

22 January 2014



Powering Success  
Pweru Llwyddiant

# The HPC Wales User Group



## 2<sup>ND</sup> USER GROUP MEETING

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

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



# The HPC Wales User Group - Agenda

Time	Agenda Item	Speaker
2:00 – 2:05	WELCOME AND BACKGROUND	Martyn Guest, HPC Wales
2:05 – 2:20	HPC WALES GATEWAY SHOWCASE - OVERVIEW OF THE LAYOUT AND ASSOCIATED INFORMATION WITHIN THE SECTOR SPECIFIC GATEWAYS OF THE HPC WALES PORTAL	Andrew Austin, HPC Wales
2:20 – 2:40	SYNFINIWAY – OVERVIEW OF THE WEB-BASED WORKFLOW INTERFACE AND ITS IMPACT ON USER PRODUCTIVITY	Ian Godfrey, Fujitsu
2:40 – 3:05	"TOP 10 ISSUES" – FEEDBACK ON ISSUES RAISED BY USERS	Martyn Guest, HPC Wales
3:05 - 3:20	SERVICE ENHANCEMENTS – ROUND TABLE DISCUSSION TO SEE WHAT CAPABILITIES USERS WOULD LIKE TO SEE ADDED TO THE CURRENT HPC WALES SERVICE	HPC Wales Users
3:20 – 3.35	THE ROLE OF FLE / NAG IN SUPPORTING THE HPC WALES USER COMMUNITY	Ross Nobes , FLE & Edward Smyth, NAG
3:35 – 3:55	"VENDOR CORNER" – A PRESENTATION BY ALLINEA ON THEIR PRODUCT OFFERING	David Lecomber, Allinea
3:55 – 4:00	FUTURE FORMAT OF THE HPC WALES USER GROUP & CLOSING	Martyn Guest, HPC Wales

- HPC Wales convened their **first project-wide user group** meeting on the afternoon of **Thursday 12<sup>th</sup> September 2013**.
- The aim of the meeting was to provide a forum for the users of the HPC Wales systems to both learn about the **range of services on offer, and to allow attendees to feedback ideas about what facilities, support and software would support the growth of their work on the HPC Wales systems.**
- Held through a **multi-site video conference** involving sites at both Hubs and all three Tier-1 sites:
- The meeting was broken out into a number of 10-20 minute updates from HPC Wales staff, followed in each case by a Q&A session that attracted a number of comments and ideas from the **25 or so** users in attendance.

The main learning points from the event were:

- Clear that the **service offerings are not very visible to users**, especially Phase 3. We presented a programme that involved the transition to Phase 2 Production service at the end of September.
- There appeared to be **little awareness of SynfiniWay**.
- From the general feedback, it was clear that more work is needed to **communicate to users**.
- A key point here is the **status of the portal** that remains sparsely populated. While the Creative Industry section is in good shape, and the Life Sciences area at least contains some content, the Advanced Manufacturing, Energy and Environment and ICT sections contained no material.
- **Visit South Wales & Aberystwyth**, to enhance requirements analysis

# Improving the Format

- Running them quarterly over VC makes sense, however it would be great to have one a year in person in order to foster a greater sense of community
- Have separate regional group meetings instead of a multi site video conference



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# HPC Wales Portal Demonstration

ADVANCED MATERIALS & MANUFACTURING  
SECTOR

ANDREW AUSTIN  
SWANSEA HUB MANAGER



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

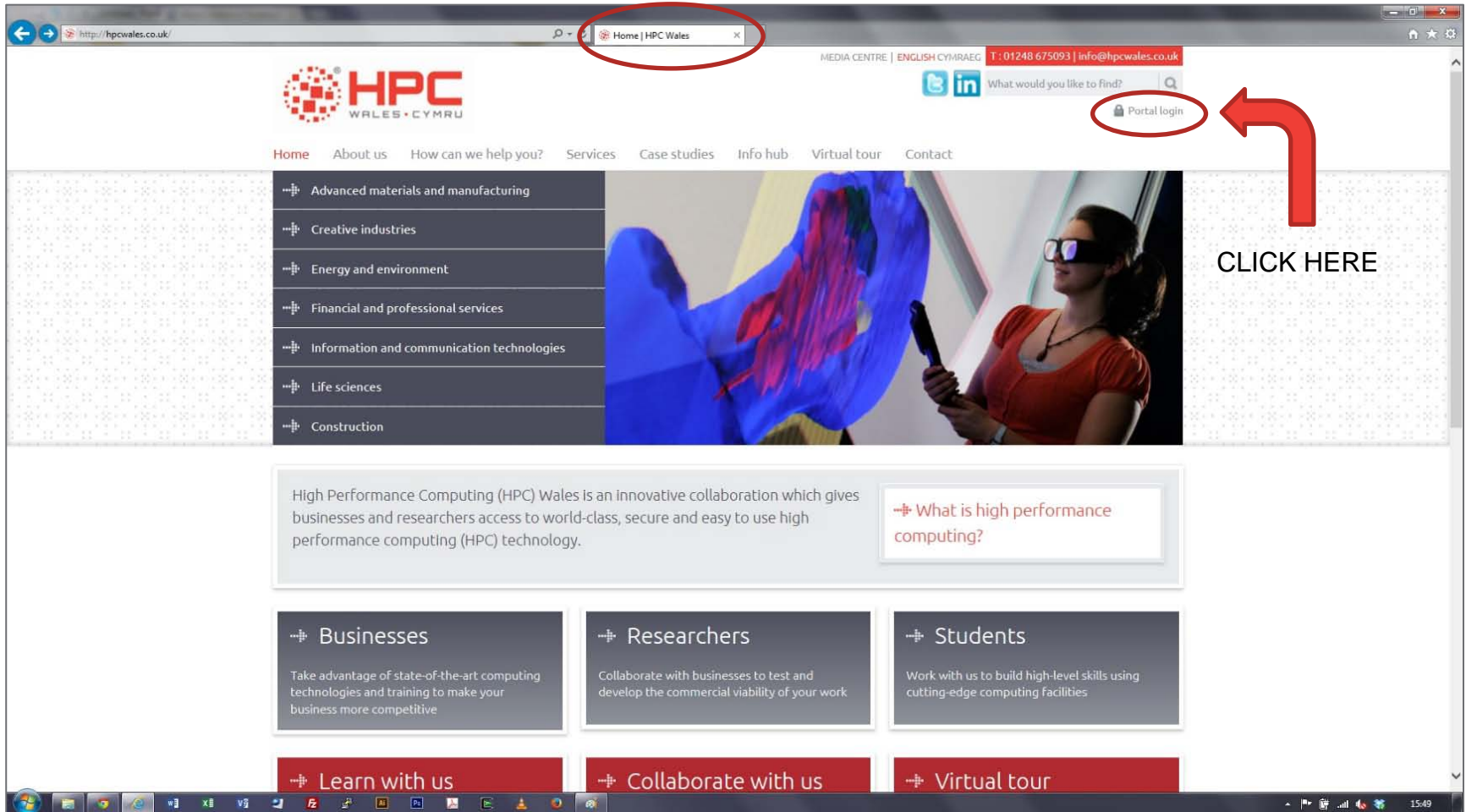
Europe & Wales:  
Investing in your future  
European Regional Development Fund



## Advanced Materials & Manufacturing Gateway (AM&M)

- Covers 'Chemistry' & 'Engineering' applications
- Instructions on how to access & use applications
- Describes Command Line & 'SynfiniWay' invocation
- Provides User / Group / Project collaboration tools
- Users / Groups / Projects can provide content...





The screenshot shows the HPC Wales website in a web browser. The address bar shows 'http://hpcwales.co.uk/' and a tab titled 'Home | HPC Wales'. The website header includes the HPC Wales logo, social media links for Twitter and LinkedIn, a search bar with the text 'What would you like to find?', and a 'Portal login' link circled in red. A large red arrow points from the 'Portal login' link to the text 'CLICK HERE'. The main navigation menu includes links for Home, About us, How can we help you?, Services, Case studies, Info hub, Virtual tour, and Contact. The main content area features a list of industries: Advanced materials and manufacturing, Creative industries, Energy and environment, Financial and professional services, Information and communication technologies, Life sciences, and Construction. Below this is a section titled 'High Performance Computing (HPC) Wales is an innovative collaboration which gives businesses and researchers access to world-class, secure and easy to use high performance computing (HPC) technology.' To the right of this text is a box titled 'What is high performance computing?'. Below the main content area are three boxes for 'Businesses', 'Researchers', and 'Students', each with a brief description of their services. At the bottom are three red buttons: 'Learn with us', 'Collaborate with us', and 'Virtual tour'.

Home | HPC Wales

MEDIA CENTRE | ENGLISH CYMRAEG T: 01248 675093 | info@hpcwales.co.uk

What would you like to find?

Portal login

CLICK HERE

Home About us How can we help you? Services Case studies Info hub Virtual tour Contact

Advanced materials and manufacturing  
Creative industries  
Energy and environment  
Financial and professional services  
Information and communication technologies  
Life sciences  
Construction

High Performance Computing (HPC) Wales is an innovative collaboration which gives businesses and researchers access to world-class, secure and easy to use high performance computing (HPC) technology.

What is high performance computing?

Businesses  
Take advantage of state-of-the-art computing technologies and training to make your business more competitive

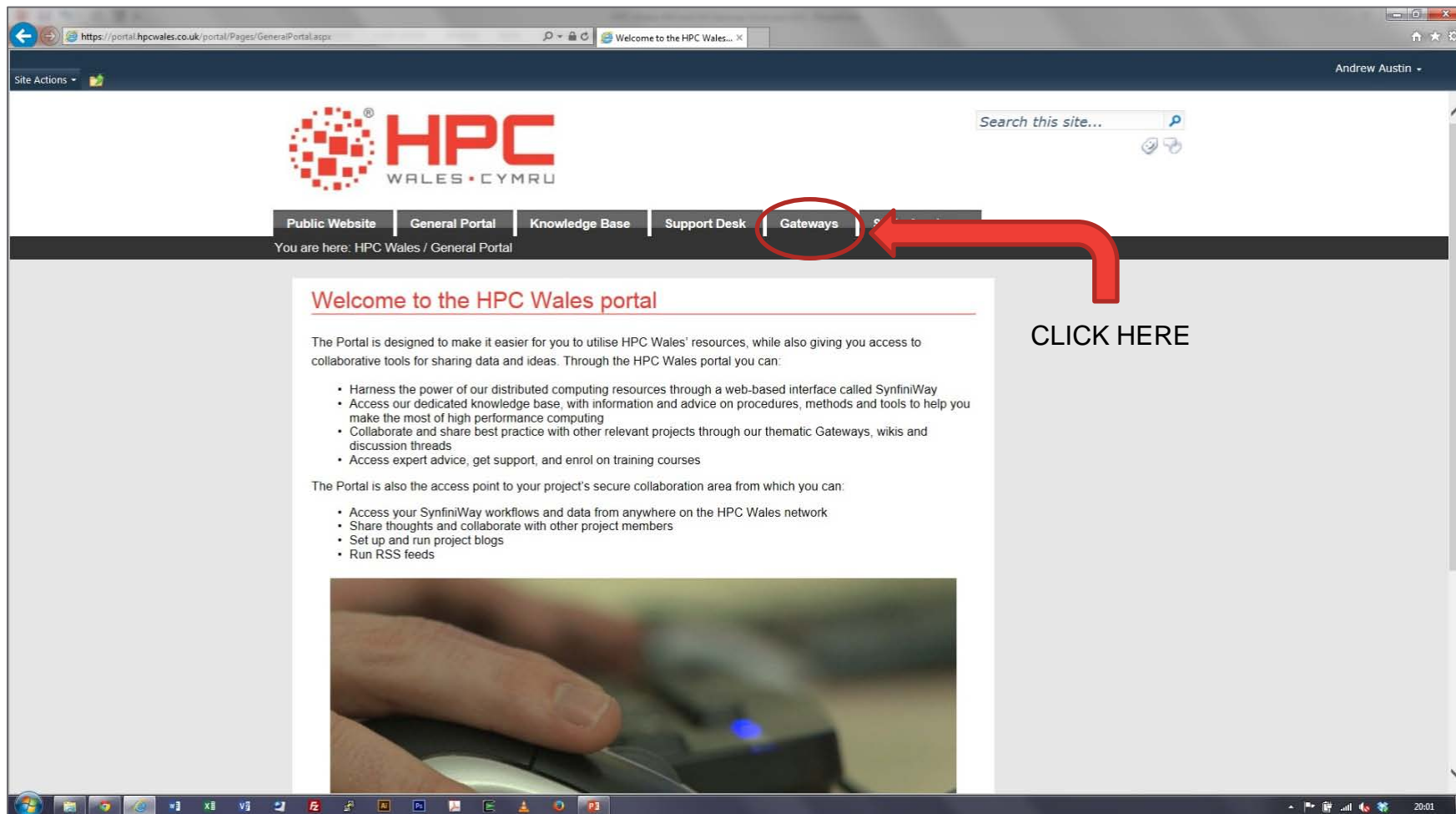
Researchers  
Collaborate with businesses to test and develop the commercial viability of your work

Students  
Work with us to build high-level skills using cutting-edge computing facilities

Learn with us Collaborate with us Virtual tour







The screenshot shows the HPC Wales portal website. The browser address bar displays <https://portal.hpcwales.co.uk/portal/Pages/GeneralPortal.aspx>. The page header includes the HPC WALES CYMRU logo and a search bar. The main navigation menu contains the following items: Public Website, General Portal, Knowledge Base, Support Desk, Gateways, and a partially visible 'SynfiniWay' item. The 'Gateways' item is circled in red, and a large red arrow points from the text 'CLICK HERE' to it. Below the navigation menu, the page content includes a welcome message, a description of the portal's purpose, a list of features, and a photograph of a hand using a computer mouse.

Site Actions

Andrew Austin

Search this site...

Public Website | General Portal | Knowledge Base | Support Desk | **Gateways** | SynfiniWay

You are here: HPC Wales / General Portal


### Welcome to the HPC Wales portal

The Portal is designed to make it easier for you to utilise HPC Wales' resources, while also giving you access to collaborative tools for sharing data and ideas. Through the HPC Wales portal you can:

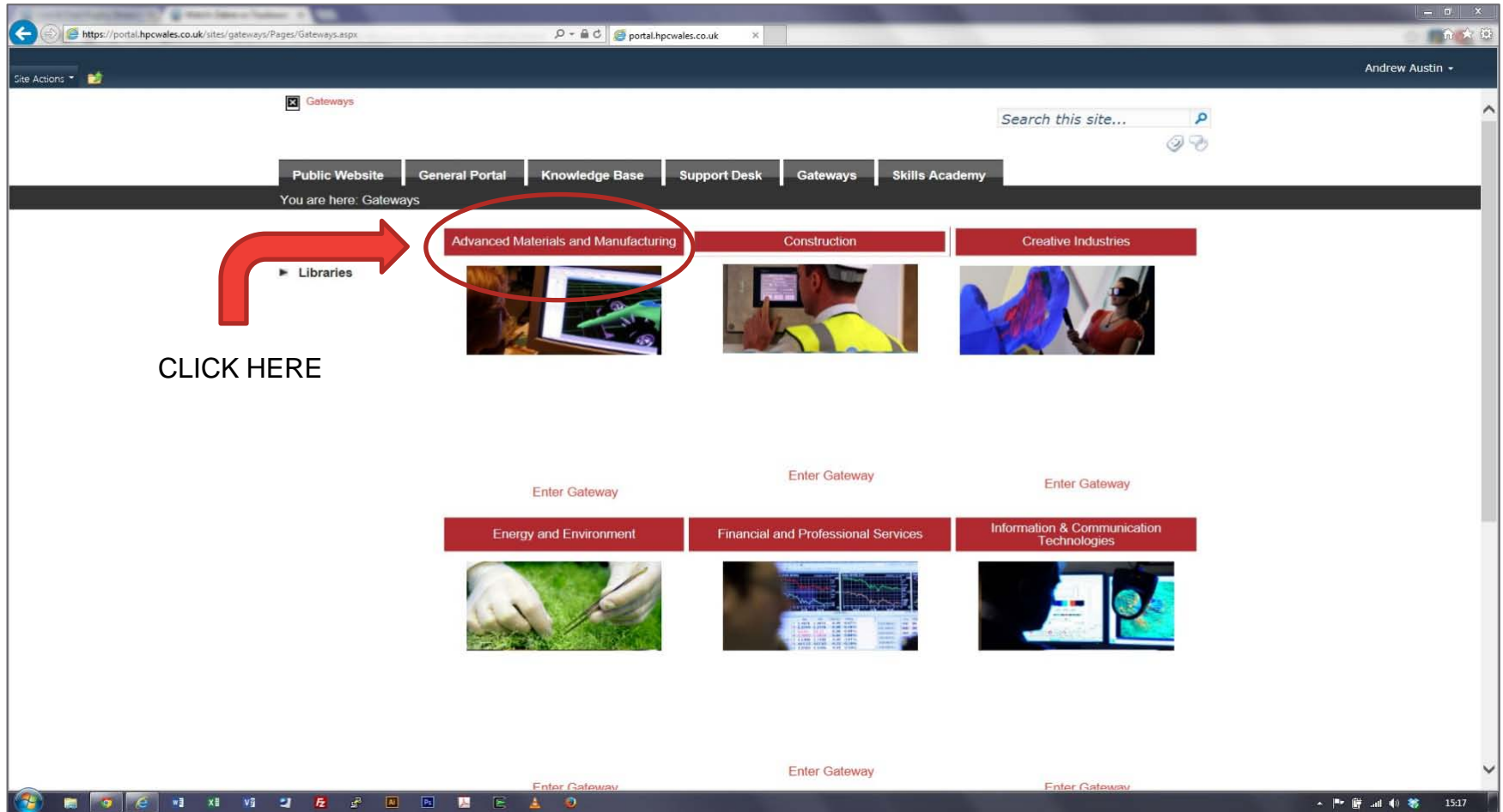
- Harness the power of our distributed computing resources through a web-based interface called SynfiniWay
- Access our dedicated knowledge base, with information and advice on procedures, methods and tools to help you make the most of high performance computing
- Collaborate and share best practice with other relevant projects through our thematic Gateways, wikis and discussion threads
- Access expert advice, get support, and enrol on training courses

The Portal is also the access point to your project's secure collaboration area from which you can:

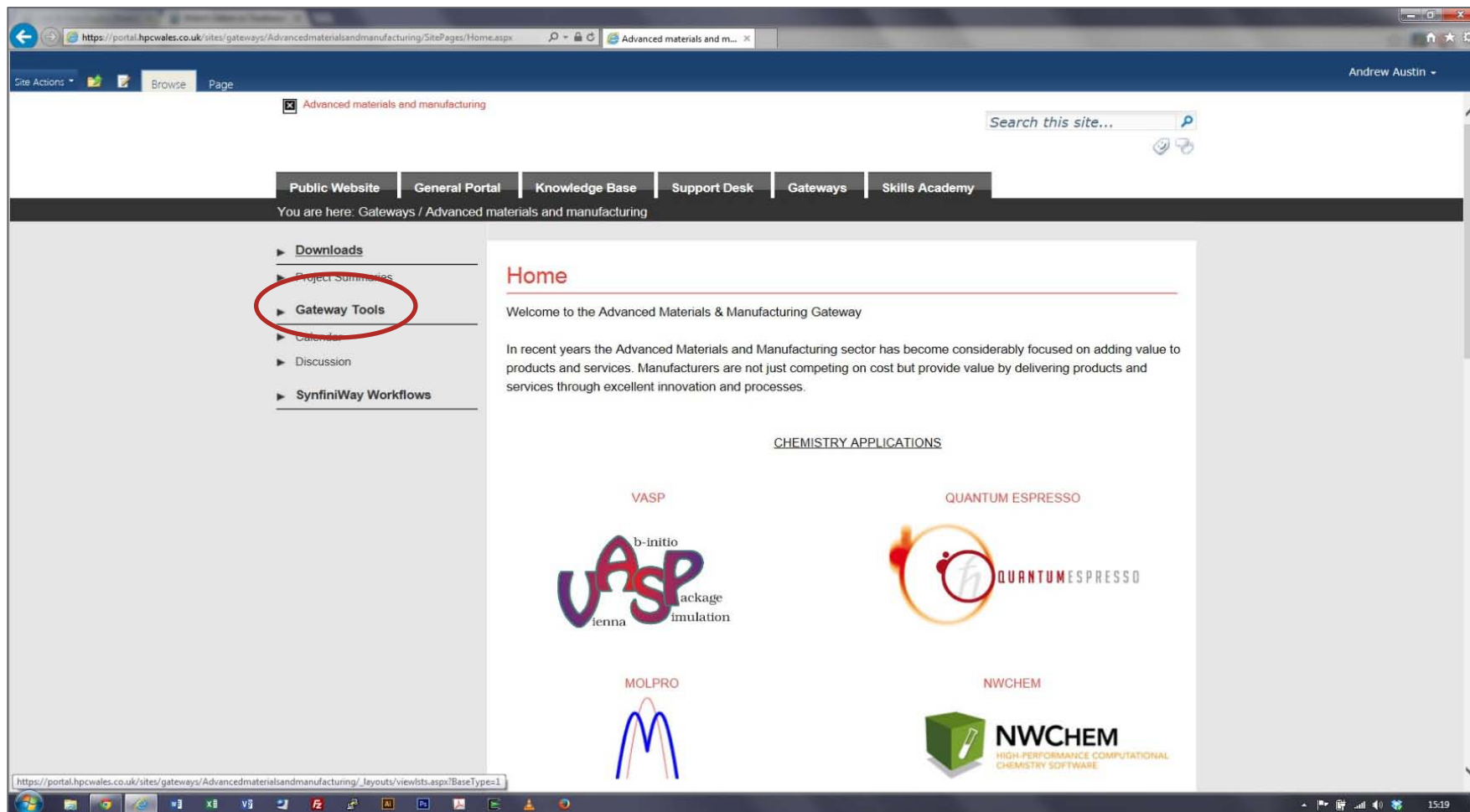
- Access your SynfiniWay workflows and data from anywhere on the HPC Wales network
- Share thoughts and collaborate with other project members
- Set up and run project blogs
- Run RSS feeds



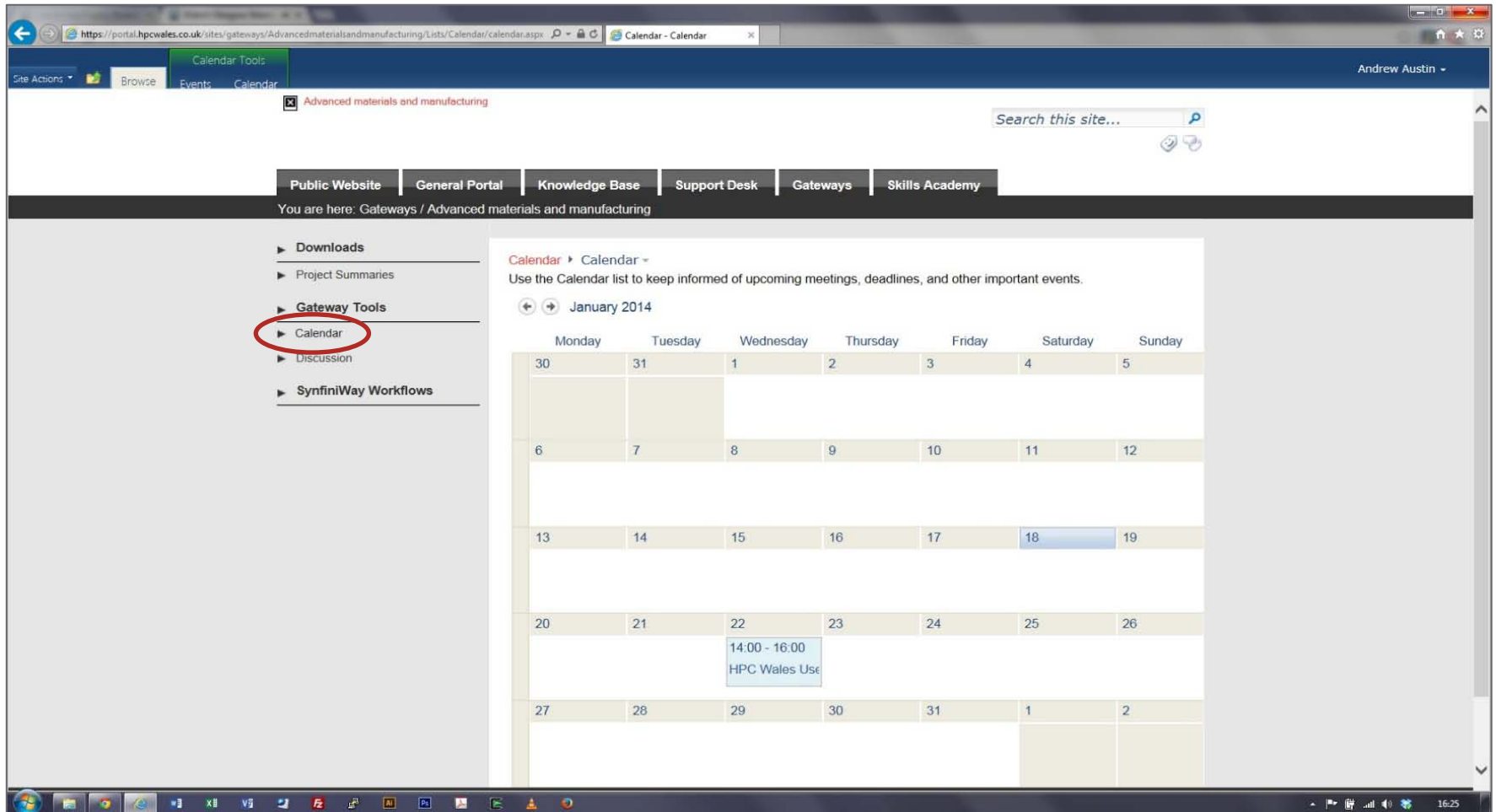
CLICK HERE



The screenshot shows the HPC Wales website interface. At the top, there is a navigation bar with links: Public Website, General Portal, Knowledge Base, Support Desk, Gateways, and Skills Academy. Below this, a search bar is visible. The main content area displays a grid of gateway categories. A red arrow points to the 'Advanced Materials and Manufacturing' gateway, which is circled in red. The text 'CLICK HERE' is placed next to the arrow. Other gateways visible include Construction, Creative Industries, Energy and Environment, Financial and Professional Services, and Information & Communication Technologies. Each gateway has a representative image and a link labeled 'Enter Gateway'.



