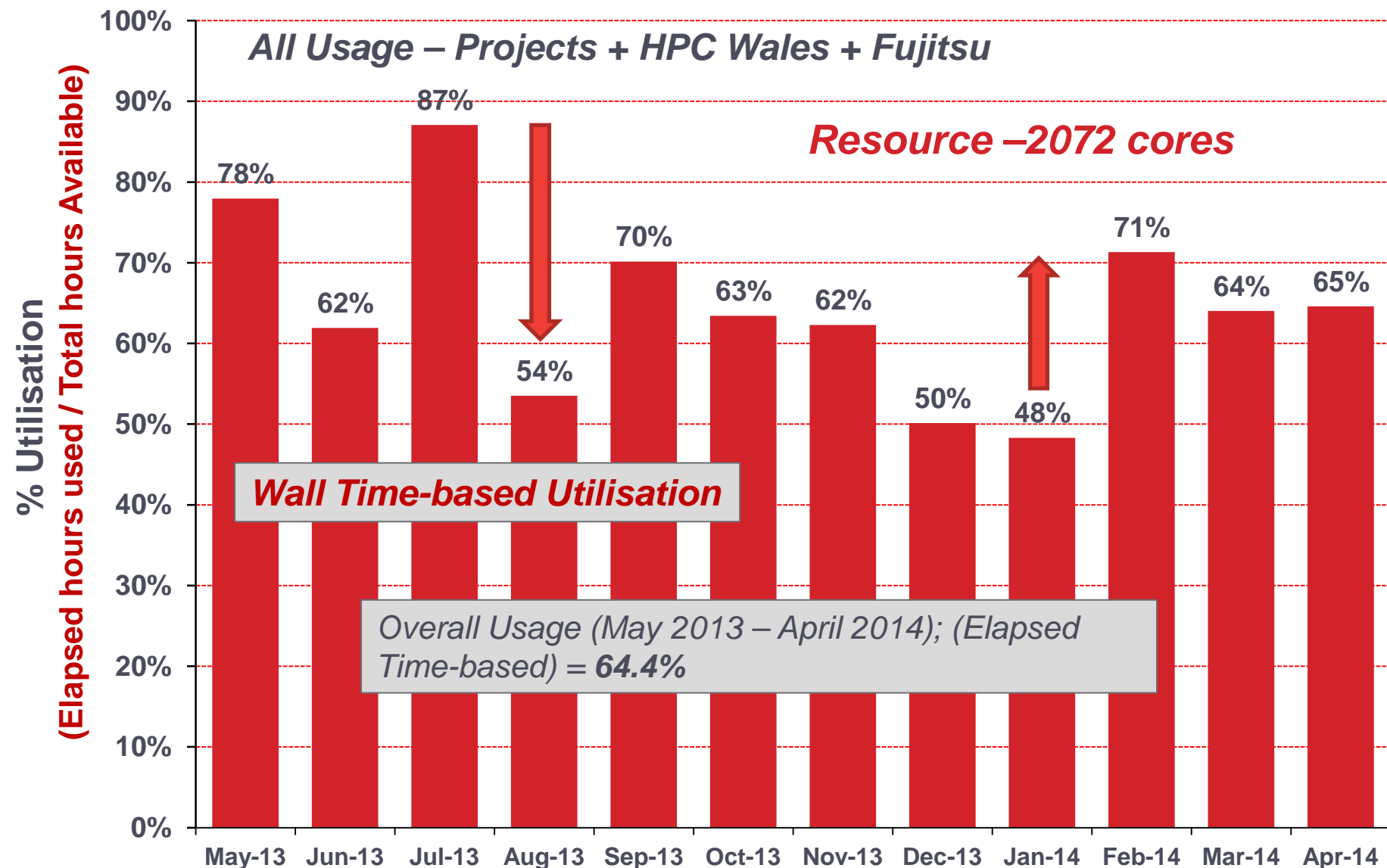
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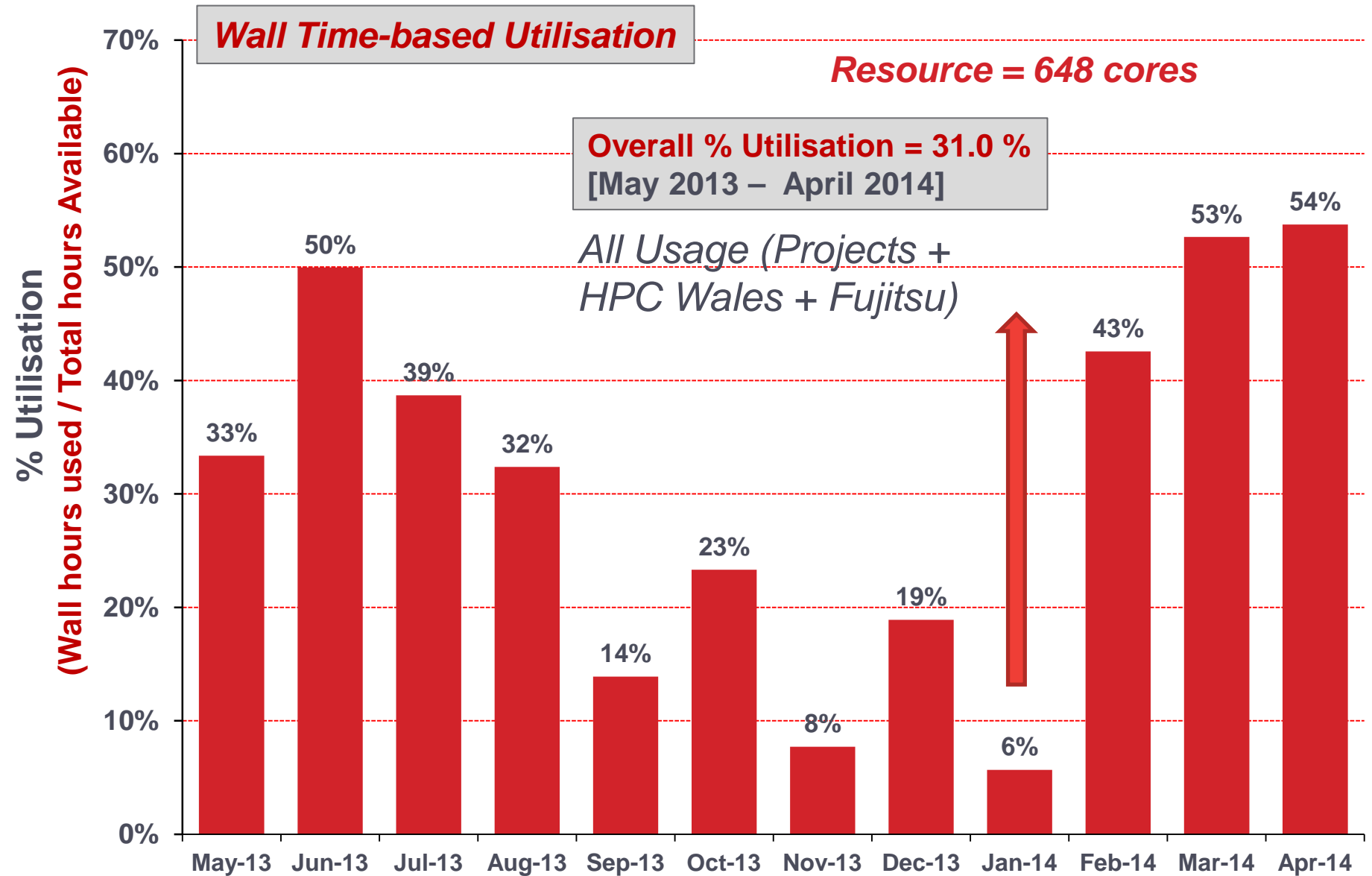


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Welsh Government

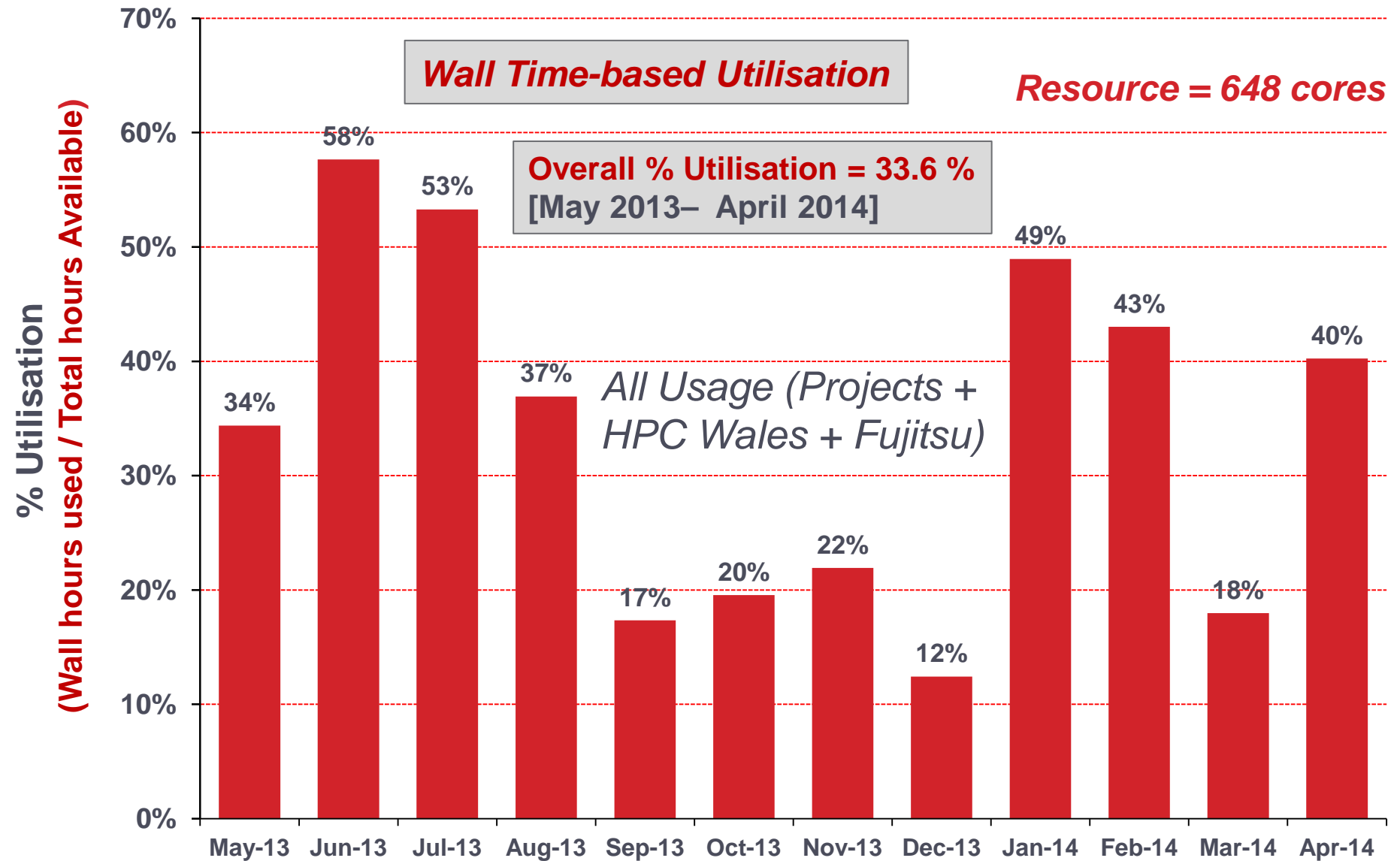
Cardiff HTC Cluster - % Utilisation (Elapsed)



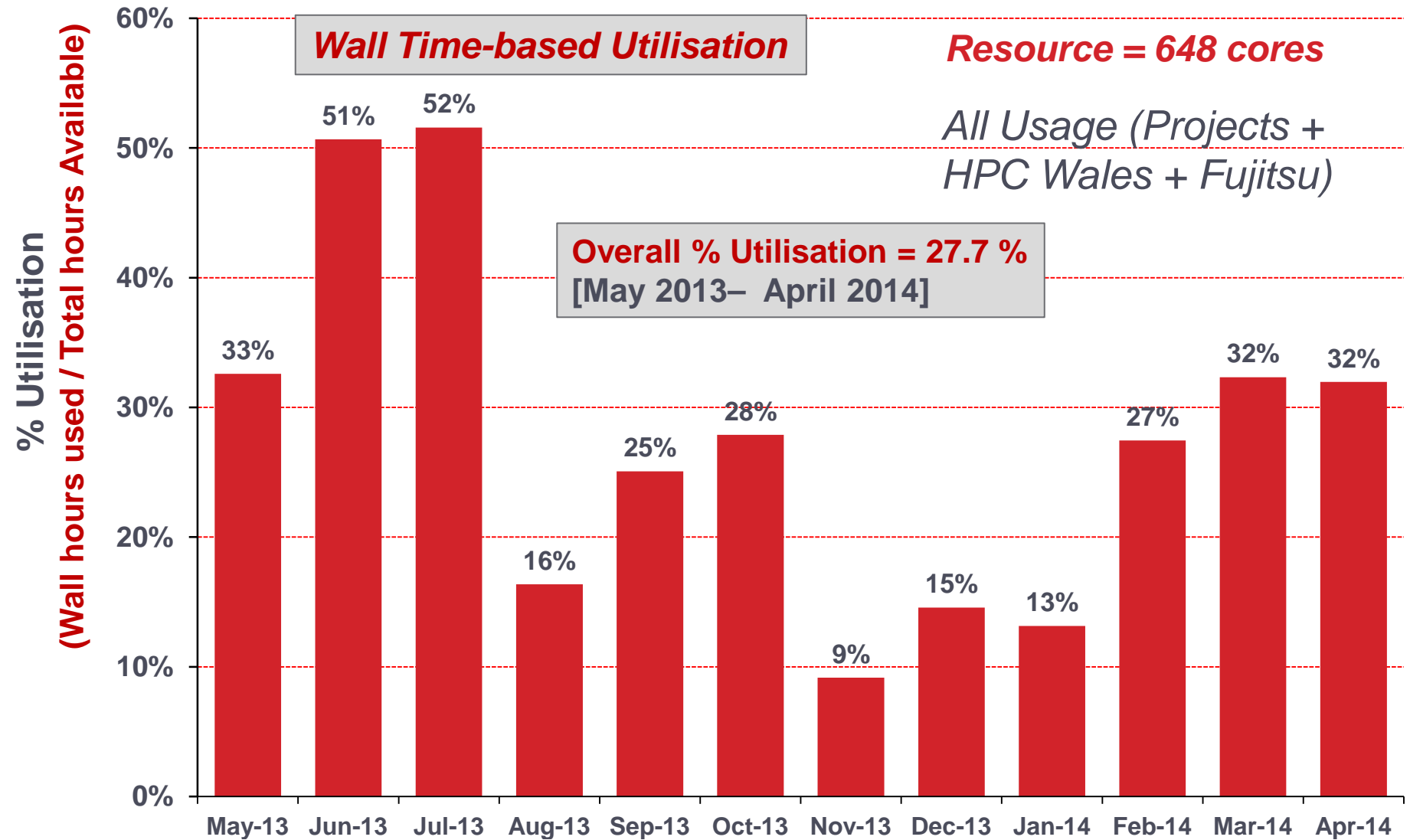
% Utilisation of the Aberystwyth T1 Cluster



