



HPC
WALES • CYMRU

Powering Success
Pweru Llwyddiant

Welsh MetUM Special Interest Group Meeting

Luke Davies, HPC Wales

HPC Wales User Group Meeting

Wednesday 22nd October 2014

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

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



Llywodraeth Cymru
Welsh Government

Overview to the UM

- The Met Office Unified Model is a world-leading weather and climate model that is used for research and operational purposes around the world.
- The term “Unified” signifies the fact the model can forecast across timescales of hours to years, allowing both short-term weather forecasts and climate studies to use fundamentally the same code.

Meeting Summary

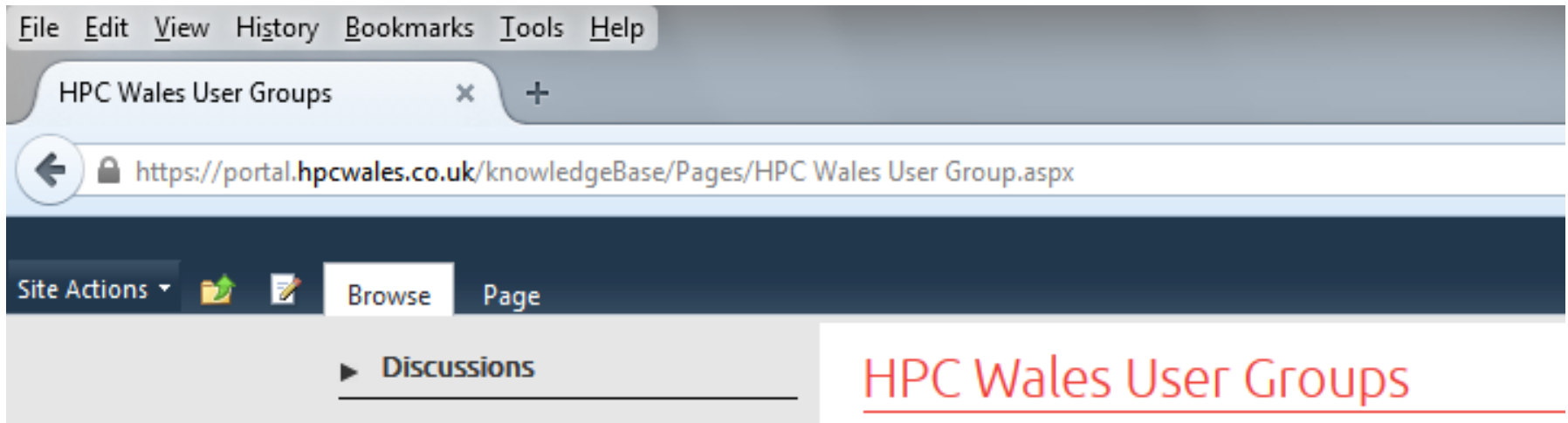
- HPC Wales organised a Special Interest Group Meeting in Cardiff on 12th September 2014 for Welsh academics with a weather modelling interest.
- Attended by: HPC Wales, Met Office, National Centre for Atmospheric Science (NCAS-CMS), Welsh academic community, Fujitsu, and Advanced Research Computing @ Cardiff (ARCCA)
- Science talks identified academic requirement and interest in the UM.
- Outcome: Met Office agreed that HPC Wales could seek and obtain an academic research license for the UM at sites not presently covered, so that Welsh academics could access UM using HPC for their research.

