

we-nmr

we-nmr

A worldwide e-Infrastructure for NMR and structural biology

EMBO Global Exchange Course, USP Sao Paulo, Jan. 19-26



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we-nmr

we-nmr The Project

A Worldwide e-Infrastructure for NMR and structural biology

Project Coordinator:
 Prof. Alexandre M.J.J. Bonvin, Utrecht University, NL

Contract n°: RI-261572
Project type: CP-CSA
Duration: 36 months (Oct.2013)
Total budget: 2'434'000 €
EC Funding: 2'150'000 €

The team:

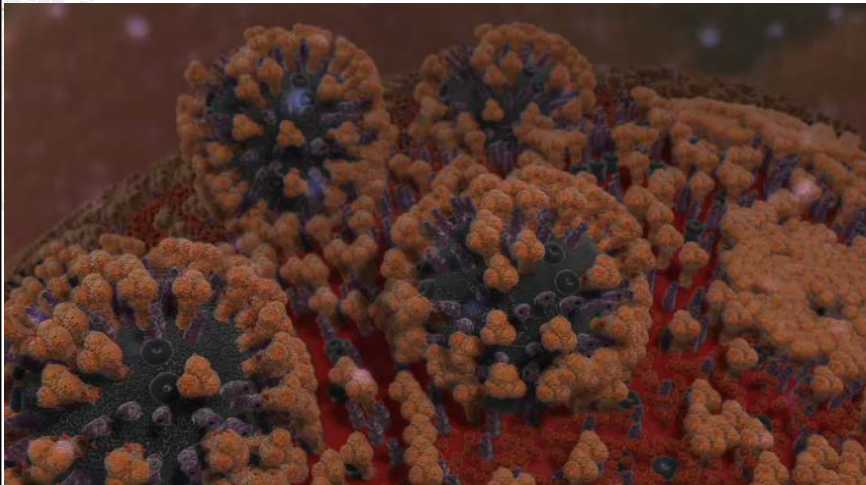
- Utrecht University, Bijvoet Center for Biomolecular Research, NL
- Johann Wolfgang Goethe Universität Frankfurt a.M., Center for Biomolecular Magnetic Resonance DE
- University of Florence, Magnetic Resonance Center, IT
- Istituto Nazionale di Fisica Nucleare, Padova, IT
- Raboud University, Nijmegen, NL
- University of Cambridge UK
- European Molecular Biology Laboratory, Hamburg, DE
- Spronk NMR Consultancy, LT
- Academia Sinica, TW






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NMR and structural biology





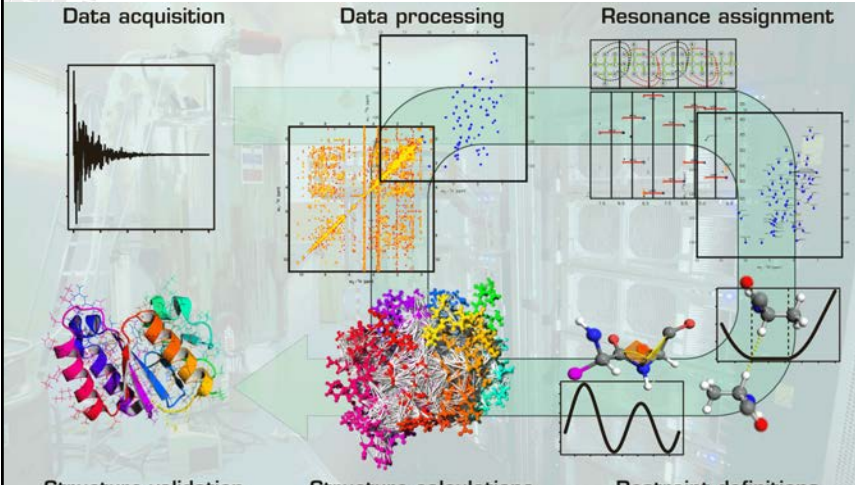



A SpronkNMR production (www.spronknmr.eu)



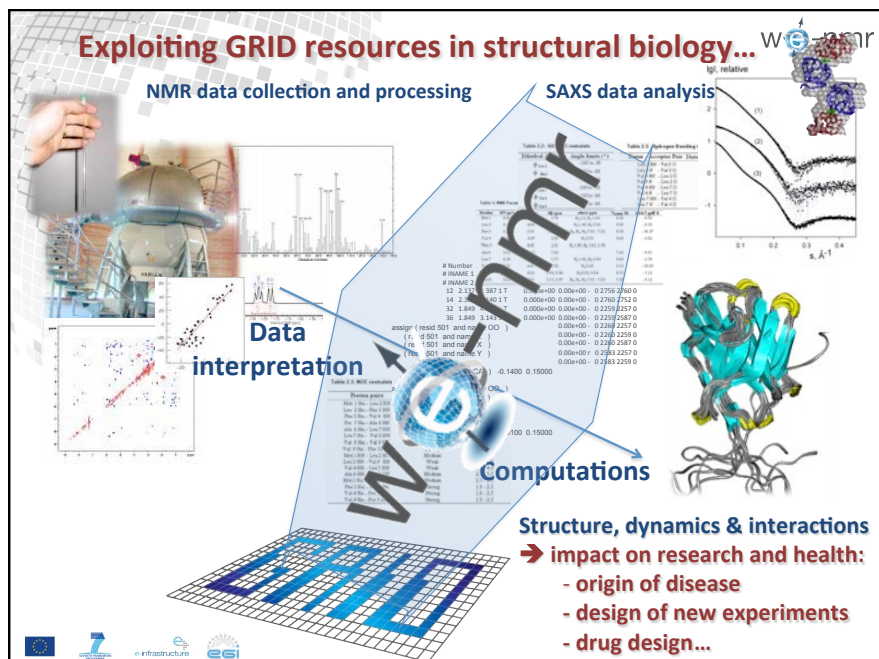
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The NMR structure determination workflow





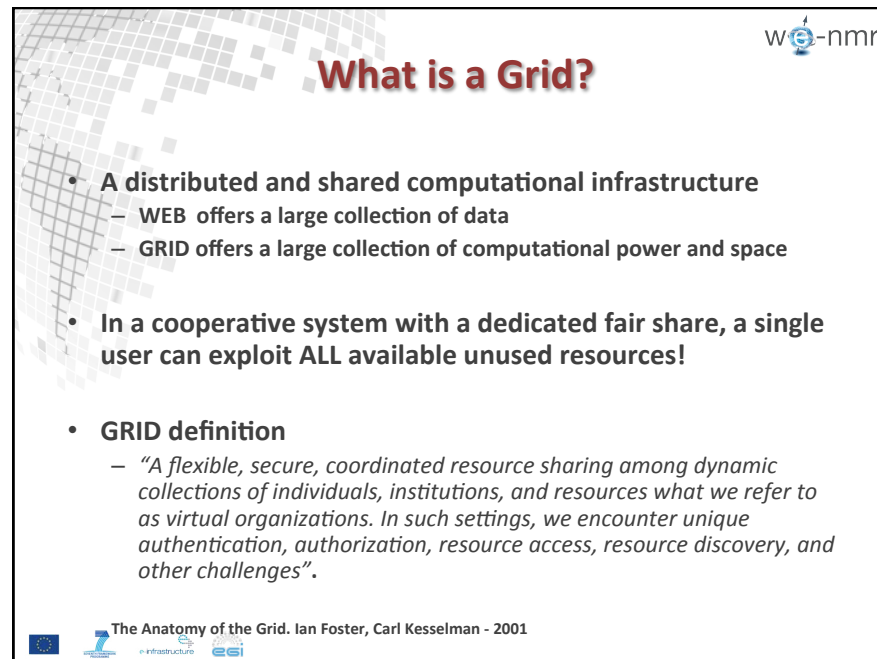


What is a Grid? 