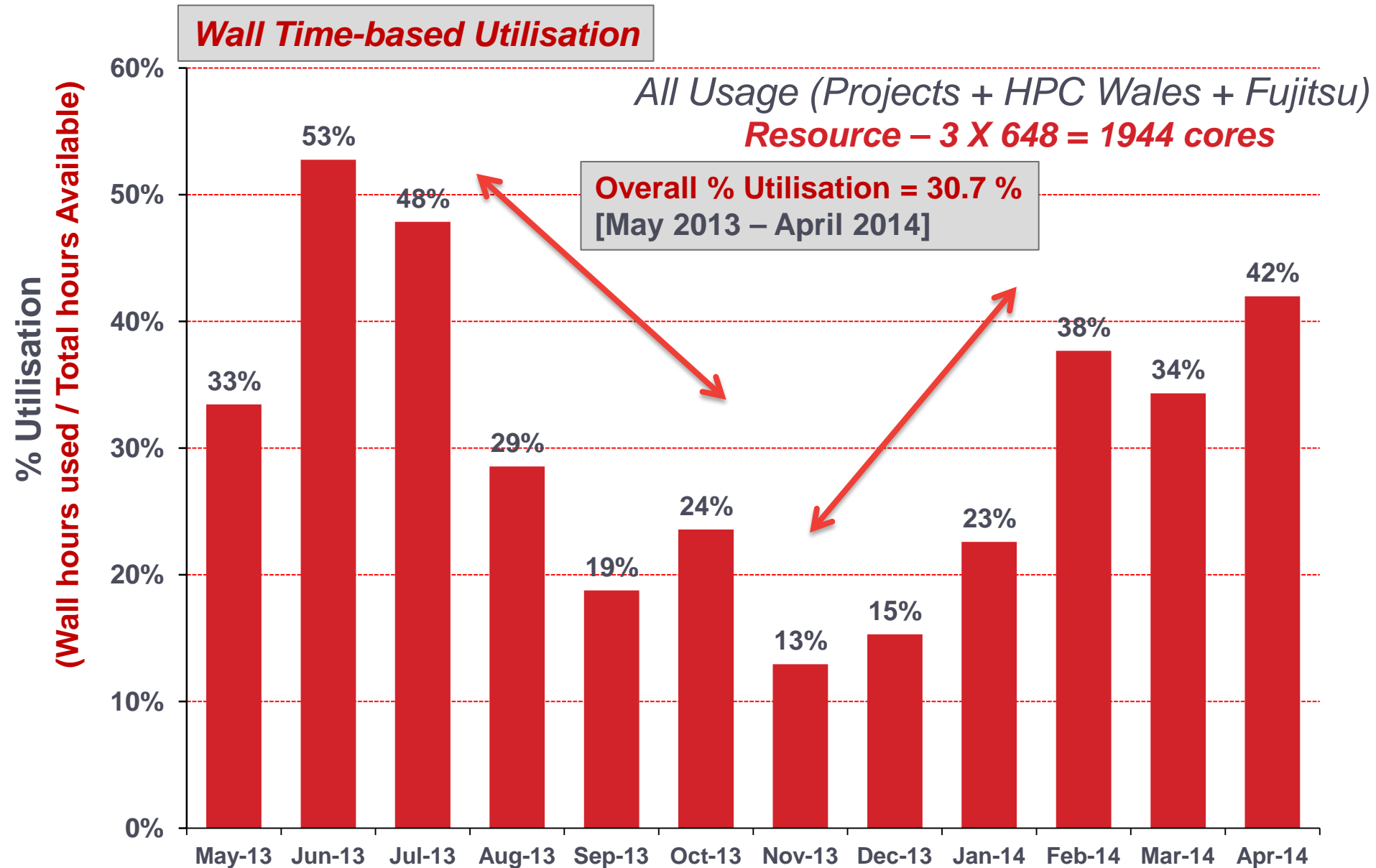
% Utilisation of the Bangor T1 Cluster



% Utilisation of the Bangor T1 Cluster

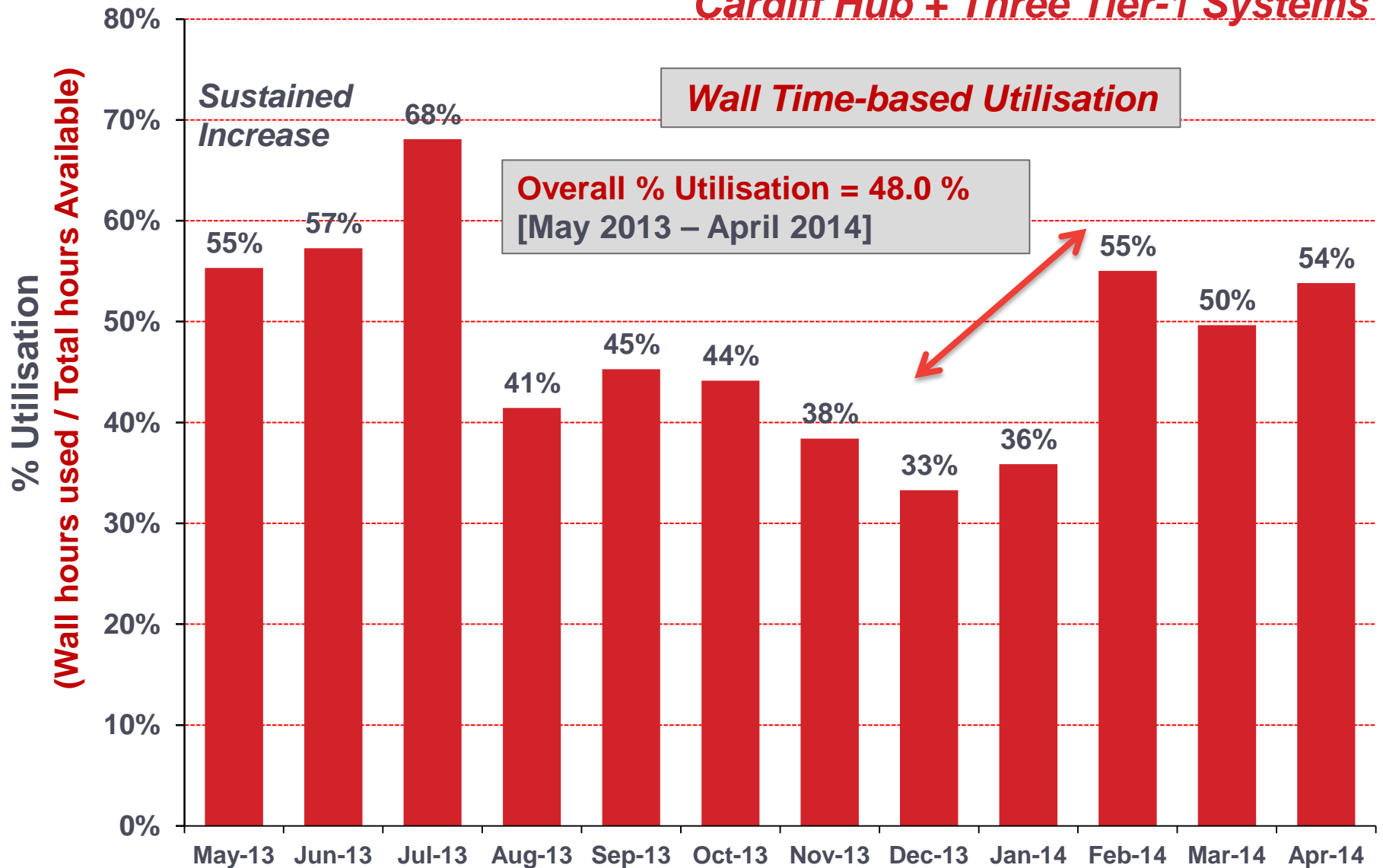


% Utilisation of the Three Tier-1 Clusters



% Utilisation of the Phase 1 Systems

Cardiff Hub + Three Tier-1 Systems





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Usage of the HPC Wales Phase 2 Systems

August 2013 – April 2014



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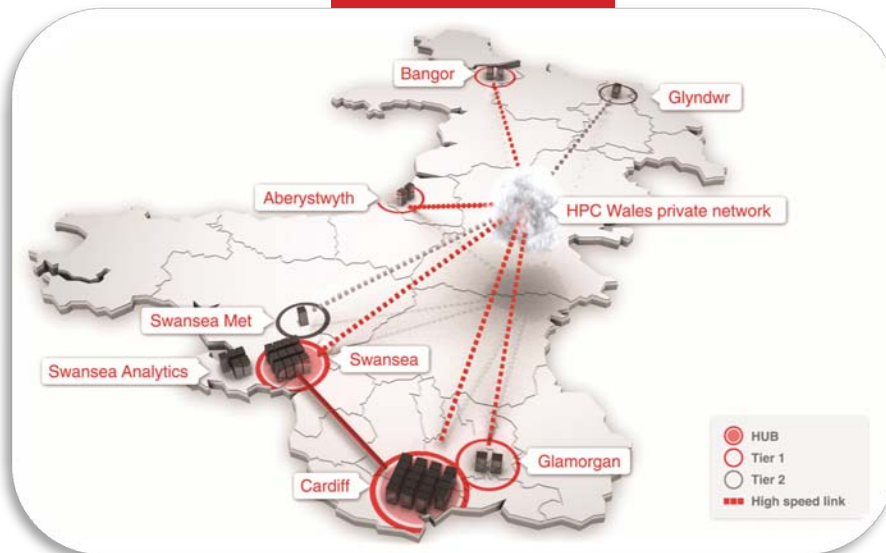
Llywodraeth Cymru
Welsh Government

Sandy Bridge and the HPC Wales Hubs

Phase 2

256 x CX250S1 E5-2690 dual processor 16-core nodes

- 240 nodes with 64GB memory
- 16 nodes with 128GB memory
- **4096 x 2.9 GHz cores with 4/8 GB memory / core**
- Infiniband non-blocking QDR network
- 95 Tflops peak performance
- 400 TB Lustre file storage and 100 TB storage for permanent filestore



Cardiff Capacity system:

- 384 x CX250S1 e5-2670 dual processor 16-core nodes
- **6144 x 2.6 GHz cores with 4 GB memory / core**
- Infiniband non-blocking QDR network
- 128 Tflops peak performance
- Filestore shared with HTC sub-system

Swansea Capacity system:

- 128 x CX250S1 E5-2670 dual processor 16-core nodes
- **2048 x 2.6 GHz cores with 4 GB memory / core**
- Infiniband non-blocking QDR network
- 43 Tflops peak performance
- Filestore shared with Capability sub-system



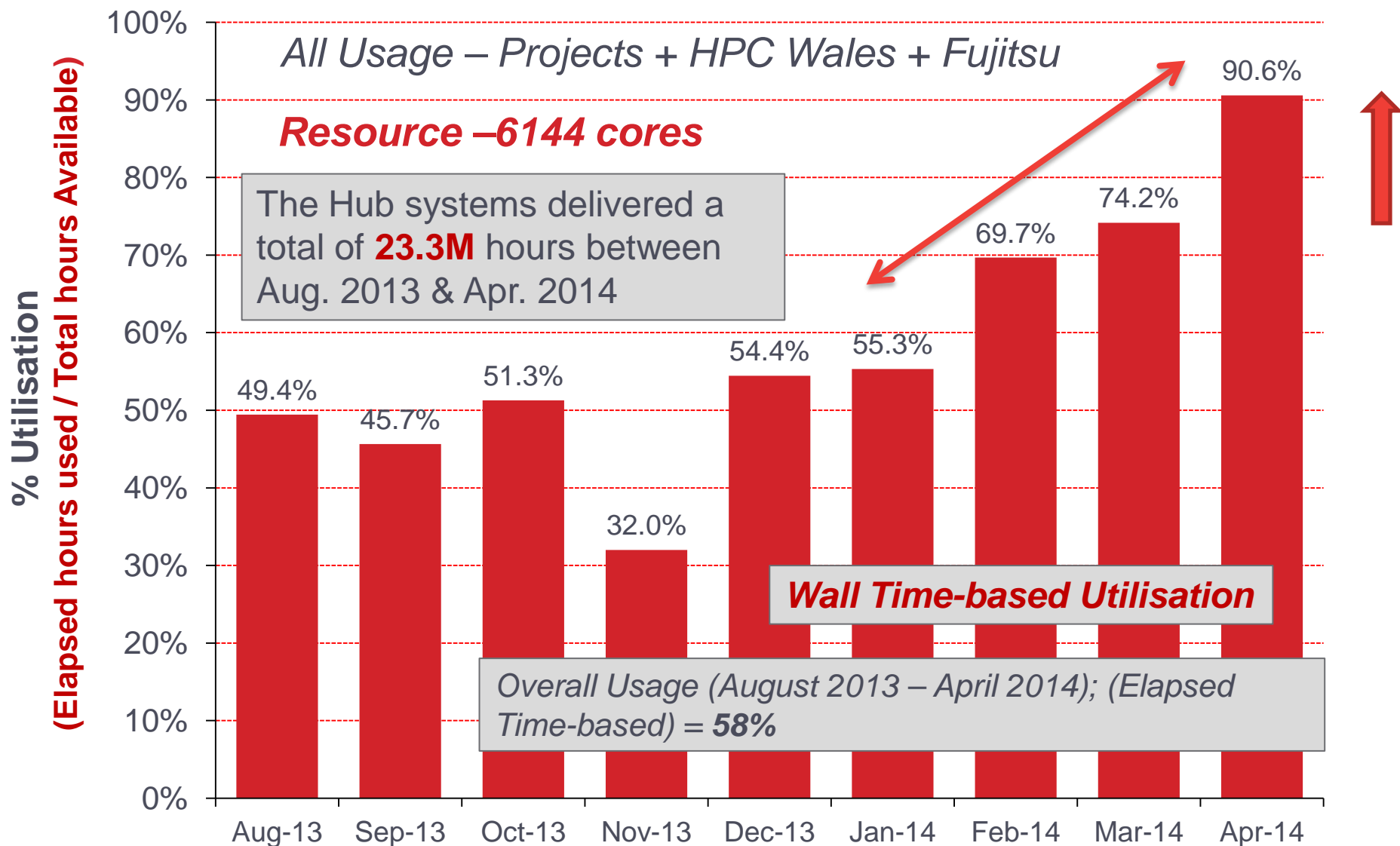
| Site | System | Number of Cores | Peak Tflops |
|--------------|-----------------------|-----------------|-------------|
| CARDIFF | HTC + Capacity | 8216 | 149.6 |
| SWANSEA | Capability + Capacity | 6144 | 137.6 |
| BOTH HUBS | GP-GPU systems | 512 | 10.6 |
| TIER-1 SITES | 3 x Medium | 1944 | 20.8 |
| All Sites | All Systems | 16816 | 318.6 |

Novel Architecture Sub-systems (at each Hub):

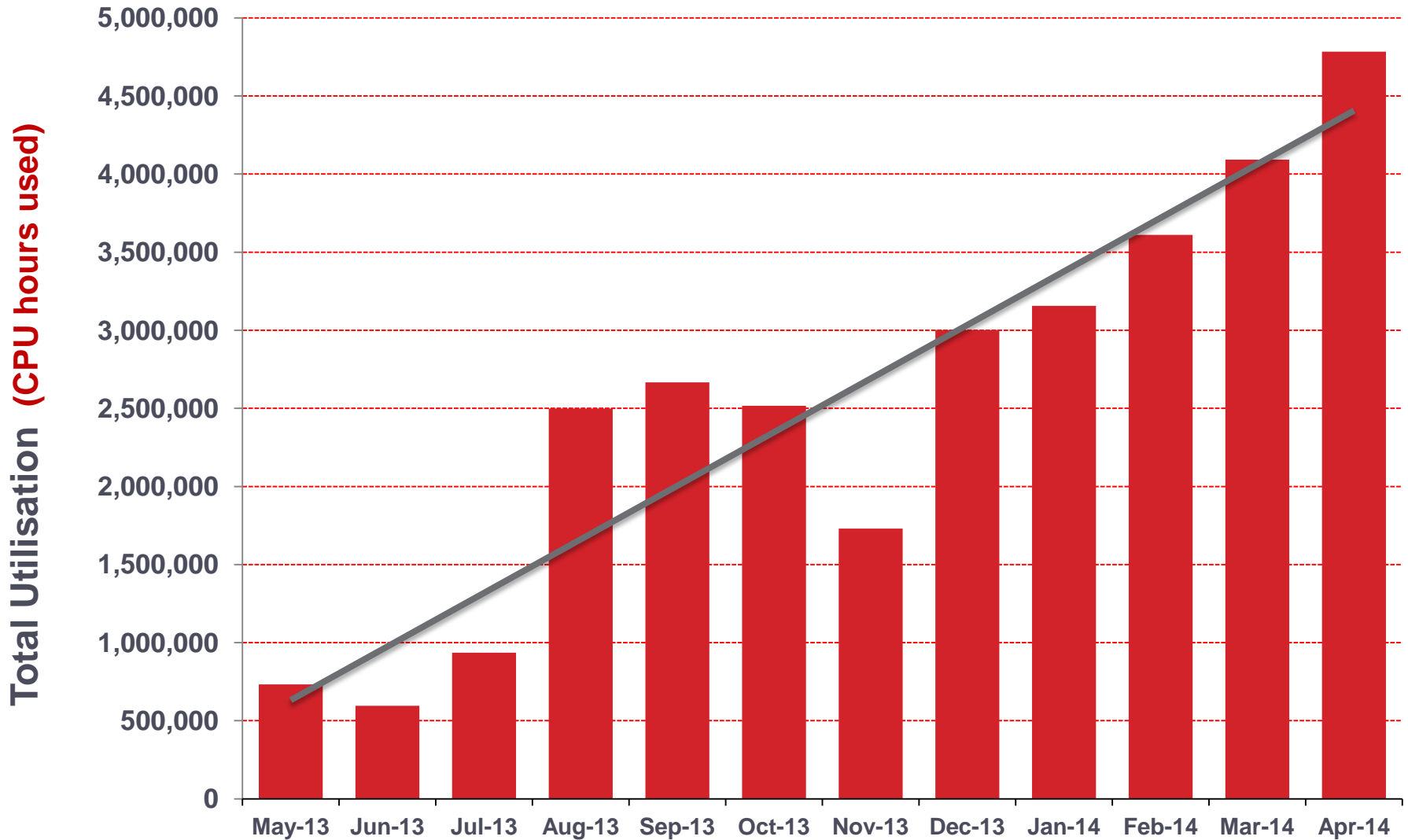
- 16 x CX270 nodes with GP-GPU capability
- 256 x 2.6 GHz cores with 4 GB memory/ core
- **each node with a M2090 GP-GPU card**
- Infiniband non-blocking QDR network

#110 in November 2013 Top 500

Swansea Cluster - % Utilisation (Elapsed)



Total CPU Utilisation – Phase 1 and Phase 2





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Phase 1 Usage Profile of the HPC Wales Projects

