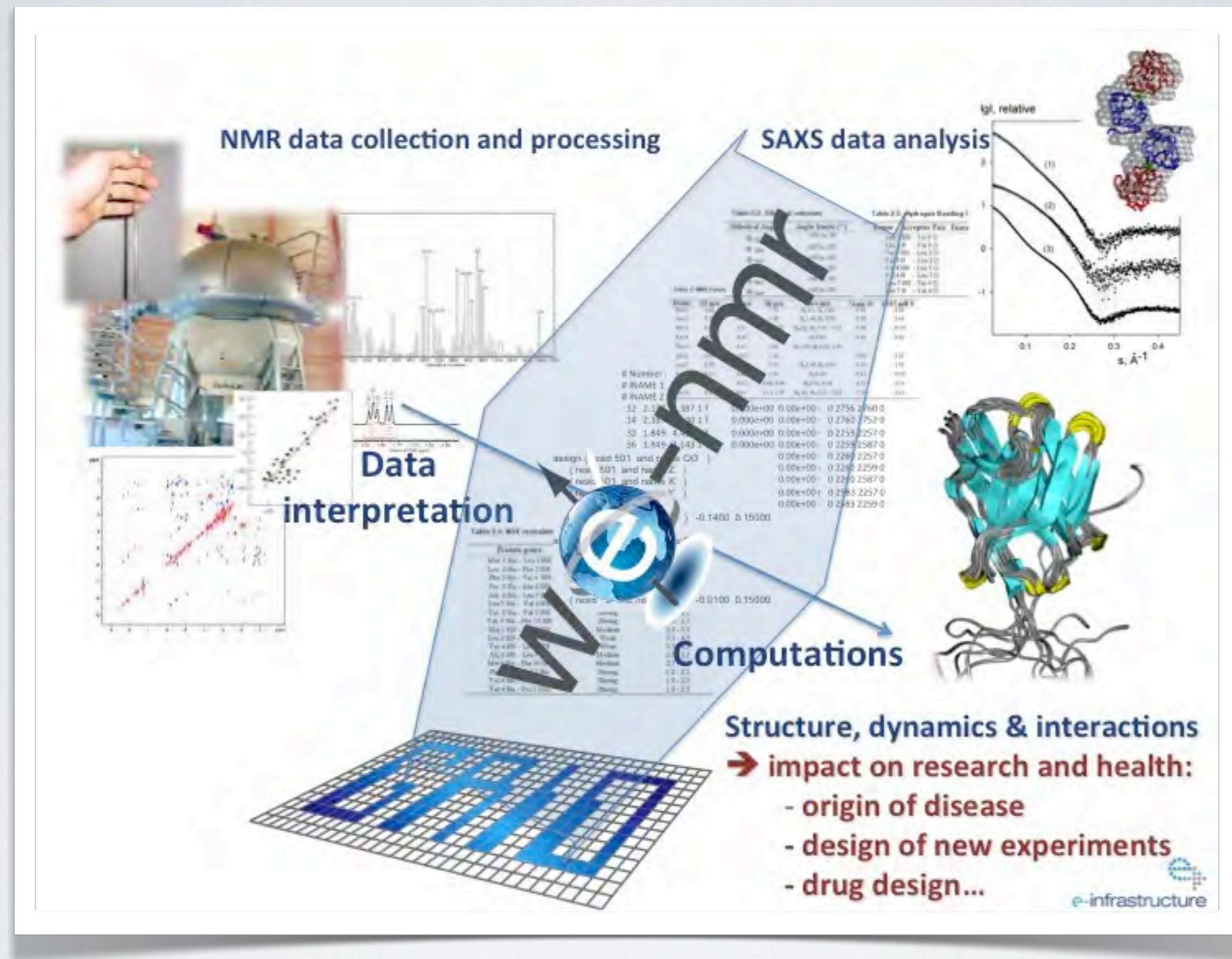


# Centralized user management and Single Sign On for the WeNMR gateway through the WeNMR Virtual Research Community



**Marc van Dijk**, Andrea Giachetti, Marco Verlato,  
Antonio Rosato, Alexandre Bonvin

EGI Technical Forum 2012



## Portals



## Scientific Expertise

The homepage of the WeNMR website features a banner image of NMR spectrometers. The header includes the WeNMR logo and a search bar. The main content area has sections for "Latest & Upcoming Events" and "Cite WeNMR".