- A distributed and shared computational infrastructure
 - WEB offers a large collection of data
 - GRID offers a large collection of computational power and space
- In a cooperative system with a dedicated fair share, a single user can exploit ALL available unused resources!
- GRID definition
 - "A flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources what we refer to as virtual organizations. In such settings, we encounter unique authentication, authorization, resource access, resource discovery, and other challenges".

The Anatomy of the Grid. Ian Foster, Carl Kesselman - 2001



Virtual Organizations and the Grid 

- Virtual Organizations:
 - groups of individuals or institutions who share the computing resources of a "grid" for a common goal, providing:
 - centralized software management on multiple Grid sites
 - users support

Virtual Organizations accessing different and overlapping sets of resources

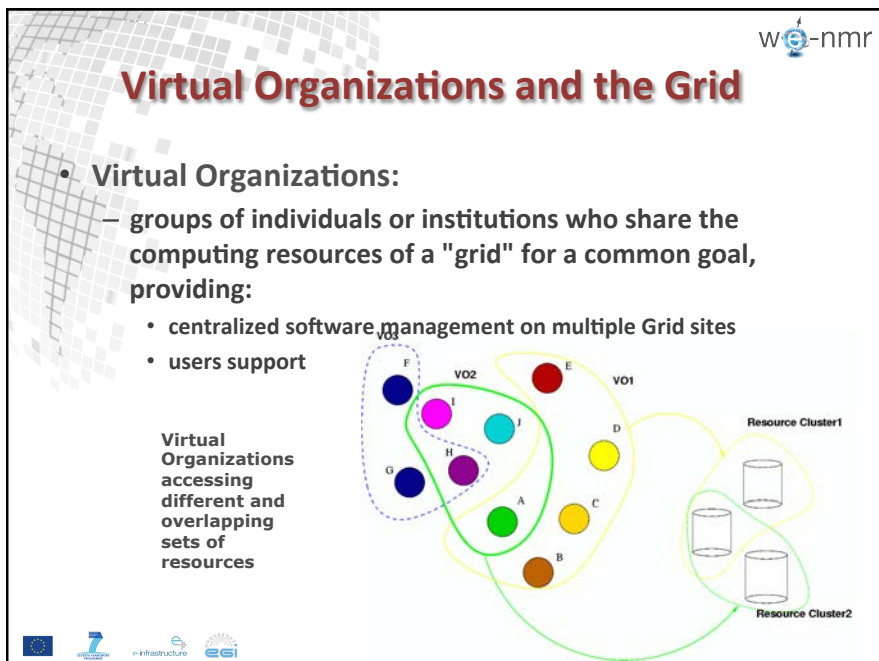
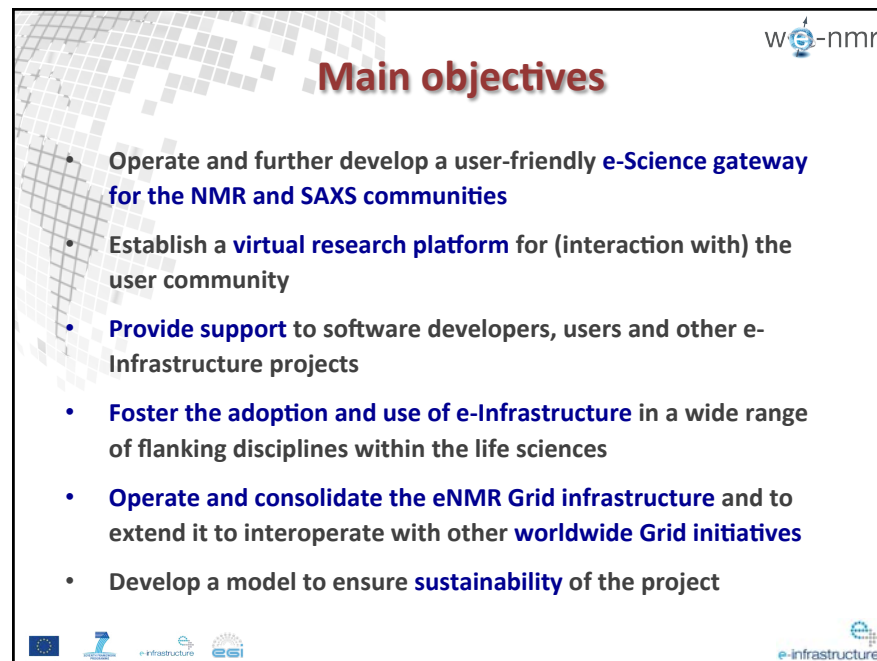


Table 1.1. Virtual Organization

Parameter	Value
Sample Name	Sample 1
Sample Concentration	1.0 mg/ml
Sample Volume	1.0 ml
Sample Temperature	300 K
Sample pH	7.0
Sample Buffer	10 mM Tris, 10 mM NaCl, 10 mM DMSO
Sample Name	Sample 2
Sample Concentration	1.0 mg/ml
Sample Volume	1.0 ml
Sample Temperature	300 K
Sample pH	7.0
Sample Buffer	10 mM Tris, 10 mM NaCl, 10 mM DMSO

Main objectives 

- Operate and further develop a user-friendly e-Science gateway for the NMR and SAXS communities
- Establish a virtual research platform for (interaction with) the user community
- Provide support to software developers, users and other e-Infrastructure projects
- Foster the adoption and use of e-Infrastructure in a wide range of flanking disciplines within the life sciences
- Operate and consolidate the eNMR Grid infrastructure and to extend it to interoperate with other worldwide Grid initiatives
- Develop a model to ensure sustainability of the project



we-nmr

The WeNMR philosophy for interacting with the Grid

- Our policy is to **shield as much as possible the end user from the Grid** and all middleware related issues and commands
- For this, we chose to develop mainly application web portals providing **"protocolized" access to the Grid**
- To facilitate operation, we **use when possible robot certificates**
- Experienced users can still interact directly with the Grid via UI and we **provide "ready-to-go" customized UI distributions (MILU) for download**