May 2013 – April 2014

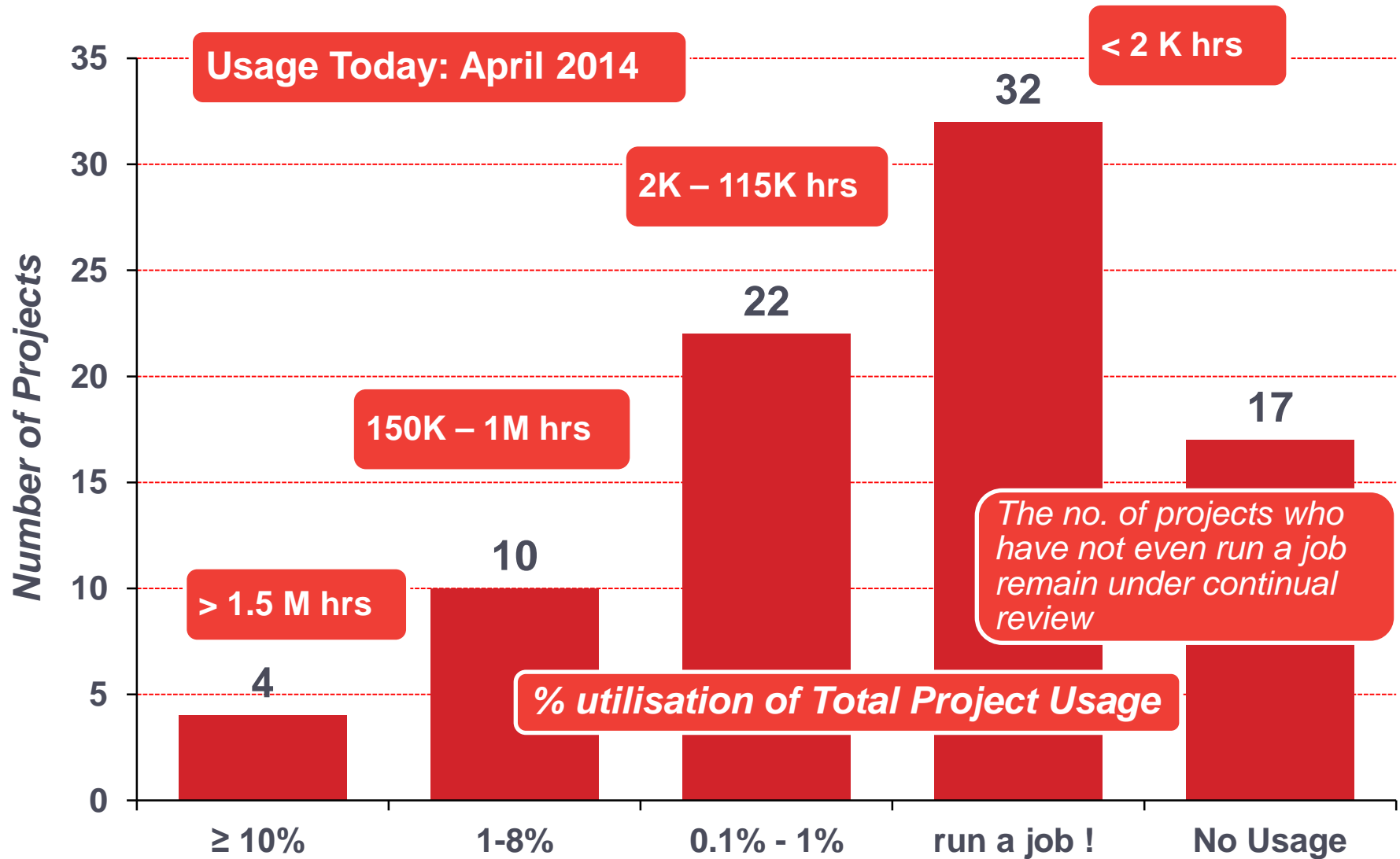


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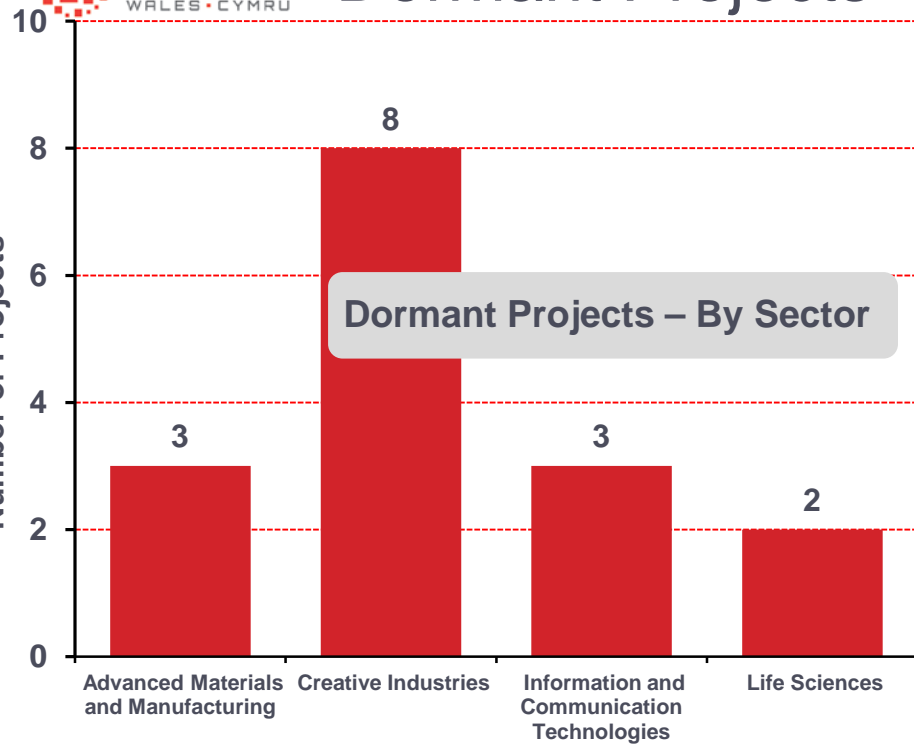
Project Utilisation Profile of the HPC Wales Phase 1 Systems



Dormant Projects

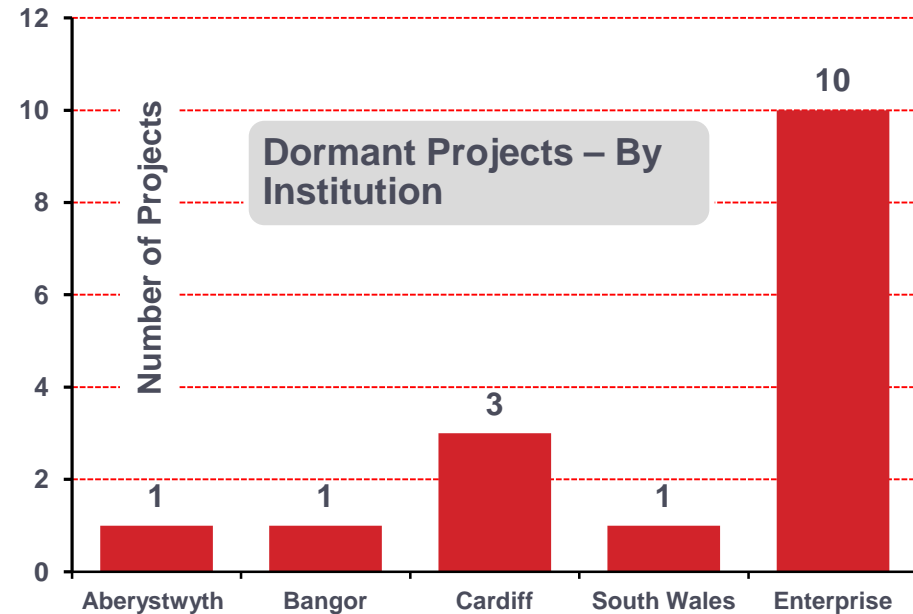
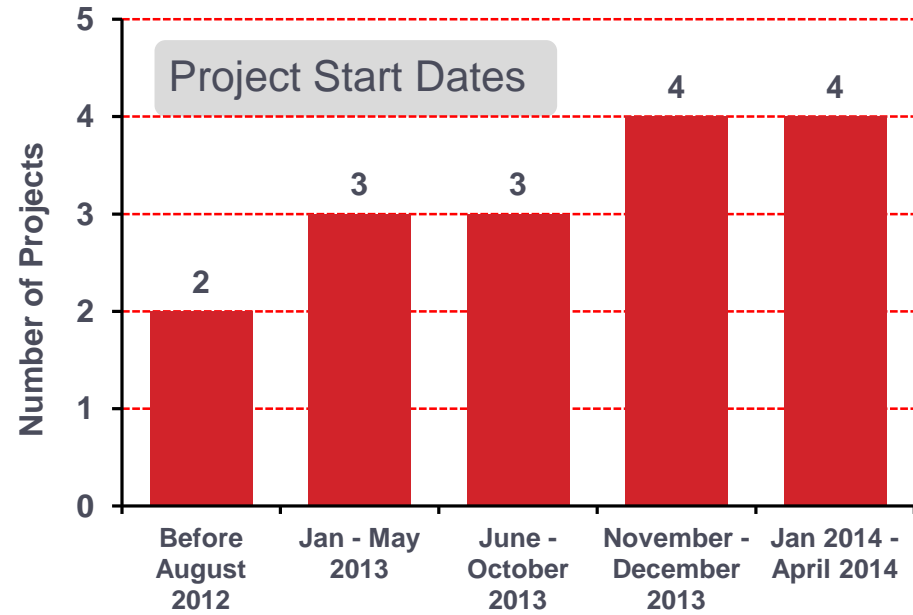
Number of Projects

Dormant Projects – By Sector



Projects that have yet to run a job on the system, going back to August 2012

Three projects activated in April – HPCW142, HPCW187 and HPCW189



Summary and Conclusions

Presented an analysis of Usage of the HPC Wales Systems

Focus on period September 2012 – April 2014. Usage presented in terms of both CPU (core) and elapsed hours

Levels of usage of Phase 1 systems initially impacted by the arrival of successful Phase 2 pilot service on Sandy Bridge. Project usage of the Cardiff HTC system increased somewhat in April - 54% (core CPU) and 65% (elapsed) of the total hours available.

Usage of the Tier-1 systems also increased in April, from 15% [March 2014] to 23 % [April] and 34 to 42% Elapsed.

Increase in number of registered users continues

Large number of active user accounts translates into modest number of users actually running jobs (1481 SAM accounts show modest usage, although SAM0043 a major user over Q3 2013)

Four new projects on the system during April, one fronted by an HEI [HPCW166], the other 3 by industry [HPCW182, 187 and 189]. Sixteen “Trial” projects now in place.

Number of HPCW pipeline projects not being activated onto the system remains an issue. Introduction of “trial” projects has helped here.

Usage by all 85 HPC Wales Projects of the HPC Wales systems

Usage dominated by a few projects e.g., HPCW070, HPCW033 and HPCW106, with HPCW107 accelerating its usage.

11 projects account for 92% of total usage. 16 projects (19%) have still to run a job on HPC Wales systems.

HPC Wales has delivered a total of 35.2M core CPUs hours to users in the period September 2012 – April 2014, 13.6M core CPU hours from its Phase-1 systems, and 21.6M from the Phase 2 Swansea & Cardiff Sandy Bridge systems.

Sandy Bridge service now delivered 1.6 X the no. of hours from August 2013 – April 2014 than the entire Phase 1 systems have delivered since the start of service in Feb 2012.



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User Concerns and Solutions



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User Concerns and Solutions

| | Issue and Concern | Resolution |
|---|--|--|
| 1 | Lack of familiarity with Linux | Training available for Linux command line and other parts of the system (further learning after On boarding) |
| 2 | Factoring in the queue system to your work schedule. Learning Linux commands. | |
| 3 | Setting things up in the first place and getting familiar with the HPC system (queue system, syntax, etc.). | |
| 4 | When I started using it I was unfamiliar with using Linux and how to run my models on the cluster so this was a big challenge to me. | Availability of NAG as part of the on-boarding process |
| 5 | Getting used to running the system, basically getting used to its language and procedures | Development of LMS as part of the Skills Academy |
| 6 | Knowing what is available | Improvements to the Gateways and Documentation |
| 7 | Improving the user's skillset from beginner to intermediate level | Training from NAG and FLE |

User Concerns and Solutions

| | Issue and Concern | Resolution |
|----|--|---|
| 8 | Prompt resolution to tickets is the main challenge, [beyond that greater availability of training materials and courses would be useful to widen my knowledge of the subject | Improved ticket monitoring and resolution Closer monitoring of NAG tickets |
| 9 | Software design | Extend available training |
| 10 | Finding support in improving the code | NAG availability Site clinics e.g. Aberystwyth |
| 11 | Reproducibility of data when running calculations on other commonly used HPC systems within UK (e.g. Hector, Archer). e.g., broadly used codes (e.g. VASP, GAMESS-UK) should be checked for that | Discussions with Code owners and ISVs; Developing links with EPCC and HPC-SIG |
| 12 | Transferring data between Cardiff and Swansea nodes | Transfer can be managed directly by the user using sftp facilities through sftp.hpcwales.co.uk Also now possible to ftp out of the HPC Wales infrastructure |
| 13 | Keeping files up to date when using the UoSW cluster and the Cardiff cluster at the same time | |
| 14 | Getting data to and from the system | |



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HPC Wales Fair Use Policy

Ade Fewings, Bangor Systems Engineer

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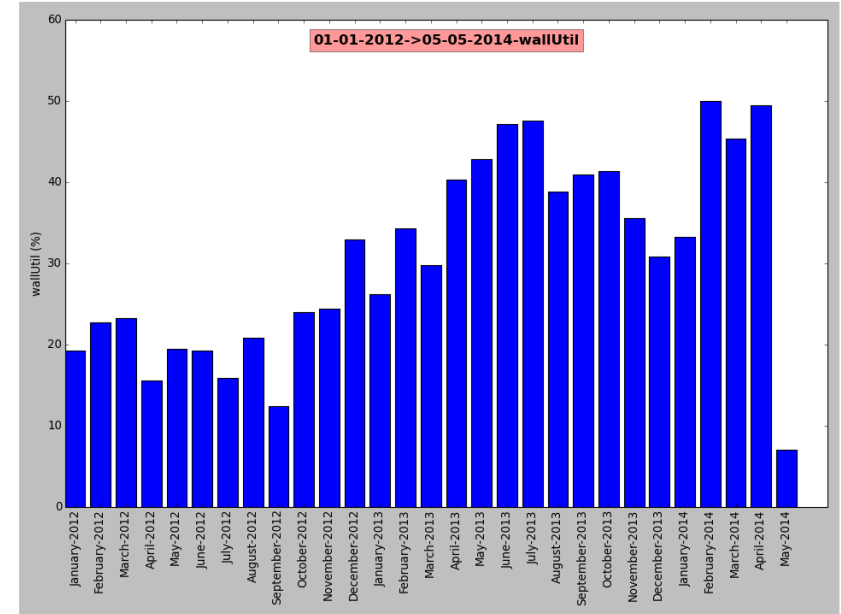
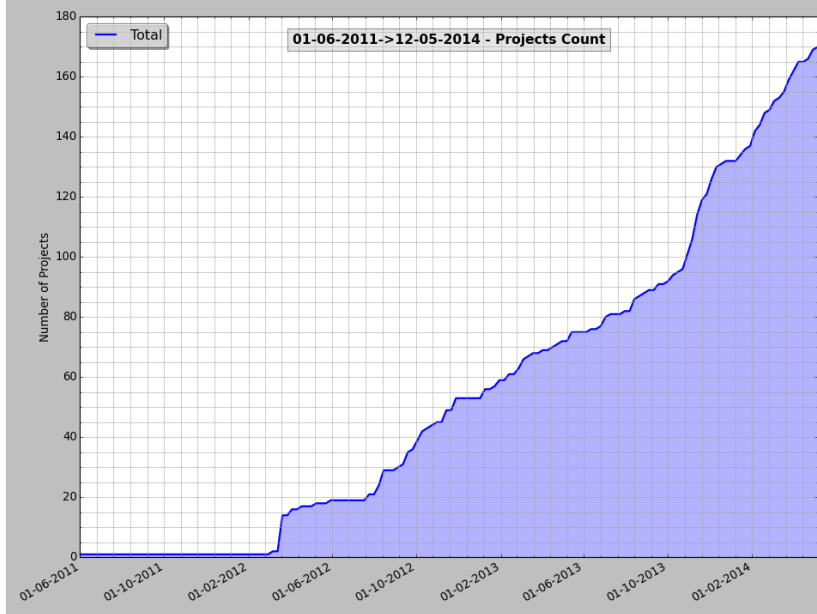