The screenshot shows a web browser window displaying the HPC Wales Advanced Materials and Manufacturing Gateway. The URL in the address bar is <https://portal.hpcwales.co.uk/sites/gateways/Advancedmaterialsandmanufacturing/SitePages/Home.aspx>. The page features a navigation bar with tabs: Public Website, General Portal, Knowledge Base, Support Desk, Gateways, and Skills Academy. A search bar is located in the top right corner. On the left side, there is a sidebar menu with the following items: Downloads, Project Summaries, Gateway Tools (highlighted with a red circle), Calendar, Discussion, and SynfiniWay Workflows. The main content area is titled "Home" and includes a welcome message: "Welcome to the Advanced Materials & Manufacturing Gateway". Below this, a paragraph states: "In recent years the Advanced Materials and Manufacturing sector has become considerably focused on adding value to products and services. Manufacturers are not just competing on cost but provide value by delivering products and services through excellent innovation and processes." Under the heading "CHEMISTRY APPLICATIONS", there are four logos: VASP (with subtext "b-initio" and "package simulation"), QUANTUM ESPRESSO, MOLPRO, and NWCHEM (with subtext "HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE"). The browser's taskbar at the bottom shows various application icons and the system clock indicating 15:19.



Calendar - Calendar

Advanced materials and manufacturing

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

**Gateway Tools**

Calendar

Discussion

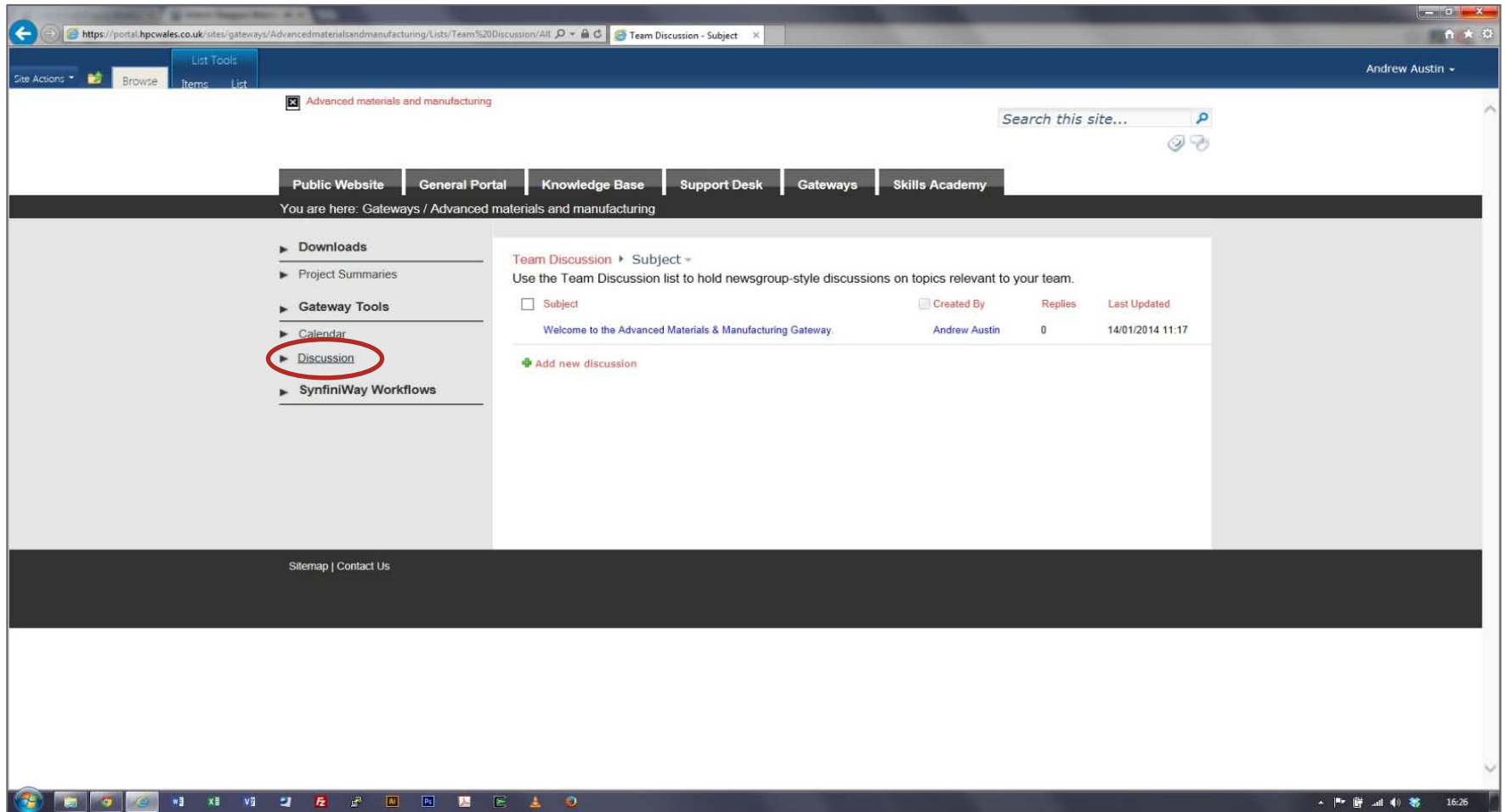
SynfiniWay Workflows

Calendar - Calendar

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

January 2014

Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday
30	31	1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22 14:00 - 16:00 HPC Wales Use	23	24	25	26
27	28	29	30	31	1	2



https://portal.hpcwales.co.uk/sites/gateways/Advancedmaterialsandmanufacturing/Lists/Team%20Discussion/All Team Discussion - Subject

Andrew Austin

Advanced materials and manufacturing

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
- Gateway Tools
  - Calendar
  - Discussion**
  - SynfiniWay Workflows

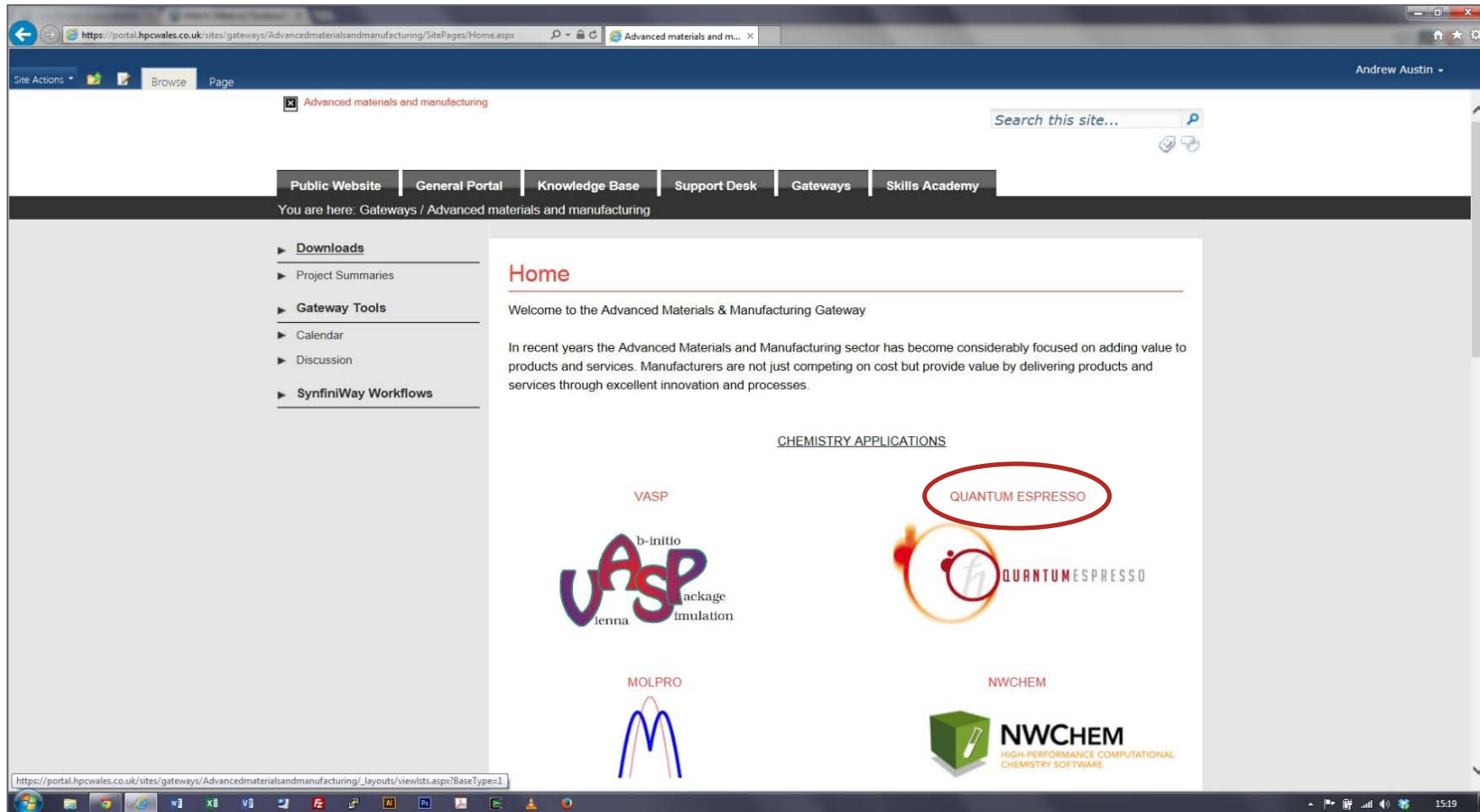
Team Discussion ▸ Subject ▾

Use the Team Discussion list to hold newsgroup-style discussions on topics relevant to your team.

<input type="checkbox"/> Subject	Created By	Replies	Last Updated
Welcome to the Advanced Materials & Manufacturing Gateway.	Andrew Austin	0	14/01/2014 11:17

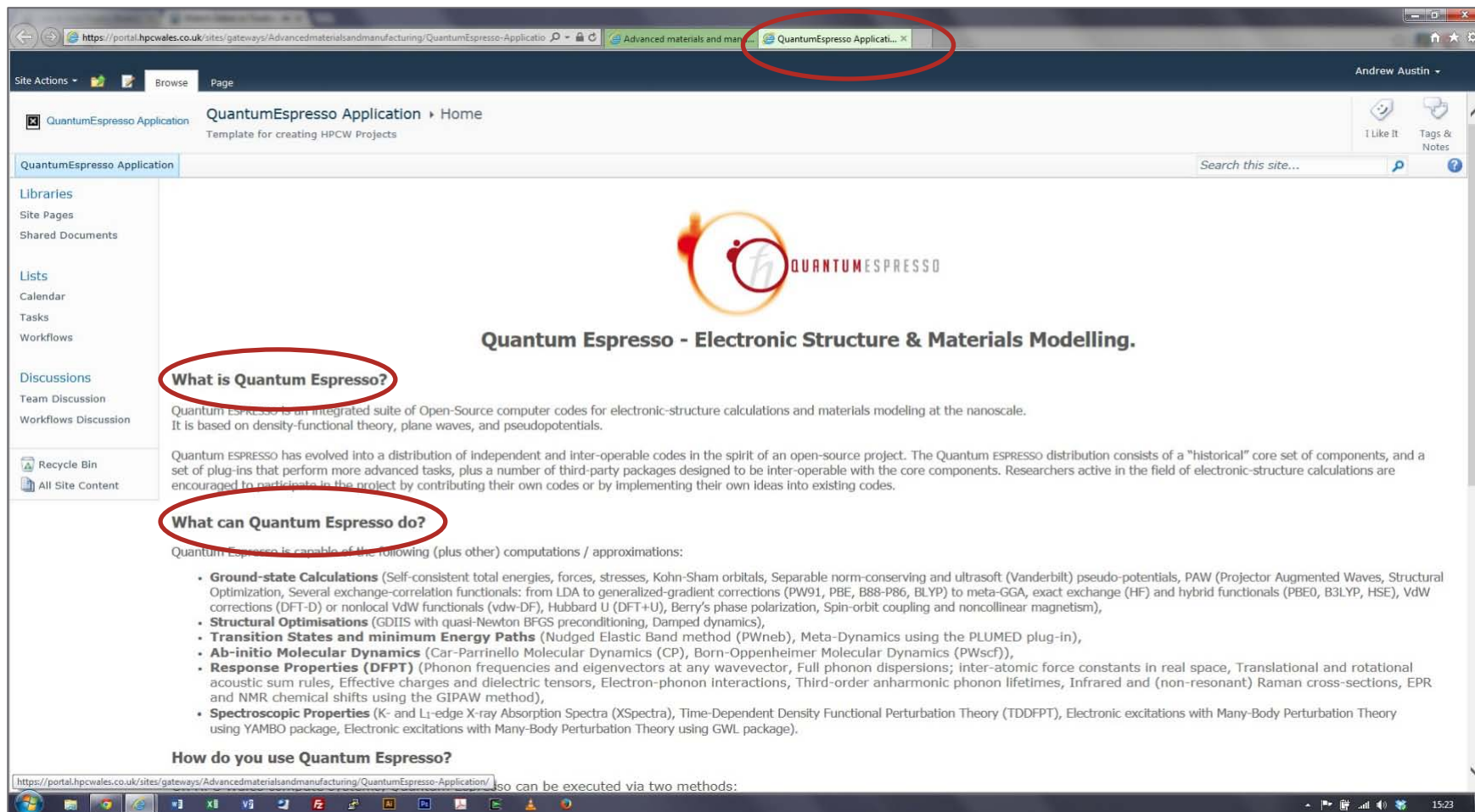
+ Add new discussion

Sitemap | Contact Us



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The screenshot shows a web browser window with the URL <https://portal.hpcwales.co.uk/sites/gateways/Advancedmaterialsandmanufacturing/QuantumEspresso-Application/>. The browser's address bar and the application's title bar are circled in red. The website header includes "Site Actions", "Browse", "Page", and "Andrew Austin". The main content area features the Quantum Espresso logo and the title "Quantum Espresso - Electronic Structure & Materials Modelling." Below this, two sections are circled in red: "What is Quantum Espresso?" and "What can Quantum Espresso do?". The "What is Quantum Espresso?" section describes it as an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale, based on density-functional theory, plane waves, and pseudopotentials. The "What can Quantum Espresso do?" section lists various capabilities: Ground-state Calculations, Structural Optimisations, Transition States and minimum Energy Paths, Ab-initio Molecular Dynamics, Response Properties (DFPT), and Spectroscopic Properties. The "How do you use Quantum Espresso?" section is partially visible at the bottom.

**What is Quantum Espresso?**

Quantum ESPRESSO is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

Quantum ESPRESSO has evolved into a distribution of independent and inter-operable codes in the spirit of an open-source project. The Quantum ESPRESSO distribution consists of a "historical" core set of components, and a set of plug-ins that perform more advanced tasks, plus a number of third-party packages designed to be inter-operable with the core components. Researchers active in the field of electronic-structure calculations are encouraged to participate in the project by contributing their own codes or by implementing their own ideas into existing codes.

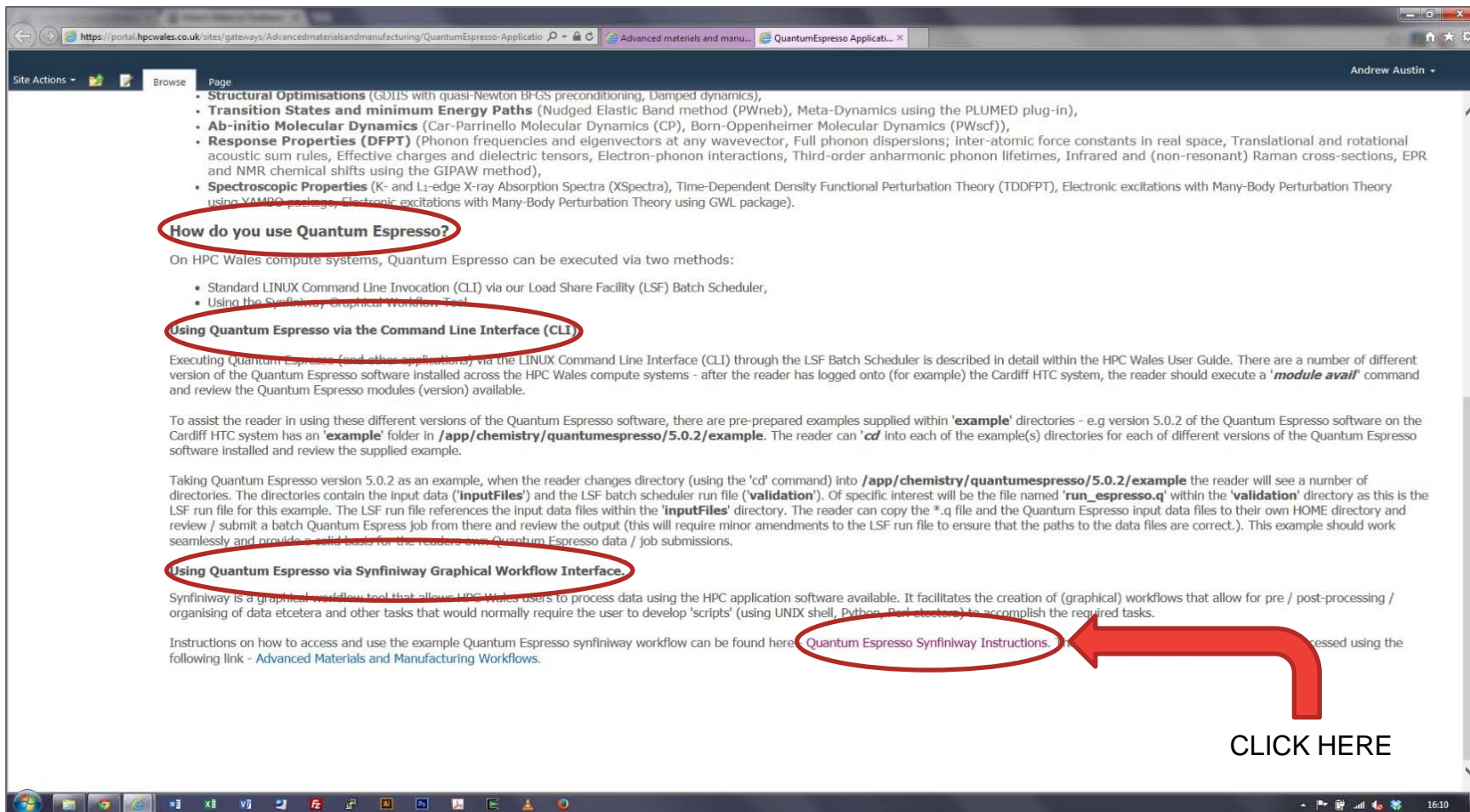
**What can Quantum Espresso do?**

Quantum Espresso is capable of the following (plus other) computations / approximations:

- **Ground-state Calculations** (Self-consistent total energies, forces, stresses, Kohn-Sham orbitals, Separable norm-conserving and ultrasoft (Vanderbilt) pseudo-potentials, PAW (Projector Augmented Waves, Structural Optimization, Several exchange-correlation functionals: from LDA to generalized-gradient corrections (PW91, PBE, B88-P86, BLYP) to meta-GGA, exact exchange (HF) and hybrid functionals (PBE0, B3LYP, HSE), VdW corrections (DFT-D) or nonlocal VdW functionals (vdw-DF), Hubbard U (DFT+U), Berry's phase polarization, Spin-orbit coupling and noncollinear magnetism),
- **Structural Optimisations** (GDIIS with quasi-Newton BFGS preconditioning, Damped dynamics),
- **Transition States and minimum Energy Paths** (Nudged Elastic Band method (PWneb), Meta-Dynamics using the PLUMED plug-in),
- **Ab-initio Molecular Dynamics** (Car-Parrinello Molecular Dynamics (CP), Born-Oppenheimer Molecular Dynamics (PWscf)),
- **Response Properties (DFPT)** (Phonon frequencies and eigenvectors at any wavevector, Full phonon dispersions; inter-atomic force constants in real space, Translational and rotational acoustic sum rules, Effective charges and dielectric tensors, Electron-phonon interactions, Third-order anharmonic phonon lifetimes, Infrared and (non-resonant) Raman cross-sections, EPR and NMR chemical shifts using the GIPAW method),
- **Spectroscopic Properties** (K- and L<sub>2</sub>-edge X-ray Absorption Spectra (XSpectra), Time-Dependent Density Functional Perturbation Theory (TDDFT), Electronic excitations with Many-Body Perturbation Theory using YAMBO package, Electronic excitations with Many-Body Perturbation Theory using GWL package).

**How do you use Quantum Espresso?**

Quantum Espresso can be executed via two methods:



Site Actions ▾ Browse Page

Advanced materials and manu... QuantumEspresso Applicati...

Andrew Austin ▾

- **Structural Optimisations** (GDIIS with quasi-Newton BFGS preconditioning, Damped dynamics),
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**How do you use Quantum Espresso?**

On HPC Wales compute systems, Quantum Espresso can be executed via two methods:

- Standard LINUX Command Line Invocation (CLI) via our Load Share Facility (LSF) Batch Scheduler,
- Using the Synfiniway Graphical Workflow Tool.

**Using Quantum Espresso via the Command Line Interface (CLI)**

Executing Quantum Espresso (and other applications) via the LINUX Command Line Interface (CLI) through the LSF Batch Scheduler is described in detail within the HPC Wales User Guide. There are a number of different version of the Quantum Espresso software installed across the HPC Wales compute systems - after the reader has logged onto (for example) the Cardiff HTC system, the reader should execute a '**module avail**' command and review the Quantum Espresso modules (version) available.

To assist the reader in using these different versions of the Quantum Espresso software, there are pre-prepared examples supplied within '**example**' directories - e.g version 5.0.2 of the Quantum Espresso software on the Cardiff HTC system has an '**example**' folder in **/app/chemistry/quantum.espresso/5.0.2/example**. The reader can '**cd**' into each of the example(s) directories for each of different versions of the Quantum Espresso software installed and review the supplied example.