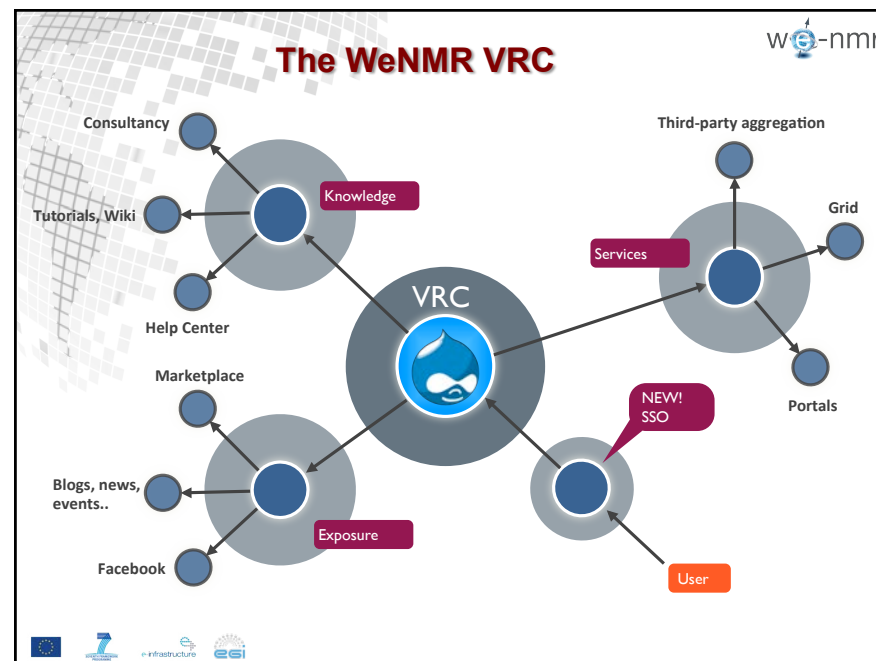
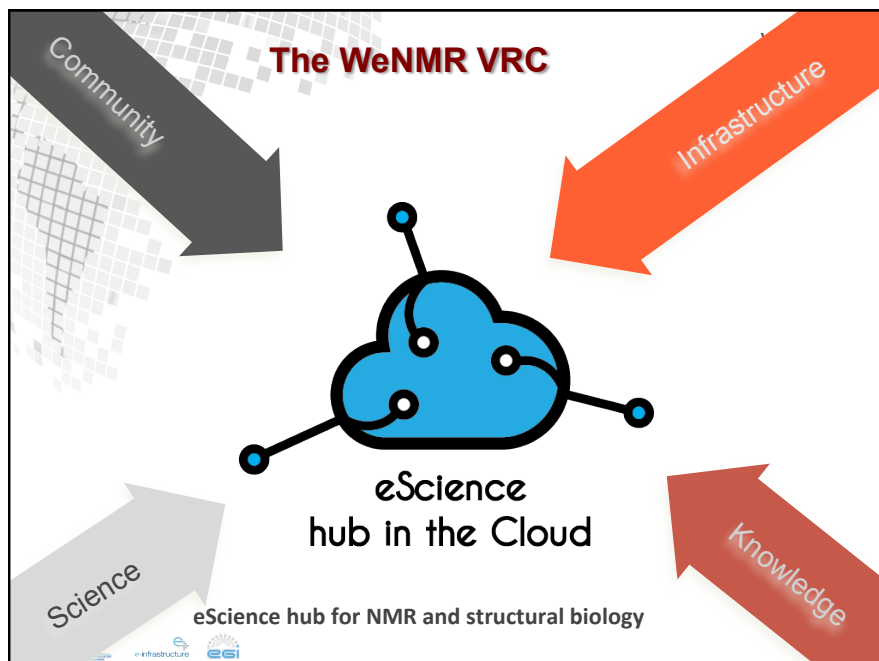

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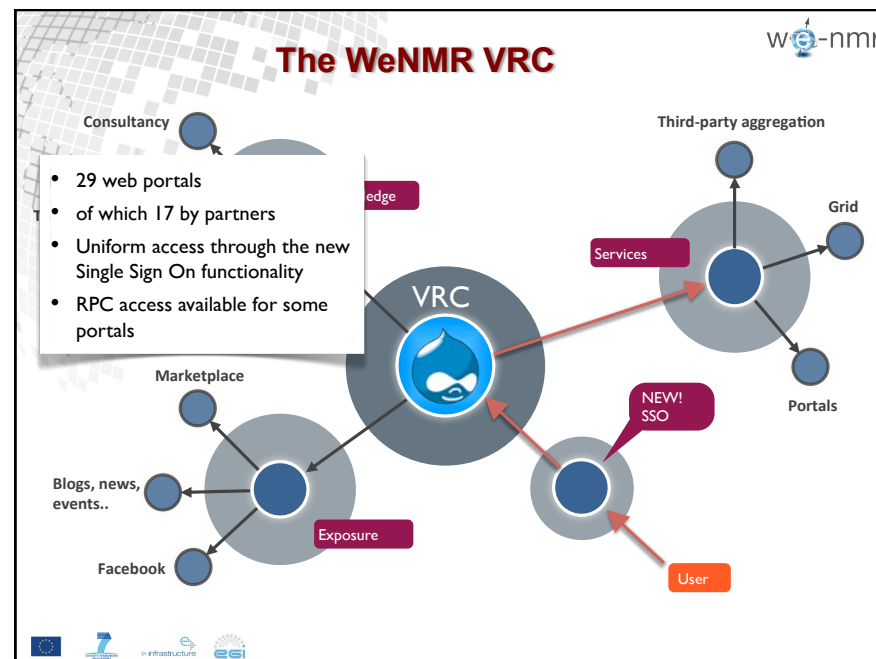
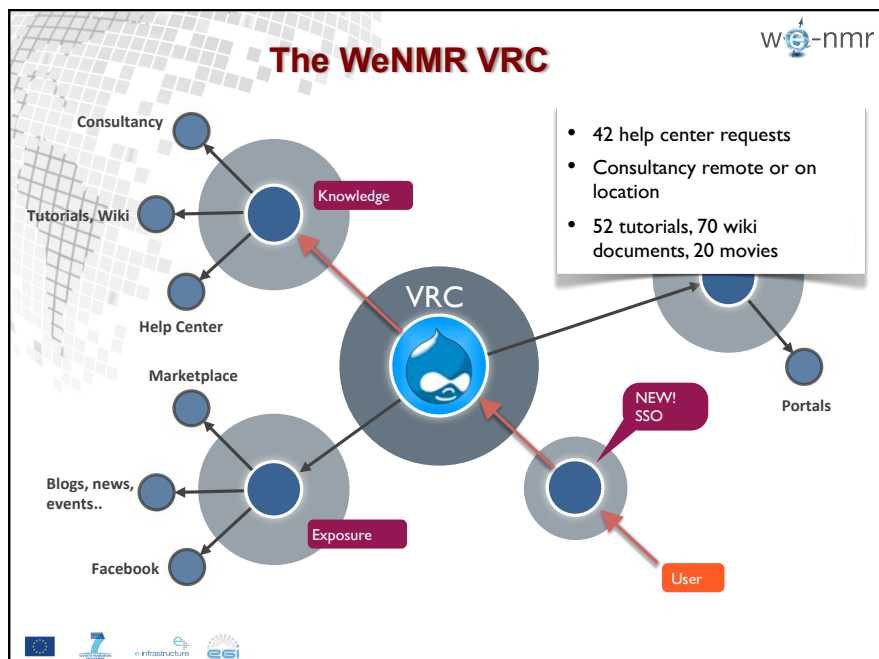
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The Virtual Research Community