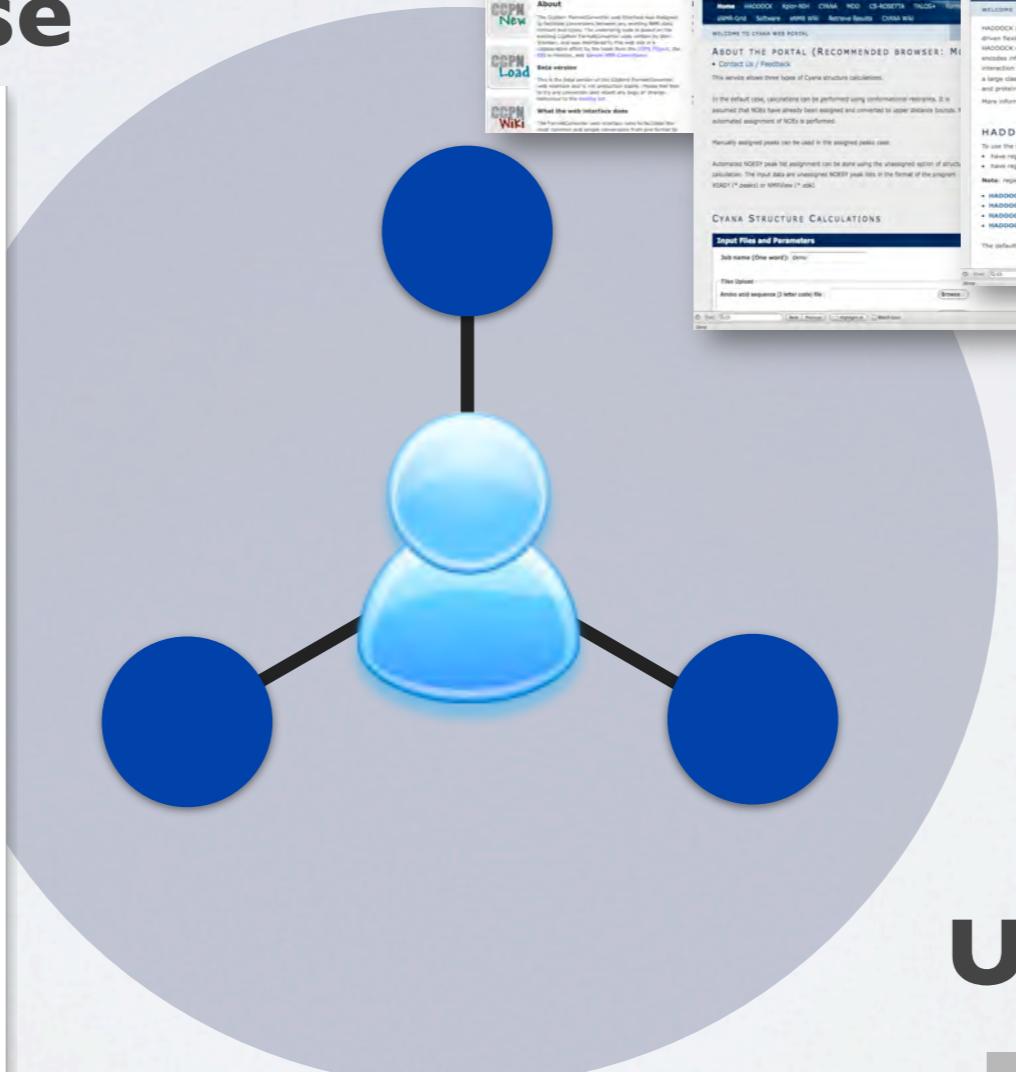
**Latest & Upcoming**

- Mar 26, 2011 - Apr 1, 2011: BioNMR Workshop: Initiatives in biological solid-state NMR
- Apr 11, 2011 - Apr 15, 2011: European Grid Infrastructure User forum
- Apr 27, 2011 - Apr 30, 2011: BioNMR Workshop: Acquisition and processing of rapidly sampled NMR data
- May 17, 2011 - May 18, 2011: Advanced topics: Protein NMR Structure Calculation and Validation
- May 22, 2011 - May 27, 2011: Gordon Conference: Computational Aspects: Biomolecular NMR

**Cite WeNMR**

Usage of the WeNMR portals should be acknowledged in any publication.

\*The WeNMR project (European FP7 e-Infrastructure grant, contract no. 261173, www.wenmr.eu) is supported by the national GRID initiatives of Belgium, Italy, Germany, The Netherlands, the Dutch BIONET project, Portugal, UK, South Africa and the Latin America GRID infrastructures via the Cluster project. Computing and storage facilities are acknowledged for the use of grid portals, computing and storage facilities.