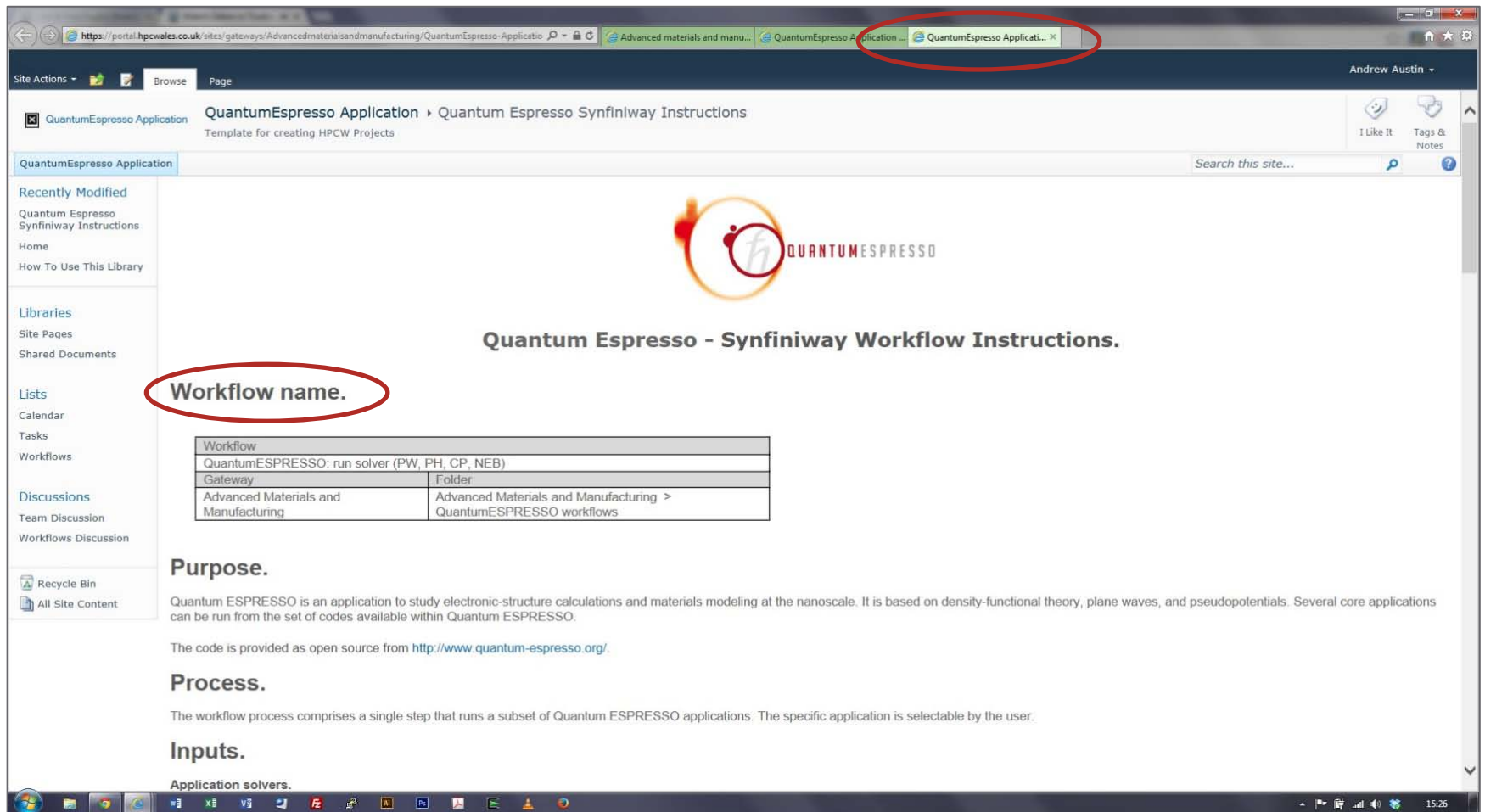
Taking Quantum Espresso version 5.0.2 as an example, when the reader changes directory (using the '**cd**' command) into **/app/chemistry/quantum.espresso/5.0.2/example** the reader will see a number of directories. The directories contain the input data ('**inputFiles**') and the LSF batch scheduler run file ('**validation**'). Of specific interest will be the file named '**run\_espresso.q**' within the '**validation**' directory as this is the LSF run file for this example. The LSF run file references the input data files within the '**inputFiles**' directory. The reader can copy the \*.q file and the Quantum Espresso input data files to their own HOME directory and review / submit a batch Quantum Espresso job from there and review the output (this will require minor amendments to the LSF run file to ensure that the paths to the data files are correct.). This example should work seamlessly and provide a solid basis for the readers own Quantum Espresso data / job submissions.

**Using Quantum Espresso via Synfiniway Graphical Workflow Interface.**

Synfiniway is a graphical workflow tool that allows HPC Wales users to process data using the HPC application software available. It facilitates the creation of (graphical) workflows that allow for pre / post-processing / organising of data etcetera and other tasks that would normally require the user to develop 'scripts' (using UNIX shell, Python, Perl etcetera) to accomplish the required tasks.

Instructions on how to access and use the example Quantum Espresso synfiniway workflow can be found here: [Quantum Espresso Synfiniway Instructions](#). The workflow can be accessed using the following link - [Advanced Materials and Manufacturing Workflows](#).

CLICK HERE



QuantumEspresso Application ▶ Quantum Espresso Synfiniway Instructions  
Template for creating HPCW Projects

QuantumEspresso Application

Recently Modified

- Quantum Espresso Synfiniway Instructions
- Home
- How To Use This Library

Libraries

- Site Pages
- Shared Documents

Lists

- Calendar
- Tasks
- Workflows

Discussions

- Team Discussion
- Workflows Discussion

Recycle Bin

All Site Content

## Quantum Espresso - Synfiniway Workflow Instructions.

**Workflow name.**

Workflow	
QuantumESPRESSO: run solver (PW, PH, CP, NEB)	
Gateway	Folder
Advanced Materials and Manufacturing	Advanced Materials and Manufacturing > QuantumESPRESSO workflows

### Purpose.

Quantum ESPRESSO is an application to study electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials. Several core applications can be run from the set of codes available within Quantum ESPRESSO.

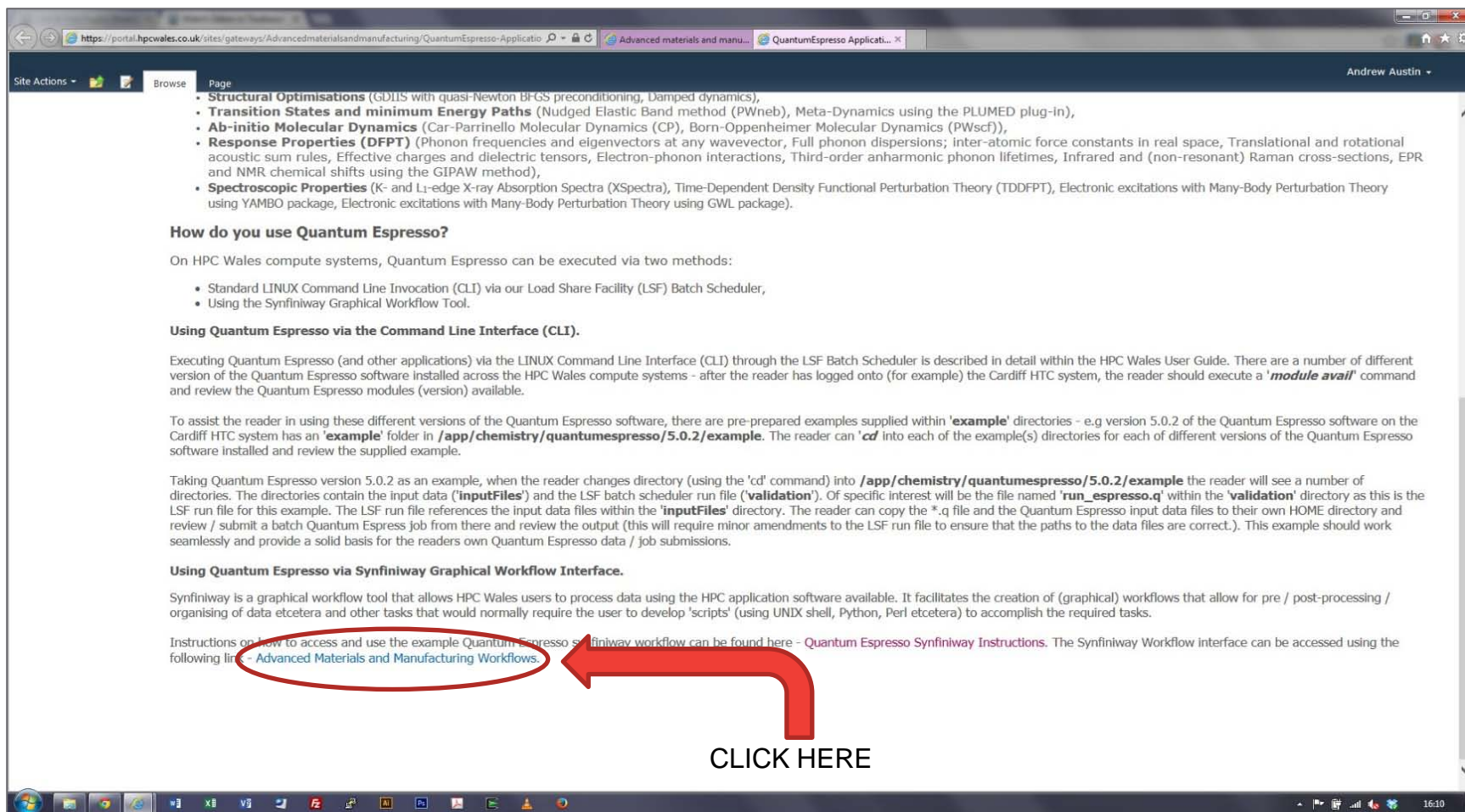
The code is provided as open source from <http://www.quantum-espresso.org/>.


### Process.

The workflow process comprises a single step that runs a subset of Quantum ESPRESSO applications. The specific application is selectable by the user.

### Inputs.

Application solvers.



Site Actions  Browse Page

Andrew Austin

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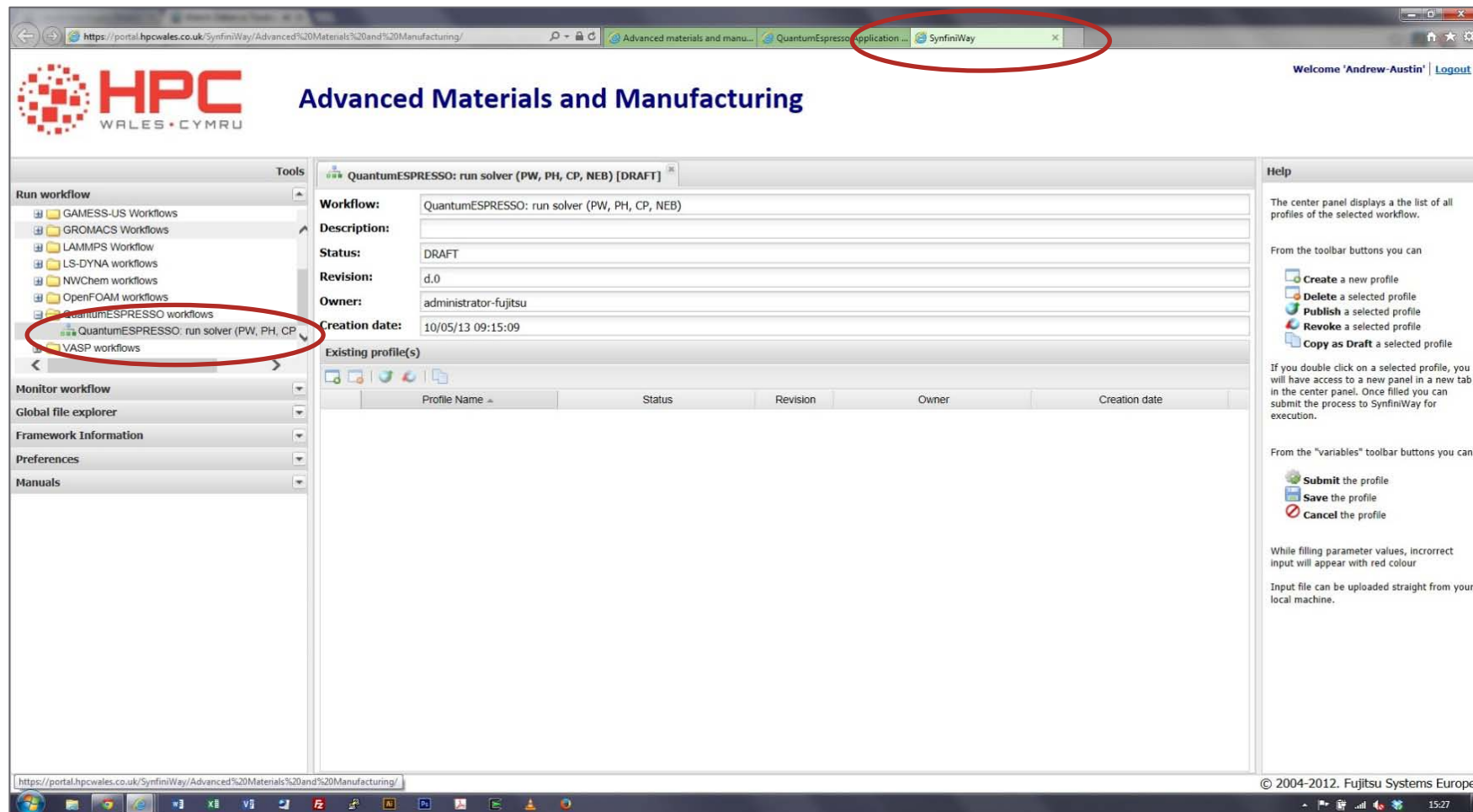
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**CLICK HERE**





https://portal.hpcwales.co.uk/SynfiniWay/AdvancedMaterials%20and%20Manufacturing/

Advanced materials and manu... QuantumESPRESSO application ... SynfiniWay

Welcome 'Andrew-Austin' | Logout

## Advanced Materials and Manufacturing

Tools

QuantumESPRESSO: run solver (PW, PH, CP, NEB) [DRAFT]

**Run workflow**

- GAMESS-US Workflows
- GROMACS Workflows
- LAMMPS Workflow
- LS-DYNA workflows
- NWChem workflows
- OpenFOAM workflows
- QuantumESPRESSO workflows
- QuantumESPRESSO: run solver (PW, PH, CP, NEB)
- VASP workflows

**Monitor workflow**

**Global file explorer**

**Framework Information**

**Preferences**

**Manuals**

**Workflow Details:**

**Workflow:** QuantumESPRESSO: run solver (PW, PH, CP, NEB)

**Description:**

**Status:** DRAFT

**Revision:** d.0

**Owner:** administrator-fujitsu

**Creation date:** 10/05/13 09:15:09

**Existing profile(s)**

Profile Name	Status	Revision	Owner	Creation date
--------------	--------	----------	-------	---------------

**Help**

The center panel displays a list of all profiles of the selected workflow.

From the toolbar buttons you can

- Create a new profile
- Delete a selected profile
- Publish a selected profile
- Revoke a selected profile
- Copy as Draft a selected profile

If you double click on a selected profile, you will have access to a new panel in a new tab in the center panel. Once filled you can submit the process to SynfiniWay for execution.

From the "variables" toolbar buttons you can

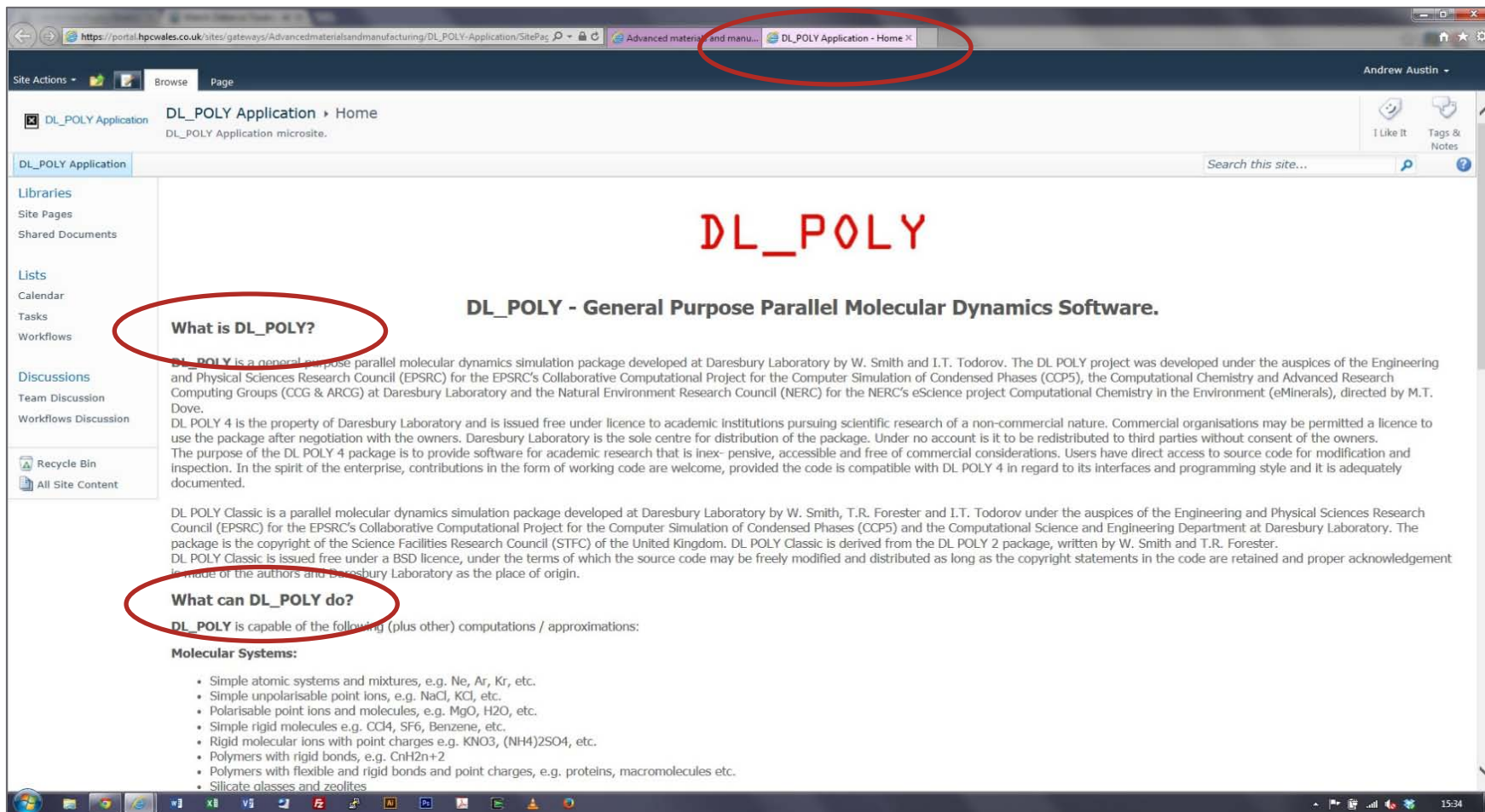
- Submit the profile
- Save the profile
- Cancel the profile

While filling parameter values, incorrect input will appear with red colour

Input file can be uploaded straight from your local machine.

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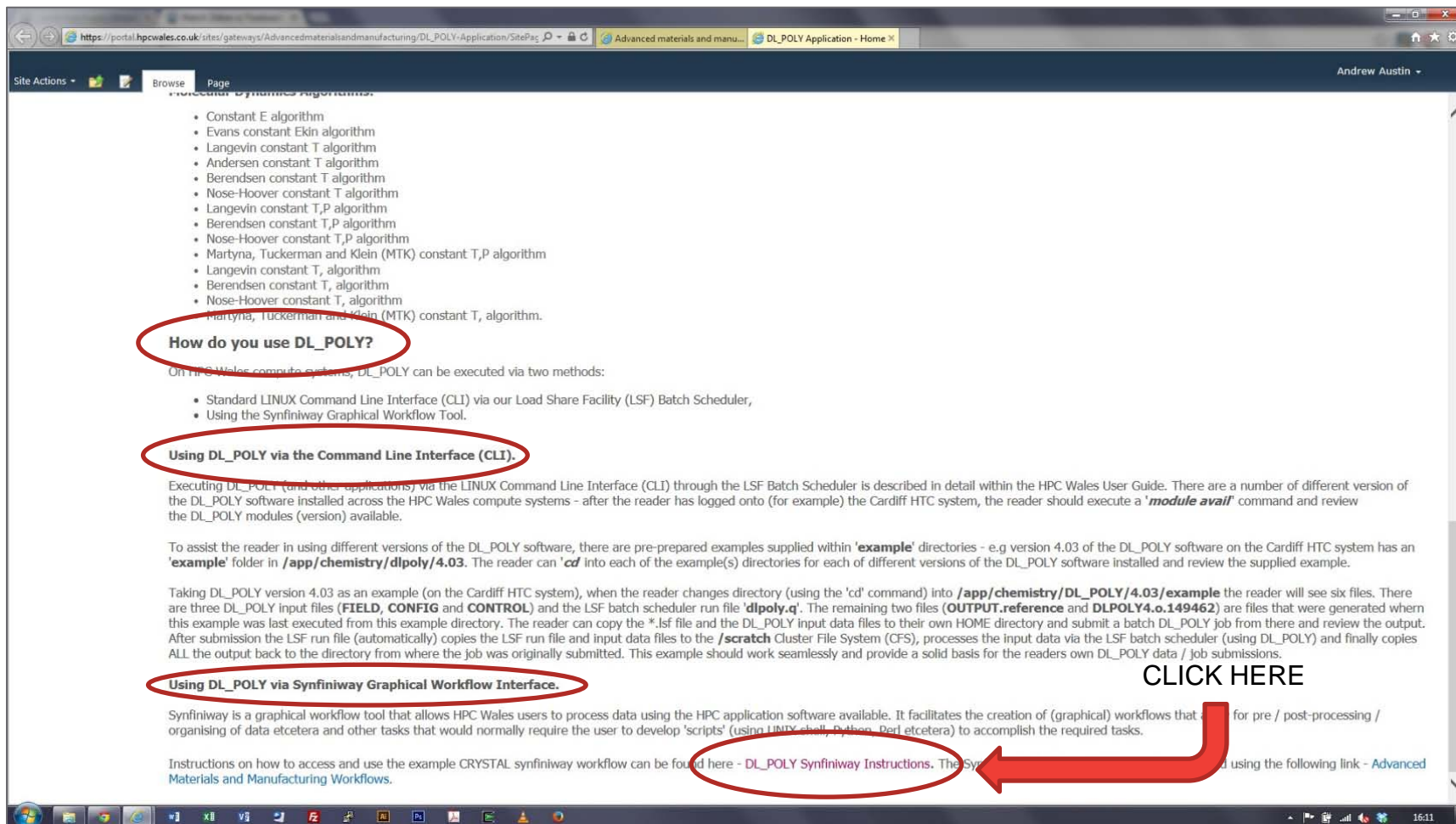




The screenshot shows a web browser window with the URL [https://portal.hpcwales.co.uk/sites/gateways/Advancedmaterialsandmanufacturing/DL\\_POLY-Application/SitePage](https://portal.hpcwales.co.uk/sites/gateways/Advancedmaterialsandmanufacturing/DL_POLY-Application/SitePage). The browser tabs show "Advanced materials and manu..." and "DL\_POLY Application - Home". The website header includes "Site Actions", "Browse", "Page", and a user profile "Andrew Austin". The main content area features the "DL\_POLY Application" microsite with a search bar and a sidebar with links like "Libraries", "Site Pages", "Shared Documents", "Lists", "Calendar", "Tasks", "Workflows", "Discussions", "Team Discussion", "Workflows Discussion", "Recycle Bin", and "All Site Content". The main heading is "DL\_POLY" in large red letters, followed by the subtitle "DL\_POLY - General Purpose Parallel Molecular Dynamics Software." Below this, the section "What is DL\_POLY?" is circled in red. The text describes DL\_POLY as a general purpose parallel molecular dynamics simulation package developed at Daresbury Laboratory by W. Smith and I.T. Todorov. It mentions the project was developed under the auspices of the Engineering and Physical Sciences Research Council (EPSRC) for the EPSRC's Collaborative Computational Project for the Computer Simulation of Condensed Phases (CCP5), the Computational Chemistry and Advanced Research Computing Groups (CCG & ARCG) at Daresbury Laboratory and the Natural Environment Research Council (NERC) for the NERC's eScience project Computational Chemistry in the Environment (eMinerals), directed by M.T. Dove. It also states that DL\_POLY 4 is the property of Daresbury Laboratory and is issued free under licence to academic institutions pursuing scientific research of a non-commercial nature. Commercial organisations may be permitted a licence to use the package after negotiation with the owners. Daresbury Laboratory is the sole centre for distribution of the package. Under no account is it to be redistributed to third parties without consent of the owners. The purpose of the DL POLY 4 package is to provide software for academic research that is inexpensive, accessible and free of commercial considerations. Users have direct access to source code for modification and inspection. In the spirit of the enterprise, contributions in the form of working code are welcome, provided the code is compatible with DL POLY 4 in regard to its interfaces and programming style and it is adequately documented. Below this, the section "What can DL\_POLY do?" is also circled in red. The text states that DL\_POLY is capable of the following (plus other) computations / approximations: **Molecular Systems:**

- Simple atomic systems and mixtures, e.g. Ne, Ar, Kr, etc.
- Simple unpolarisable point ions, e.g. NaCl, KCl, etc.
- Polarisable point ions and molecules, e.g. MgO, H<sub>2</sub>O, etc.
- Simple rigid molecules e.g. CCl<sub>4</sub>, SF<sub>6</sub>, Benzene, etc.
- Rigid molecular ions with point charges e.g. KNO<sub>3</sub>, (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, etc.
- Polymers with rigid bonds, e.g. CnH2n+2
- Polymers with flexible and rigid bonds and point charges, e.g. proteins, macromolecules etc.
- Silicate glasses and zeolites





Site Actions ▾ Browse Page

DL\_POLY Application - Home

Andrew Austin ▾

- Constant E algorithm
- Evans constant Ekin algorithm
- Langevin constant T algorithm
- Andersen constant T algorithm
- Berendsen constant T algorithm
- Nose-Hoover constant T algorithm
- Langevin constant T,P algorithm
- Berendsen constant T,P algorithm
- Nose-Hoover constant T,P algorithm
- Martyna, Tuckerman and Klein (MTK) constant T,P algorithm
- Langevin constant T, algorithm
- Berendsen constant T, algorithm
- Nose-Hoover constant T, algorithm
- Martyna, Tuckerman and Klein (MTK) constant T, algorithm.