The screenshot shows the WeNMR website homepage. The header includes the WeNMR logo and the tagline "A worldwide e-Infrastructure for NMR and structural biology". The navigation menu includes: WeNMR, Services, Market & Resources, Support, Access, and a search bar. The main content area features a large image of a molecular structure and a text box stating: "WeNMR is both a three years project funded under the European Commission's 7th Framework Programme (e-Infrastructure RI-261571) and a Virtual Research Community supported by EGI, the largest one within the life science area. WeNMR aims at bringing together complementary research teams in the structural biology and life science area into a virtual research community at a worldwide level and provide them with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modelling." Below this is a "Get Started >>" link and the text "Harness the power of the GRID". The footer includes a "Highlights" section with a list of recent events and the website URL "www.wenmr.eu".

www.wenmr.eu

The screenshot shows the WeNMR Support page. The header includes the WeNMR logo and the tagline "A worldwide e-Infrastructure for NMR and structural biology". The navigation menu includes: WeNMR, Services, Market & Resources, Support, Access, and a search bar. The main content area is titled "WeNMR Support" and includes sections for: Getting Started, Tutorials, Wiki, Help Center & Forums, and Blogs. The "Getting Started" section includes a link to "Learn about WeNMR services and how to get started." The "Help Center & Forums" section includes a link to "Post your questions and problems on WeNMR services and get fast and reliable answers from our Help Center associated experts." The "Blogs" section includes a link to "Read opinions and news from experts, and write your own blogs about anything related to your NMR and SAXS research or interests." The footer includes the EGI logo and the text "European Grid Infrastructure Towards a sustainable grid infrastructure".

www.wenmr.eu

A worldwide e-Infrastructure for NMR and structural biology

a.m.j.bonvin | Logout

WeNMR
Services
Market & Resources
Support
Access

Support
Getting Started
Tutorials
Wiki
Help Center & Forums
Surveys
GRID related
General services

View
Edit
Outline
Panel layout
Track
Panel content
Clone

Home » Support

Tutorials and use cases

NMR Tutorials +
Learn and get started quickly with our NMR tutorials and use cases.

SAXS Tutorials +
Learn and get started quickly with our SAXS tutorials and use cases.

GRID Tutorials +
Learn more about GRID technology with our GRID tutorials.

General Tutorials +
Get familiar with the WeNMR website, its general usage, services and functionality.

Search tutorials
Enter your keywords:

Latest tutorials

- Create new tutorial**
- Anisofit webserver tutorial 44 weeks 21 hours ago on Anisofit
- Almost 44 weeks 22 hours ago on Almost
- CS-ROSETTA web server tutorial 47 weeks 4 hours ago on chemical shifts, CS-ROSETTA, CS-Rosetta, structure calculations, TACS, WebNMR

All tutorials

Cite WeNMR
Usage of the WeNMR portals should be acknowledged in any publication.
*The WeNMR project (European FP7 e-Infrastructure grant, contract

EGI-approved
The WeNMR Virtual Research Community has been the first to be officially recognized by the EGI.

European Union
WeNMR is an e-Infrastructure project funded under the 7th framework of the EU. Contract no. 261572

A worldwide e-Infrastructure for NMR and structural biology

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WeNMR
Services
Market & Resources
Support
Access

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Getting Started
Tutorials
Wiki
Help Center & Forums
Surveys
GRID related
General services

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Edit
Outline
Panel layout
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Panel content
Clone

Home » Support

Wiki

About GRID technology +
Find general background information about GRID technology.

About NMR +
Find general background information about NMR.

About SAXS +
Find general background information about SAXS.

Grid Services +
Read detailed explanations and information about GRID services.

NMR Services +
Find out about our NMR services. Detailed background information, and explanations of softwares.

SAXS Services +
Find out about our SAXS services. Detailed background information and explanations of softwares.

Search Documentation:
Enter your keywords:

Advanced search

Latest articles

- Create new document page**
- FCC Clustering 21 weeks 8 days ago on clustering, contacts, HADDOCK, protein complex
- Useful interface predictions for HADDOCK 39 weeks 4 days ago on Haddock, HADDOCK, interface predictions
- HADDOCK scriptorium - chemical shift scoring 40 weeks 2 days ago on analysis, chemical shifts, Haddock, HADDOCK, scoring
- HADDOCK scriptorium - geometrical properties of a molecule 41 weeks 1 day ago on HADDOCK
- Getting started with FANDAS 41 weeks 1 day ago on FANDAS
- FANDAS web server documentation 40 weeks 2 days ago on FANDAS

All Documentation Articles

A worldwide e-Infrastructure for NMR and structural biology

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WeNMR
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Help Center & Forums

Issue Categories

NMR Services Issues

- 3D-DART +
- AMBER +
- Antechamber +
- ASDP +
- Auto Assign +
- CcpNmr-Analysis +
- CING +
- CNS +
- CS-ROSETTA +
- CS23D +
- CYANA +
- DisMeta +
- FANDAS +
- Format Converter +
- GaNMR +
- GROMACS +
- HADDOCK +
- MARS +
- MaxOCC +
- MOD NMR +
- PREDITOR +
- PROSA +
- PROSESS +
- RCI +
- ResProx +

Latest Open Issues

- Create new issue**
- Defining Side chain flexibility using Haddock webserver 10 weeks 22 hours ago on HADDOCK
- mRNA truncated 16 weeks 8 days ago on HADDOCK
- Clustering error 37 weeks 1 day ago on HADDOCK
- pdf-format issue: residue numbers 38 weeks 1 day ago on HADDOCK
- Problem loading pdf file 42 weeks 6 days ago on AMBER

Latest Closed Issues

- error message 14 weeks 1 day ago on CS-ROSETTA
- Simulation has frozen 28 weeks 6 days ago on CYANA

All issues

A worldwide e-Infrastructure for NMR and structural biology

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WeNMR
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General services

View
Edit
Webform
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Results
Revisions
Track
Access control
Clone

Home » Access

Registration

In order to make use of the WeNMR GRID platform, one needs to obtain a GRID user certificate and register at the e-NMR VO (Virtual Organisation) using that certificate. Always use the same web-browser for requesting, obtaining and registering the personal GRID certificate. Although most web-browsers are suitable, we would recommend to use Mozilla Firefox.