Next Steps...Route of Access to UM

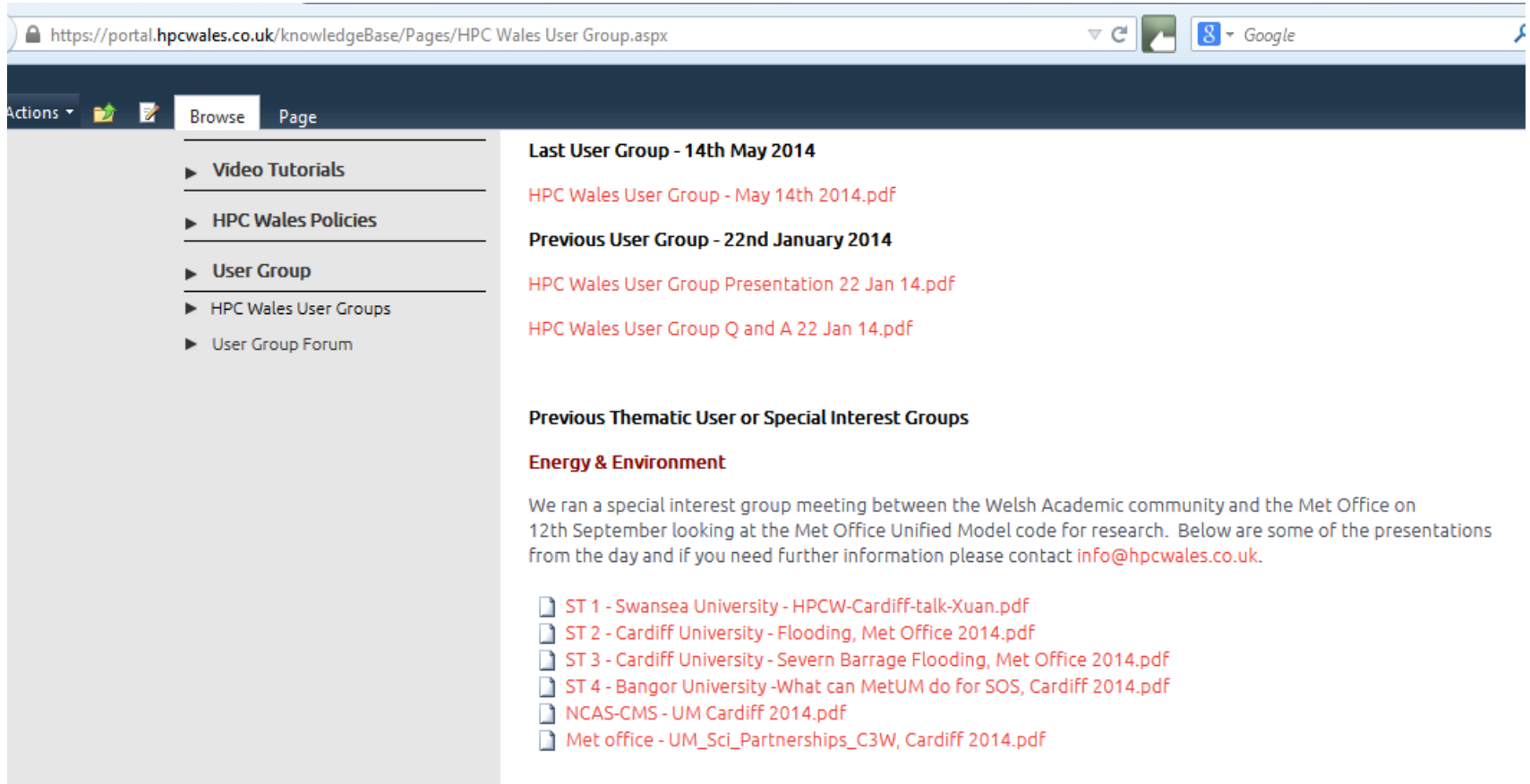
- NCAS offers 'PUMA' (Providing Unified Model Access) as a service to reduce maintenance of running the UM and as a centralized Unified Model User Interface (UMUI).
 - A common server and user interface
 - Access to all the versions available on PUMA
 - Ease of sharing jobs and local files

- PUMA only provides access to the UM source code and user interface, the UM jobs are run on other systems such as a hub at HPC Wales or Raven at ARCCA using standard ssh access and copying of scripts across to the respective systems.

Access the presentations at The Knowledge Base on our Portal...