**How do you use DL\_POLY?**

On HPC Wales compute systems, DL\_POLY can be executed via two methods:

- Standard LINUX Command Line Interface (CLI) via our Load Share Facility (LSF) Batch Scheduler,
- Using the Synfiniway Graphical Workflow Tool.

**Using DL\_POLY via the Command Line Interface (CLI).**

Executing DL\_POLY (and other applications) via the LINUX Command Line Interface (CLI) through the LSF Batch Scheduler is described in detail within the HPC Wales User Guide. There are a number of different version of the DL\_POLY software installed across the HPC Wales compute systems - after the reader has logged onto (for example) the Cardiff HTC system, the reader should execute a '**module avail**' command and review the DL\_POLY modules (version) available.

To assist the reader in using different versions of the DL\_POLY software, there are pre-prepared examples supplied within '**example**' directories - e.g version 4.03 of the DL\_POLY software on the Cardiff HTC system has an '**example**' folder in **/app/chemistry/dlpoly/4.03**. The reader can '**cd**' into each of the example(s) directories for each of different versions of the DL\_POLY software installed and review the supplied example.

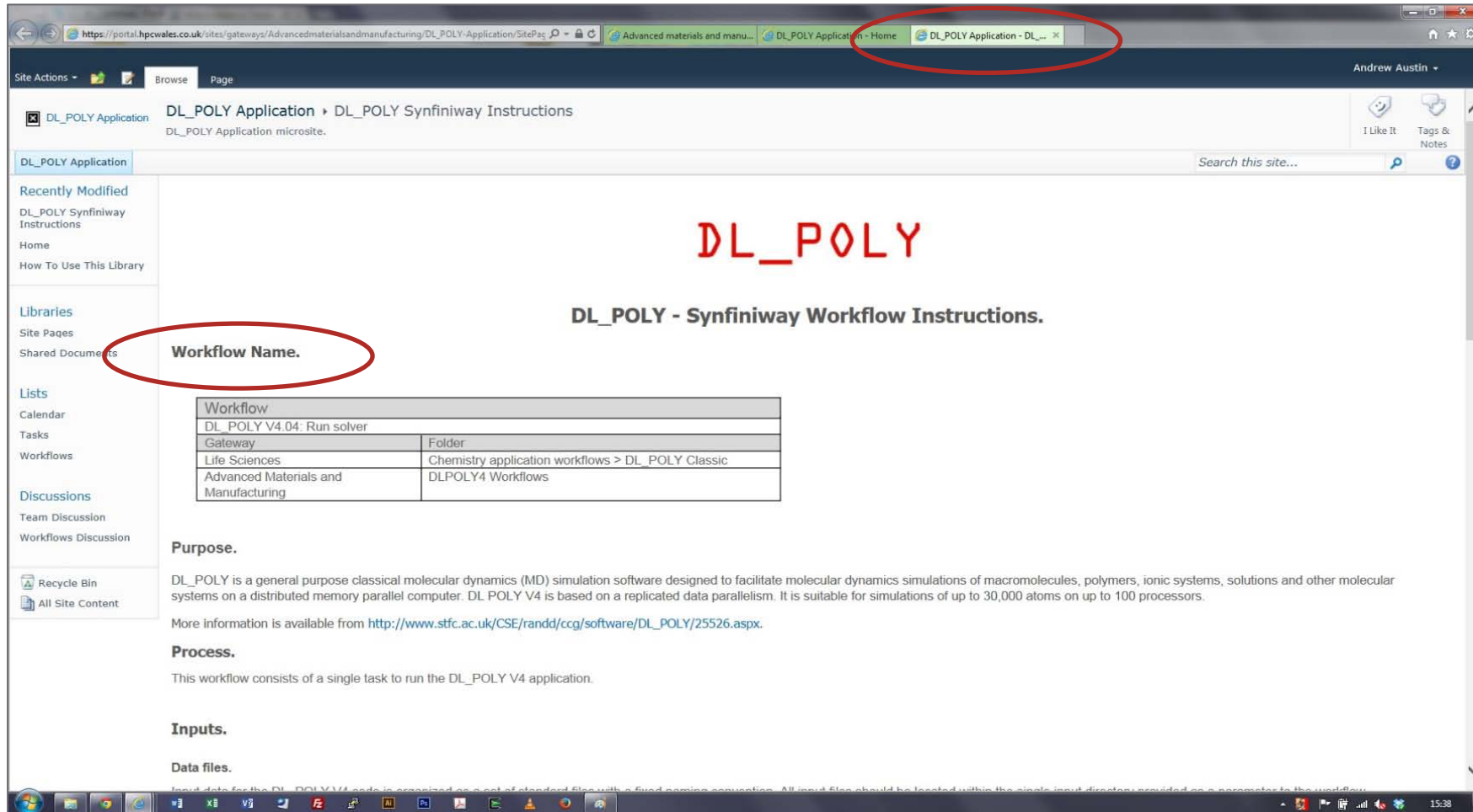
Taking DL\_POLY version 4.03 as an example (on the Cardiff HTC system), when the reader changes directory (using the '**cd**' command) into **/app/chemistry/DL\_POLY/4.03/example** the reader will see six files. There are three DL\_POLY input files (**FIELD**, **CONFIG** and **CONTROL**) and the LSF batch scheduler run file '**dlpoly.q**'. The remaining two files (**OUTPUT.reference** and **DLPOLY4.o.149462**) are files that were generated when this example was last executed from this example directory. The reader can copy the \*.lsf file and the DL\_POLY input data files to their own HOME directory and submit a batch DL\_POLY job from there and review the output. After submission the LSF run file (automatically) copies the LSF run file and input data files to the **/scratch** Cluster File System (CFS), processes the input data via the LSF batch scheduler (using DL\_POLY) and finally copies ALL the output back to the directory from where the job was originally submitted. This example should work seamlessly and provide a solid basis for the readers own DL\_POLY data / job submissions.

**Using DL\_POLY via Synfiniway Graphical Workflow Interface.**

Synfiniway is a graphical workflow tool that allows HPC Wales users to process data using the HPC application software available. It facilitates the creation of (graphical) workflows that can be used for pre / post-processing / organising of data etcetera and other tasks that would normally require the user to develop 'scripts' (using LINUX shell, Python, Perl etcetera) to accomplish the required tasks.

Instructions on how to access and use the example CRYSTAL synfiniway workflow can be found here - [DL\\_POLY Synfiniway Instructions](#). The Synfiniway application can be accessed using the following link - [Advanced Materials and Manufacturing Workflows](#).

**CLICK HERE**



DL\_POLY Application - DL\_POLY Synfiniway Instructions

DL\_POLY Application microsite.

DL\_POLY Application

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DL\_POLY Synfiniway Instructions

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# DL\_POLY

## DL\_POLY - Synfiniway Workflow Instructions.

**Workflow Name.**

Workflow	Folder
DL_POLY V4.04: Run solver	
Gateway	
Life Sciences	Chemistry application workflows > DL_POLY Classic
Advanced Materials and Manufacturing	DLPOLY4 Workflows

**Purpose.**

DL\_POLY is a general purpose classical molecular dynamics (MD) simulation software designed to facilitate molecular dynamics simulations of macromolecules, polymers, ionic systems, solutions and other molecular systems on a distributed memory parallel computer. DL\_POLY V4 is based on a replicated data parallelism. It is suitable for simulations of up to 30,000 atoms on up to 100 processors.

More information is available from [http://www.stfc.ac.uk/CSE/randd/ccg/software/DL\\_POLY/25526.aspx](http://www.stfc.ac.uk/CSE/randd/ccg/software/DL_POLY/25526.aspx).

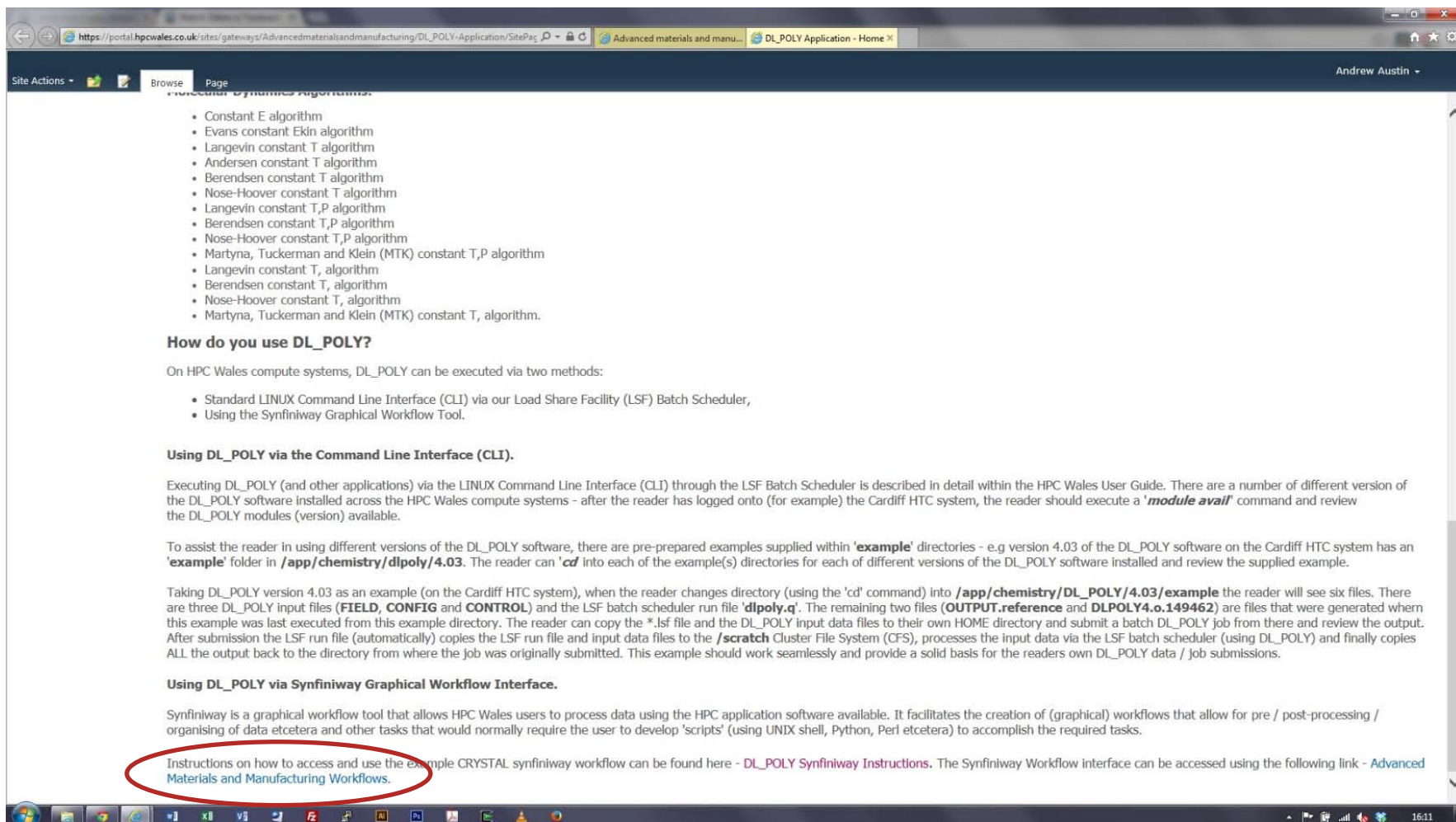
**Process.**

This workflow consists of a single task to run the DL\_POLY V4 application.

**Inputs.**

**Data files.**

Input data for the DL\_POLY V4 code is organized as a set of standard files with a fixed naming convention. All input files should be located within the single input directory provided as a parameter to the workflow.



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Advanced materials and manu... DL\_POLY Application - Home X

Andrew Austin -

**Molecular Dynamics Algorithms:**

- Constant E algorithm
- Evans constant Ekin algorithm
- Langevin constant T algorithm
- Andersen constant T algorithm
- Berendsen constant T algorithm
- Nose-Hoover constant T algorithm
- Langevin constant T,P algorithm
- Berendsen constant T,P algorithm
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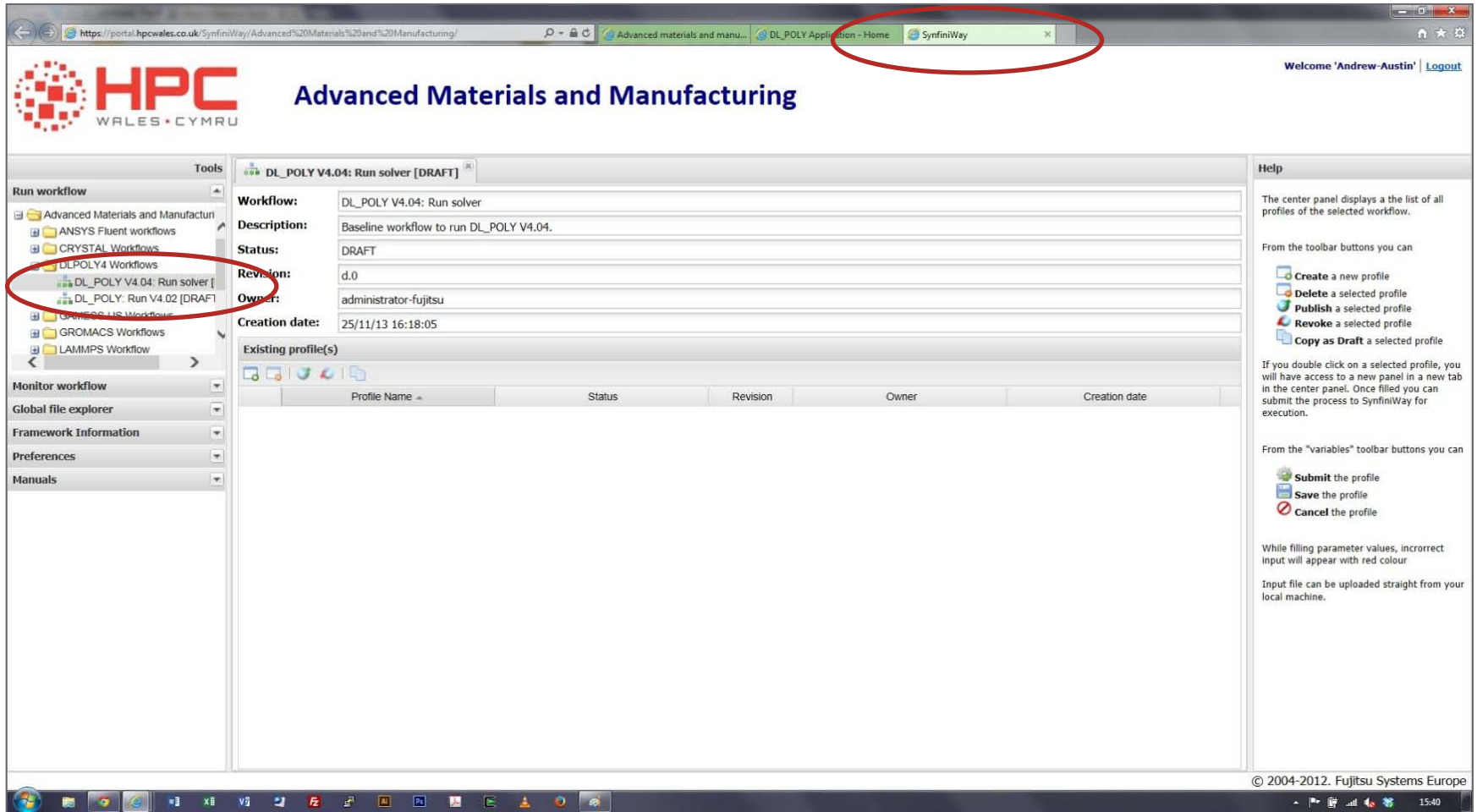
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**Using DL\_POLY via Synfiniway Graphical Workflow Interface.**

Synfiniway is a graphical workflow tool that allows HPC Wales users to process data using the HPC application software available. It facilitates the creation of (graphical) workflows that allow for pre / post-processing / organising of data etcetera and other tasks that would normally require the user to develop 'scripts' (using UNIX shell, Python, Perl etcetera) to accomplish the required tasks.

Instructions on how to access and use the example CRYSTAL synfiniway workflow can be found here - [DL\\_POLY Synfiniway Instructions](#). The Synfiniway Workflow interface can be accessed using the following link - [Advanced Materials and Manufacturing Workflows](#).



https://portal.hpcwales.co.uk/SynfiniWay/Advanced%20Materials%20and%20Manufacturing/

Advanced Materials and Manufacturing

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**Tools**

**Run workflow**

- Advanced Materials and Manufacturing
  - ANSYS Fluent workflows
  - CRYSTAL Workflows
  - DLPOLY4 Workflows
    - DL\_POLY V4.04: Run solver [DRAFT]**
    - DL\_POLY: Run V4.02 [DRAFT]
  - GROMACS US Workflows
  - GROMACS Workflows
  - LAMMPS Workflow

**Monitor workflow**

**Global file explorer**

**Framework Information**

**Preferences**

**Manuals**

**DL\_POLY V4.04: Run solver [DRAFT]**

**Workflow:** DL\_POLY V4.04: Run solver

**Description:** Baseline workflow to run DL\_POLY V4.04.

**Status:** DRAFT

**Revision:** d.0

**Owner:** administrator-fujitsu

**Creation date:** 25/11/13 16:18:05

**Existing profile(s)**

Profile Name	Status	Revision	Owner	Creation date
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**Help**

The center panel displays a list of all profiles of the selected workflow.

From the toolbar buttons you can

- Create a new profile
- Delete a selected profile
- Publish a selected profile
- Revoke a selected profile
- Copy as Draft a selected profile

If you double click on a selected profile, you will have access to a new panel in a new tab in the center panel. Once filled you can submit the process to SynfiniWay for execution.

From the "variables" toolbar buttons you can

- Submit the profile
- Save the profile
- Cancel the profile

While filling parameter values, incorrect input will appear with red colour

Input file can be uploaded straight from your local machine.

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15:40

https://portal.hpcwales.co.uk/sites/gateways/Advancedmaterialsandmanufacturing/SitePages/Home.aspx

Advanced materials and m... x

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LAMMPS

GROMACS

ONETEP

CRYSTAL

DL\_POLY

SIESTA

NAMD

MATERIALS APPLICATIONS

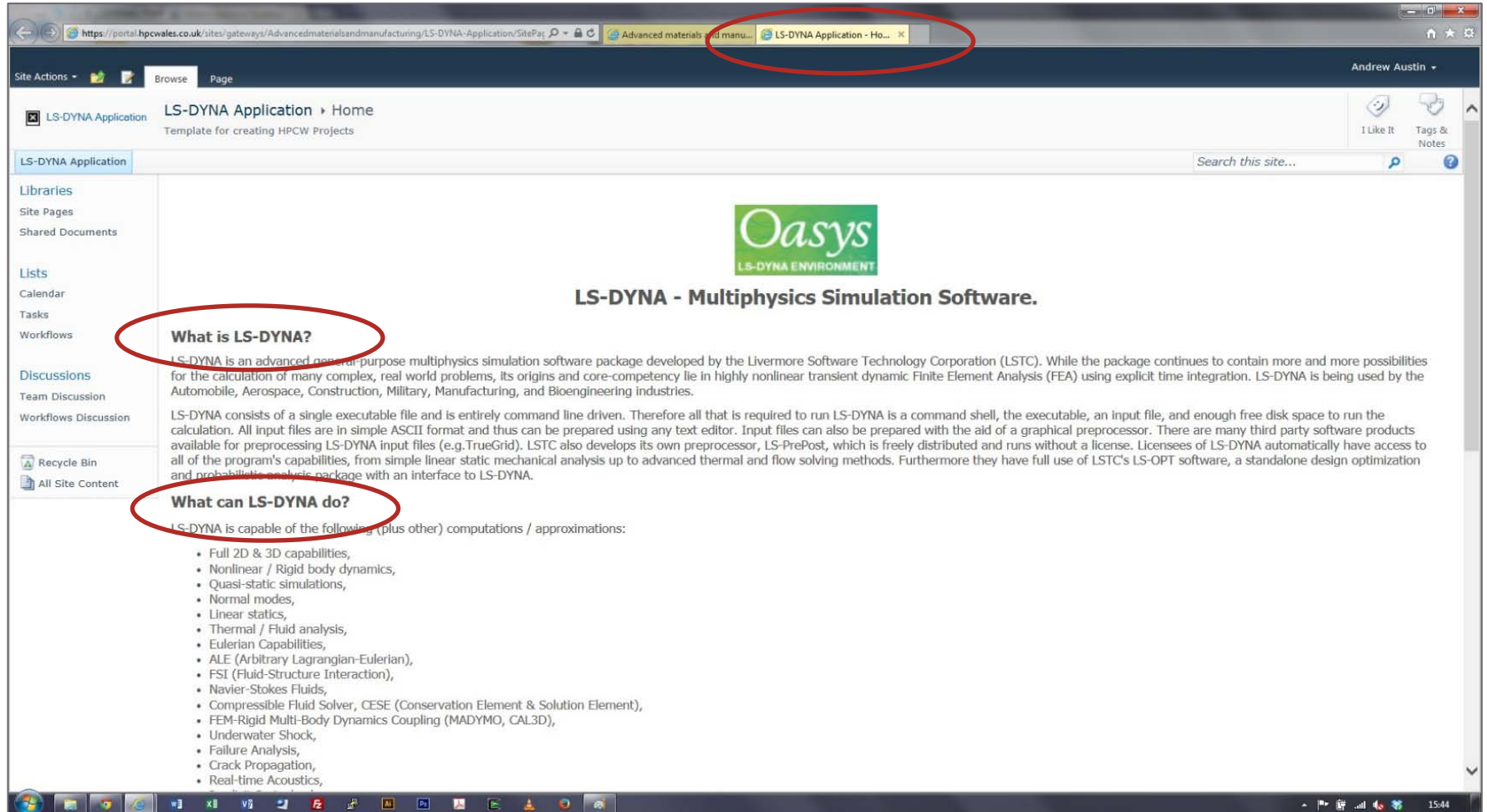
Oasys

OPENFOAM

ANSYS FLUENT

ANSYS MAXWELL-3D





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LS-DYNA Application

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Template for creating HPCW Projects