To register and start using the WeNMR services the following steps should be taken:

1. Request a personal GRID certificate (and load it into your web browser, see e.g. [how to do it](#))
2. Register with the e-nmr.eu VO (using the web browser in which you loaded your certificate)

In case of trouble registering, see the following [troubleshooting page](#) on the WeNMR wiki

3. Register individually to each service (Web Portal) you want to use.

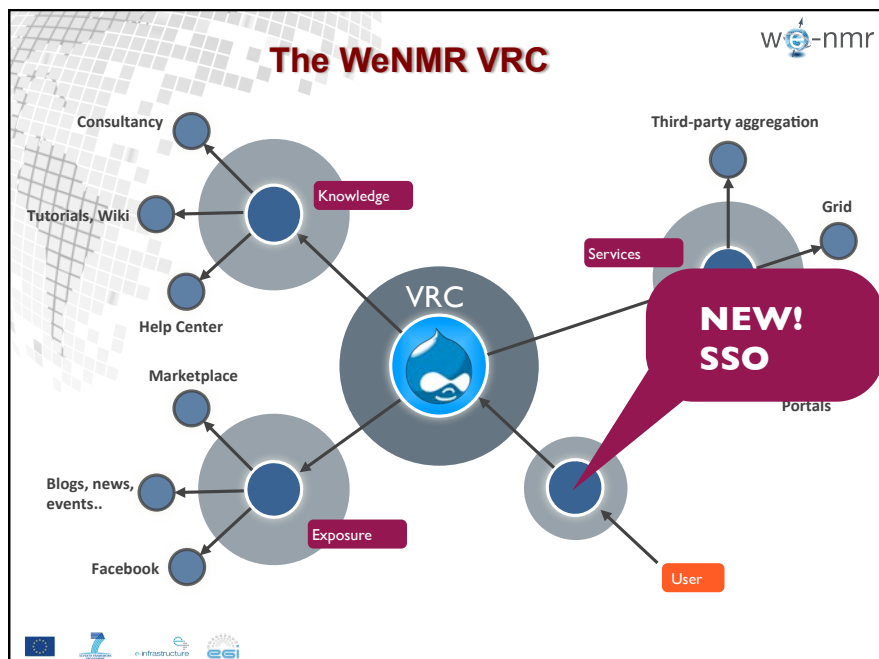
Once using our services, please cite WeNMR in any resulting publication.

Request a personal GRID certificate:

When from Europe, visit the website of the European GRID Policy Management Authority (EUGridPM) to find the Certification Authority (CA) of your country. International users can visit the website of the International Grid Trust Federation (IGTF). Useful information about CAs can also be found from the CHAIN project web site. Click on your region of interest to find more information about regional CAs and other useful links.

Direct links to some of the Certificate Authorities in Europe (for a more complete list see the before mentioned links):

- The Netherlands (DutchGrid-NIKHEF)
- Germany (GermanGrid-GridKa or DFN-Grid)
- Italy (INFN)
- Switzerland (SwissGrid or CERN)
- Austria (AustrianGrid)
- Poland (Polish Grid)
- Czechia (CESNET)
- Slovakia (SlovakGrid)
- Hungary (HUP)
- Ukraine (UGRID)



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Welcome to your personal WeNMR services subscription page listing all the services that you can subscribe to. A subscription allows you to use your WeNMR login credentials to authenticate to the service. Subscribing is as simple as checking the subscription checkbox and submitting the form. Some services require subscription approval, you can follow the approval process on this page. Your subscription status to the available services is indicated by the color of service boxes as:

not subscribed (grey) subscribed (green) pending (orange)

Service	Subscribed since	Total jobs	Active jobs
HADDOCK	13-Sep-2012	1	0
UNIO	13-Sep-2012	0	0
AMBER	AMBER Molecular Dynamics WEB Portal		
GROMACS	13-Sep-2012	0	0
ATLAS	ATLAS Grid Portal		
XPLOR-NH	Xplor-NIH is a generalized software for biomolecular structure determination from experimental NMR data combined with geometric data. This is achieved by seeking the minimum of a target function comprising terms for the experimental NMR restraints.		

Buttons: **SUBSCRIBE** (for AMBER, ATLAS, XPLOR-NH) **Submit**

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UNIO	13-Sep-2012	0	0
AMBER	AMBER Molecular Dynamics WEB Portal		
GROMACS			

Grid certificate 1 **License agreement 2** **Submit request 3**

You are 2 steps away from subscribing to this service

Follow the steps listed in the menu on the left to subscribe

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UNIO	13-Sep-2012	0	0
AMBER	AMBER Molecular Dynamics WEB Portal		
GROMACS			

Grid certificate 1 **License agreement 2** **Submit request 3**

Step 1 This service requires you to have a valid Grid certificate

Congratulations, you have a valid GRID certificate still valid for 159 days

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Home > My account

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not subscribed subscribed pending

	Subscribed since	Total jobs	Active jobs
HADDOCK	13-Sep-2012	1	0
UNIO	13-Sep-2012	0	0
AMBER	AMBER Molecular Dynamics WEB Portal		

SUBSCRIBE

Grid certificate 1

License agreement 2

Submit request 3

Step 2 This service requires approval of a license agreement

License agreement

AMBER 12 SOFTWARE LICENSE AGREEMENT

IMPORTANT: This Amber license Agreement is a legal agreement between you, the end user (either an individual or an entity), and the University of California.

AMBER Software License

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	Subscribed since	Total jobs	Active jobs
HADDOCK	13-Sep-2012	1	0
UNIO	13-Sep-2012	0	0
AMBER	AMBER Molecular Dynamics WEB Portal		

SUBSCRIBE

Grid certificate 1

License agreement 2

Submit request 3

All steps complete, submit the request

Submit

	Subscribed since	Total jobs	Active jobs
GROMACS			

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Home > My account

WeNMR services for amjibonvin

Your subscription to service AMBER is active

Welcome to your personal WeNMR services subscription page listing all the services that you can subscribe to. A subscription allows you to use your WeNMR login credentials to authenticate to the service. Subscribing is as simple as checking the subscription checkbox and submitting the form. Some services require subscription approval, you can follow the approval process on this page. Your subscription status to the available services is indicated by the color of service boxes as:

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	Subscribed since	Total jobs	Active jobs
HADDOCK	13-Sep-2012	1	0
UNIO	13-Sep-2012	0	0
AMBER	15-Mar-2013	0	0
GROMACS	13-Sep-2012	0	0
ATSAS	ATSAS Grid Portal		
XPLOR-NH	Xplor-NH is a generalized software for biomolecular structure determination from experimental NMR data combined with geometric data. This is achieved by seeking the minimum of a target function comprising terms for the experimental NMR restraints.		