Finite Resources

- Hardware & Software
 - Processors, Memory, disk, Licenses

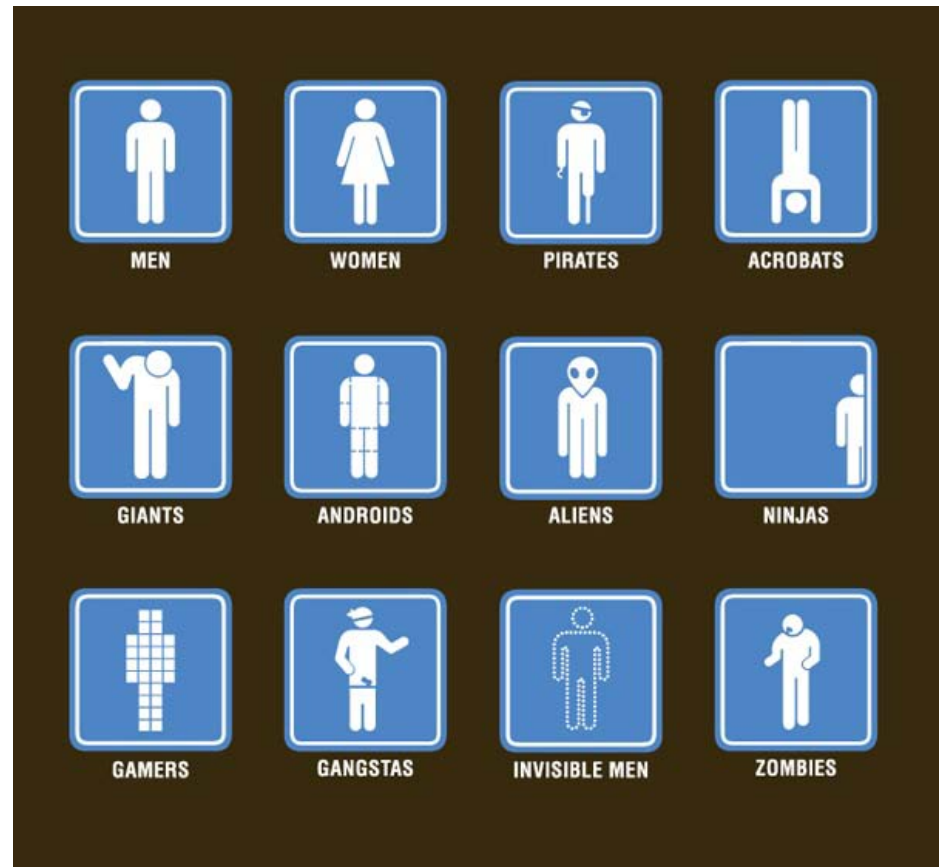


Increasing Consumption



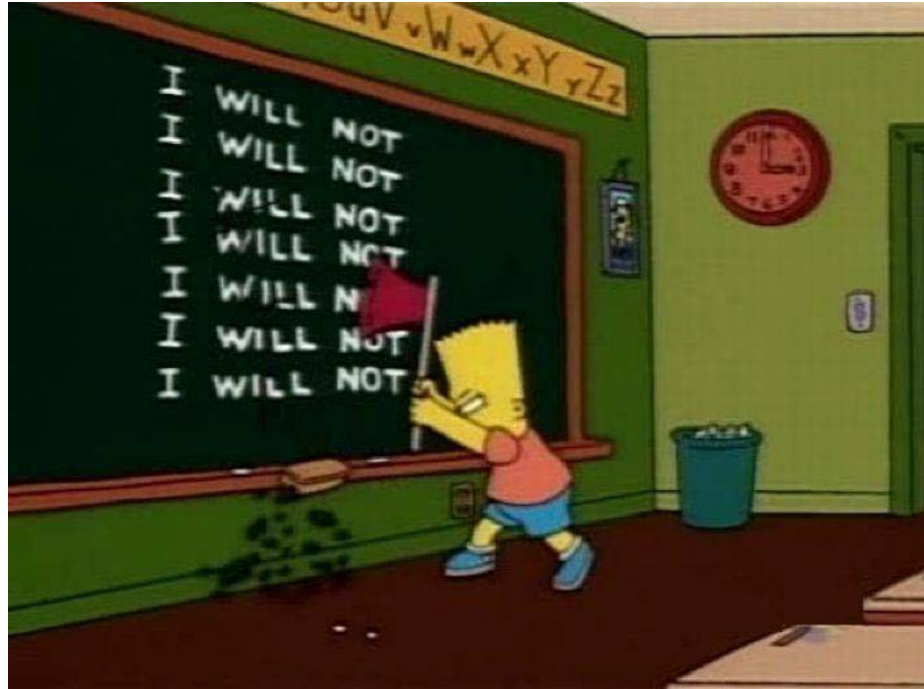
Diverse User Base

- Academia & Commercial
- Huge variety of applications
- Differing Requirements
 - Devil is in the detail



What is 'Fair Usage'?

- We operate an open system
 - We do not want to impose draconian limits
- Set of guidelines, with just a few rules
- Broadly encouraging user awareness
- Improve service & predictability for all
 - Large proportion of usage by small proportion of users
 - More resources will come



A Few Highlights

- Computation must happen through the scheduler
- Storage is not intended for long-term dataset archival
- Keep it secure



The screenshot displays the 'Fair Usage Policy' document from HPC Wales. The document is titled 'Fair Usage Policy' and includes a section for 'Rules and guidelines'. It outlines the following points:

- 1: The home directory is for code, scripts, and small data sets**
The home directories are designed for availability and safety, but not so much for performance. If your job makes a lot of disk access (reading and/or writing files), then it should do so in either a local temporary space on a compute node or a file scratch. Please do not use the cluster file systems for long-term storage of data. Once data is not being actively used it should be moved elsewhere to free up space for other cluster users. We do not routinely operate a data archive or provide a long-term storage service; this will only be possible in special circumstances.
- 2: The scratch directory is for temporary data created/ utilised by a job**
The scratch directories are designed to be able to accommodate large amounts of data very rapidly. They are for a job to store temporary data and should be cleaned after the job has finished. They are not for storing data, as scratch directories are subject to arbitrary cleaning at any moment.
- 3: The login nodes are for compiling, debugging, and file editing activities**
The login nodes are intended for interactive SSH sessions, file editing, compiling, debugging and managing jobs in the job scheduler. They are reserved for activities which do not consume lots of processing or memory resource. Any job dedicated to computing must be run on a compute node.

At the bottom of the document, there is a footer with the HPC Wales logo, the website 'hpcwales.co.uk', and logos for the Welsh Government, the European Union, and the UK Government.



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Progress on Gateways

Charlie Godfrey, Skills Academy Manager



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Topics

- HPC Wales User Portal
- Knowledge Base (additions and changes)
 - User Group
 - Video Tutorials
 - Other Guides
- Gateways
 - Project Summaries
 - Calendars
 - Team Discussions

Knowledge Base

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Knowledge Base
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 - ▶ Command Line Environment
 - ▶ Data Storage & Management
 - ▶ University Access to HPCW Systems
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- ▶ **Video Tutorials**


Knowledge Base



The Knowledge Base contains a variety of documentation on the HPCW project and use of the systems and services. Please access the links to the left in order to learn more.


Recent Software Updates & Additions


| Name | Version & Build Details |
|-------------------------------|--|
| LS-DYNA | Version R6.1.1. |
| MAXWELL-3D | Version 16.0. |
| CRYSTAL09 | 2.01 built with the Intel Compiler v11.1, and Intel MPI 4.0. For the MPP version, the Intel Scalapack libraries have been used. |
| gaussian | 09d01 |
| fastx_toolkit | version 0.0.13.2 It requires libgtextutils version 0.6.x which was built separately). Both were compiled using GNU compiler. |





 Video Tutorials

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- ▶ **Video Tutorials**

Video Tutorials

The links below are to the video tutorials we have on how to use HPC Wales' services.

Note: Further tutorials can also be found within the Gateways section of the portal, where they relate to an industry or sector application.

Tutorials

Starting Out

- [How to Access the Portal](#)
- [How to Access the Gateway](#)

SynfiniWay Workflows

- [How to Access SynfiniWay](#)
- [How to Access a Workflow](#)
- [How to set up Profiles in SynfiniWay](#)
- [How to Submit a Maya Workflow](#)
- [How to Monitor a Workflow](#)

Support Desk

- [How to Raise a Support Call in Service Now](#)
- [How to Monitor and Update a Support Call in Service Now](#)

PuTTY

- [Part 1 of 3 – Installation](#)
- [Part 2 of 3 – First Connection and Configuration](#)
- [Part 3 of 3 – Running Top](#)

FileZilla

- [Part 1 of 3 – Installation](#)
- [Part 2 of 3 – First Connection and Configuration](#)
- [Part 3 of 3 – Uploading, Deleting and Downloading Files](#)



How to Access the Portal - YouTube

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How to Access the Portal

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- Zeeko Ltd: us precision eng by hpcwales 33 views 3:37
- How supercor Bloodhound - by hpcwales 53 views 3:05
- Xodus Group to explore the by hpcwales 38 views 3:11
- Calon Cardio supercomputi by hpcwales 17 views 3:27

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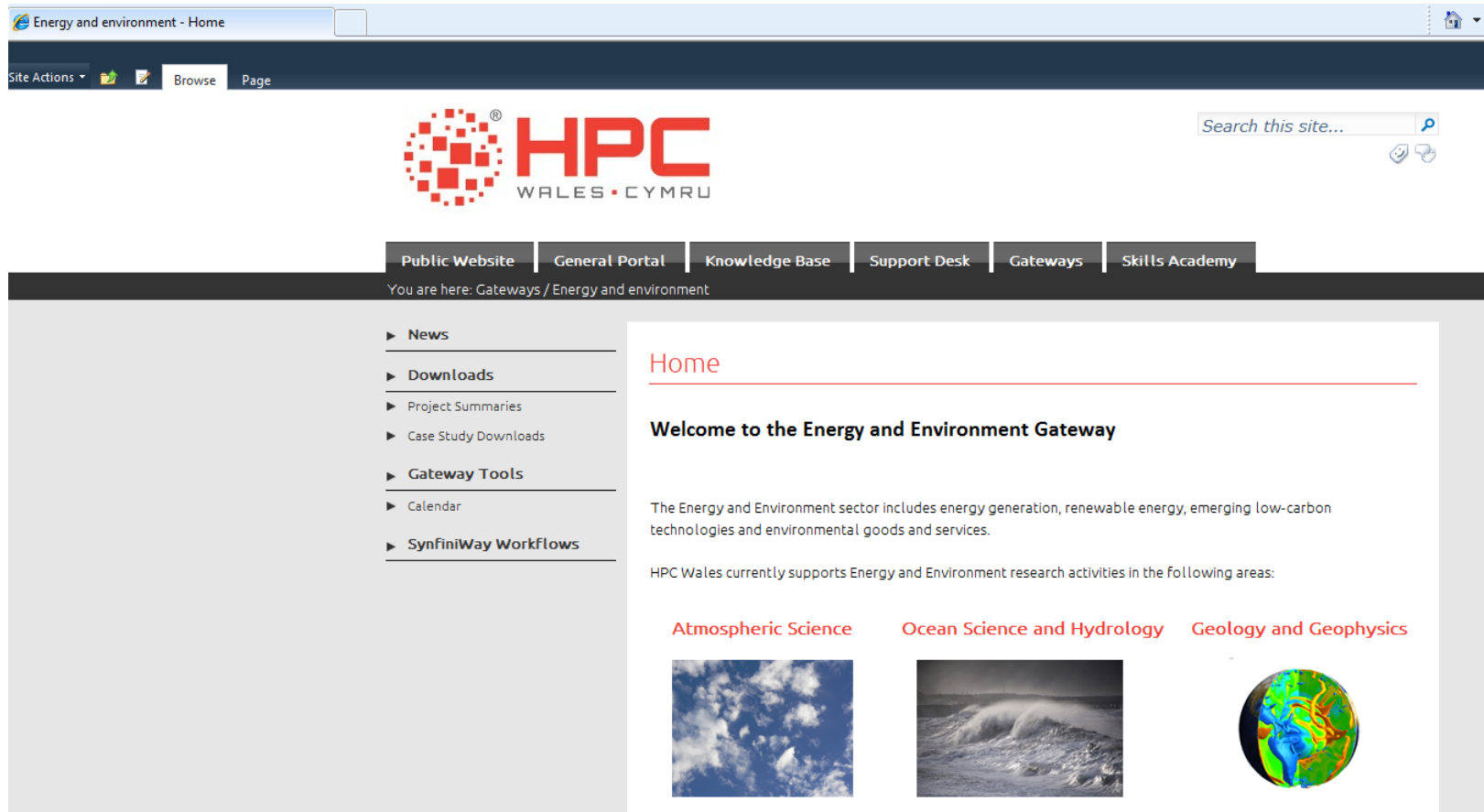
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Other Guides

This page contains links to other reference guides to help use HPC Wales' services.


| Topic | Description | Document Link |
|--------------------|--|---|
| ddt | is a graphical debugger for parallel codes written using MPI and OpenMP. This guide will take you through the process of using DDT on HPC Wales. | Using ddt.pdf |
| Emacs | This guide provides a summary of the Emacs commands and links to other reference materials for Emacs. | Quick Reference Guide Using Emacs.pdf |
| FileZilla - Set up | This guide will take you through the process of setting up FileZilla for use on HPC Wales. | FileZilla setup.pdf |
| FileZilla - Using | This guide will take you through the process of usingup FileZilla on HPC Wales. | Using FileZilla.pdf |
| IPM | Integrated Performance Monitoring (IPM) is a portable profiling infrastructure that provides a low-overhead framework for measuring the performance and resource utilization of parallel codes. | Using ipm.pdf |
| Linux | This guide provides a summary of Linux commands and links to other reference materials for Linux. | Quick Reference Guide Using Linux.pdf |
| OSS | [Open]SpeedShop is a profiling tool built on top of a number of open-source applications (such as PAPI and Vampirtrace) that can be used to gather performance data about serial and parallel codes. This guide will take you through the process of using OSS on HPC Wales. | Using oss.pdf |

[Scalable performance Analysis of Large Scale Applications] is a software tool that supports the performance optimisation of

A screenshot of the HPC Wales Energy and Environment Gateway website. The browser address bar shows 'Energy and environment - Home'. The website header includes the HPC Wales Cymru logo and a search bar with the text 'Search this site...'. A navigation menu contains links for 'Public Website', 'General Portal', 'Knowledge Base', 'Support Desk', 'Gateways', and 'Skills Academy'. Below the menu, a breadcrumb trail reads 'You are here: Gateways / Energy and environment'. The left sidebar lists categories: 'News', 'Downloads' (with sub-items 'Project Summaries' and 'Case Study Downloads'), 'Gateway Tools' (with sub-items 'Calendar' and 'SynfiniWay Workflows'), and 'SynfiniWay Workflows'. The main content area has a red 'Home' link, followed by the heading 'Welcome to the Energy and Environment Gateway'. The text describes the sector and lists supported research areas: 'Atmospheric Science', 'Ocean Science and Hydrology', and 'Geology and Geophysics'. Each area is accompanied by a representative image: clouds for atmospheric science, ocean waves for ocean science, and a globe for geology and geophysics.

Project Summaries - All Items

Site Actions ▾ Browse List Tools Items List



 Search this site... 🔍

Public Website | General Portal | Knowledge Base | Support Desk | Gateways | Skills Academy

You are here: Gateways / Energy and environment

- News
- Downloads
- [Project Summaries](#)
- Case Study Downloads
- Gateway Tools
- Calendar
- SynfiniWay Workflows

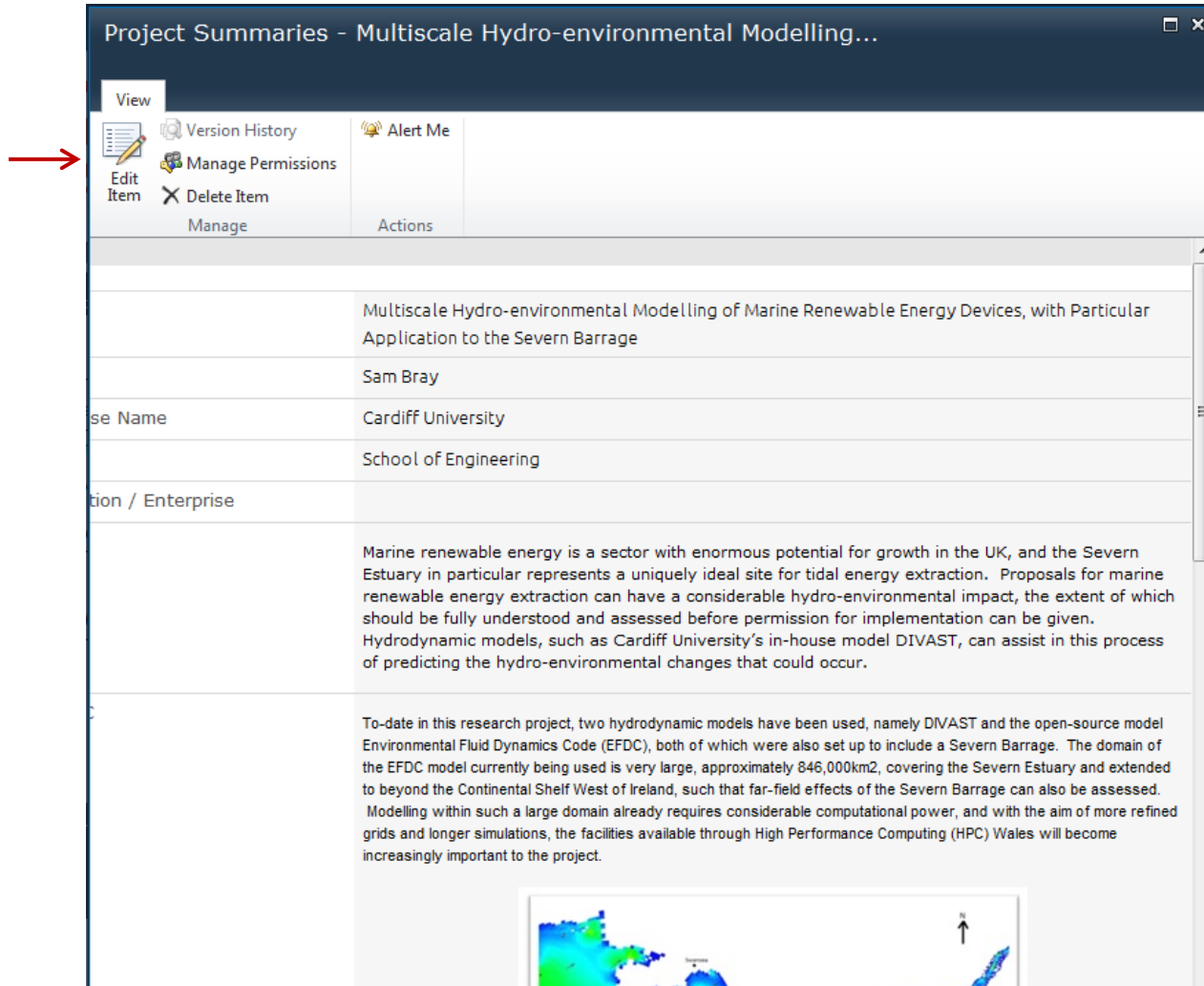
Project Summaries ▸ All Items ▾

|   Title | Project Lead | Institution / Enterprise Name |
|---|------------------|-------------------------------|
| Feedbacks between tidal stream farm operation and the marine environment | Dr Simon Neill | Bangor University |
| Improving Hydrocarbon Exploration by Assimilating Seismic Data | J. H. Davies | Cardiff University |
| Multiscale Hydro-environmental Modelling of Marine Renewable Energy Devices, with Particular Application to the Severn Barrage | Sam Bray | Cardiff University |
| Simulating the impacts of climate change on estuarine dynamics using an integrated catchment-to-coast model | Dr Reza Hashemi | Bangor University |
| Tide-ice sheet interaction in a Future Climate | Dr Mattias Green | Bangor University |

➕ Add new item



Gateways – Project Summaries




Project Summaries - Multiscale Hydro-environmental Modelling...