Access the presentations at The Knowledge Base on our Portal...



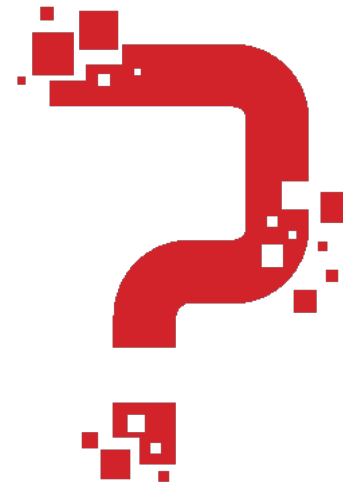
The screenshot shows a web browser window with the URL [https://portal.hpcwales.co.uk/knowledgeBase/Pages/HPC Wales User Group.aspx](https://portal.hpcwales.co.uk/knowledgeBase/Pages/HPC%20Wales%20User%20Group.aspx). The page has a dark blue header with 'Actions', 'Browse', and 'Page' tabs. A left-hand navigation menu lists: Video Tutorials, HPC Wales Policies, User Group (selected), HPC Wales User Groups, and User Group Forum. The main content area is titled 'Last User Group - 14th May 2014' and lists a PDF: [HPC Wales User Group - May 14th 2014.pdf](#). Below this is 'Previous User Group - 22nd January 2014' with two PDFs: [HPC Wales User Group Presentation 22 Jan 14.pdf](#) and [HPC Wales User Group Q and A 22 Jan 14.pdf](#). A section for 'Previous Thematic User or Special Interest Groups' includes 'Energy & Environment' with a paragraph: 'We ran a special interest group meeting between the Welsh Academic community and the Met Office on 12th September looking at the Met Office Unified Model code for research. Below are some of the presentations from the day and if you need further information please contact info@hpcwales.co.uk.' This is followed by a list of six PDFs: [ST 1 - Swansea University - HPCW-Cardiff-talk-Xuan.pdf](#), [ST 2 - Cardiff University - Flooding, Met Office 2014.pdf](#), [ST 3 - Cardiff University - Severn Barrage Flooding, Met Office 2014.pdf](#), [ST 4 - Bangor University -What can MetUM do for SOS, Cardiff 2014.pdf](#), [NCAS-CMS - UM Cardiff 2014.pdf](#), and [Met office - UM_Sci_Partnerships_C3W, Cardiff 2014.pdf](#).