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home >> AMPS-NMR

AMPS-NMR

(installing paramagnetic restraints plugin)

WeNMR GRID-enabled web portal

WebNMR home NMR services SAXS services WeNMR Support Center

WELCOME ALEXANDRE BONVIN

My Account Amber Jobs Projects Logout

HOW TO START? (QUICK RUN)

To quickly create a new calculation, use the Amber drop down menu from the blue bar above and select New calculation. Then follow the four-steps procedure to input all of your data. Check also the AMPS-NMR paper in bioinformatics. Pubmed link

TUTORIAL

We would like to show the very basic of Amps-nmr in a short, simple and interactive tutorial. This tutorial is designed to give you a good basic understanding of the use of mainly functionality of this web portal without loading you down with too much technical details.

Click here to read this tutorial.

WebNMR home NMR services SAXS services WeNMR Support Center

© 2008 by NMR Spectroscopy Center, All rights reserved. Version 1.0.0.0

The WeNMR services portfolio

we-nmr

The collage displays a wide range of computational chemistry and structural biology services available through the WeNMR infrastructure. Each service is represented by a thumbnail of its respective web interface, showing various input forms, data visualizations, and user guides.

3D-DART

SHIFTX2

ASOP

Antechamber

AdisoFIT

GROMACS

CCPN format

MDD

APTASign

TALOS

MAXOCC

CS-ROSETTA

CYANA

AMBER

Haddock

EMBL HAMBURG

Biological Small Angle Scattering

BIOSSAXS

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ATSAS Grid

Home > Software > ATSAS Grid

ATSAS Grid Portal

DAMMIN - *ab initio* shape determination by simulated annealing using a bead model
DAMMIF - rapid *ab initio* bead model shape determination
GASBOR - *ab initio* reconstruction of protein structure by a chain-like ensemble of dummy residues

You will need to authenticate yourself. Please use your [ATSAS online](#) email address as user name.

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And SAXS services as well!

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WeNMR NMR SAXS Market Support