View

Version History Alert Me

Edit Item Manage Permissions Delete Item Manage Actions

| | |
|-------------------|---|
| | Multiscale Hydro-environmental Modelling of Marine Renewable Energy Devices, with Particular Application to the Severn Barrage |
| | Sam Bray |
| se Name | Cardiff University |
| | School of Engineering |
| tion / Enterprise | |
| | <p>Marine renewable energy is a sector with enormous potential for growth in the UK, and the Severn Estuary in particular represents a uniquely ideal site for tidal energy extraction. Proposals for marine renewable energy extraction can have a considerable hydro-environmental impact, the extent of which should be fully understood and assessed before permission for implementation can be given. Hydrodynamic models, such as Cardiff University's in-house model DIVAST, can assist in this process of predicting the hydro-environmental changes that could occur.</p> |
| | <p>To-date in this research project, two hydrodynamic models have been used, namely DIVAST and the open-source model Environmental Fluid Dynamics Code (EFDC), both of which were also set up to include a Severn Barrage. The domain of the EFDC model currently being used is very large, approximately 846,000km², covering the Severn Estuary and extended to beyond the Continental Shelf West of Ireland, such that far-field effects of the Severn Barrage can also be assessed. Modelling within such a large domain already requires considerable computational power, and with the aim of more refined grids and longer simulations, the facilities available through High Performance Computing (HPC) Wales will become increasingly important to the project.</p>  |

Calendar - Calendar


Site Actions

Browse

Calendar Tools

Events

Calendar



Search this site...

Public Website

General Portal

Knowledge Base

Support Desk

Gateways

Skills Academy

You are here: Gateways / Energy and environment

News

Downloads

Project Summaries

Case Study Downloads

Gateway Tools

Calendar

SynfiniWay Workflows

Calendar

Calendar

Use the Calendar list to keep informed of upcoming meetings, dead lines, and other important events.




May 2014





| Monday | Tuesday | Wednesday | Thursday | Friday | Saturday | Sunday |
|-----------------------------------|-----------------------------------|-----------|----------|--------|----------|--------|
| 28 MIKE by DHI | 29 | 30 | 1 | 2 | 3 | 4 |
| 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| 12 | 13 16th MIKE by DHI User Group | 14 | 15 | 16 | 17 | 18 |
| 19 | 20 | 21 Add | 22 | 23 | 24 | 25 |
| 26 | 27 | 28 | 29 | 30 | 31 | 1 |
| 2014 ROMS User Workshop (Croatia) | | | | | | |

Done

Internet

Welcome to the Advanced Materials Manufacteri...

Site Actions  Browse  List Tools  List

 Search this site...   


Public Website | General Portal | Knowledge Base | Support Desk | Gateways | Skills Academy


You are here: Gateways / Advanced materials and manufacturing

- ▶ Downloads
 - ▶ Project Summaries
 - ▶ Shared Documents
- ▶ Gateway Tools
 - ▶ Calendar
 - ▶ Team Discussion
- ▶ SynfiniWay Workflows

Team Discussion ▶ Welcome to the Advanced Materials Manufacturing Gateway ▶ Flat ▾
Use the Team Discussion list to hold newsgroup-style discussions on topics relevant to your team.

Posted By Post

Started: 14/01/2014 11:17 [View Properties](#)  [Reply](#)


Andrew Austin

Welcome to the Advanced Materials & Manufacturing Gateway.
Welcome to the Advanced Materials & Manufacturing Gateway.

Use this area to post tips, tricks and requests for help from other Advanced Materials & Manufacturing users about using any of the applications in this section.

Note that for HPC Wales technical support, please send an email to support@hpcwales.co.uk with a description of your issue.

Thank you.

HPC Wales Technical Support.

There are no items to show in this view of the "Team Discussion" discussion board.

[Sitemap](#) | [Contact Us](#)



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Powering Success
Pweru Llwyddiant

Thematic User Groups

Charlie Godfrey, Skills Academy Manager



Ewrop & Chymru:
Buddsoddi yn eich dyfodol
Cronfa Datblygu Rhanbarthol Ewrop

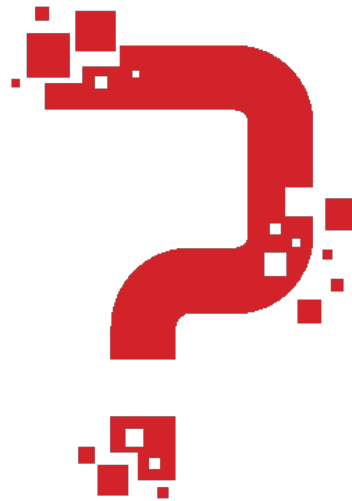
Europe & Wales:
Investing in your future
European Regional Development Fund



Thematic User Groups – What's Being Considered

- Life Sciences
 - Genomics (8th -9th Oct 2014)
 - Bio-molecular Simulation
- ICT
 - Big Data
- Advanced Materials & Manufacturing
 - Chemistry
 - Computational Dynamics
- Energy & Environment
- Creative Industry
- Optimising Tools & Libraries

What Would You Like To See?





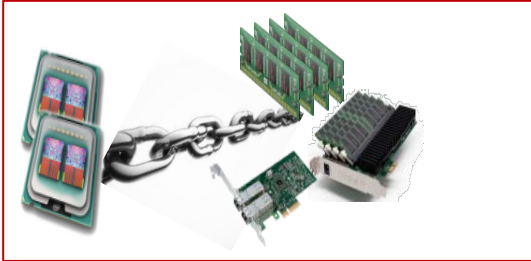
shaping tomorrow with you

HPC Wales User Group, 14th May 2014

Vendor Technology Presentation

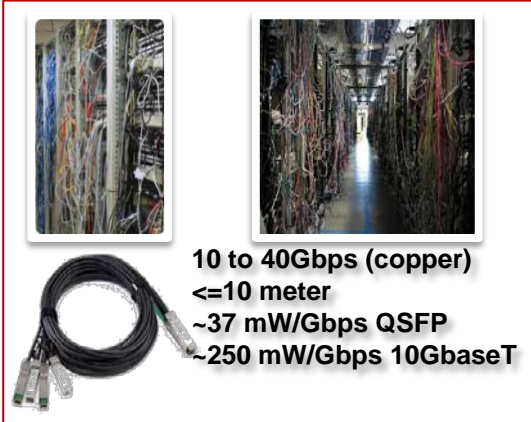
Application Optimized Server Design

Server Design Evolvment



- From chained memory and I/O to flexible pool of resources.

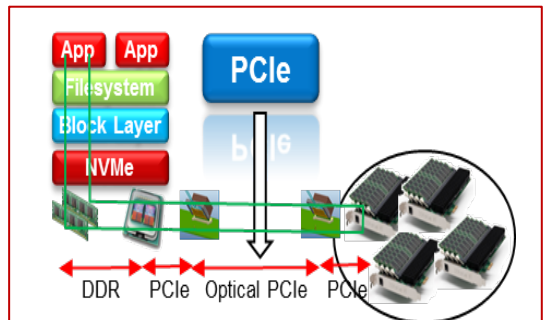
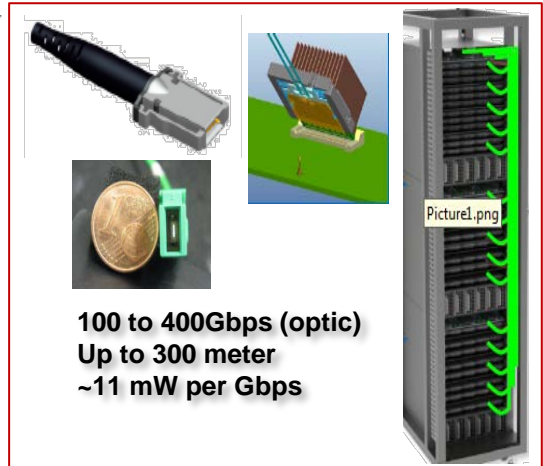
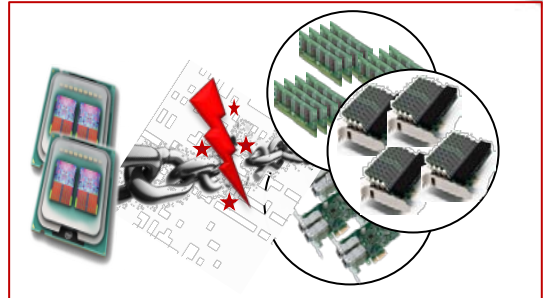
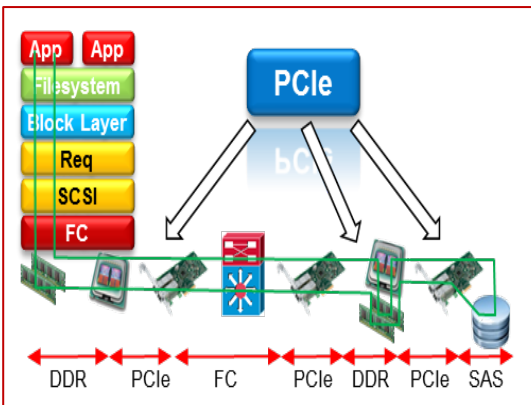
- From complex, fault-prone and costly cable management to thin fail-safe wired once cabling.



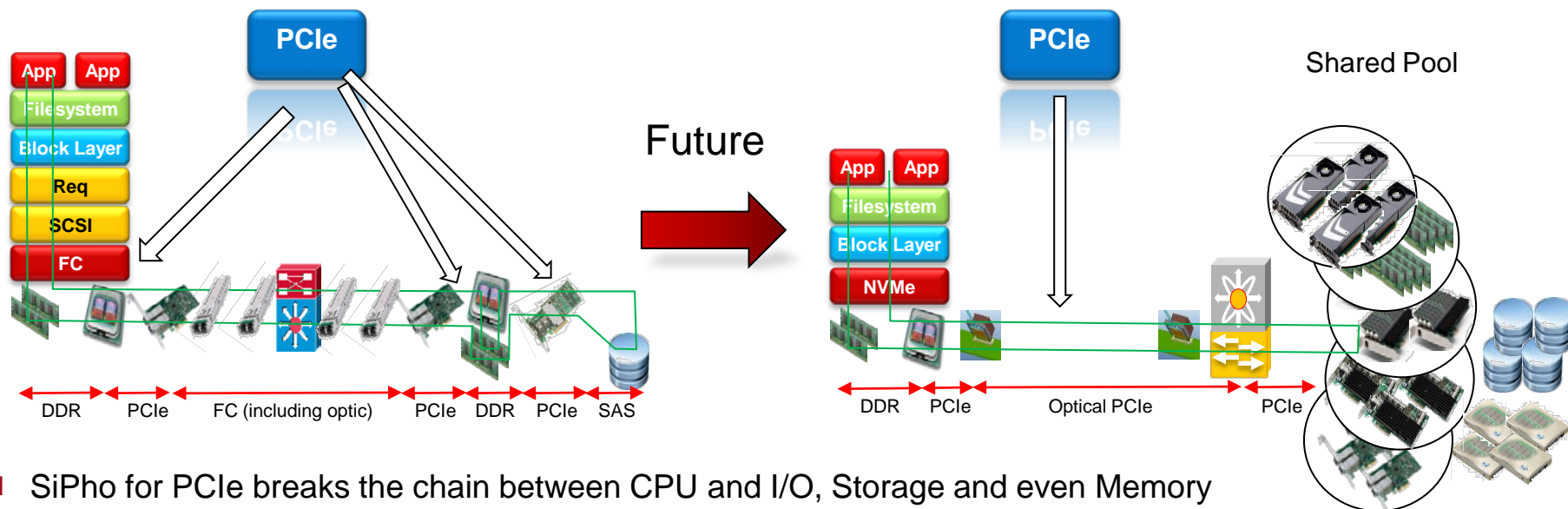
- From limited copper cable bandwidth to boundless high bandwidth optical cable.

- From big power hungry copper interconnects to lean power saving optical interconnect.

- From heavy and compute intensive protocols to lightweight low latency protocols and connections.



From chained Memory and I/O to flexible Pool of Resources



■ SiPho for PCIe breaks the chain between CPU and I/O, Storage and even Memory

- SiPho for PCIe is able to provide enough bandwidth (hundreds of Gbps) low overall latency as well as huge distance (up to 300 meter).
- Allows great part and therefore cost reductions in CAPEX (parts) as well as OPEX(cabling, maintenance, power).
- Enable new data-center architectures with pooled resources flexible available on demand.
 - No overprovision at individual server instead lean server with remote pooled I/O

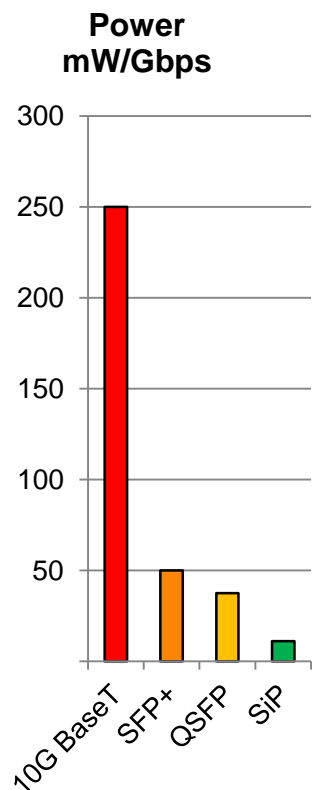
■ PCIe on the way to be the major storage interface

- NVMe, SATAExpress, SCSI over PCIe they all rely on PCIe interface.
- With PCIe SFF even traditional HDD's gets it PCIe based counterparts

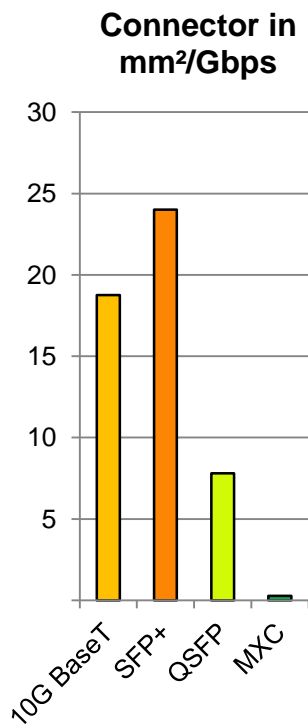
Some SiP Metrics

Comparison done on major network interfaces in the Data-Centre.