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**What is LS-DYNA?**

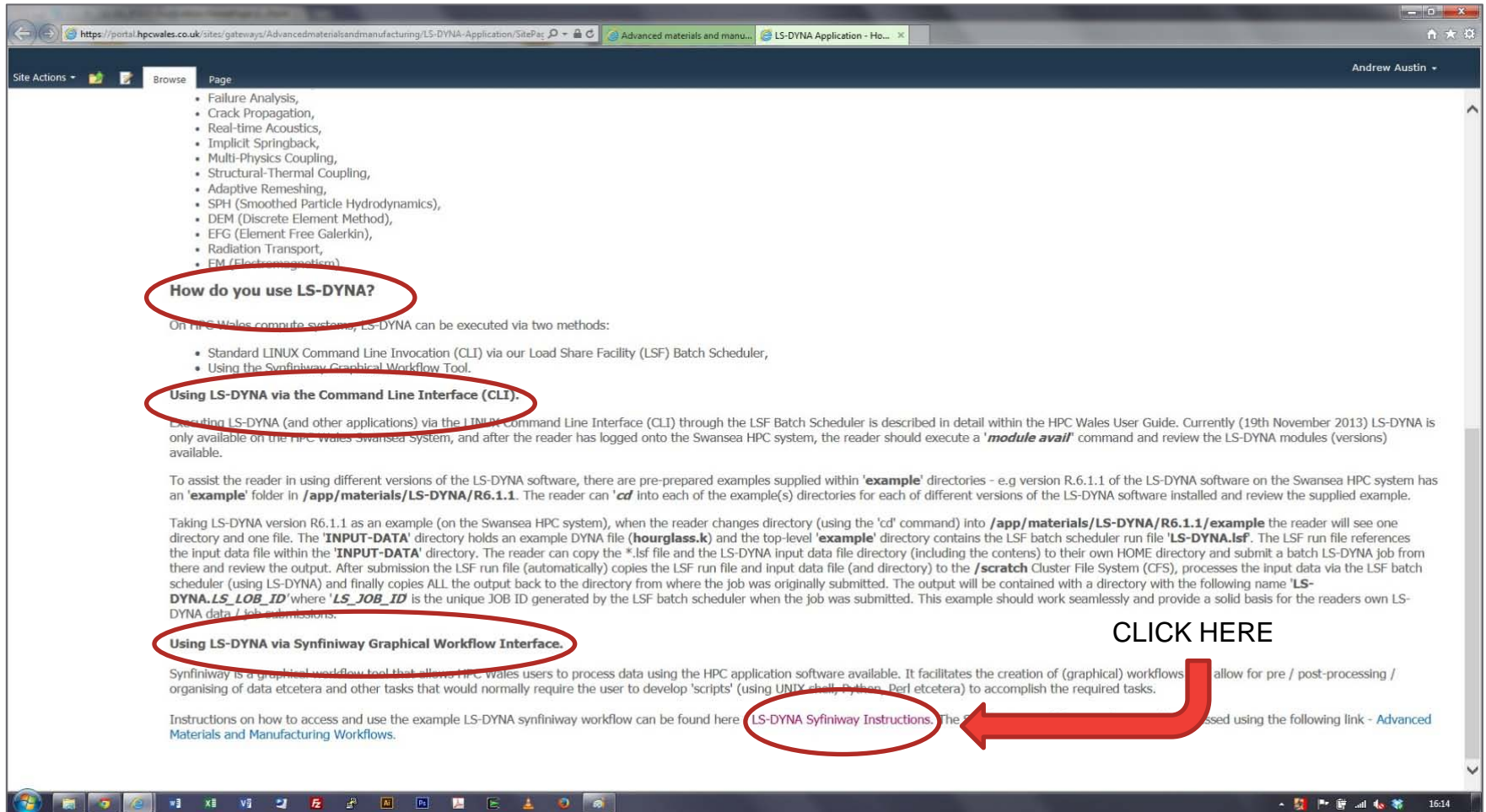
LS-DYNA is an advanced general-purpose multiphysics simulation software package developed by the Livermore Software Technology Corporation (LSTC). While the package continues to contain more and more possibilities for the calculation of many complex, real world problems, its origins and core-competency lie in highly nonlinear transient dynamic Finite Element Analysis (FEA) using explicit time integration. LS-DYNA is being used by the Automobile, Aerospace, Construction, Military, Manufacturing, and Bioengineering industries.

LS-DYNA consists of a single executable file and is entirely command line driven. Therefore all that is required to run LS-DYNA is a command shell, the executable, an input file, and enough free disk space to run the calculation. All input files are in simple ASCII format and thus can be prepared using any text editor. Input files can also be prepared with the aid of a graphical preprocessor. There are many third party software products available for preprocessing LS-DYNA input files (e.g. TrueGrid). LSTC also develops its own preprocessor, LS-PrePost, which is freely distributed and runs without a license. Licensees of LS-DYNA automatically have access to all of the program's capabilities, from simple linear static mechanical analysis up to advanced thermal and flow solving methods. Furthermore they have full use of LSTC's LS-OPT software, a standalone design optimization and probabilistic analysis package with an interface to LS-DYNA.

**What can LS-DYNA do?**

LS-DYNA is capable of the following (plus other) computations / approximations:

- Full 2D & 3D capabilities,
- Nonlinear / Rigid body dynamics,
- Quasi-static simulations,
- Normal modes,
- Linear statics,
- Thermal / Fluid analysis,
- Eulerian Capabilities,
- ALE (Arbitrary Lagrangian-Eulerian),
- FSI (Fluid-Structure Interaction),
- Navier-Stokes Fluids,
- Compressible Fluid Solver, CESE (Conservation Element & Solution Element),
- FEM-Rigid Multi-Body Dynamics Coupling (MADYMO, CAL3D),
- Underwater Shock,
- Failure Analysis,
- Crack Propagation,
- Real-time Acoustics,



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- Failure Analysis,
- Crack Propagation,
- Real-time Acoustics,
- Implicit Springback,
- Multi-Physics Coupling,
- Structural-Thermal Coupling,
- Adaptive Remeshing,
- SPH (Smoothed Particle Hydrodynamics),
- DEM (Discrete Element Method),
- EFG (Element Free Galerkin),
- Radiation Transport,
- EM (Electromagnetism)

**How do you use LS-DYNA?**

On HPC Wales compute systems, LS-DYNA can be executed via two methods:

- Standard LINUX Command Line Invocation (CLI) via our Load Share Facility (LSF) Batch Scheduler,
- Using the Syfiniway Graphical Workflow Tool.

**Using LS-DYNA via the Command Line Interface (CLI).**

Executing LS-DYNA (and other applications) via the LINUX Command Line Interface (CLI) through the LSF Batch Scheduler is described in detail within the HPC Wales User Guide. Currently (19th November 2013) LS-DYNA is only available on the HPC Wales Swansea system, and after the reader has logged onto the Swansea HPC system, the reader should execute a **'module avail'** command and review the LS-DYNA modules (versions) available.

To assist the reader in using different versions of the LS-DYNA software, there are pre-prepared examples supplied within **'example'** directories - e.g version R6.1.1 of the LS-DYNA software on the Swansea HPC system has an **'example'** folder in **/app/materials/LS-DYNA/R6.1.1**. The reader can **'cd'** into each of the example(s) directories for each of different versions of the LS-DYNA software installed and review the supplied example.

Taking LS-DYNA version R6.1.1 as an example (on the Swansea HPC system), when the reader changes directory (using the **'cd'** command) into **/app/materials/LS-DYNA/R6.1.1/example** the reader will see one directory and one file. The **'INPUT-DATA'** directory holds an example DYNA file (**hourglass.k**) and the top-level **'example'** directory contains the LSF batch scheduler run file **'LS-DYNA.lsf'**. The LSF run file references the input data file within the **'INPUT-DATA'** directory. The reader can copy the \*.lsf file and the LS-DYNA input data file directory (including the contents) to their own HOME directory and submit a batch LS-DYNA job from there and review the output. After submission the LSF run file (automatically) copies the LSF run file and input data file (and directory) to the **/scratch** Cluster File System (CFS), processes the input data via the LSF batch scheduler (using LS-DYNA) and finally copies ALL the output back to the directory from where the job was originally submitted. The output will be contained with a directory with the following name **'LS-DYNA\_LS\_JOB\_ID'** where **'LS\_JOB\_ID'** is the unique JOB ID generated by the LSF batch scheduler when the job was submitted. This example should work seamlessly and provide a solid basis for the readers own LS-DYNA data / job submissions.

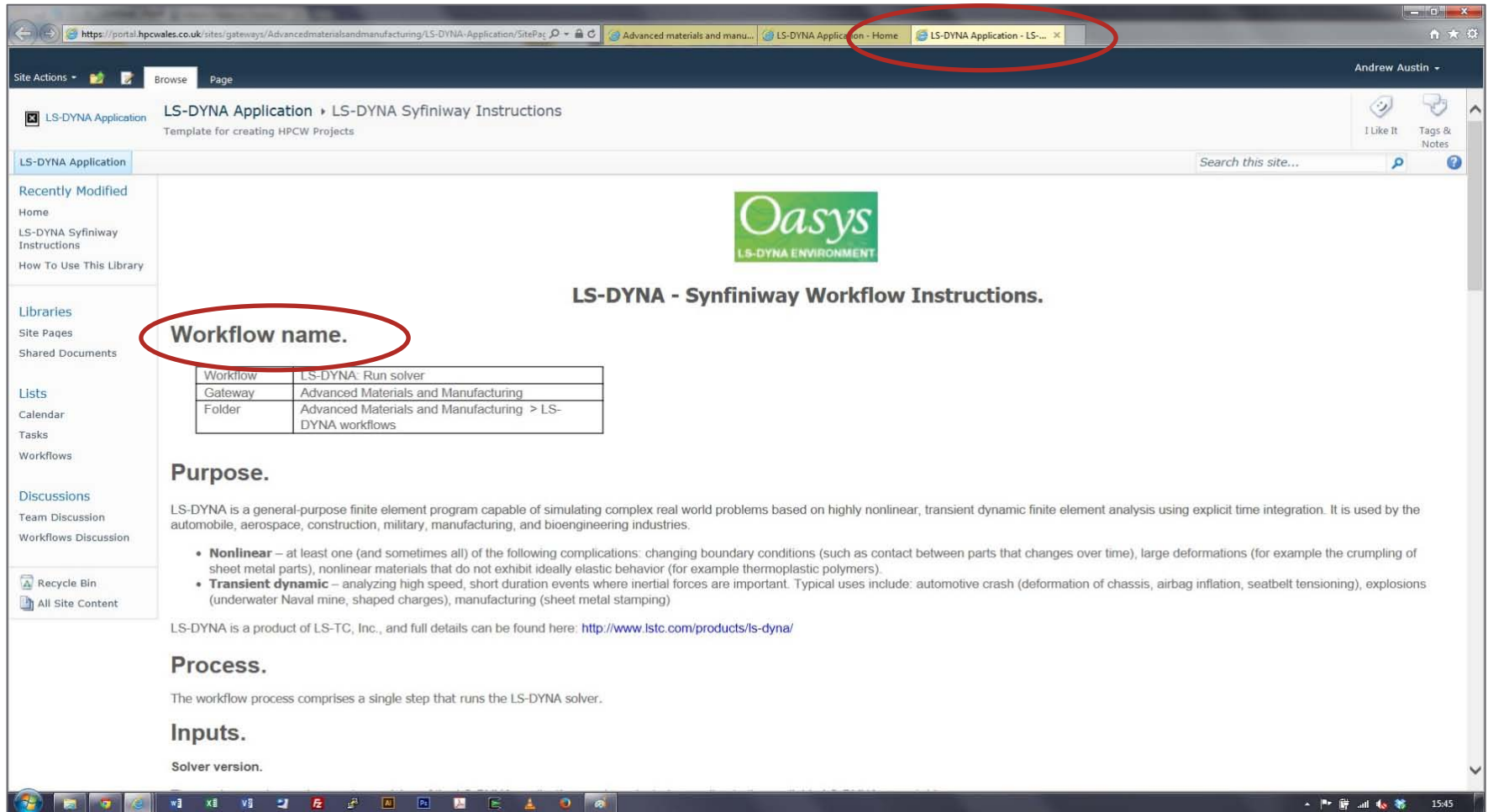
**Using LS-DYNA via Syfiniway Graphical Workflow Interface.**

Syfiniway is a graphical workflow tool that allows HPC Wales users to process data using the HPC application software available. It facilitates the creation of (graphical) workflows that allow for pre / post-processing / organising of data etcetera and other tasks that would normally require the user to develop 'scripts' (using UNIX shell, Python, Perl etcetera) to accomplish the required tasks.

Instructions on how to access and use the example LS-DYNA syfiniway workflow can be found here [LS-DYNA Syfiniway Instructions](#). The workflow can be accessed using the following link - [Advanced Materials and Manufacturing Workflows](#).

**CLICK HERE**





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LS-DYNA Application | LS-DYNA Syfiniway Instructions  
Template for creating HPCW Projects

LS-DYNA Application

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All Site Content

**Workflow name.**

Workflow	LS-DYNA: Run solver
Gateway	Advanced Materials and Manufacturing
Folder	Advanced Materials and Manufacturing > LS-DYNA workflows

**Purpose.**

LS-DYNA is a general-purpose finite element program capable of simulating complex real world problems based on highly nonlinear, transient dynamic finite element analysis using explicit time integration. It is used by the automobile, aerospace, construction, military, manufacturing, and bioengineering industries.

- Nonlinear** – at least one (and sometimes all) of the following complications: changing boundary conditions (such as contact between parts that changes over time), large deformations (for example the crumpling of sheet metal parts), nonlinear materials that do not exhibit ideally elastic behavior (for example thermoplastic polymers).
- Transient dynamic** – analyzing high speed, short duration events where inertial forces are important. Typical uses include: automotive crash (deformation of chassis, airbag inflation, seatbelt tensioning), explosions (underwater Naval mine, shaped charges), manufacturing (sheet metal stamping)

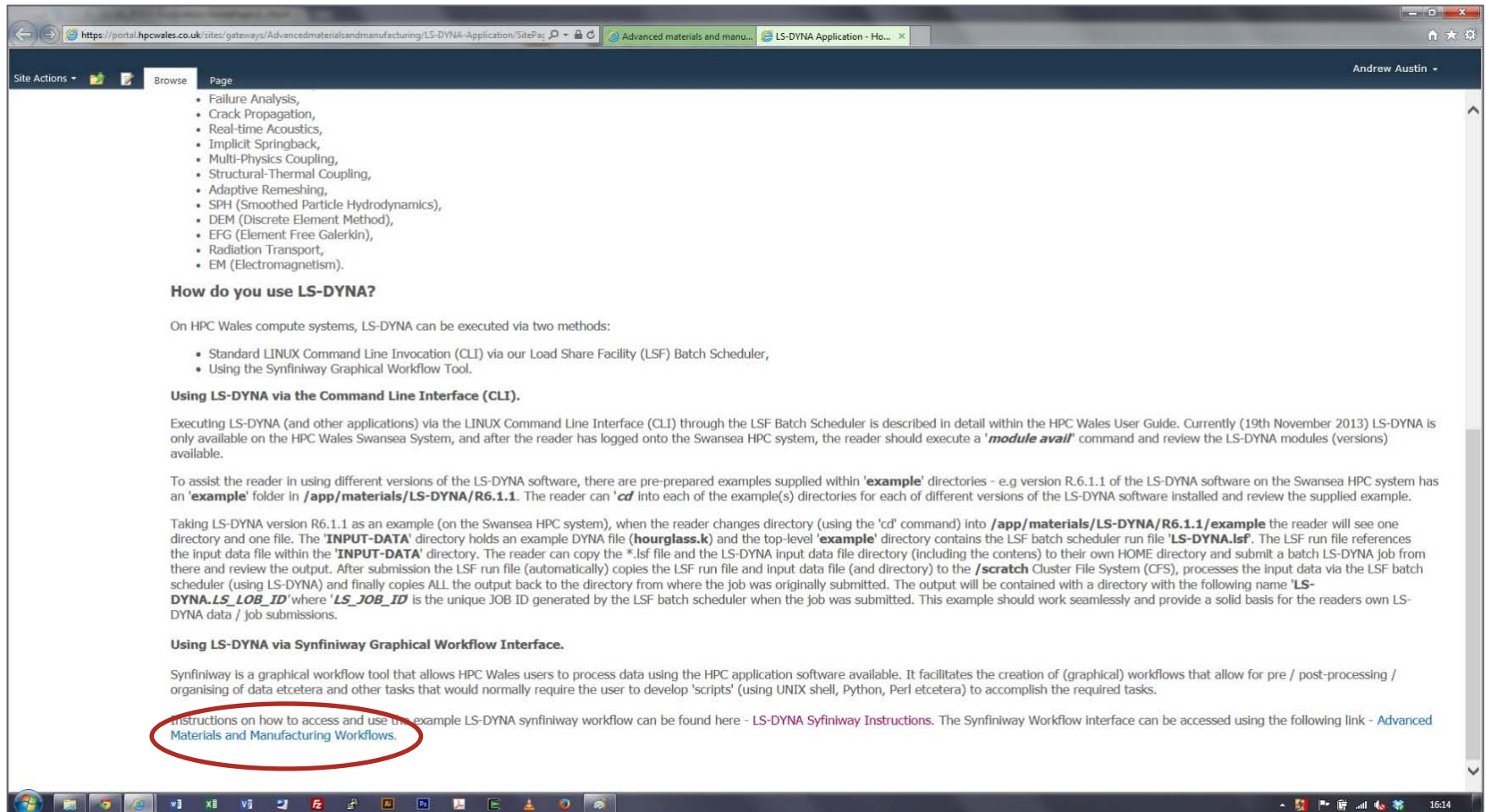
LS-DYNA is a product of LS-TC, Inc., and full details can be found here: <http://www.lstc.com/products/ls-dyna/>



**Process.**

The workflow process comprises a single step that runs the LS-DYNA solver.

**Inputs.**

Solver version.



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- Failure Analysis,
- Crack Propagation,
- Real-time Acoustics,
- Implicit Springback,
- Multi-Physics Coupling,
- Structural-Thermal Coupling,
- Adaptive Remeshing,
- SPH (Smoothed Particle Hydrodynamics),
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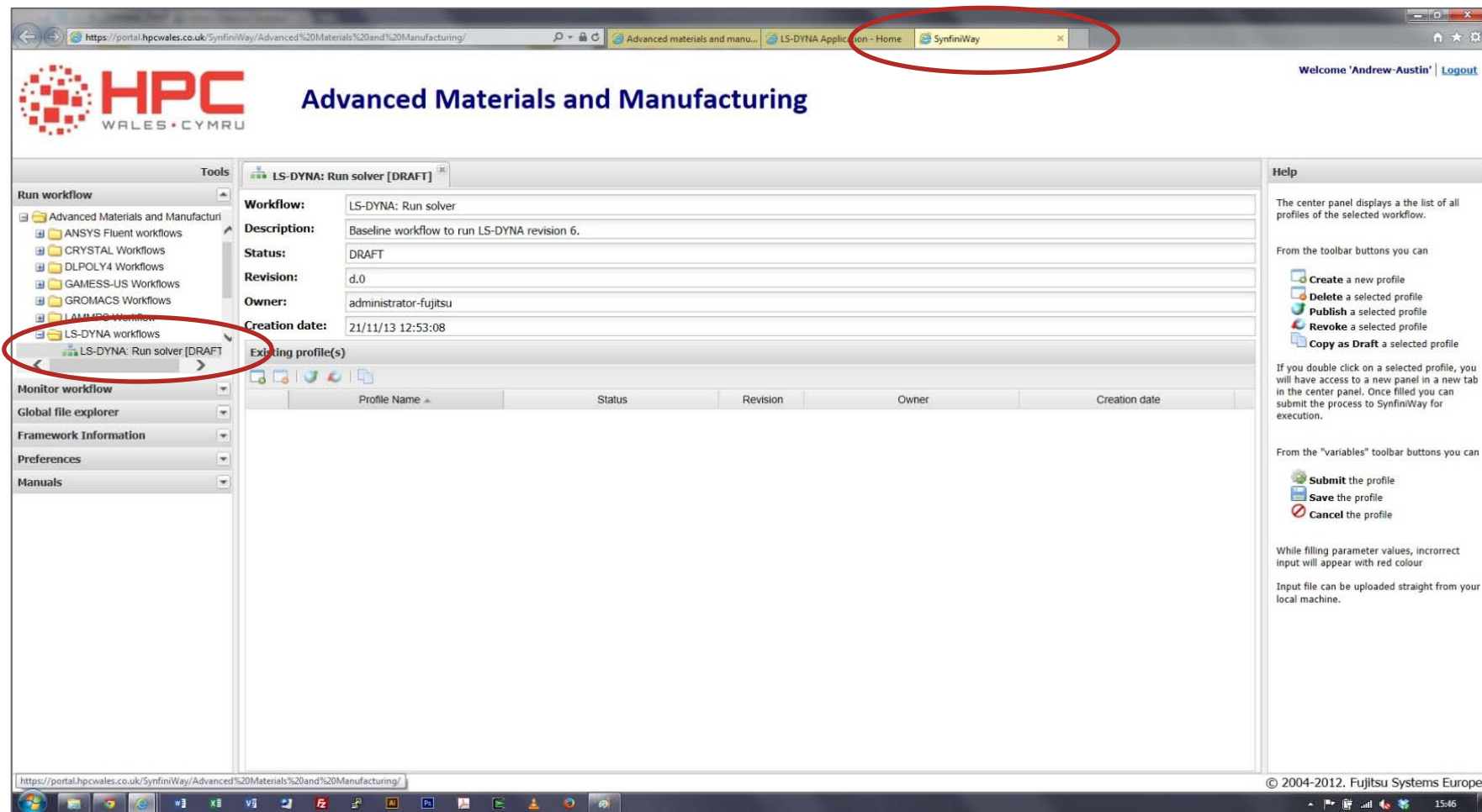
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## Advanced Materials and Manufacturing

Tools

Run workflow

- Advanced Materials and Manufacturing
  - ANSYS Fluent workflows
  - CRYSTAL Workflows
  - DLPOLY4 Workflows
  - GAMMESS-US Workflows
  - GROMACS Workflows
  - LAMMPS Workflows
  - LS-DYNA workflows
    - LS-DYNA: Run solver [DRAFT]

Monitor workflow

Global file explorer

Framework Information

Preferences

Manuals

Workflow: LS-DYNA: Run solver

Description: Baseline workflow to run LS-DYNA revision 6.

Status: DRAFT

Revision: d.0

Owner: administrator-fujitsu

Creation date: 21/11/13 12:53:08

Existing profile(s)

Profile Name	Status	Revision	Owner	Creation date
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Help

The center panel displays a list of all profiles of the selected workflow.