## User Community

[www.wenmr.eu](http://www.wenmr.eu)

## The challenge

- Flexible authentication from a user perspective
- Flexible user management from a portal perspective
- Powerful accounting functionality from a project perspective

## The solution

**Centralized user management and Single Sign On module for  
the Drupal based WeNMR VRC**

### The portal perspective

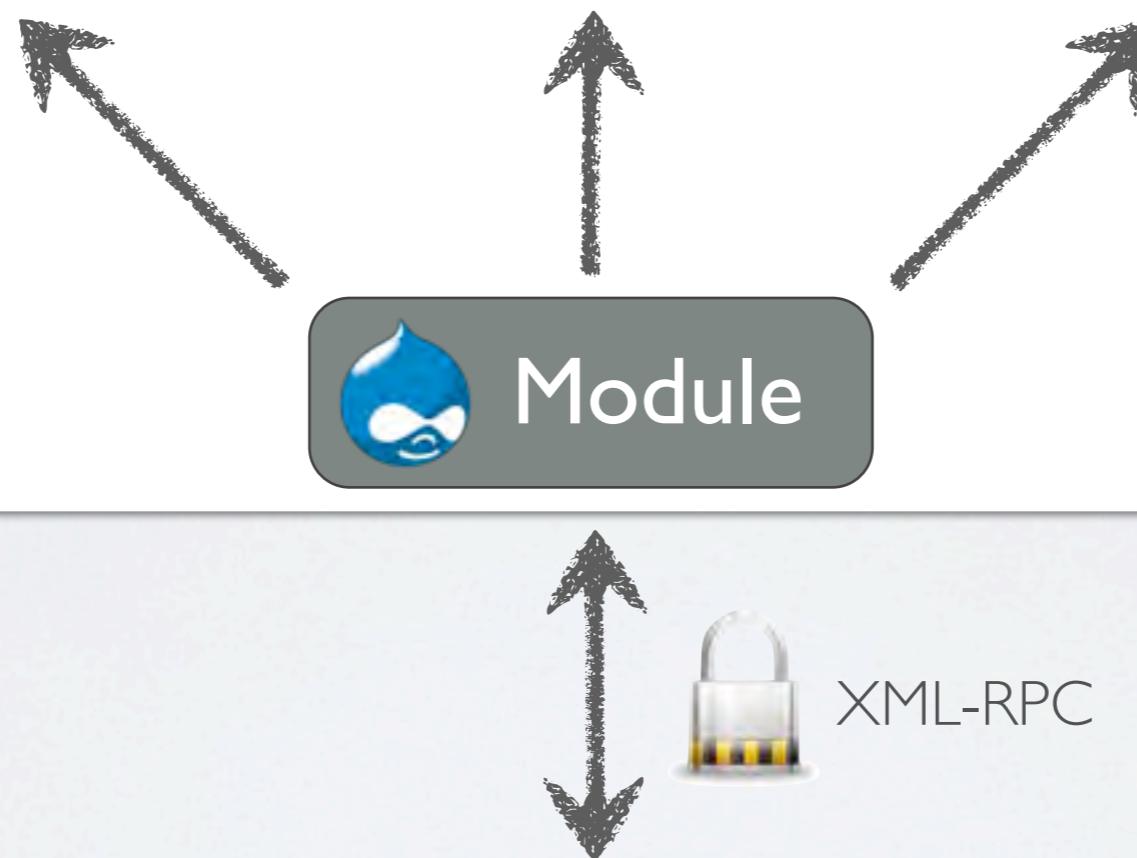
- Register portals
- Manage users

### The user perspective

- Easy subscription to portals
- Manage job submissions

### The project perspective

- Detailed portal accounting



### The portal perspective

- Secure authentication and accounting

- Written as true Drupal module; PHP + JavaScript + CSS
- Makes use of Drupal ‘hooks’ to extend Drupal Core functions;
  - authentication, permissions, user accounts
- Stores data in a backup enabled, secure MySQL DB, local or remote
- Makes use of BlowFish encrypted, XML-RPC function calls for communication between portals and VRC



### Flexible authentication

- Social media credentials: Facebook, LinkedIn, Google, Twitter ...
- SAML and Shibboleth authentication
- phpCAS SSO authentication
- Robot certificates no problem!