Diolch yn fawr - Thank you

HPC Wales

- Luke Davies
- Luke.Davies@hpcwales.co.uk
- 07850 771289

- Laura Redfern
- Laura.Redfern@hpcwales.co.uk
- 07850 771287





HPC
WALES • CYMRU

Powering Success
Pweru Llwyddiant

HPC User Presentation

James Jackson, Horde Labs

HPC Wales User Group Meeting

Wednesday 22nd October 2014

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

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



HORDE
LABS

James Jackson



2nd Year Computer Science

Background in Web Development



Student Lead - Horde Labs



Professional Perspectives



Professionalism Module - Delivered by Chris Headleand

Research and Report Assignment



Presentation



RES



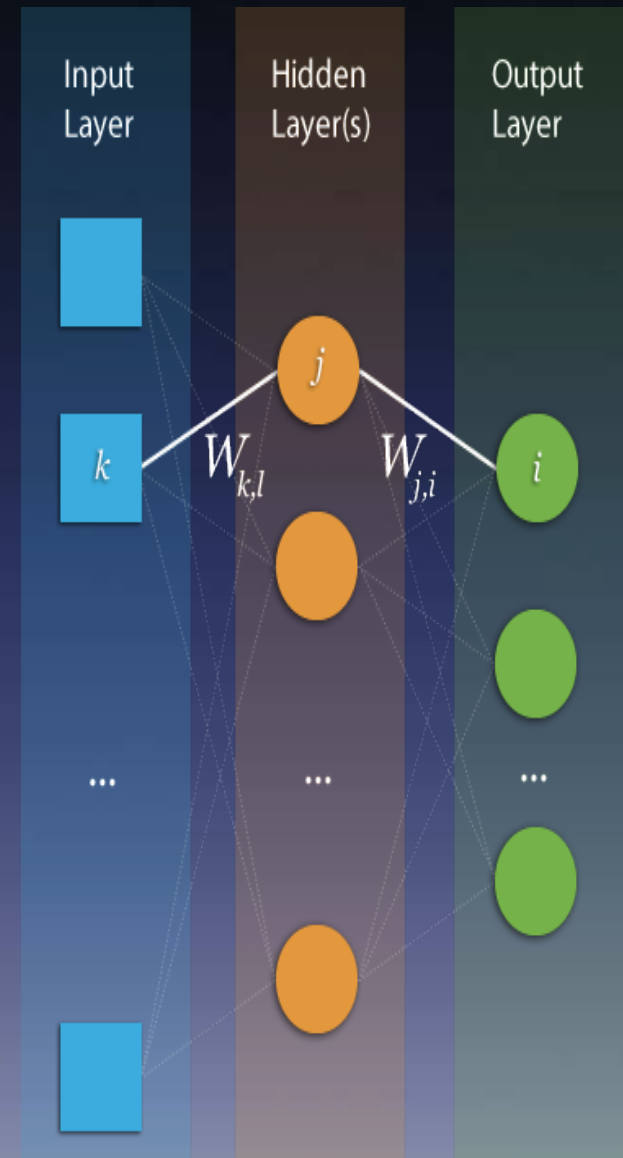
High Speed Prediction System.



Predicting potential outcomes of changes in ecosystems.



Allow companies and organisations to adhere to legislations and make informed decisions.



HPC Wales

Introduction



Training - MPI, Unix Shell



Bursaries



Project Mercury



Visual Agent/ Environment Editor



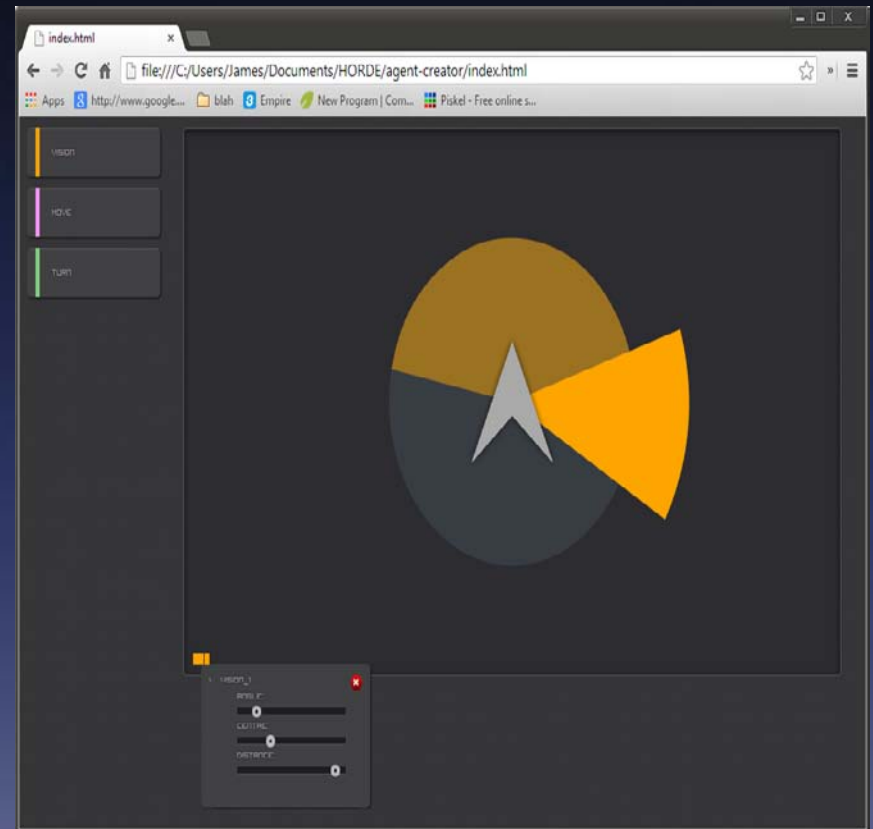
Interpreter



Python (MPI) simulation software



Data visualisation module



Where Now?