From the toolbar buttons you can

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- Delete a selected profile
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- Save the profile
- Cancel the profile

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## Advanced Materials & Manufacturing Gateway (AM&M)

- Not all AM&M applications yet covered
- Further development required (e.g. 'User Expertise')
- More SynfiniWay example workflows to be added

Now for a SynfiniWay Workflow  
Demonstration



**HPC**  
WALES • CYMRU

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# SynfiniWay – Workflow impact on the Research Agenda

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Buddsoddi yn eich dyfodol  
Cronfa Datblygu Rhanbarthol Ewrop

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



# SynfiniWay role in HPC Wales user environment

HPC web-based gateways  
with workflow automation



Access from anywhere

Data access and movement

Workflow service orchestration

HPC infrastructure abstraction

HPC Wales Framework



Hub



Hub



Tier 1



Tier 2A

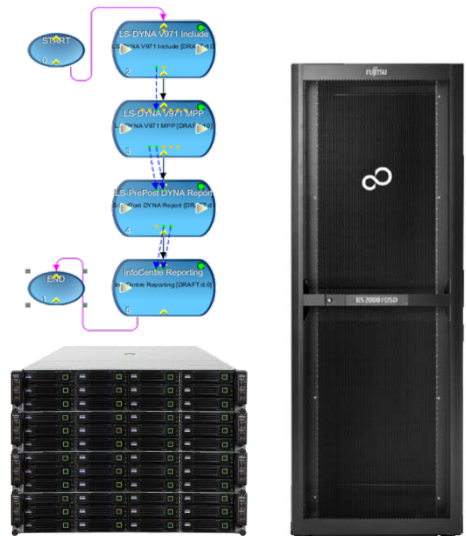
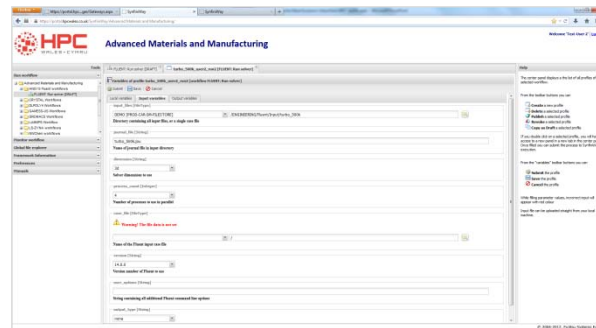


# How SynfiniWay workflows help

Structure and encode business processes as automated transferable workflows

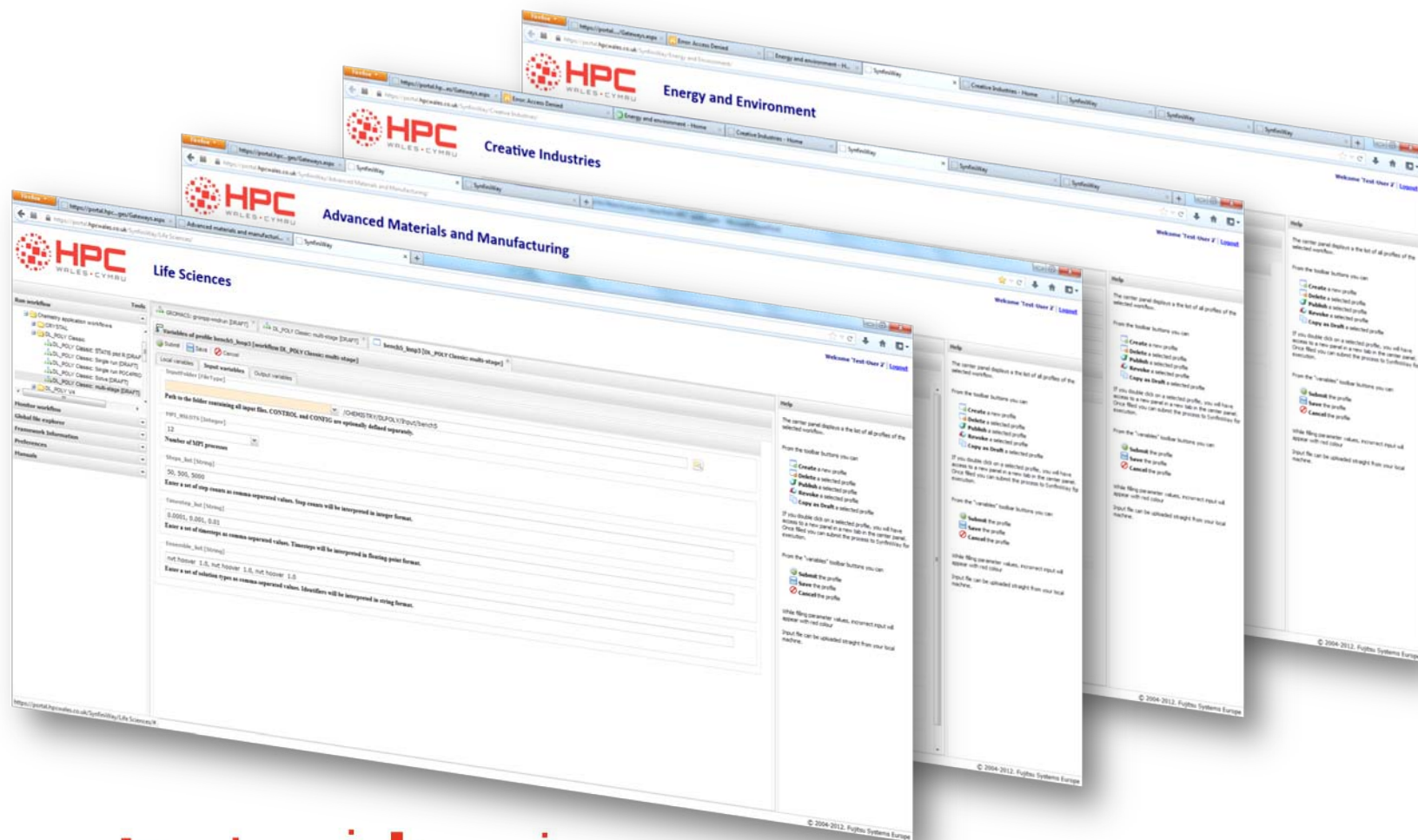
Allows users to focus on research and analysis – eliminates low-level actions, increases productivity

Systematic deployment of best practice and expert methods, to non-experts and other experts





# SynfiniWay Gateways available to date



# Applications

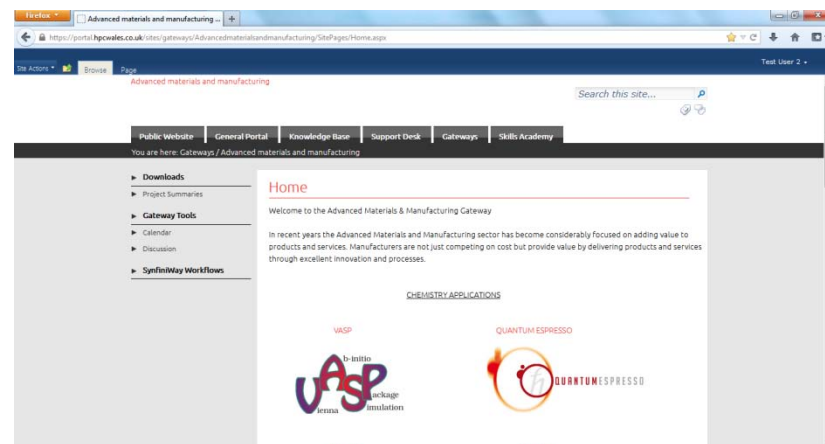
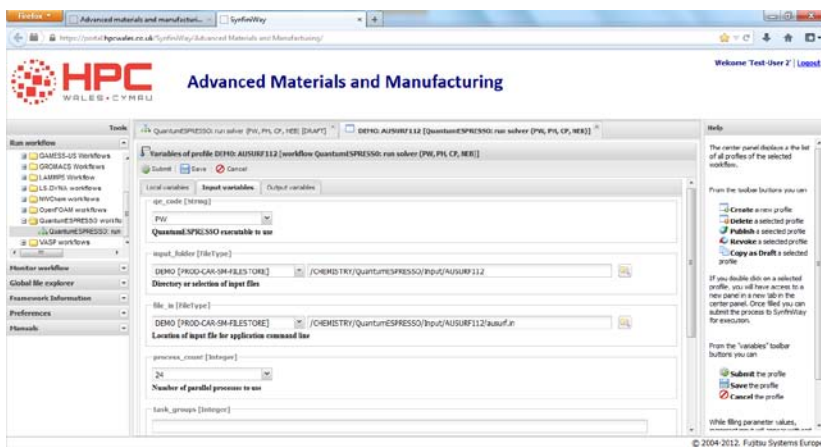
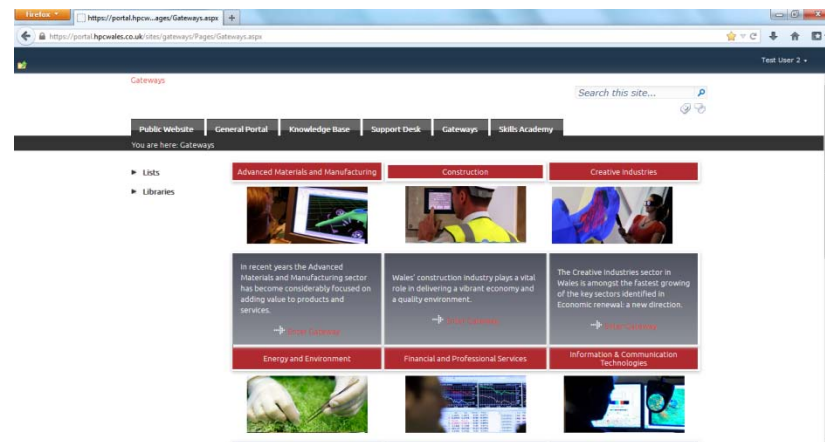
Wide range of applications are already available for use through the Gateway and SynfiniWay baseline workflows.

Advanced Manufacturing & Materials	Creative Industries	Energy & Environment	Life Sciences – Chemistry	Life Sciences - Genomics	Multi-Sector
ANSYS Fluent CRYSTAL DL_POLY 4 GAMESS-US GROMACS LS-DYNA NWChem OpenFOAM QuantumESPRESSO VASP	Arnold Lightwave MentalRay	ROMS SWAN	DL_POLY 4 DL_POLY Classic GAMESS-UK GAMESS-US Gromacs LAMMPS NAMD NWCHEM QuantumESPRESSO VASP	ABYSS Biskit BLAST Bowtie BWA CABOG CURVES+ MRBAYES PLINK SATSUMA SOAP2 T-Coffee TELEMAT	R

# Simplified HPC usage

Locate chosen application  
in thematic Gateway >>>

Define, submit and monitor application  
process all through web interface

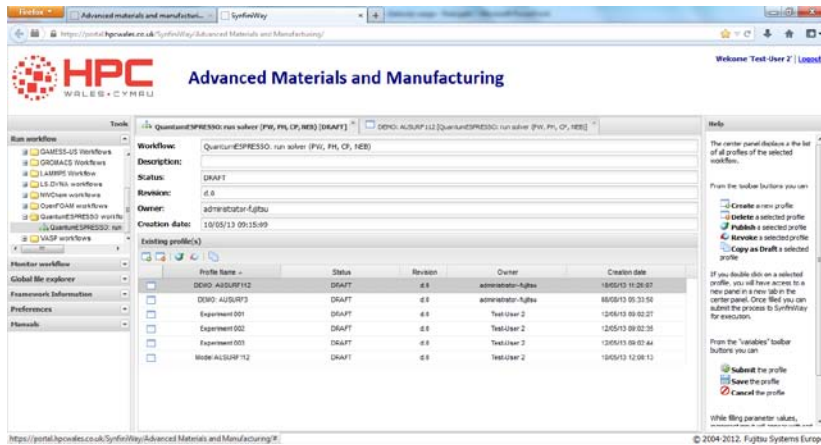


## New users

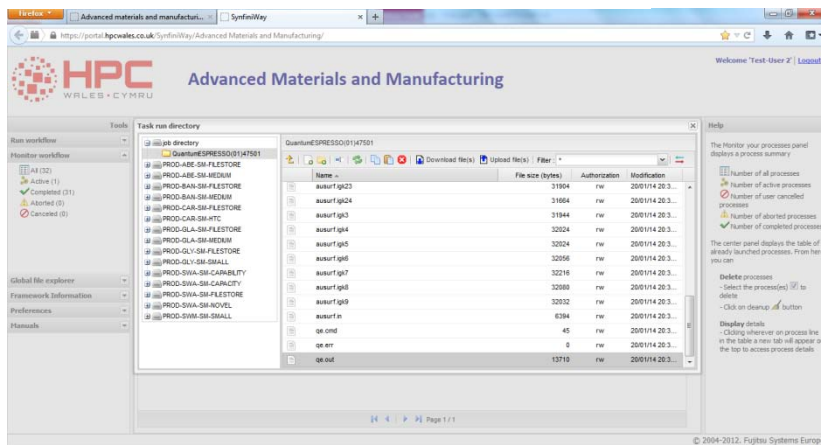
- Identify the application you need to use under the associated Gateway
- Review existing usage guides for this on-boarded process
  - The baseline interface should offer most common parameters
  - If additional parameters are required these can be rapidly added by the HPC Wales technical team
- If additional applications or tools are required a simple interface can be quickly created
  - Contact the Gateway owner or technical team

# Graphical job management

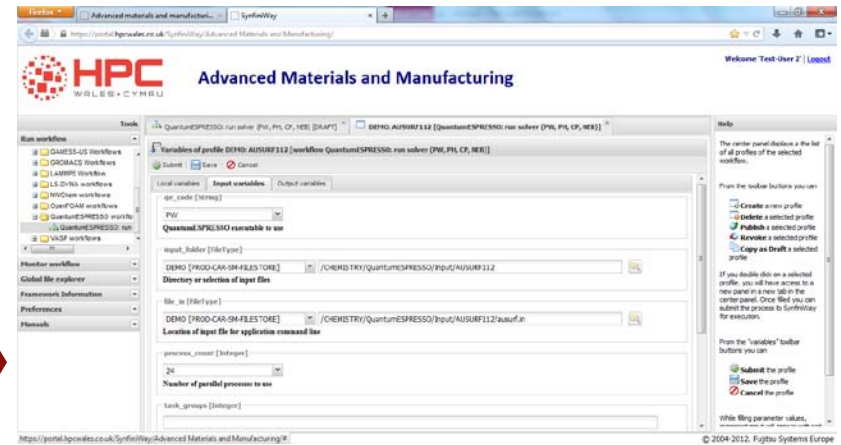
Select workflow and create input profile



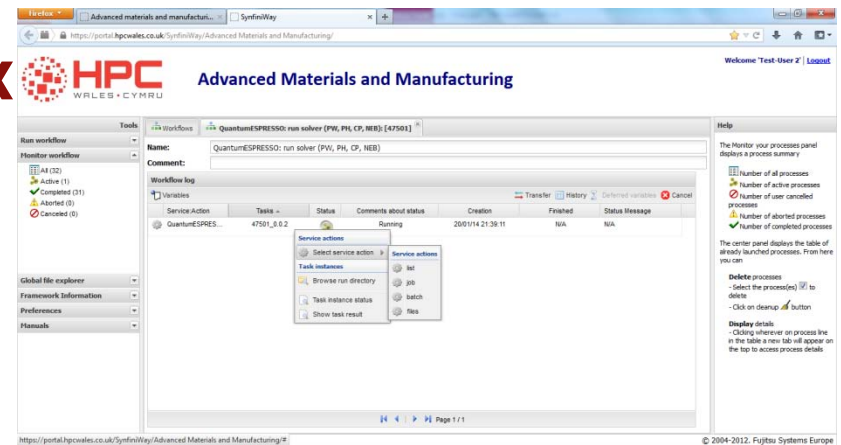
Download files, workflow copied to persistent store



Define input values and submit



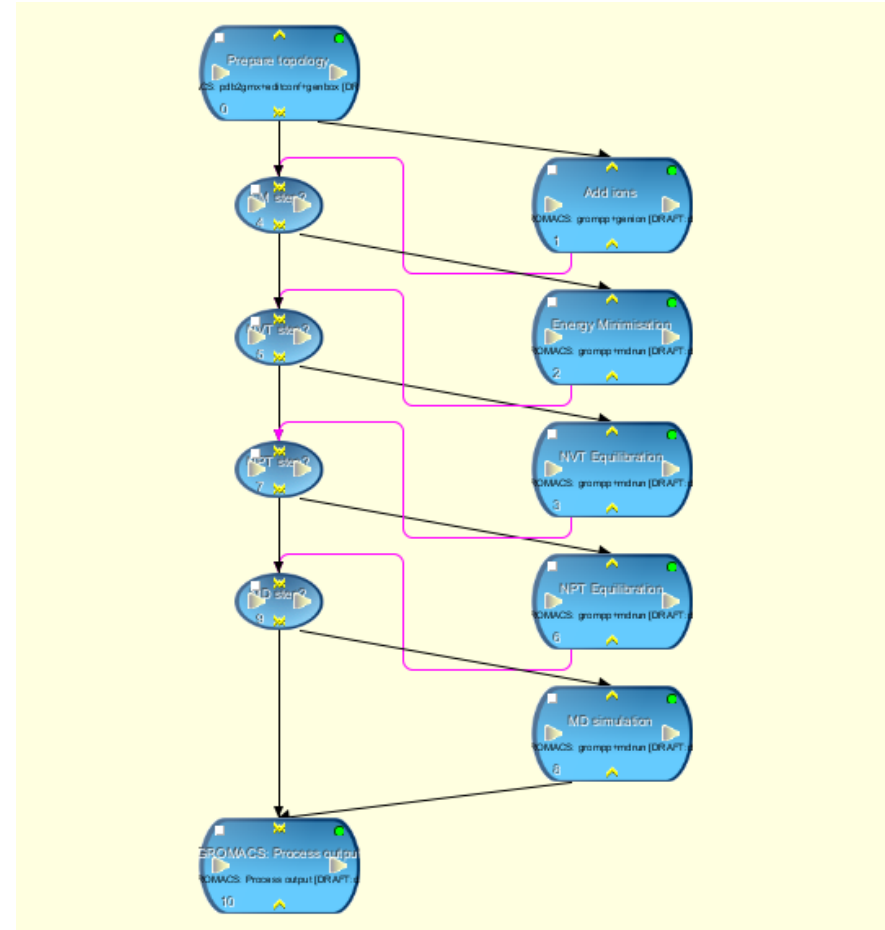
Control status, inspect files, monitor key values





# Complete workflows

- More extended workflows enable programming a multi-step process
- Tasks can be selected by user input controls or based on output variables
- Allows generalisation of the process to accommodate different input scenarios or an evolving computation



## Workflow advantages

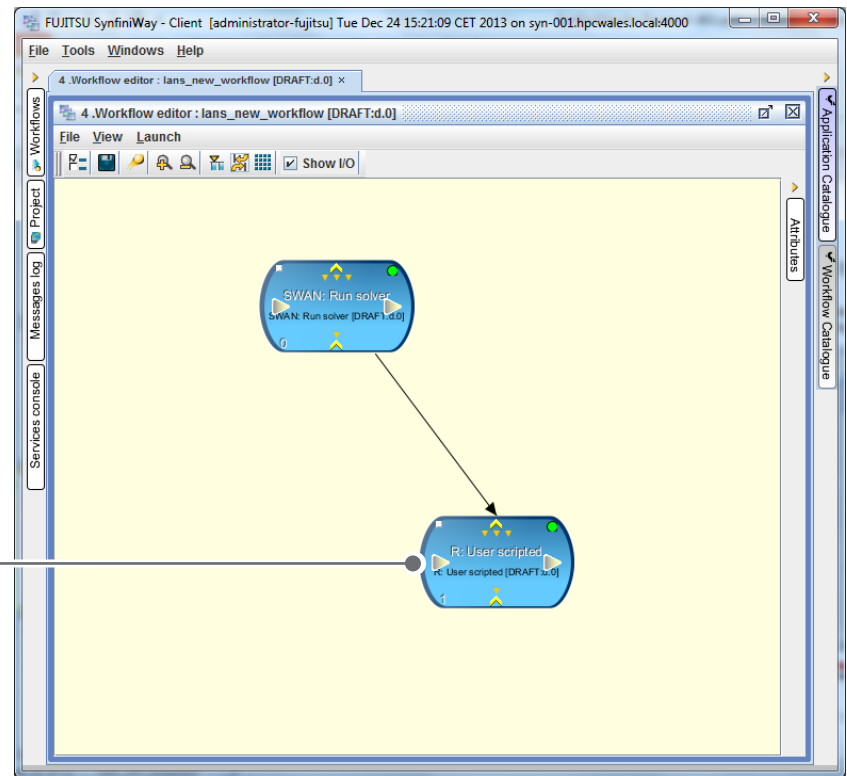
- Decouple HPC outcome from IT activity
  - Workflow tasks are system and location independent
- Encode and automate practically any business process
  - Complex conditionals, iterative
- Provide the foundation for global optimisation
  - Automated data movement between HPC Wales sites
- Promote reusability and sharing
  - Incorporate sub-flows for re-use of tried and tested best practice templates and IP protection
- Increases security
  - Fine-grained authorisation control on workflows and tasks based on role and groups

# Assemble workflow from pre-built interfaces

Certain components are already available. Check the function and interface for consistency with your process.

New components can be added as required. You could integrate your own scripts as workflow services.

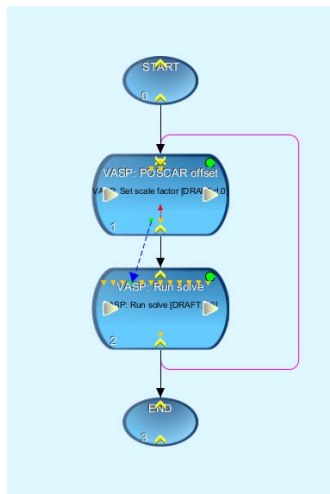
Name	Revision	Last Modification
Mental Ray : Final Gather	d.0	24-Jul-2013
Mental Ray : Final Gather Merge	0.1	23-Apr-2013
Mental Ray : Proxy Adjustment	d.0	25-Apr-2013
NAMD: solver	d.0	10-Apr-2013
NWCHEM: Run solver	d.0	21-Aug-2012
NWCHEM: Run solver	d.1	26-Nov-2013
OpenFOAM: 2D plot data	d.0	12-May-2013
OpenFOAM: Decomposition	d.0	12-May-2013
OpenFOAM: Meshing	d.0	12-May-2013
OpenFOAM: Solving	d.0	20-May-2013
PLINK3	0.1	17-Sep-2011
PLINK4	d.0	19-Aug-2011
PLINK: Analysis	d.0	15-Mar-2012
PLINK_ade_app	d.0	23-Sep-2011
PLINK_andrew_app	d.0	23-Sep-2011
QuantumESPRESSO: run solver	d.0	10-May-2013
R: CAN	d.0	08-Jul-2013
R: CAN test	d.0	31-May-2013
R: User scripted	d.0	24-May-2013
R: xyplot	d.0	24-May-2013
R: xyplot with type	d.0	05-Jul-2013
ROMS: Run oceanM	d.0	18-Jan-2013
ROMS: Run oceanM old	d.0	15-Jan-2013
ROMS: Run oceanM old variables	d.0	18-Jan-2013
ROMS: Tile count	d.0	12-Dec-2012



# Common workflow structures (1)

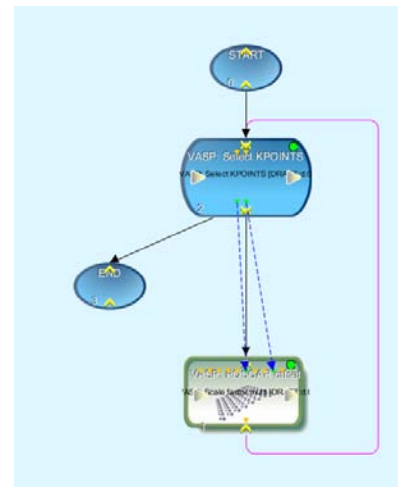
## Single level loop methods

The experiment comprises a series of different value on one dimension, either defined individually or incremented across a range. A loop workflow provides a robust method to define such processes for optimisation or ranging studies.



## Multi-level loop methods with embedded process

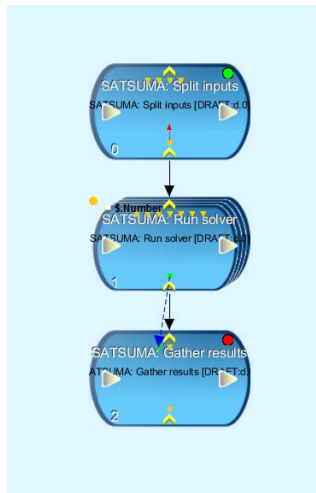
The experiment comprises a two-dimensional variation. We can re-use an existing workflow for the inner dimension with results being output from each computation on both dimensions.



# Sample workflow structures (2)

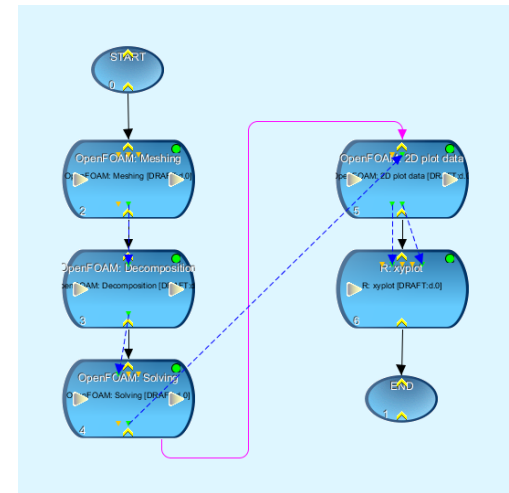
## Multi-tasked methods

The experiment builds a set of inputs that can be simulated concurrently. At the end of the process all results need to be assimilated and analysed to produce either a statistical summary or an optimised design point.