### Flexible Framework

- Allot of functionality for free in Drupal
- XML-RPC enables a flexible API to expose functionality to the portals

[www.drupal.org](http://www.drupal.org)

# Subscribe to portals and manage submissions all from one page

The screenshot shows a user interface for managing subscriptions to scientific portals. On the left, there's a sidebar with three items: 'Grid certificate' (with a green checkmark), 'License agreement' (with a blue '2'), and 'Submit request' (with a blue '3'). The main area displays two subscribed portals:

- HADDOCK**: Subscribed since 17-Aug-2012, with 0 total jobs and 0 active jobs.
- GROMACS**: Subscribed since 06-Sep-2012, with 3 total jobs and 0 active jobs.

For the HADDOCK portal, there's a 'SUBSCRIBE' button. Below the HADDOCK section, a message states: "Step 1 This portal requires you to have a valid Grid certificate". It also says: "Congratulations, you have a valid GRID certificate still valid for 114 days".

- Access Control List
- Portal specific Step-by-Step signup
- Grid certificate validation
- Portal submission management

# Easy registration and management of portals and their users

WeNMR SSO							
ID	URL	Status	Registration date	Administrator	Users	Operations	[more help...]
1	HADDOCK	active	19 Jul 2012	Marc van Dijk	2	   	
2	UNIO	active	20 Jul 2012	Marc van Dijk	3	   	
3	3D-DART	active	14 Jun 2010	weAdmin	-	   	
4	FANDAS	active	01 Jan 2012	weAdmin	-	   	
11	AMBER	active	21 Aug 2012	Andrea Giachetti	3	   	
12	GROMACS	active	06 Sep 2012	Marc van Dijk	3	   	

# Easy registration and management of portals and there users

WeNMR SSO

This page provides an overview of all WeNMR portals registered to make use of the WeNMR Single Sign On and accounting facility. Please use the Admin menu to register new portals.

## GROMACS

– Edit user subscriptions –

Batch edit the subscriptions of all users for which the *Edit* checkbox is selected.

Change subscription status to:

Active

Group the user belongs to (group):

Default

User permission level (permission):

Easy

Submit

Edit	ID	Name	Subscription	Total jobs	Active jobs	group	permission
<input type="checkbox"/>	3	amijbonvin	active	0	0	DEF	EASY
<input type="checkbox"/>	9	Marc van Dijk	active	3	0	ADM	EXPERT
<input type="checkbox"/>	14	Antonio Rosato	active	0	0	DEF	EASY

Basic portal information  
Define the name and URL of your portal and provide a basic description of its purpose for display on the user page

**Portal name:** \*  
  
Specify the portal name (machine name = gromacs)

**Portal URL:** \*  
  
Specify the URL of the portal.

**Portal IP address:** \*  
  
Drupal will allow this IP address to make XML-RPC calls to the server

**The public status of the server:**  
 :  
Public status of the portal as: active, paused, stopped

**Portal description:**  
  
Provide a short description of the portals purpose

**Roles**  
Choose which roles may use this portal. An *anonymous user* will open the portal to everybody and thus requires no authentication but you can still use the accounting functionality. A *authenticated user* will allow all VRC registered users to signup for the portal

anonymous user  
 authenticated user  
 project partners  
 site managers

- → [Signup requirements](#)  
- → [Variable data fields](#)

Portal registration. Define:

- How to reach the portal
- Who may use the portal
- Signup requirements
- Any custom user account variables?

## The modules accounting functionality enables powerful statistics

### GROMACS accounting

List of all jobs accounted for by the portal. The results can be filtered by date and/or user name. Please note that the job ID often links to the job results page but it might no longer exist.

[more help...]

#### Filter jobs

Filter the portals jobs by date range or user name

##### Start:

1970 : Jan : 1 :

##### End:

2012 : Sep : 16 :

##### User:

Filter on user name

5 records:

Job ID	User	Status	Start date	Finish date	Message
645326	Anonymous	done	Thu, 1970-01-01 02:00	Sat, 2012-09-15 09:47	
344188	Marc van Dijk	submitted	Sat, 2012-09-15 17:44		
275630	Marc van Dijk	done	Thu, 2012-09-06 13:58	Thu, 2012-09-06 14:23	
135837	Anonymous	done	Thu, 1970-01-01 02:00	Sat, 2012-09-15 09:47	
68265	Marc van Dijk	failed	Thu, 1970-01-01 02:00	Sat, 2012-09-15 09:47	

## The mod

### GROMACS

List of all jobs accounted for in the results page but it might not be up to date.

Filter jobs

Filter the portals jobs by

Start:  
1970 : Jan : 1970

End:  
2012 : Sep : 2012

User:

Filter on user name

Submit

5 records:

Job ID	User
645326	Anonym
344188	Marc van
275630	Marc van
135837	Anonym
68265	Marc van



**Thank you for your attention**