Ab Initio Modelling
Advanced Modelling
Instrument Access

EMBL HAMBURG Biological Small Angle Scattering

BIOSSAXS we-nmr ATSAS Grid

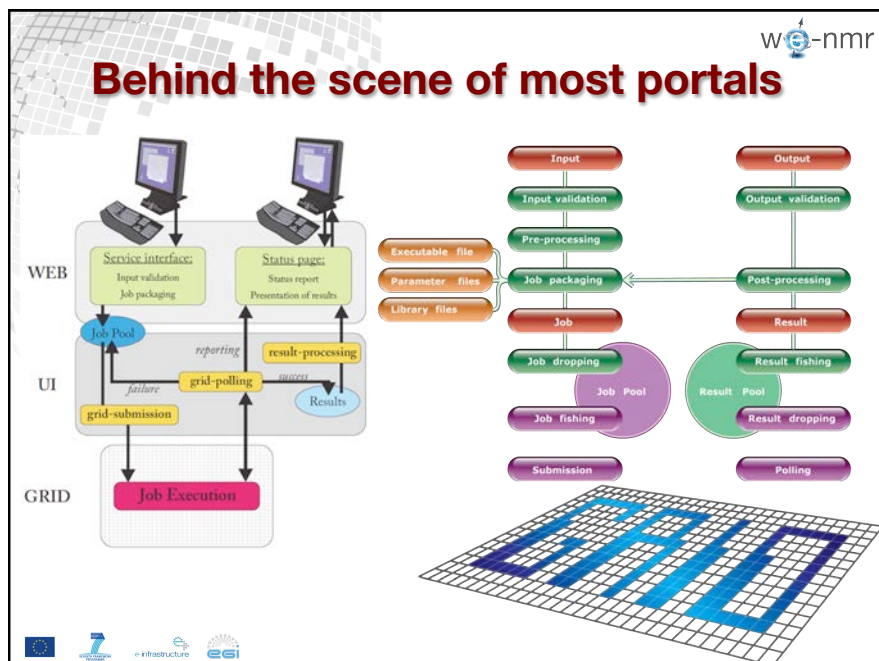
Home > Software > ATSAS Grid

ATSAS Grid Portal

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Services and Usage

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Services and Usage

EMBL HAMBURG

Biological Small Angle Scattering

BIOSSAXS

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ATSAS Grid

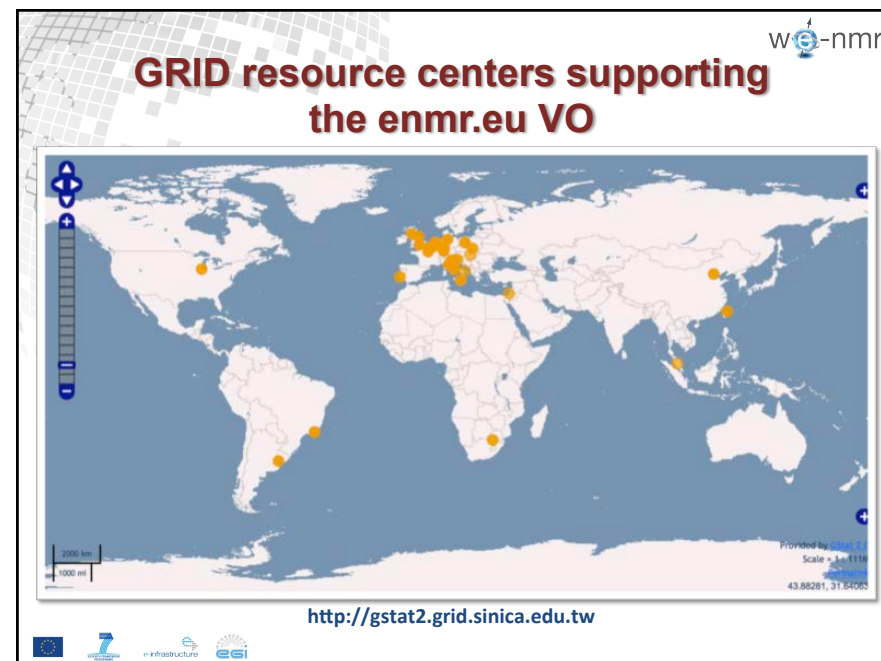
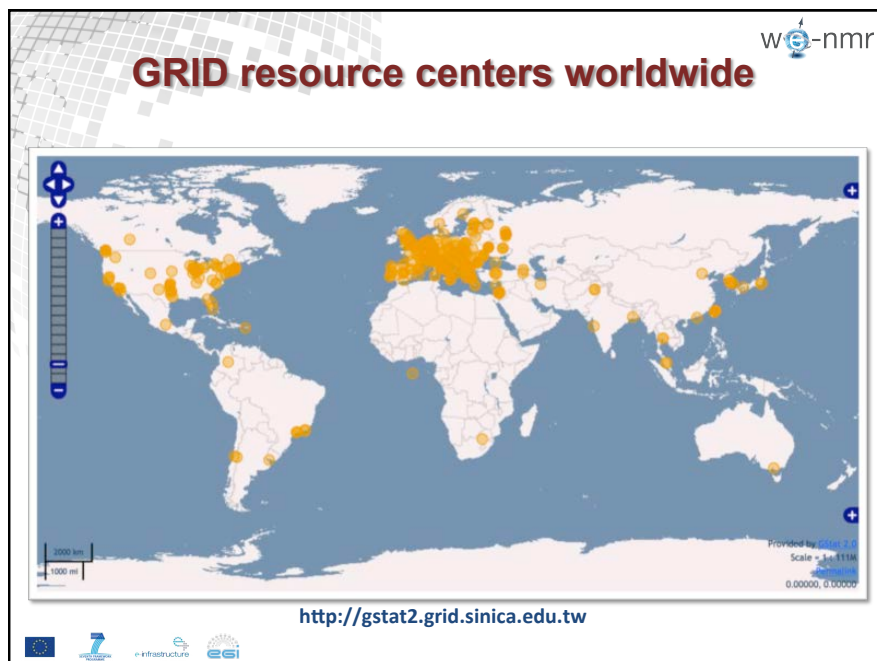
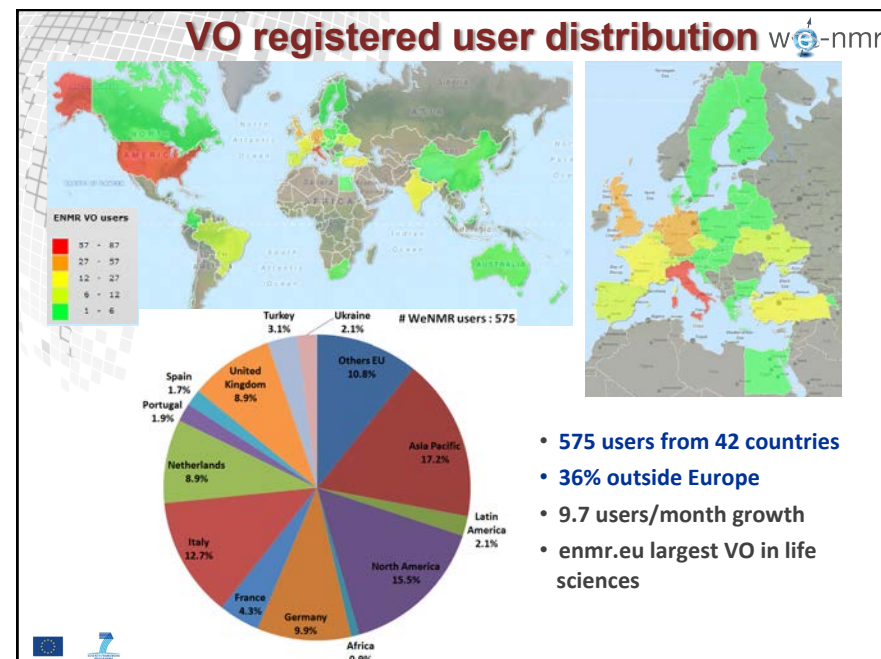
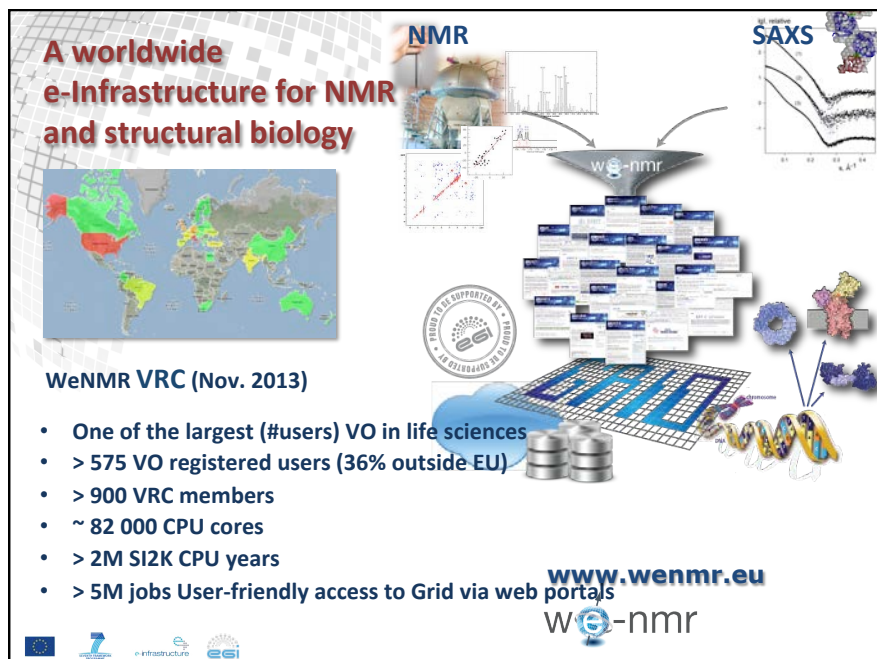
Home > Software > ATSAS Grid