## Pre-Solve-Post methods

Common in CAE, the pre-solve-post process automates the meshing/decomposition, followed by the simulation stage. Post-processing may include first-pass analysis, data filtering and compression, and report generation, including plots and images.

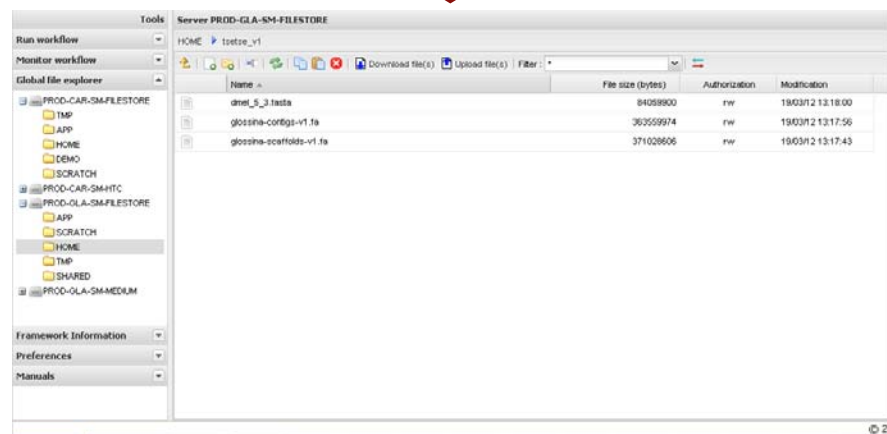
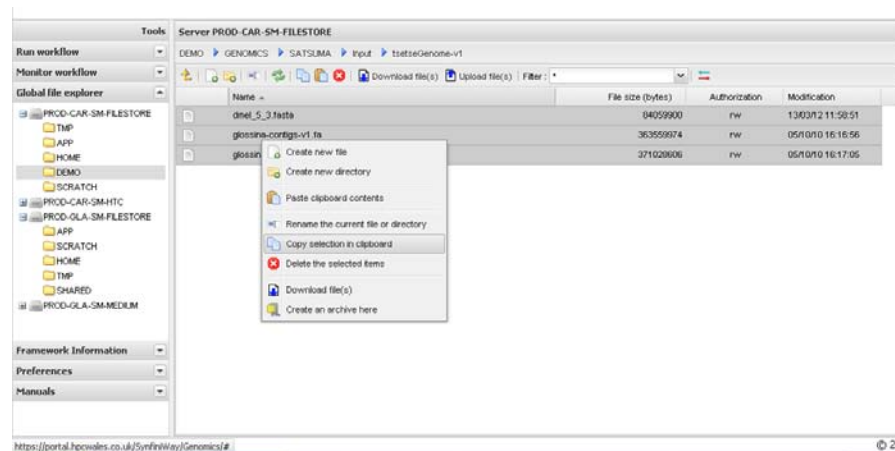


Methods can further address error handling (fix, resubmit) and could include appropriate utility tasks (archive, filter, chart). Tasks for these normally depend on the application.



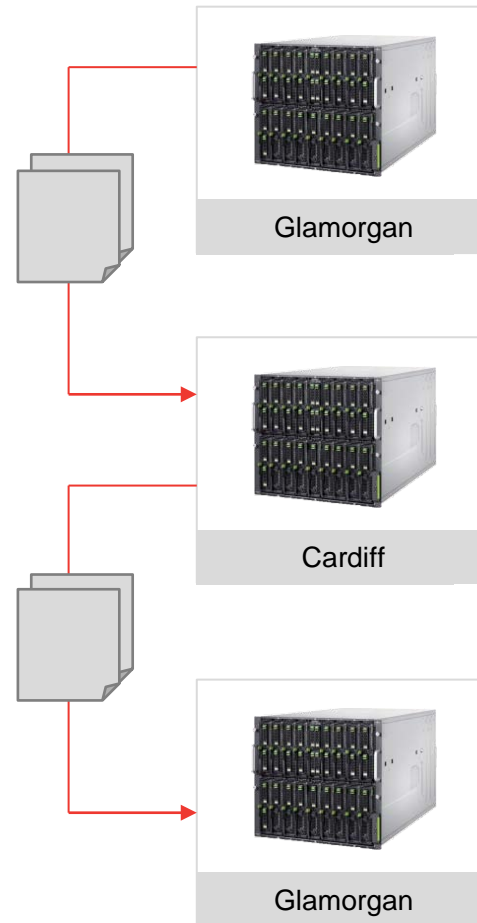
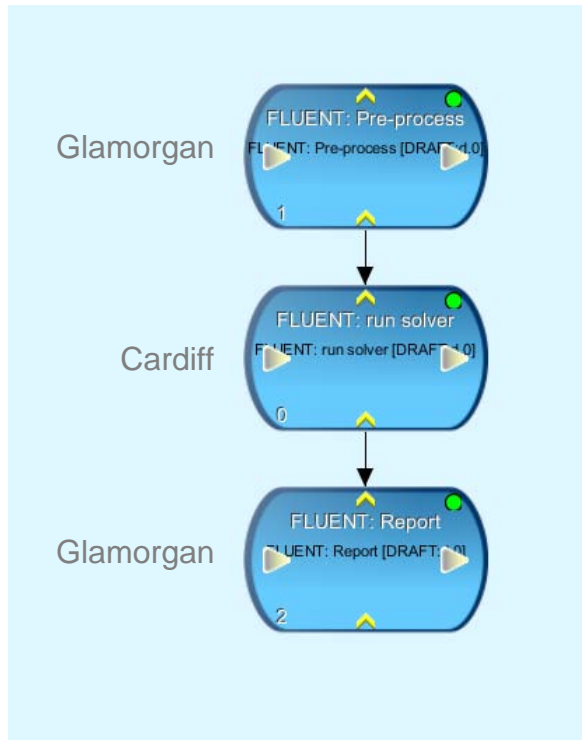
# Global data access and movement (1)

Through the global file explorer you can cut and past files between HPC Wales sites.



## Global data access and movement (2)

Within a workflow the data movement between sites of systems is handled automatically.



Advantage is that user located in Glamorgan need only handle input and output files from their local site filesystems.

# Workflow impact

Democratization

Process-oriented

Systematic methods

Service based

Organized activity

Multi-application

Dynamic scale

Network neutral



Broaden individual and team access to HPC applications and methods

## Next steps

- Which applications in this list do you use?
  - Which need to be added?
- Do you run basically the same script each time
  - Other than changes to input files, executables options, environment
- Are you using any types of multi-stage process?

22 January 2014



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# The HPC Wales User Group

## THE “TOP 10” ISSUES



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Europe & Wales:  
Investing in your future  
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Llywodraeth Cymru  
Welsh Government



# Survey Outcomes: Main challenges

1. **Lack of familiarity with Linux.**
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.**
5. **Getting used to running the system, basically getting used to its language and procedures.**
6. **Knowing what is available.**
7. **Improving the user's skillset from beginner to intermediate level.**

8. **Getting prompt resolution to tickets is the main challenge, beyond that greater availability of training materials and courses would be useful in terms of widening my knowledge of the subject.**
9. **Software design.**
10. **Finding support in improving the code.**
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.**
12. **Transferring data between Cardiff and Swansea nodes.**
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.**

# ServiceNow: The Support Desk

1. Accessing the Support Desk can be either via email ([support@hpcwales.co.uk](mailto:support@hpcwales.co.uk)), telephone ([01248 675093](tel:01248675093)) or self-service through the Portal or directly via the URL: <http://hpcwprod.service-now.com>
2. Users must login using their HPC Wales credentials



IT Service Management Suite

Login

User name: ANother

Password: .....

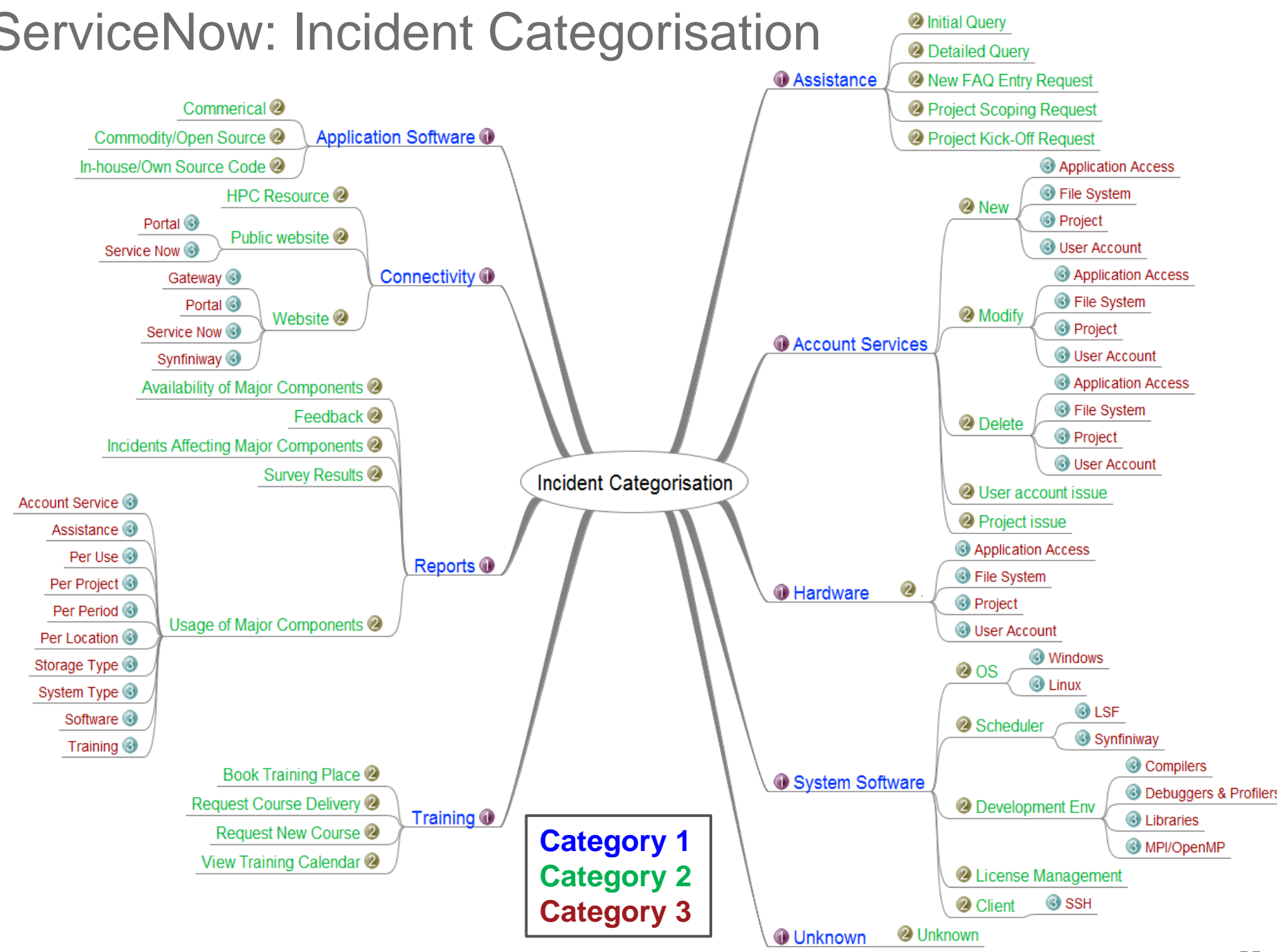
☒ Remember me

Login

Welcome to ServiceNow

3. The Support desk provides an interface for customers to monitor the status of calls raised with HPC Wales

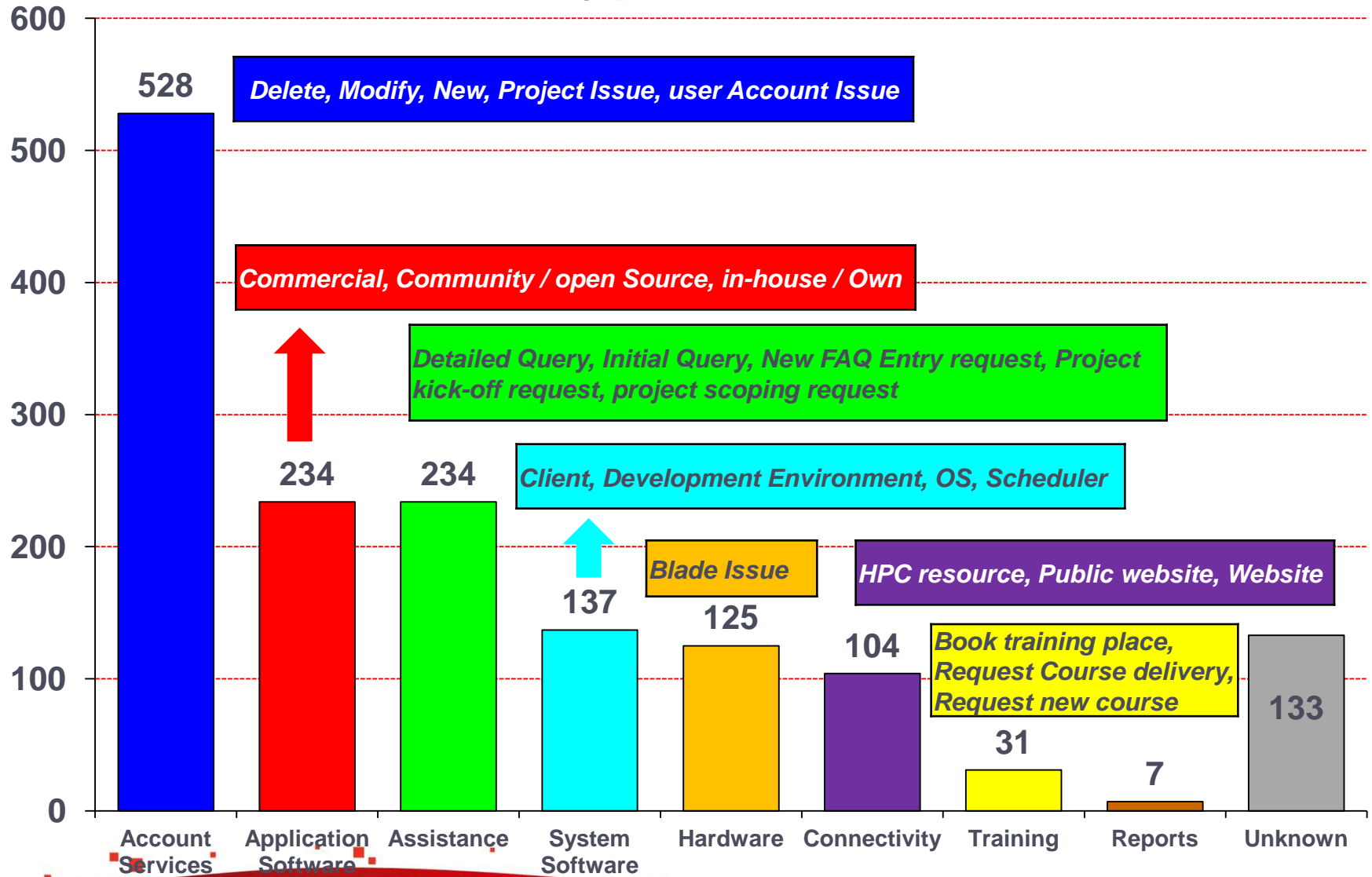
# ServiceNow: Incident Categorisation



Incident Categorisation

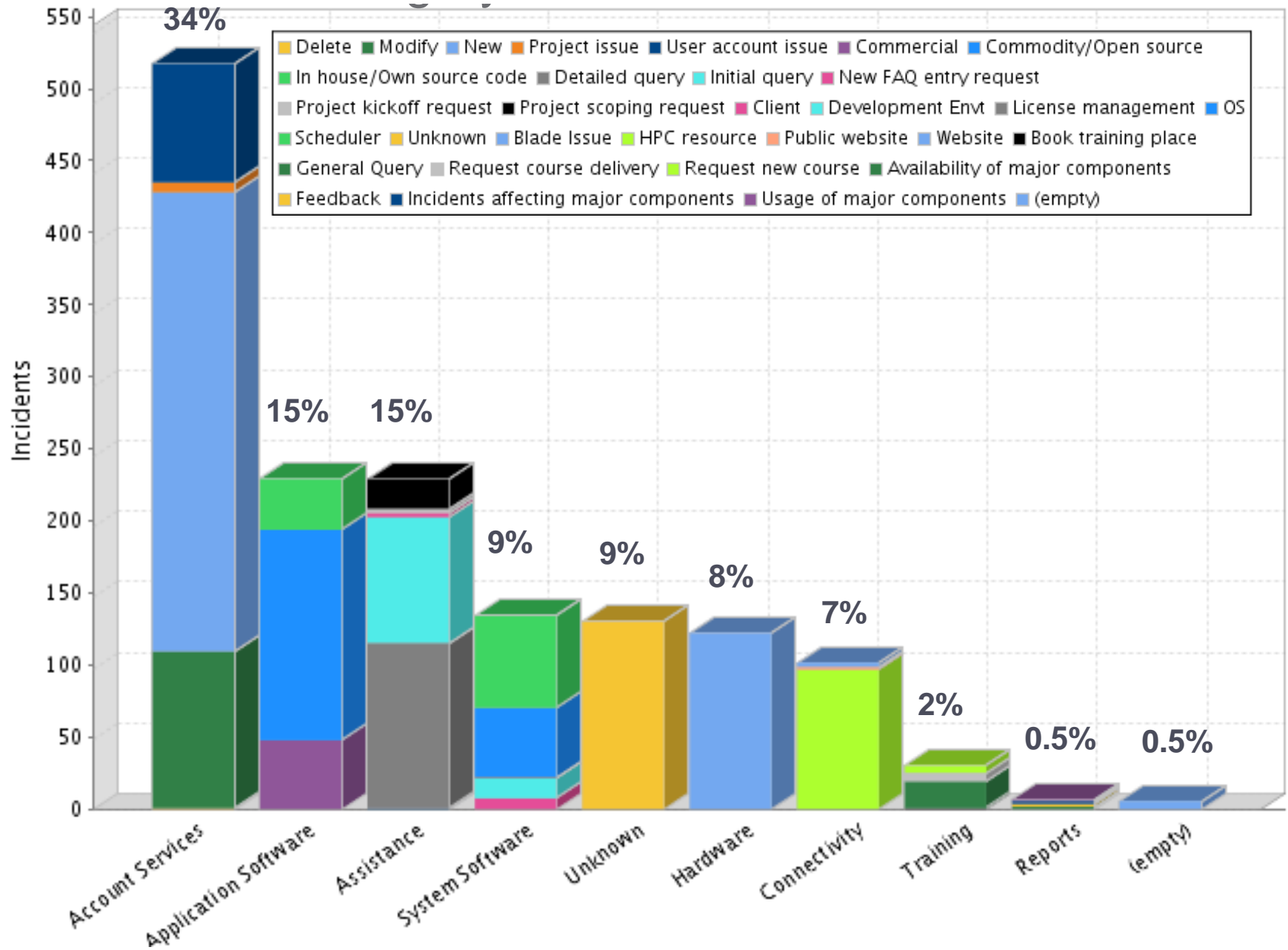
Category 1  
Category 2  
Category 3

# Incident Types over last 12 months

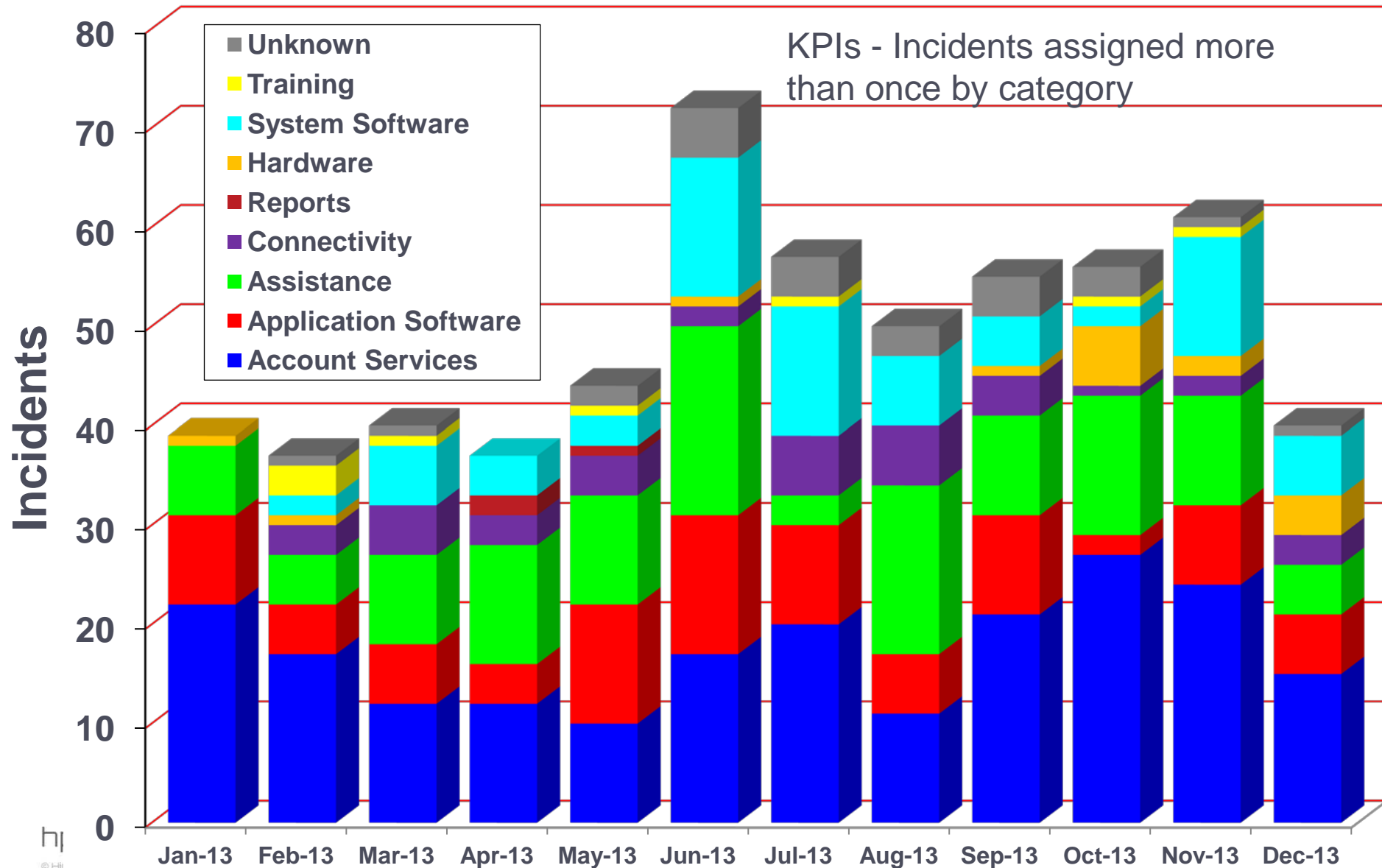




# Category 1 & 2 Calls over last 12 months



# Support Calls over last 12 months



# Major Support Call Categories

Category 1	%	Category 2
Account Services	34%	Delete, Modify, <b>New</b> , Project Issue, user Account Issue
Application Software	15%	Commercial, <b>Community / open Source</b> , in-house / Own
Assistance	15%	<b>Detailed Query, Initial Query</b> , New FAQ Entry request, Project kick-off request, project scoping request
Hardware	8%	<b>Blade Issues</b>
System Software	9%	Client, Development Environment, OS, <b>Scheduler</b>
Connectivity	7%	<b>HPC resource</b> , Public website, Website
Training	2%	Book training place, <b>General Query</b> , Request Course delivery, Request new course

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# The HPC Wales User Group

## SERVICE ENHANCEMENTS



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- **Streamlining of job submission** from uploading, to running jobs and results extraction.
- **Sandy Bridge** system progress.
- Whether there will be a fair use policy implemented on **Sandy Bridge**.
- Using the **GP-GPU** queues
- Better indication on the website of what **tools are available**, whom they are available to and examples of how to use them
- **Amount of storage** currently available / Concerns over large data sets.
- Submission script for an **Ansys FSI** analysis.
- Shortage of **Ansys CFX** licenses is resulting in long wait times.
- What about collaboration with non-profit research companies outside Wales but within EU. Is there such a possibility ?