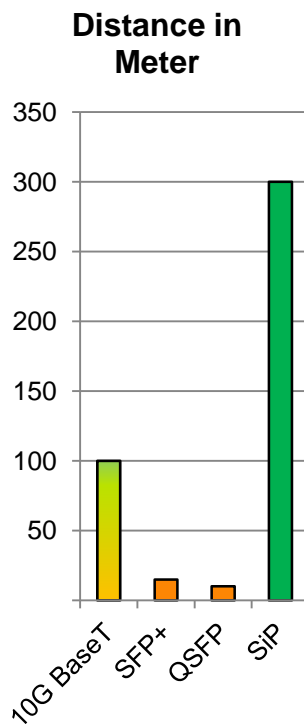
10GbaseT, SFP+, QSFP are copper based (Cat5/6Twinax), ClearCurve/MXC



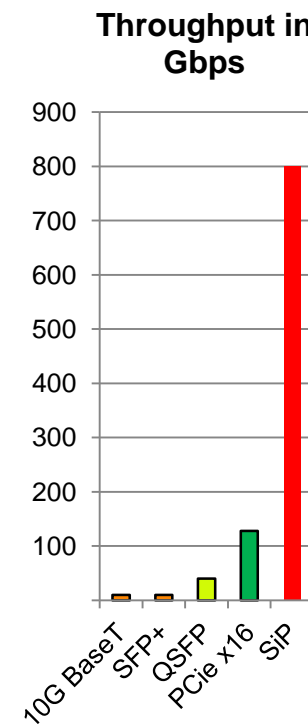
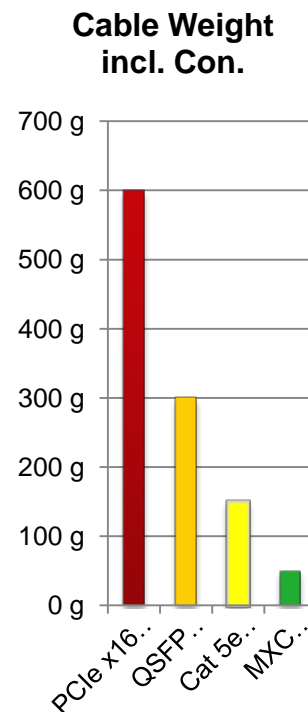
OPEX



Density



DC Concepts



Performance

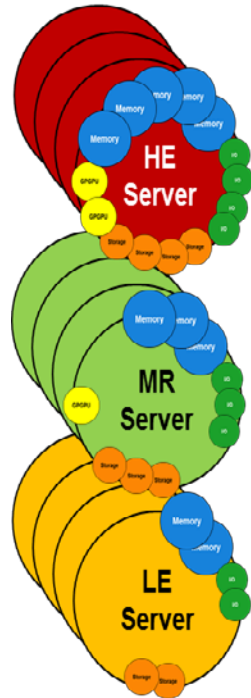
Benefits enabled by SiP based Architectures



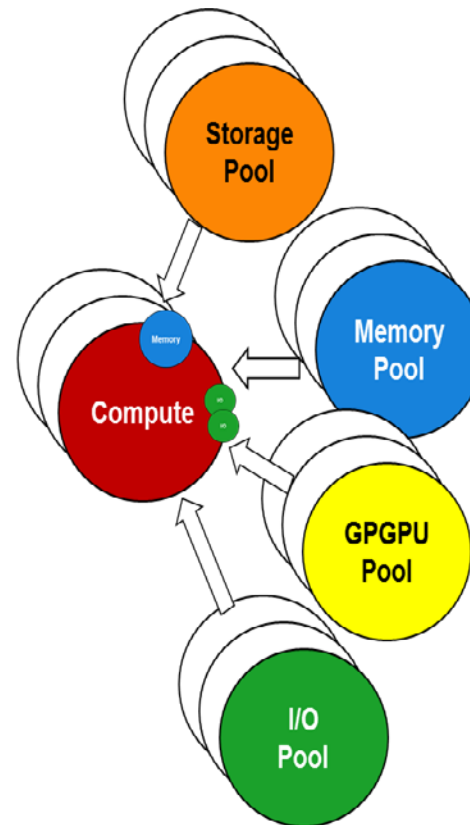
- Rack scale resource provisioning to accomplish app-optimized server build
- Business-driven (re-) build of IT-Infrastructure at any time
- Lowest TCO by disaggregation of compute, memory, storage and networking
- High Bandwidth, long reach, very dense and power efficient Interconnects

Traditional versus Disaggregation

Traditional



Disaggregated



- From fixed server for different workloads towards slim compute nodes flexible configured for different application demands

New IT Usage Models

■ New IT usage models require business driven build of IT HW

■ Cloud

on customer demand compute, storage and network resources

■ XaaS

HW resource usage model changes over system lifetime

■ Big Data

varying compute, network and storage requirements
(hot, cold, dark)

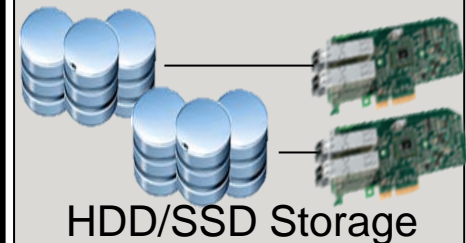
■ HPC

from static to application optimized system configuration

Compute / Memory

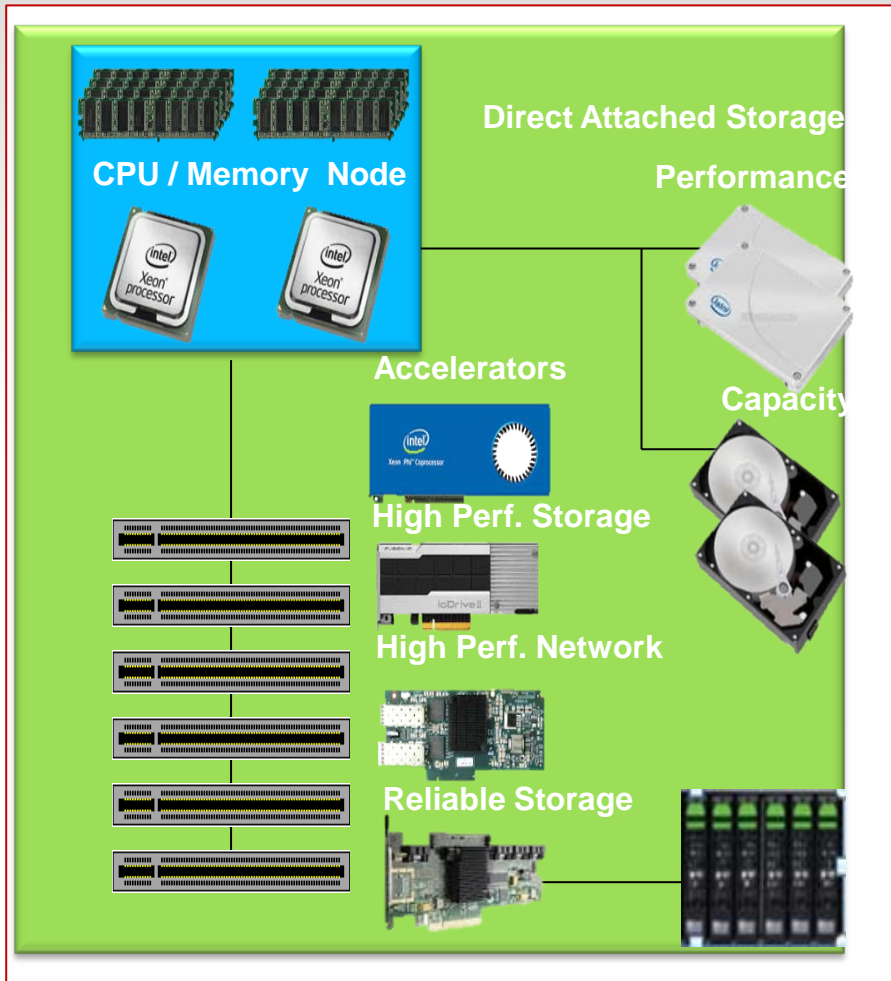


Pool of

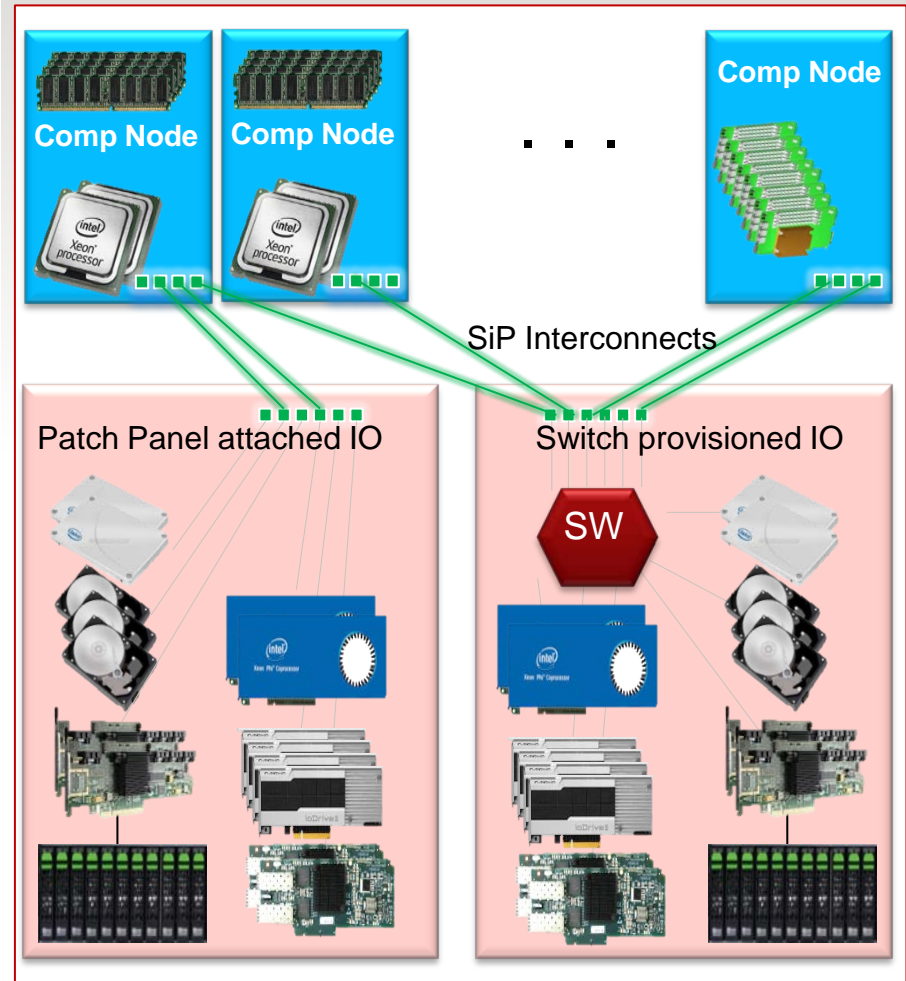


State of Art vs. App. Optimized Server

State of Art



App optimized



Server Features: State of Art vs. App. optimized



State of Art Server

One enclosure for multi purpose usage

- Optimized for sweet spot of deployments
- Complex design w/ config options to extend server range of use

Mostly oversized for dedicated usage

- IO Slots, Disk space, PSU capacity, ...
- more space consuming than required
- CAPEX, OPEX disadvantages

IO config Limitations

- High Power/Space demanding Devices like GPGPUs, PCIe SSD
- Full Height, full Length slots

Common Life Cycle for Server Resources

App optimized Server

Server build from rack level resource pools

- Optimized for individual Application and Business
- More Simple design by building block (re-)usage
- HW attached and/or SW provisioned Resources
- enabled by Intels SiP opt.IF Technology

Optimized for dedicated user application

- Compute, Storage, Network, .. deployed as needed from dense packaged, resource pool offerings
- CAPEX, OPEX advantages

Support of App Specific HW Requirements

- more Space/Power for CPU/Memory by disaggregation
- diverse resource pool offerings to cover broad range of individual App specific requirements

Individual Life Cycles of Server Resources

- e.g. CPU Technology update w/o side impacts

Silicon Photonics enables Resource Pool provided NV Storage Benefits



■ Flexible provisioning of new NV storage TIERs required

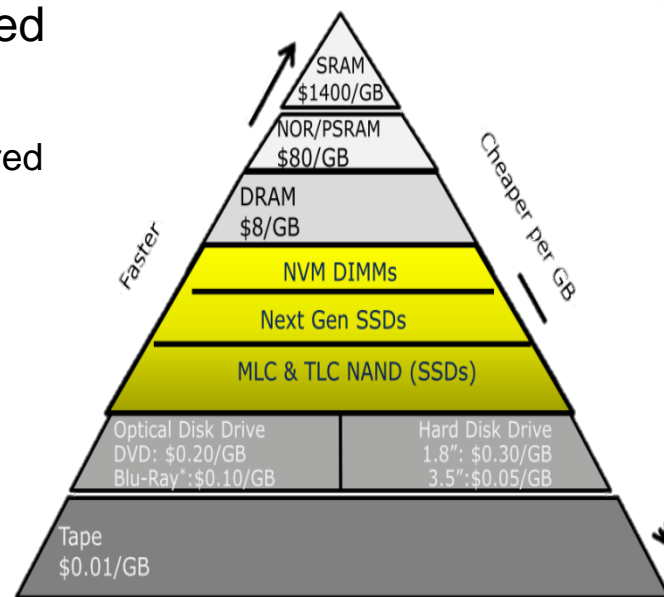
- Significant cost/performance differences between storage TIERs
- Demand for business driven provisioning of different TIERs required
 - Especially in Cloud, XaaS, Big Data environments

■ Usage model of NV storage is changing

- from caching to storage of important system and application data
 - new Kernel OS and Application APIs emerging
- No High Availability for Server local only accessible NV storage

■ Resource Pool provided new NV Storage becoming obvious to meet new IT usage requirements

- On-demand assignability of resources to Compute Nodes
- Failover support by Multi Node accessibility



Source: Bernstein 2013

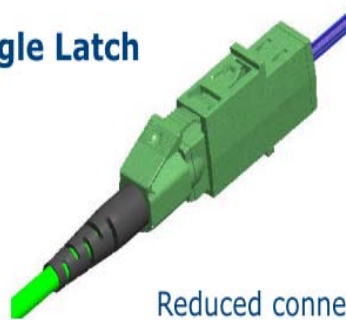
MXC Optic Connector - Presented at IDF 2013



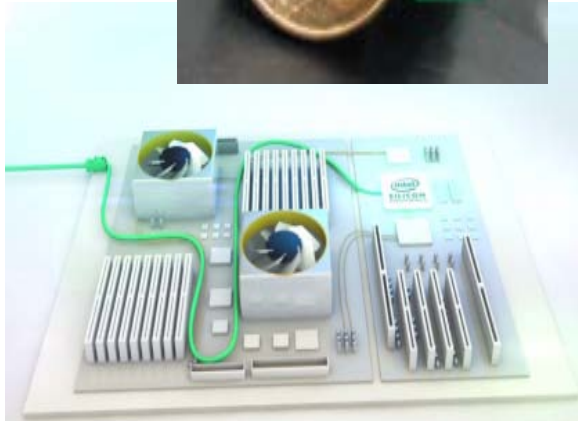
- up to 25Gbps per Fiber
- Up to 64 fibers/connector
- 1.6Tbps, up to 300m via LX MMF cable