Valuable experience in HPC computing and programming

Continued effort on project mercury



Possibility of Dissertation, Postgraduate projects in the form of additional modules for Mercury.



Thank You

Any Questions?



HPC
WALES • CYMRU

Powering Success
Pweru Llwyddiant

HPC User Presentation

Dr David Willock, Cardiff University

HPC Wales User Group Meeting

Wednesday 22nd October 2014

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

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





HPC
WALES • CYMRU

Powering Success
Pweru Llwyddiant

HPC User Presentation

Bela Paizs, Bangor University

HPC Wales User Group Meeting

Wednesday 22nd October 2014

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

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

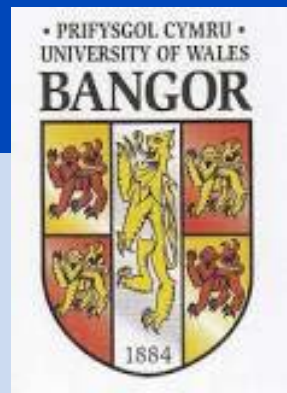


Llywodraeth Cymru
Welsh Government

Computational Proteomics

Bela Paizs

School of Chemistry, Bangor University, Bangor, LL57 2UW, UK



Overview

- Proteomics
- Mass spectrometry in proteomics
- HPC & proteomics

Why is Research on Proteins Important?

Determination of the genome (hereditary information encoded in DNA) is only the first step towards understanding biology.

Why is Research on Proteins Important?

Determination of the genome (hereditary information encoded in DNA) is only the first step towards understanding biology.