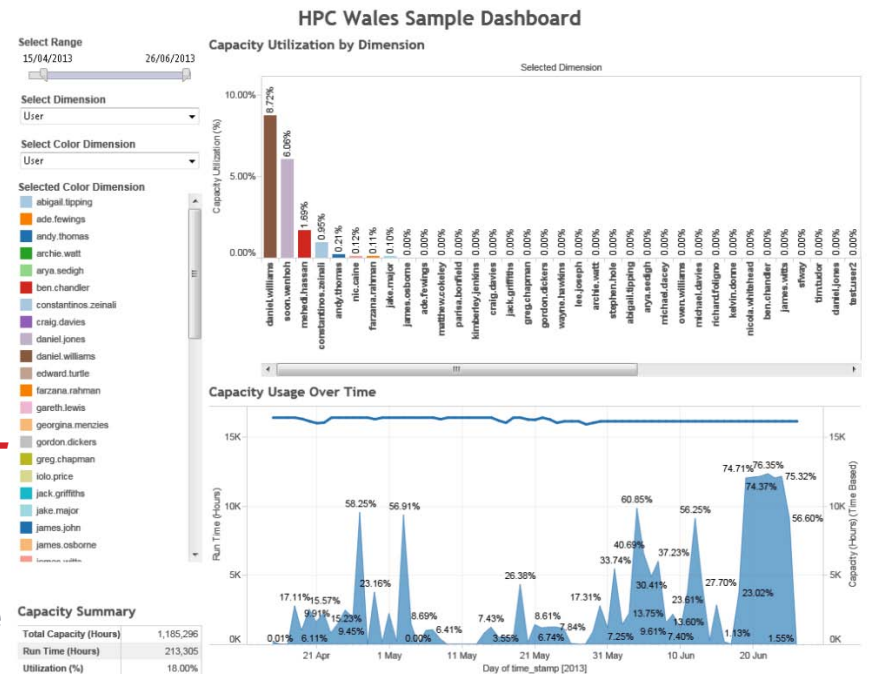
<http://www-03.ibm.com/systems/technicalcomputing/platformcomputing/products/lsf/analytics.html>

- HPC Wales operational service has a long standing requirement for features such as:
  - Job and resource reporting
  - Usage reporting for chargeback accounting
  - Operational reporting and analysis
  - Resource and service-level analysis
  - Intuitive, customizable interfaces
- Initial discussions with Platform and subsequent demonstrations suggested that IBM Platform Analytics provided much of the required functionality, but at a cost.
- After a long wait, the final costs were presented to HPC Wales on September 19th. These included the associated professional services to tailor the solution plus H/W costs involved in its deployment.



# Advanced Workload Data Analytics

- The final figure confirmed our primary concerns (i) that the proposed solution would not provide a value-for-money solution, and (ii) would still require considerable work to be fully fit for purpose.
- The Technical Team considered possible alternatives, and are convinced that *an in-house solution was the optimum way forward*, building on some preliminary work to design and rollout an open-source solution based on e.g. Gold Algorithm.



- While a major piece of work, **Ade Fewings and Jay Davies** have undertaken the project through a Three phase program – (0) Project Code Enforcement and Application Profiles, (1) Data Base and Parser, and (2) Internal User Views.
- Good progress to date, with the possible demo of Management data by the mid-term audit.

# FLE's Role in HPC Wales

HPC Wales User Group

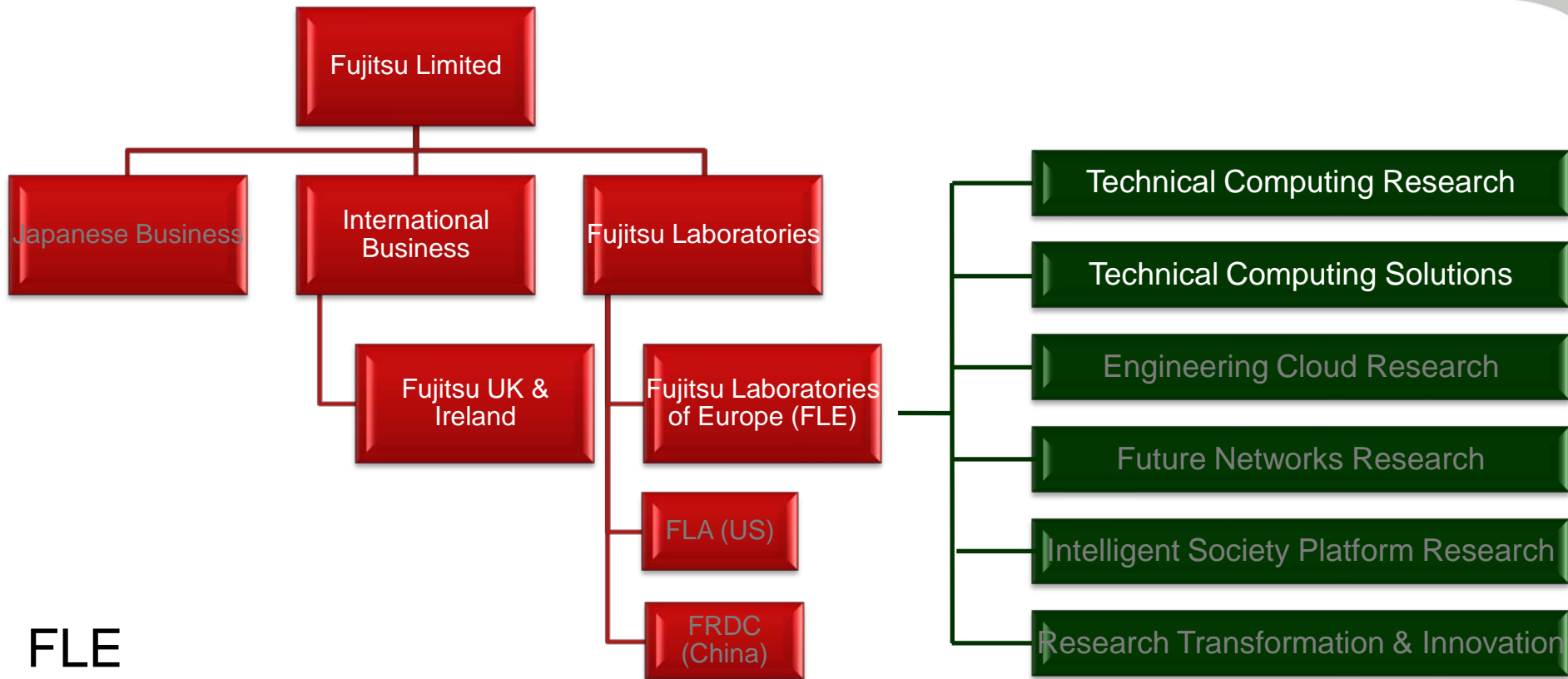
22 January 2014

*Ross Nobes*

*Senior Research Fellow,*

*Fujitsu Laboratories of Europe*

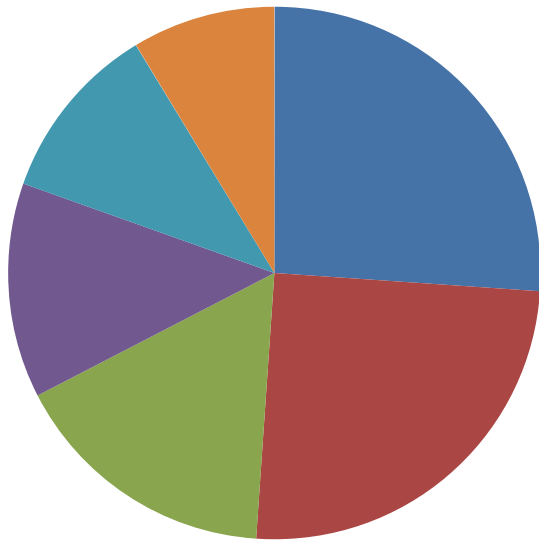
# Fujitsu Laboratories of Europe



## FLE

- Established 2001 and based in West London
- ~45 employees
- Strong track record in European and other collaborative projects
- Technical Computing groups contribute to HPC Wales project
  - 'Services' as a subcontractor to Fujitsu UK & Ireland
  - Research collaboration overseen by Fujitsu Laboratories

# FLE's Services Role



- Support to new/potential projects; user groups; case studies
- Studentships and research & innovation calls
- Software installation, documentation, benchmarking; Support Desk activities (with NAG)
- Skills Academy contributions
- Participation in working groups
- Business engagement events; development of funding bids

## *Example 1: Studentships*

- Worked with HPC Wales to put 20 PhD Studentships in place
- Involvement in six-monthly review meetings and reporting
- Development of 'case studies' highlighting student's work

## *Example 2: ONETEP Benchmarking*

- Worked with HPC Wales technical team to optimise performance of ONETEP on Sandy Bridge
- Led to HPC Wales winning external contract

# FLE's Research Collaboration Role

## ■ Software for future architectures

- Application performance on NVIDIA GPGPU, Intel Xeon Phi, etc.
  - Open-source codes (OpenFOAM, Gromacs, Quantum ESPRESSO, WRF, pBWA) and other applications of importance to HPC Wales and/or Fujitsu

## ■ Strategic applications: Extreme weather impacts in Wales

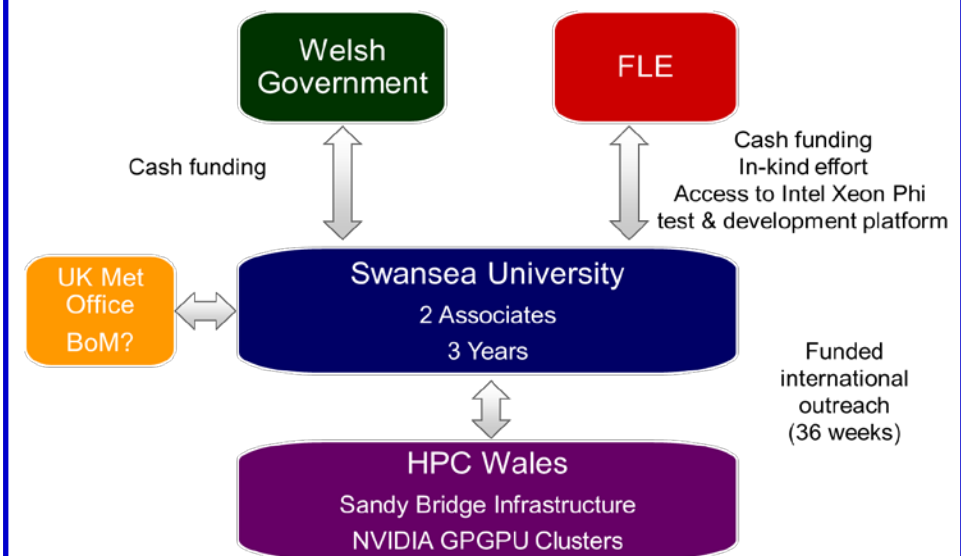
- Establish climate modelling codes and other applications on HPC Wales

## ■ HPC Wales infrastructure development

### *Example 1: Genomics with South Wales*

- Develop parallel algorithms for motif detection in bioinformatics
- M. Triska, D. Grocutt, J. Southern, D.J. Murphy & T. Tatarinova, "cisExpress: Motif Detection in DNA Sequences", Bioinformatics, 29, 2203-2205, 2013

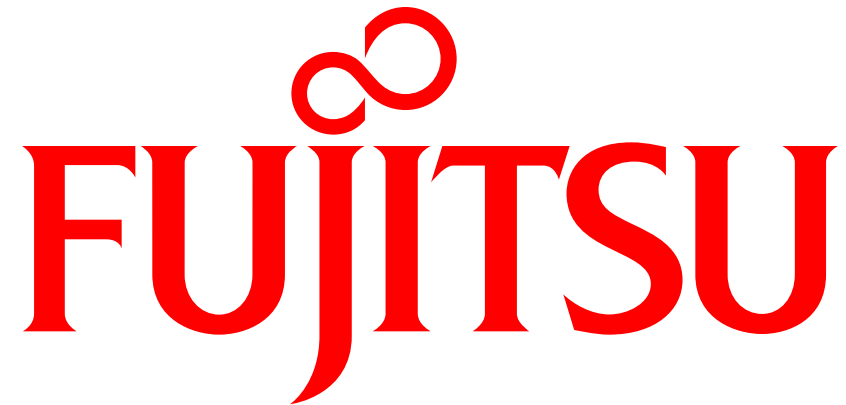
### *Example 2: Swansea Knowledge Transfer Project*



# Summary

- FLE is an active partner in the HPC Wales project
- We can offer services both to HPC Wales and to end users
  - Do you have an application that needs to be ported to HPC Wales?
  - Do you need help in optimising the application's performance?
  - Should FLE and HPC Wales be setting up thematic user groups (e.g. in life sciences, energy & environment, computational chemistry)?
  - Would you like tutorial material to be created for the portal and/or Skills Academy?
- We are also seeking partners for research collaboration activities
  - Are you working to develop future software technologies to overcome scalability barriers, to enhance robustness and eliminate programming complexity?
  - Are you interested in working with FLE to develop European Horizon 2020 bids?





shaping tomorrow with you



# NAG and HPC Wales

Ed Smyth

[edwards@nag.co.uk](mailto:edwards@nag.co.uk)

*HPC Wales user meeting*

*Jan 2014*



Experts in numerical algorithms  
and HPC services

# Introduction to NAG

- Started in 1970, not for profit company since 1976.
- NAG Library products and NAG Fortran compiler:
  - Libraries can be used from Fortran, C, C++, Matlab, Python, Java, Excel, ...
- Involvement in Fortran, MathML and OpenMP standardisation activities.
- Consultancy and service activities:
  - CSE support for HPC Wales, HECToR, CHPC (South Africa)
  - Work with Intel and AMD on math libraries
  - Consultancy for academia, finance, engineering, oil&gas
- See [www.nag.co.uk](http://www.nag.co.uk) for further information.

# NAG's role in HPC Wales

- Computational Science & Engineering (CSE) support:
  - Working with HPC Wales and Fujitsu.
  - Helping users get the most benefit from their time allocation on the system.
- Three main areas:
  - Service requests: e.g. software installation, debugging, etc.
  - Collaborative Partnership Team (CPT): In-depth performance analysis and optimisation work on important applications.
  - Skills academy: training courses and support for new users.

# Service request and CPT work

## ■ Service requests:

- Installing software e.g. PETSc, Python (with numpy+scipy), Octave, R, Delft3d, WRF, UCSC GenomeBrowser, Autodock, OpenFOAM+swak4Foam, Gaussian, ...

## ■ CPT projects:

- Initial work started on three codes:
  - FLITE CFD software used for Bloodhound SSC project
  - Computational Rheological Modelling code
  - TERRA mantle circulation code
- Performance profiled, areas for potential improvement identified.

# Skills academy

- NAG has delivered for HPC Wales courses on:
  - Parallel Programming with MPI
  - OpenMP and Mixed-mode Programming
  - Debugging and Profiling (inc. online guides for tools used)
- We have provided the following on HECToR:
  - Fortran 95
  - Optimisation
  - Scientific Visualisation
  - Parallel I/O
  - ...
  - Details at [www.hector.ac.uk/cse/training/courselist/](http://www.hector.ac.uk/cse/training/courselist/)



# How can we help you?

- “Onboarding” – training and advice for users getting started on the system.
- What codes would you like installed?
- What training courses do people want?
- What codes need in-depth support via CPT mechanism?
- Contact [info@hpcwales.co.uk](mailto:info@hpcwales.co.uk) to request support.



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# Allinea Software

Powering Success... via HPC Software

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European Regional Development Fund



# About Allinea Software

- **The Company**

- Warwick, UK - HQ and research and development team
- Offices in USA and Germany

- **Allinea Performance Reports**

- Application analysis to uncover missing performance

- **Allinea DDT and Allinea MAP**

- Development tools for debugging and profiling HPC applications

- **Interesting facts**

- Allinea developed the first tool to debug over 100,000 cores – still unbeaten
- The most powerful supercomputers in Europe and America rely on Allinea

# Who can Alinea Software help?

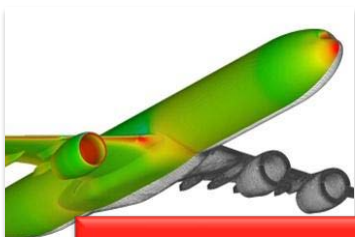
- **System Users and Managers**

- Improve application performance with Alinea Performance Reports
- More results for less machine time

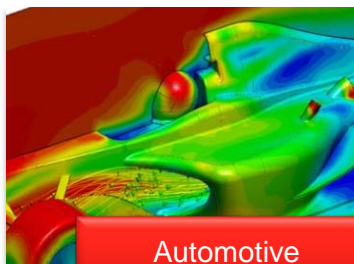
- **Software Developers and Computational Scientists**

- Fix software errors quickly
- Analyse performance at source level
- Single unified tool environment
- Saving time by using tools designed for parallel applications

# Allinea's Core Markets



Aerospace and Space



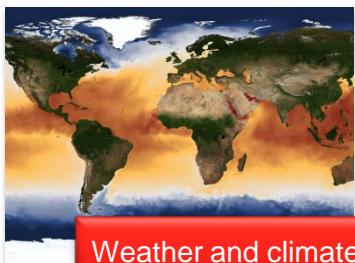
Automotive



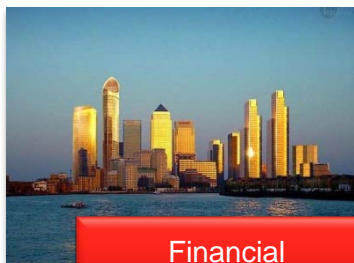
Oil and Gas



EDA



Weather and climate



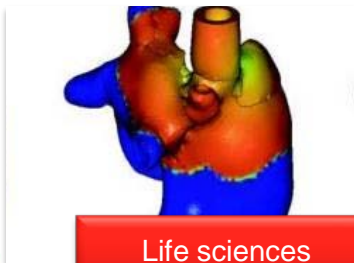
Financial



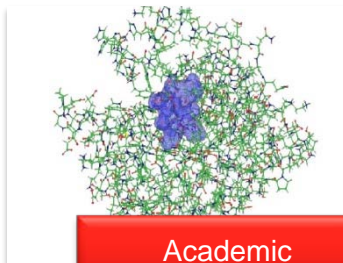
Defence



Government Labs



Life sciences



Academic

# A snapshot of Allinea users





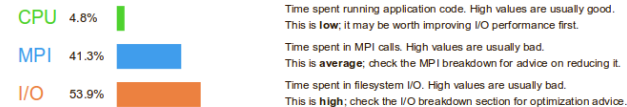
# Allinea Performance Reports

- A simple way to run any HPC application and characterize performance
  - No changes to application
  - As easy as running the job itself
- .. A fast route to uncover missing performance



Summary: MADbench2 is **I/O-bound** in this configuration

The total wallclock time was spent as follows:



This application run was **I/O-bound**. A breakdown of this time and advice for investigating further is in the **I/O** section below.

**CPU** A breakdown of how the 4.8% total CPU time was spent:

**MPI** Of the 41.3% total time spent in MPI calls:

Scalar numeric ops 4.8%  
Vector numeric ops 0.0%  
Memory accesses 99.0%  
Other 0.0%

The per-core performance is low. Identify time-consuming operations. No time was spent in vectorization advice to speed up.

**I/O** A breakdown of how the 53.9% total I/O time was spent:

Time in reads 3.7%  
Time in writes 96.3%  
Estimated read rate 272 Mb/s  
Estimated write rate 7.06 Mb/s

Most of the time is spent in write operations, which have a very low transfer rate. This may be caused by contention for the filesystem or inefficient access patterns. Use an I/O profiler to investigate which write calls are affected.

**I/O**

A breakdown of how the 53.9% total I/O time was spent:

Time in reads	3.7%	
Time in writes	96.3%	██████████
Estimated read rate	272 Mb/s	██████████
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Most of the time is spent in **write operations**, which have a very low **transfer rate**. This may be caused by contention for the filesystem or inefficient access patterns. Use an I/O profiler to investigate which write calls are affected.

# Why development tools matter

## Technology is beyond the tipping point for developers

- Extreme complexity: highly parallel processors and systems
- Print-style debugging does not scale
- Application performance is a mystery

## Scalable systems need scalable tools

- Development tools can enable software to exploit the hardware
- .. but tools must simplify the complexity of today's systems

## Allinea provides the solution

- Modern scalable tools for highly parallel systems and software
- Proven on the world's largest supercomputers

# Key Benefits: Debugging with Alinea DDT

## Simplicity

Applications are hard to understand

Alinea DDT simplifies parallel information

Alinea DDT highlights differences

## Completeness

Application fail for complex reasons

Alinea DDT's memory debugging makes random bugs reproducible

Alinea DDT masters HPC datasets with filtering and visualization

## Scalability

Many tools fail to scale

Alinea DDT has a scalable architecture and GUI

Alinea DDT is full-size proven on the #1 system

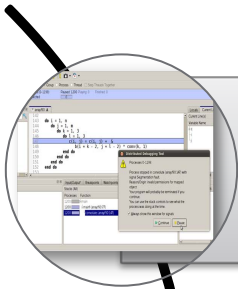
## Efficiency

Bugs cost machine and developer time

Alinea DDT is lightning fast – at any scale

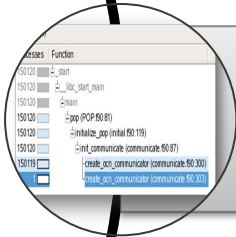
Alinea DDT's offline mode finds bugs whilst you sleep

# Allinea DDT: Debugging for HPC developers



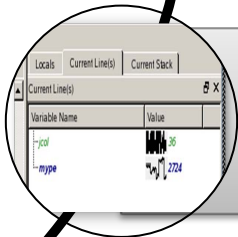
## Where?

- Leaps to source automatically
- Powerful instantaneous memory debugging



## How?

- Real-time data comparison and consolidation
- Identify outliers and unusual threads



## Why?

- “Smart Highlighting” of differences and changes
- Sparklines comparing data across processes

# Key Benefits: Performance Profiling with Alinea MAP

## Simplicity

Many tools target the expert

Alinea MAP is for scientist and analyst alike

No complex setup and compilation

## Clarity

Many tools overwhelm with too much information

Alinea MAP merges data intelligently

Alinea MAP displays performance in the source code

## Scalability

Performance at scale is a mystery

Alinea MAP handles the most complex applications

Alinea MAP scales to extreme machines

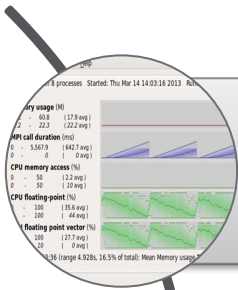
## Accuracy

Profiling overheads destroy accuracy

Alinea MAP does not create large data files

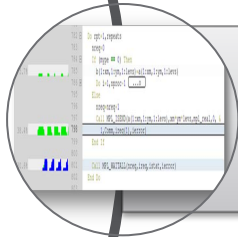
Alinea MAP achieves <5% slowdown

# Allinea MAP: Performance made easy



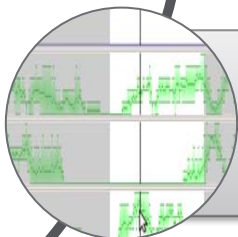
## Low overhead measurement

- Accurate, non-intrusive application performance profiling
- Seamless – no recompilation or relinking required



## Easy to use

- Source code viewer pinpoints bottleneck locations
- Zoom in to explore iterations, functions and loops



## Deep

- Measures CPU, communication, I/O and memory to identify problem causes
- Identifies vectorization and cache performance

## What our users are saying



“My group routinely debugs code at over 100,000 processes using Allinea DDT. No other debugger comes close – obviously it’s a hit with users,” Oak Ridge National Laboratory



“Allinea’s experience and tools will make a big impact in the speed at which scientists can complete their research,” NCSA Blue Waters



“Previous experiences with other profilers had left us more confused than informed. Allinea MAP is the opposite”



## Allinea at HPC Wales

- **Allinea's development tools are available on HPC Wales systems**
  - Develop, debug, and optimize your C, C++ or Fortran applications
- **Allinea Performance Reports will be available soon**
  - To be launched as a product in April 2014
- **How can Allinea help you to get more from HPC and HPC Wales?**