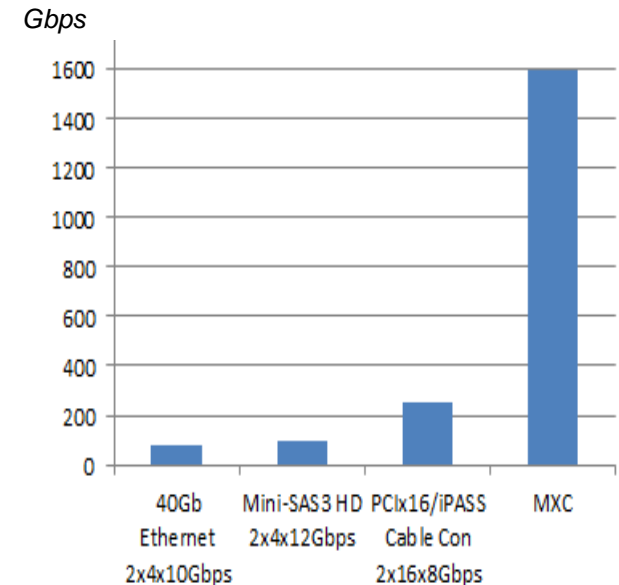
Single Latch



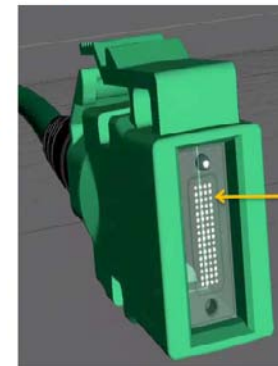
Reduced connector and adapter footprint



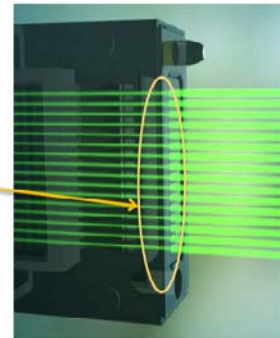
Different Interconnect Bandwidths



Expanded Beam Interconnects

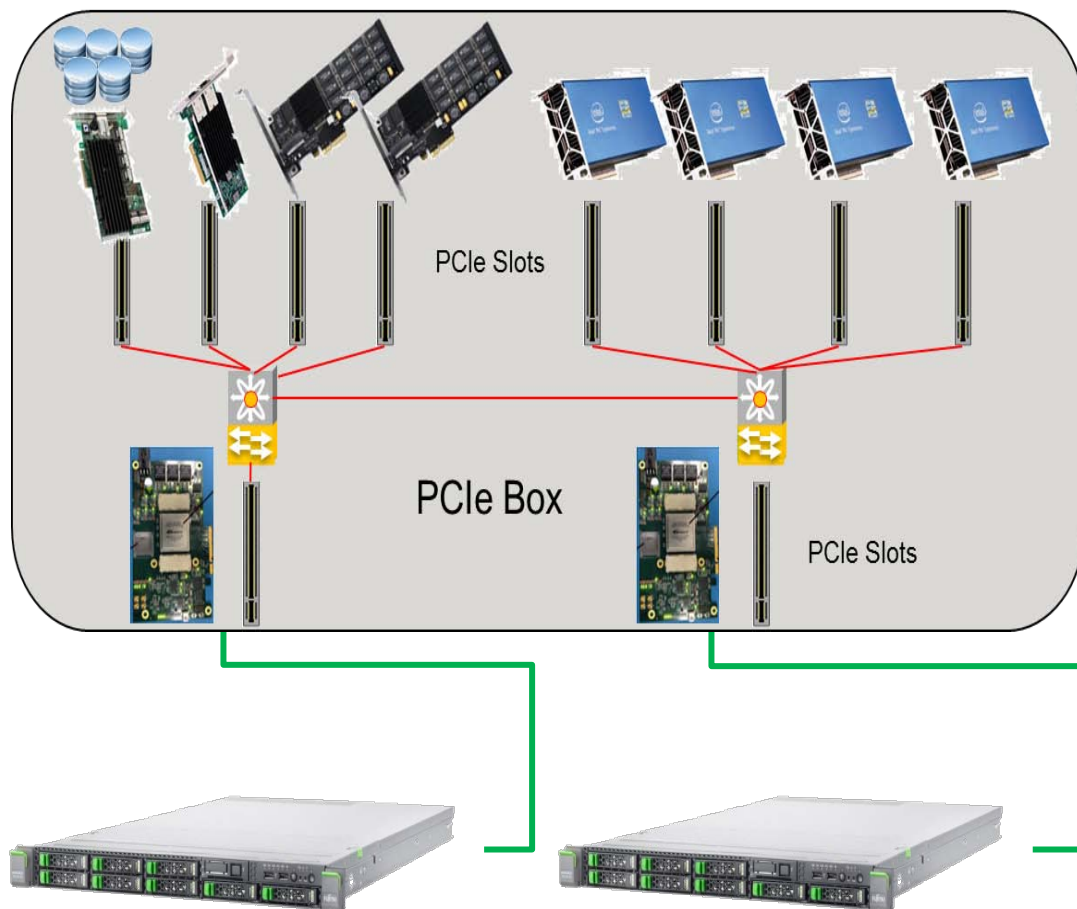


Recessed Integrated beam expander



MXC and Clear Curve Fiber Video: http://www.youtube.com/watch?v=EBM6mmSbe_8

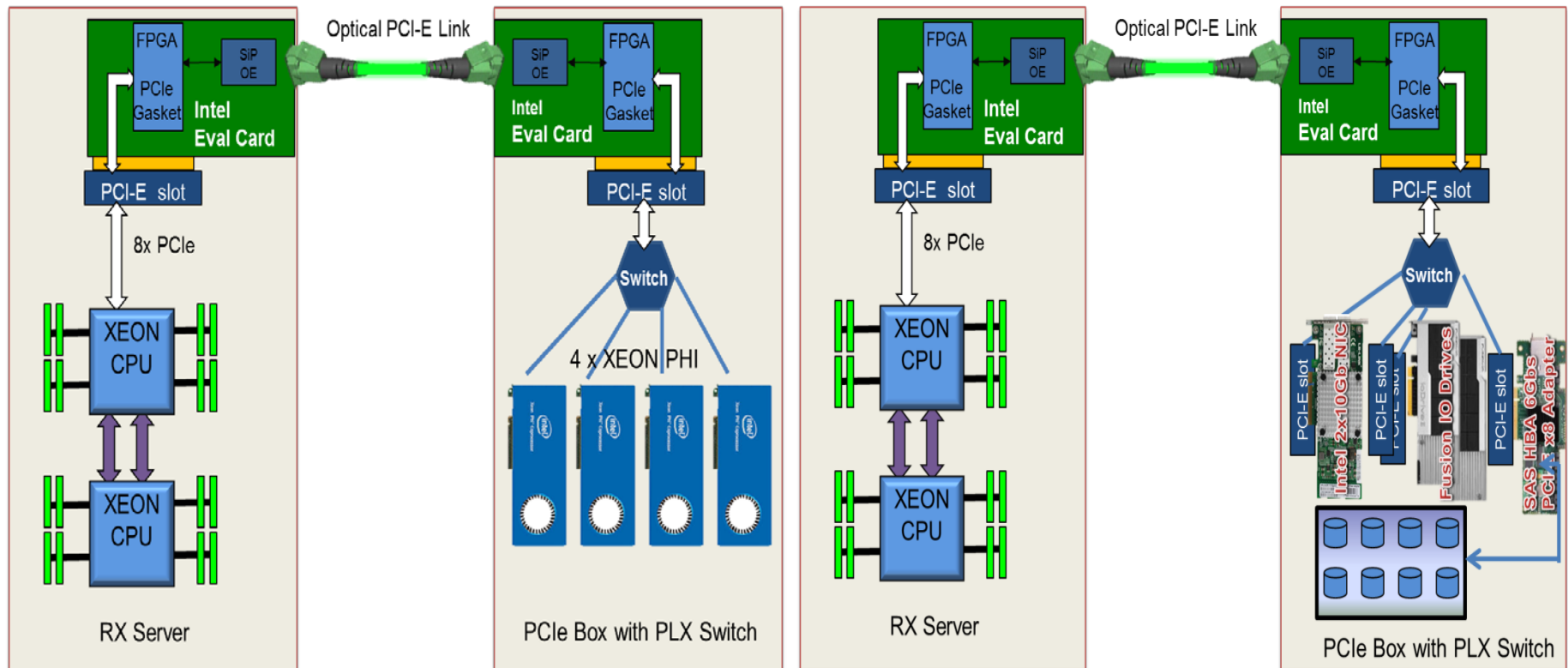
Proof of Concept Configuration



- 2 x PRIMERGY RX200 S8 as Compute Nodes
- 2 x MXC Connector and ClearCurve® Fibre
- 1 x PCIe I/O Box
- 4 x Optical Engine and FPGA PCIe gasket on PCIe card
 - Placed inside the server and the PCIe I/O Box
- Two PLX PCIe Switches inside the PCIe I/O Box
- 1 x 10GbBaseT adapter from Intel
- 1 x Cougar LSI RAID Controller connected to 8 HDD'S inside the PCIe I/O Box.
- Two Fusion I/O PCIe SSD's with 1,5 and 1 Terabyte connected to the PRIMERGY RX200 S8
- 4 x Intel XEON Phi™ connected to the PRIMERGY RX200 S8
- Microsoft Windows 2012 R2 for the video workload
- Linux RedHat 6.4 for the GPGPU workload

Opt. PICE Demo Scenarios

Erläuterungen B.Sch.

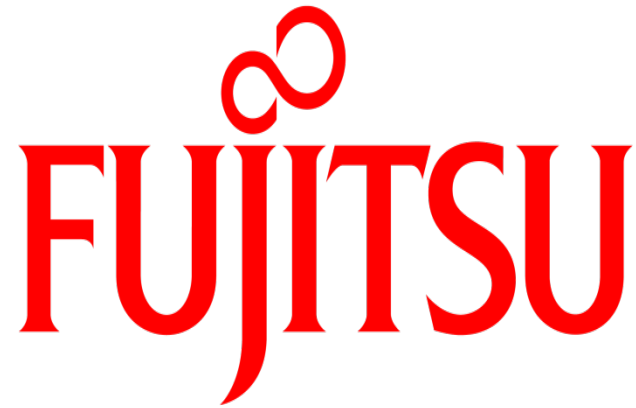


Remote pool of XEON PHIs



Remote Pool of Storage





shaping tomorrow with you



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Powering Success
Pweru Llwyddiant

SME Case Study

Ben Barton, Knowtra

Ewrop & Chymru:
Buddsoddi yn eich dyfodol
Cronfa Datblygu Rhanbarthol Ewrop

Europe & Wales:
Investing in your future
European Regional Development Fund



Applying physical oceanography for business problems – from the Nigerian creeks to global renewables

Ben Barton
Knowtra Limited

My background

- Studied the MSci in Oceanography at Southampton
 - Particle tracking simulation of radioactivity pollution
 - Experience in using range of data sources including satellite data
 - Sound grounding to ocean physics and data collection
- Now for working for Knowtra on metocean problems

Dr Steve Spall's background

- Maths graduate
- Studied the MSc in Oceanography at Southampton
- PhD at Southampton - modelling the impact of ocean fronts of plankton growth
- Work at the Met Office for 9 years
 - Climate change modelling
 - Managing modelling projects for MoD
- Now freelance working on metocean problems

The talk

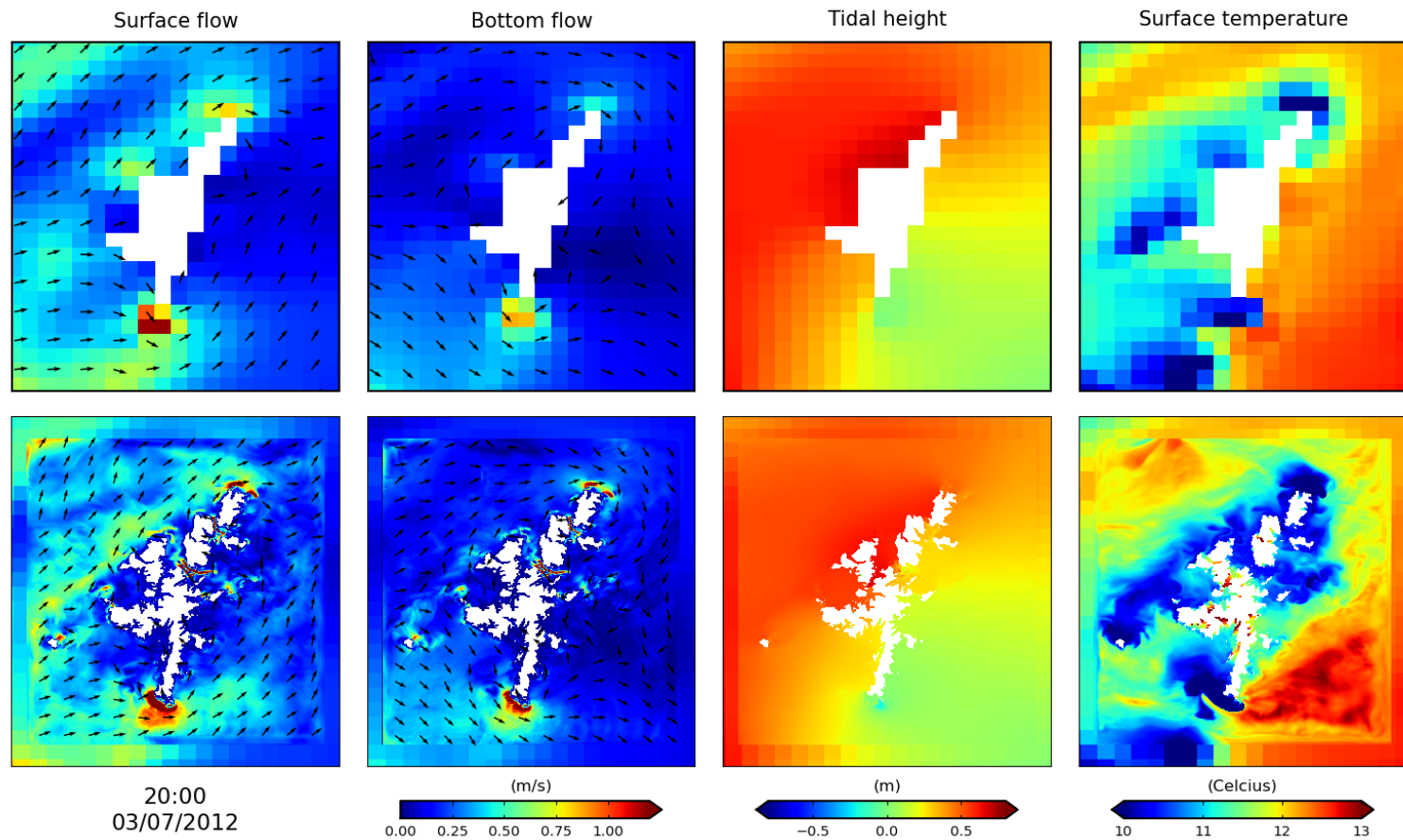
- Usage and Benefits of HPCWales
- Modelling Shetland for oil spill response
- Challenges of projects in Nigeria

HPCWales usage

- Regional Ocean Modelling System (ROMS)
- SWAN wave model
- Python (for data analysis)

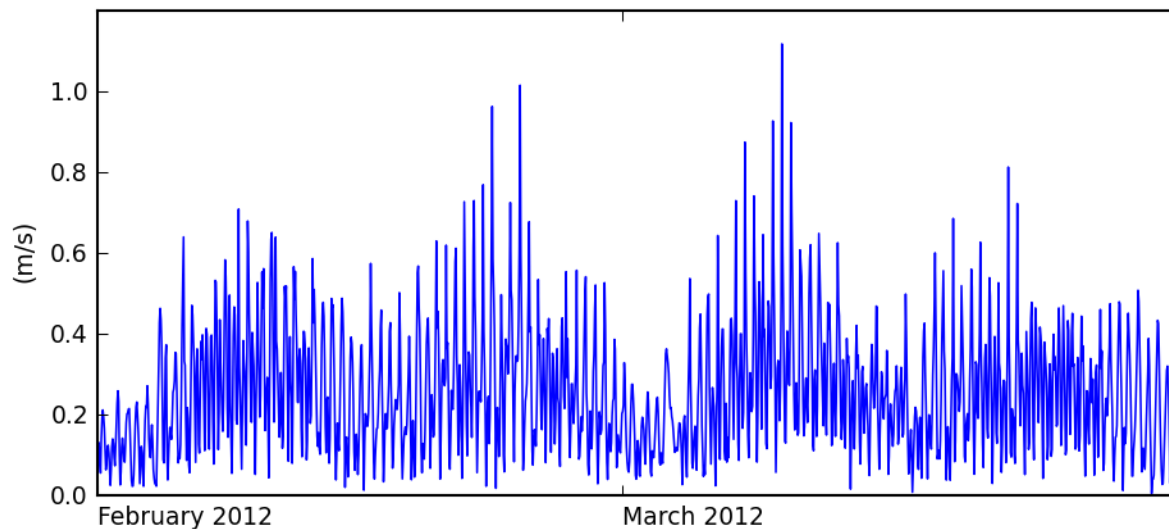
Benefits of HPCWales

High resolution model for Shetland



High resolution model for Shetland

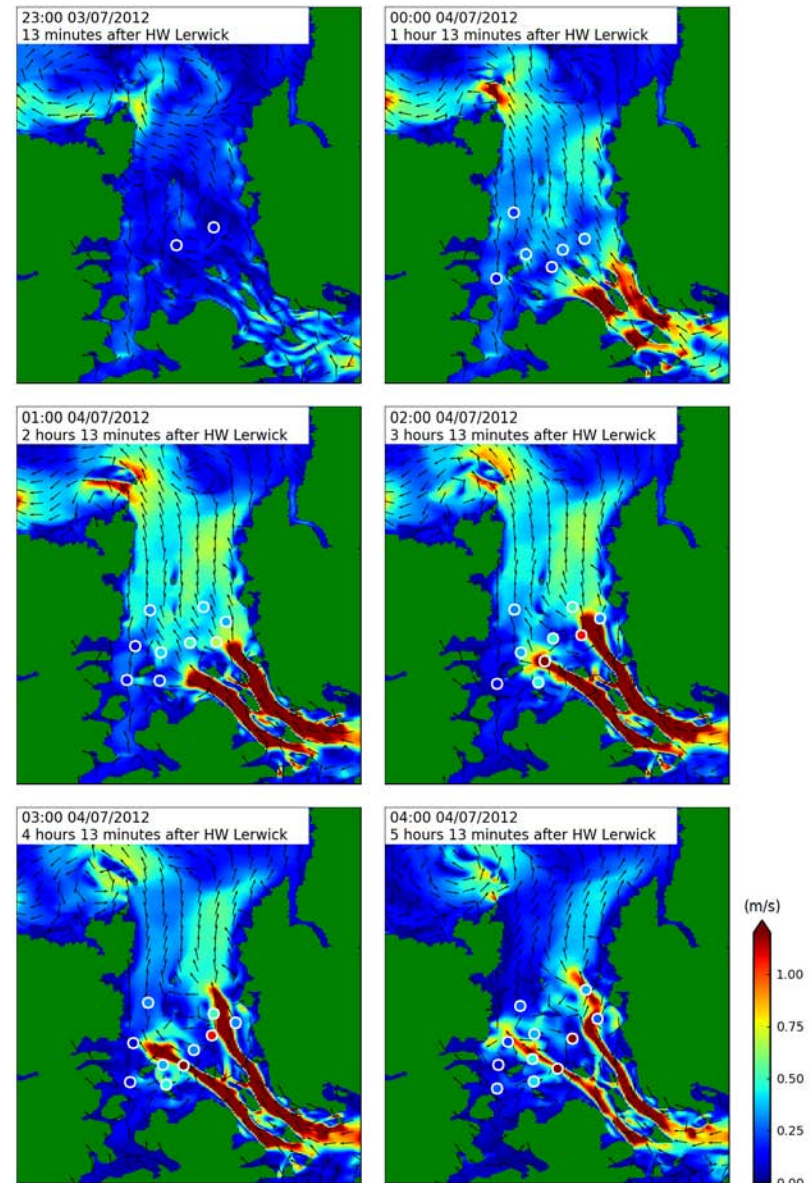
- Using the ROMS model and HPC Wales for computing
- Forced with North West European (NWE) Shelf currents
- Hourly current forcing at top, middle and bottom
- Wind forcing from the ECMWF model