The same genome



different expressed proteins

Typical Protein Identification Workflow



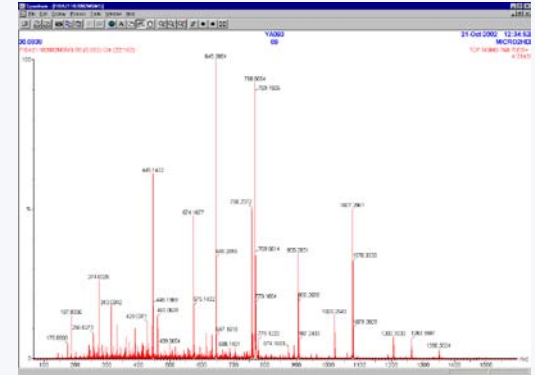
Protein
mixture

Digestion
→

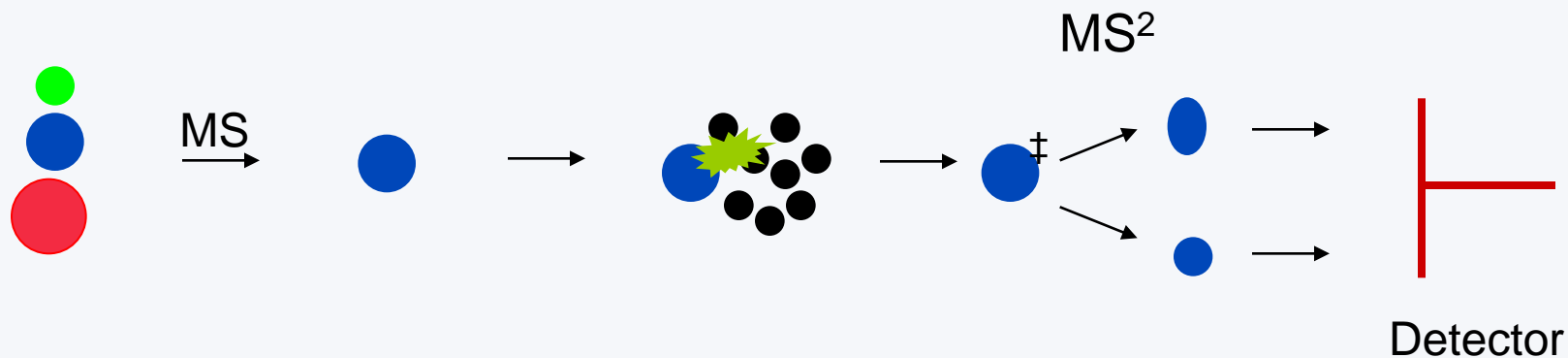
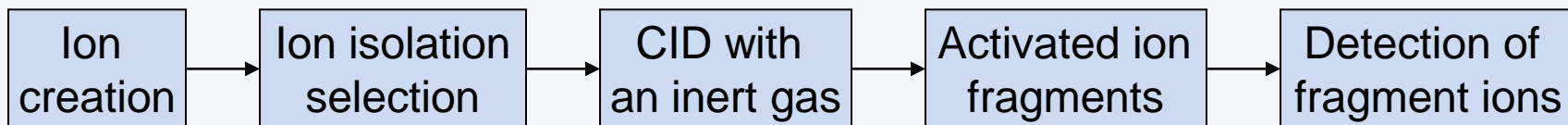


Peptide
mixture

Mass
spectrometry
→



Collision Induced Dissociation (CID)



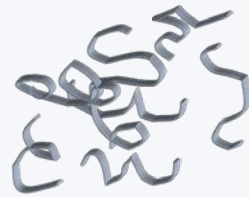
Two or more stages of MS:
tandem mass spectrometry

Typical Protein Identification Workflow



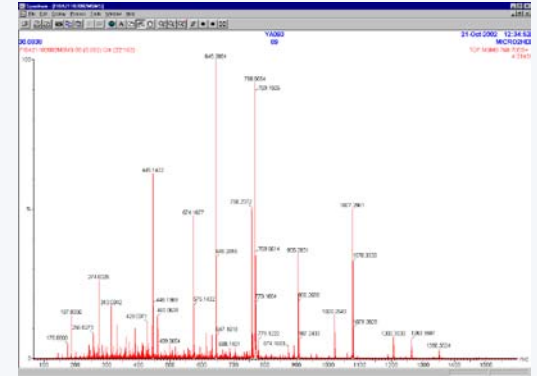
Protein mixture

Digestion

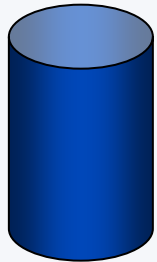


Peptide mixture

Mass spectrometry



Compare & rank

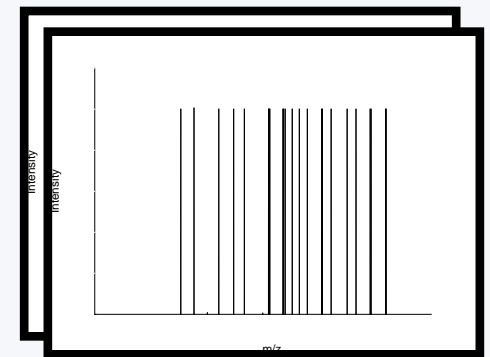


Protein database

Peptide m/z

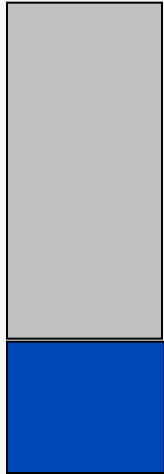
Candidate peptide sequences

Fragmentation model



Theoretical (*in silico*) spectra

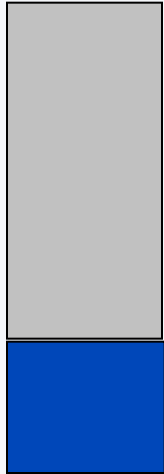
Current Sequencing Software Performs Poorly



~50 % unassigned
Related biological information is lost

~50 % assigned, but with some error rate

Current Sequencing Software Performs Poorly



~50 % unassigned
Related biological information is lost

~50 % assigned, but with some error rate

NewsFocus

‘Proteomics Ponders Prime Time’

„... most errors in MS-based analyses arise not because the technology cannot spot the proteins researchers are looking for but because software programs often misidentify them.“

Science, 26 September 2008, page 1758.