- Ocean, weather and climate expertise
- IT and training solutions

High resolution model for Shetland

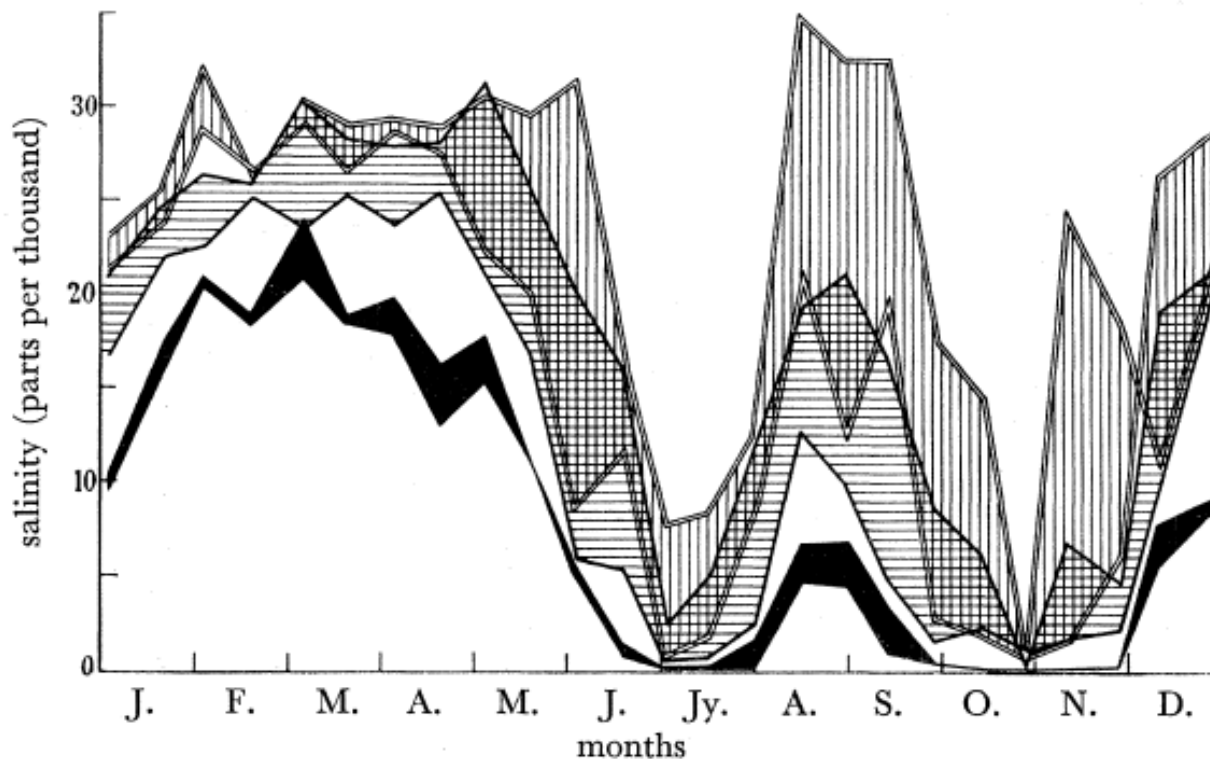
- Compared surface currents to the Admiralty tidal atlas for Shetland
- Coloured circles show the flow speeds from the atlas
- Example of adding detail as needed for local spill modelling



Challenges for Nigeria

- Lack of historic accessible data
- Complex creek systems
- Security issues
- Restricted project budgets
- Need to make the most of what information there is

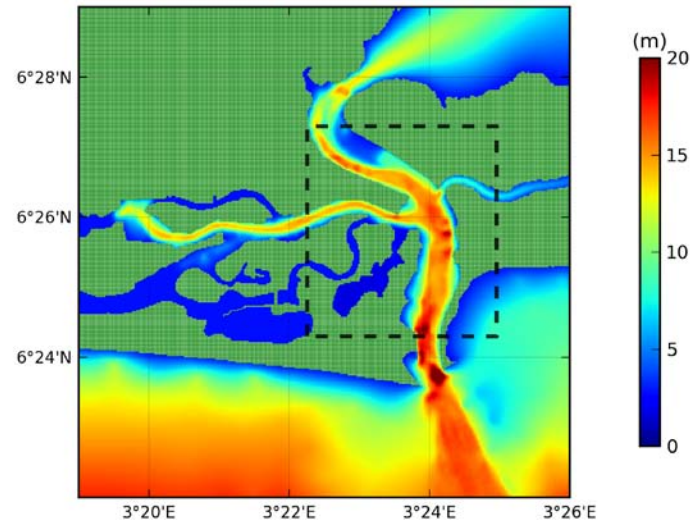
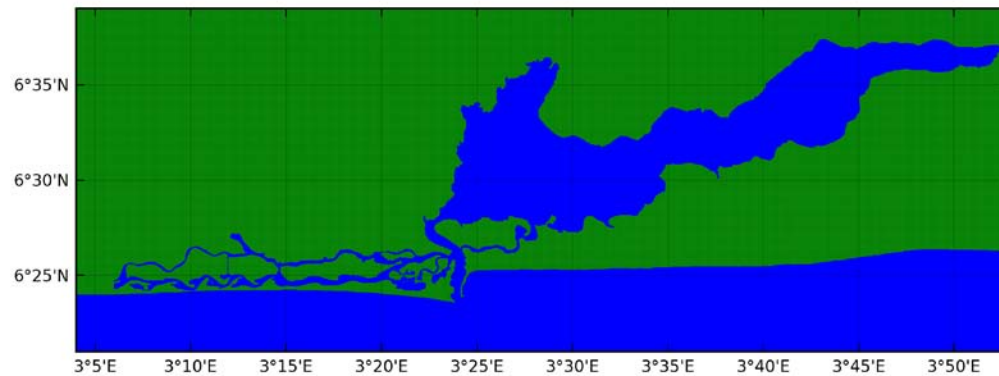
Lagos Harbour salinity



Salinity data
collected in
Lagos Harbour
in 1954

Hill and Webb
Phil. Trans. R. Soc.
Lond. B 1958
241, 319-333

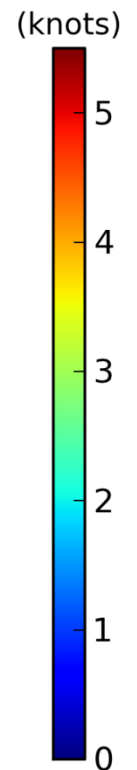
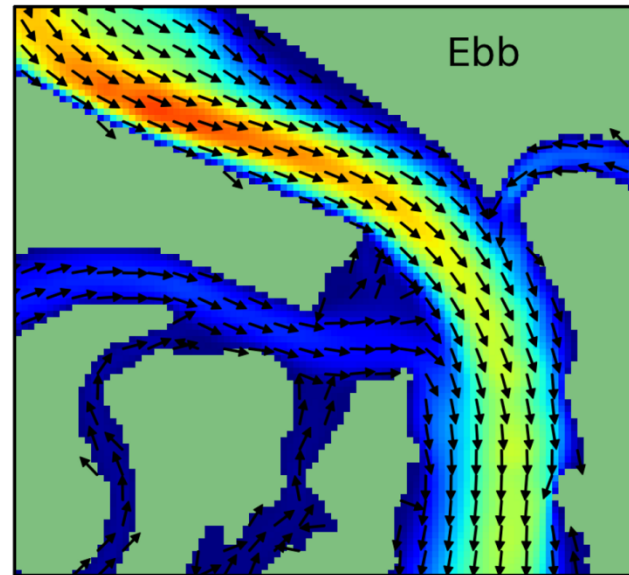
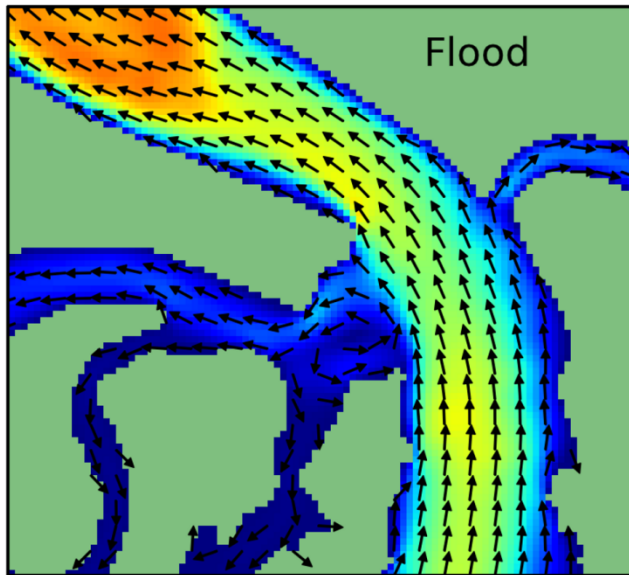
Hydrodynamic models



Lagos Harbour

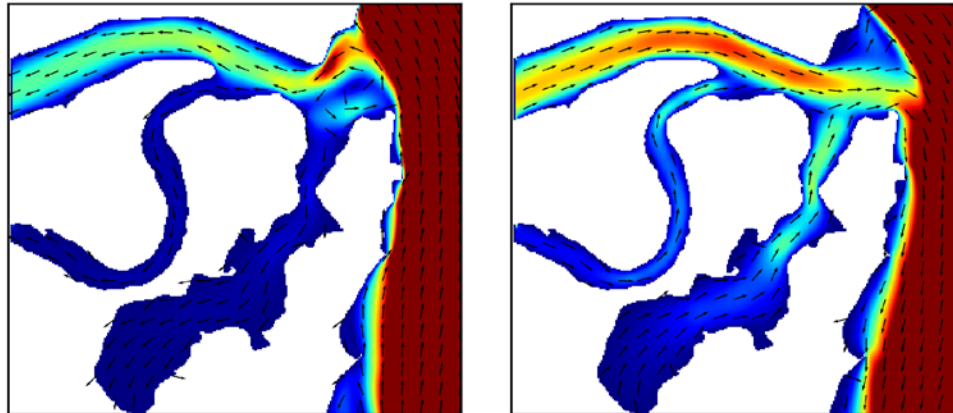
- Ocean, weather and climate expertise
- IT and training solutions

Hydrodynamic models



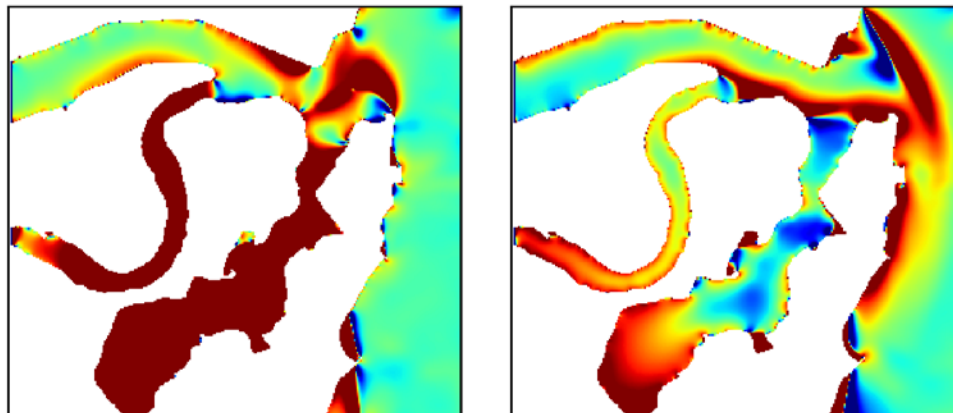
Flood - spring tides

Ebb - spring tides



Surface flow (knots)

0.0 0.5 1.0



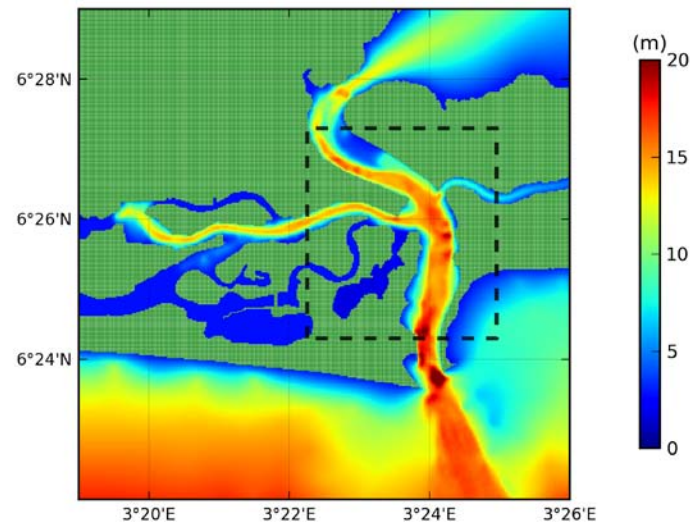
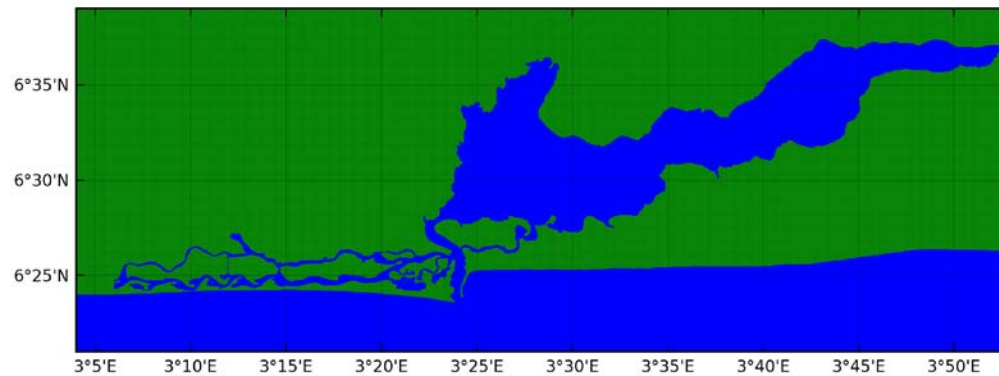
Bottom flow (% of surface flow)

50 70 90

Higher resolution nested model

- Interesting top to bottom differences in flow
- What are the implications for sediment transport?

Wave models

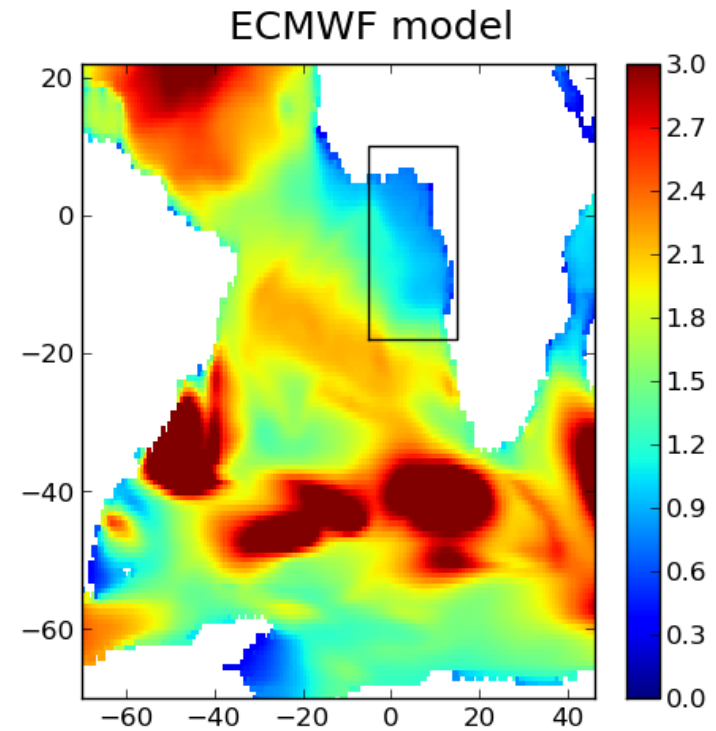
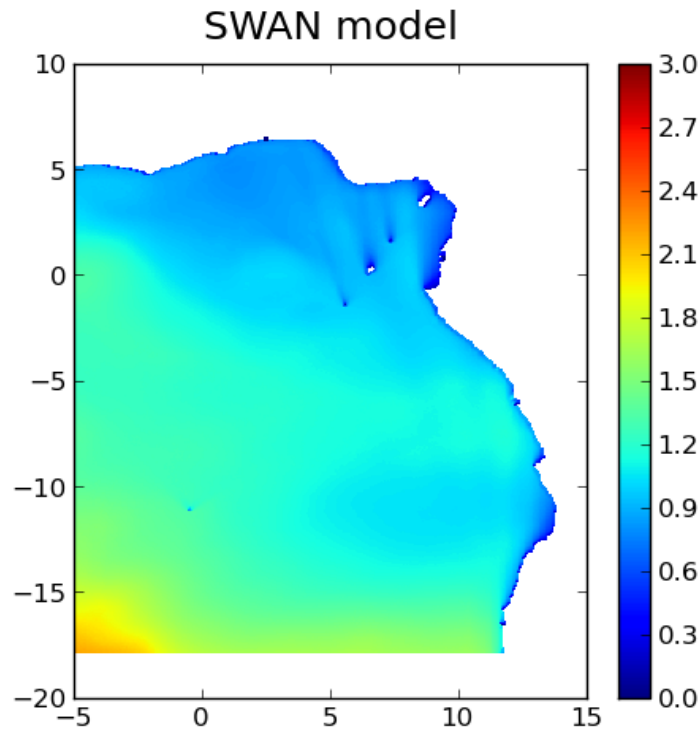


Lagos Harbour

- Ocean, weather and climate expertise
 - IT and training solutions
-

Wave models

Our future use of HPCWales



- Ocean, weather and climate expertise
- IT and training solutions

I hope it has been interesting -
and thank you for listening

Questions welcome



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Studentship Video

Farzana Rahman

Ewrop & Chymru:
Buddsoddi yn eich dyfodol
Cronfa Datblygu Rhanbarthol Ewrop

Europe & Wales:
Investing in your future
European Regional Development Fund



Studentship Case Study, Farzana Rahman

- PhD student, Farzana Rahman from Bangladesh, has been selected by EPSRC to compete in the prestigious UK ICT pioneer 2014 competition
- Combatting Bacterial Toxicity: Using Super Computing to Transform Health Services



- Video produced by the University of South Wales – [Link to video](#)



HPC
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Powering Success
Pweru Llwyddiant

Forum Discussion

Ewrop & Chymru:
Buddsoddi yn eich dyfodol
Cronfa Datblygu Rhanbarthol Ewrop

Europe & Wales:
Investing in your future
European Regional Development Fund