Typical Protein Identification Workflow



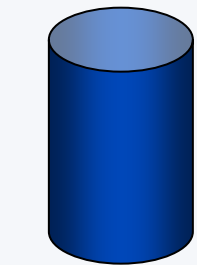
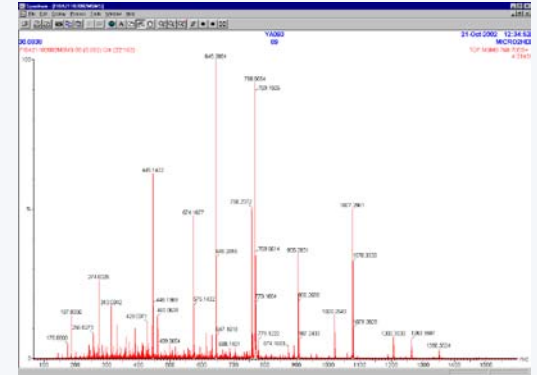
Protein mixture

Digestion



Peptide mixture

Mass spectrometry

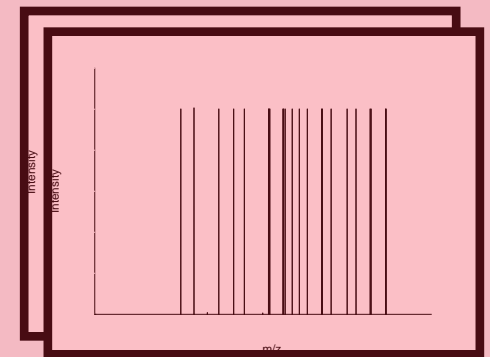


Protein database

Peptide
m/z

Candidate
peptide
sequences

Fragmentation
model



Theoretical (*in silico*)
spectra

Compare
& rank

Need for Deeper Understanding of Peptide Fragmentation

- Current software uses *oversimplified* fragmentational models
- We need to develop a new generation of score functions that utilizes advanced peptide fragmentation chemistry
- Fragmentation chemistry is computed at HPC Wales



HPC
WALES • CYMRU

Powering Success
Pweru Llwyddiant

The importance of the forthcoming User Surveys

Professor Martyn Guest, HPC
Wales

HPC Wales User Group Meeting

Wednesday 22nd October 2014

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

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



HPC User Surveys

- Survey 1 – to all HPC Wales Users
 - Purpose: monitor customer satisfaction and inform service delivery
 - Plan: release on the 22nd Oct. 10 day turnaround
 - Prize to be confirmed

<https://www.surveymonkey.com/s/KCH8TFS>

- Survey 2 – to HPC PI's in Wales
 - Purpose: identify the needs of the HPC community over the next 5 years to inform the business planning process
 - Plan: release on the 3rd Nov. 10 day turnaround
 - Prize to be confirmed

<https://www.surveymonkey.com/s/WLF5VB5>



HPC
WALES • CYMRU

Powering Success
Pweru Llwyddiant

Forum Discussion

HPC Wales User Group Meeting

Wednesday 22nd October 2014

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

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



Llywodraeth Cymru
Welsh Government

User Group Forum - Questions

- What special interest groups do people think would be beneficial?
- Is there anyone in attendance who would be willing to champion a local or SIG?
- Would those champions be happy to sit on the advisory committee?
- Are there any service issues people would like to discuss?

Q&A & Close