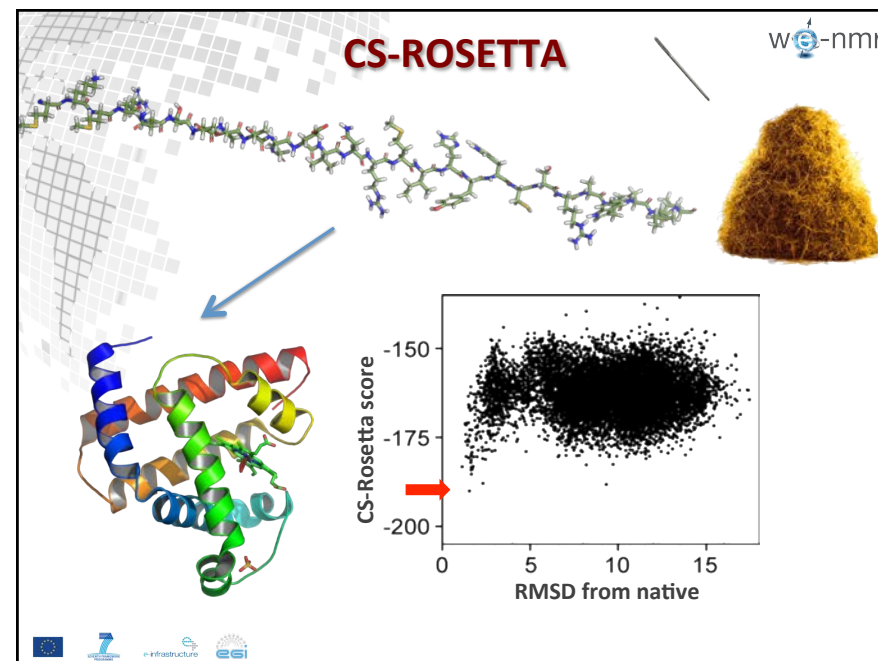
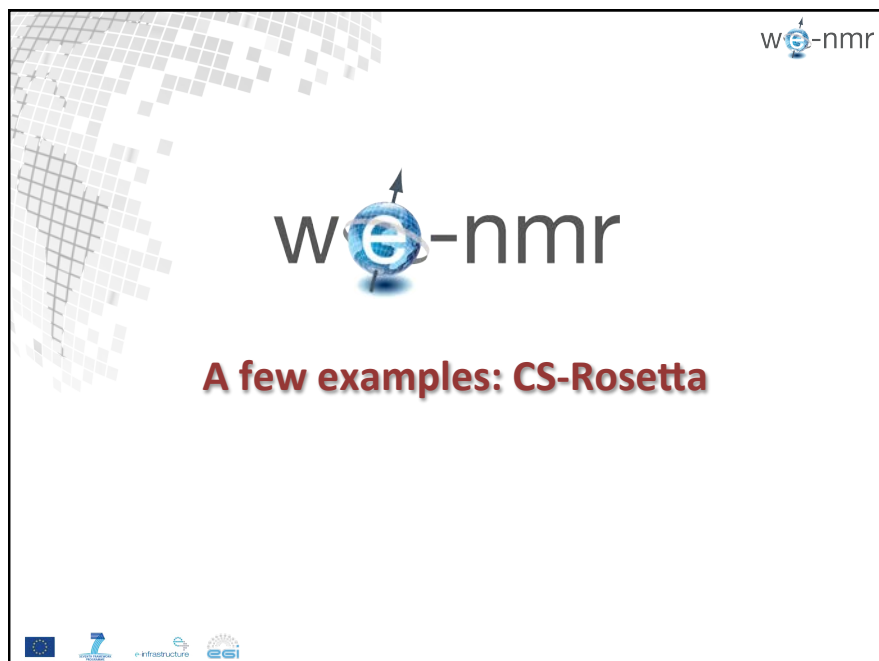
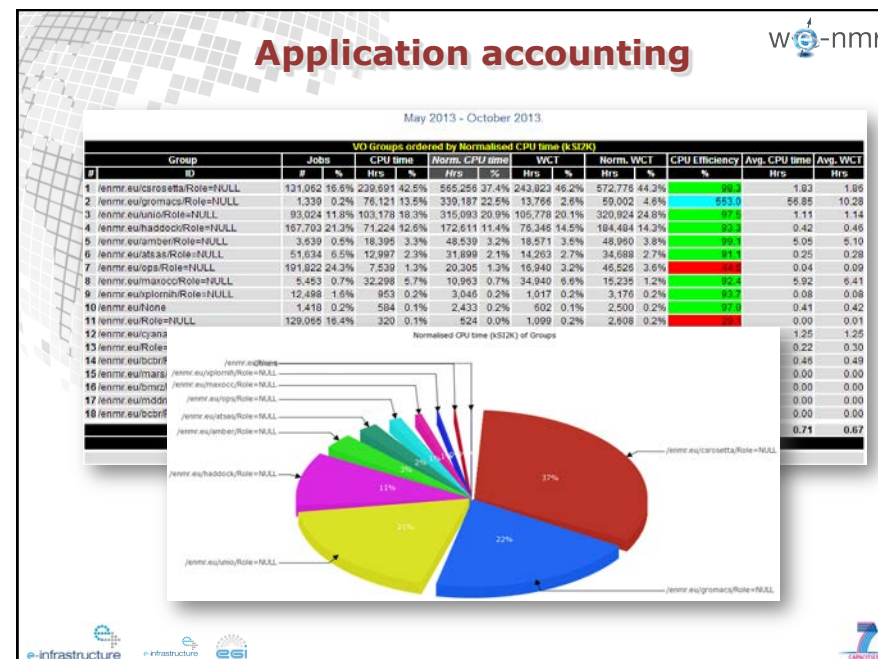
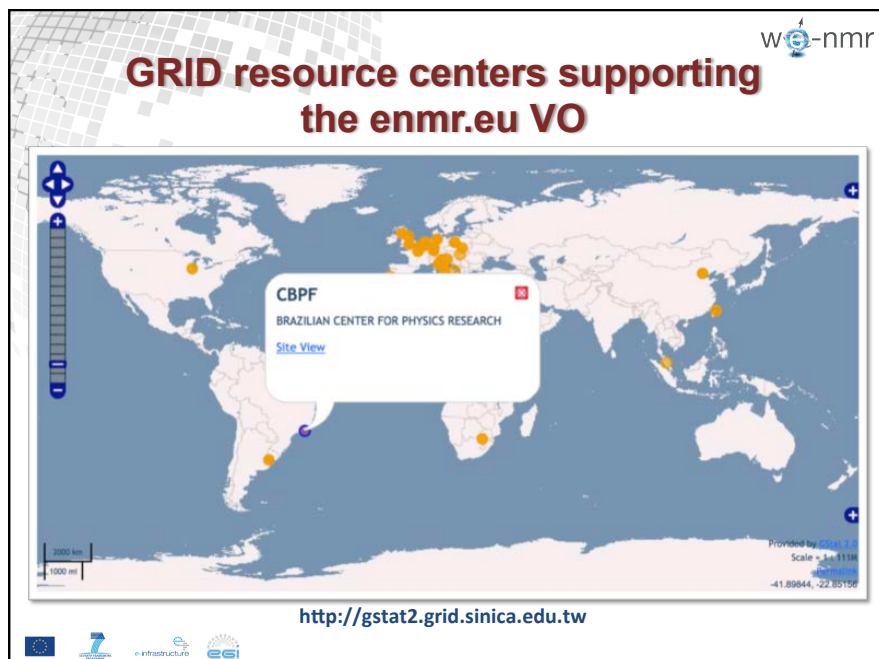
ATSAS Grid Portal

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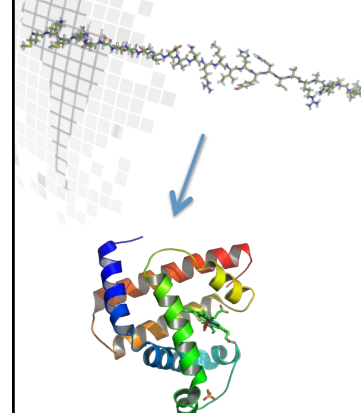
CS-ROSETTA (not) web portal



```
/Volumes/Home/Users/christophe/minirosetta_svn/bin/minirosetta.macosgccrelease -abinitio::increase_cycles
1 -nstruct 10 -database /Volumes/Home/Users/christophe/minirosetta_database -frag3 /Volumes/Home/Users/
christophe/Dropbox/minirosetta_pcs_file/DATA/1NKU/FRAG_CS-ROSETTA/frag3.t000.rosetta.tab.gz -frag9 /
Volumes/Home/Users/christophe/Dropbox/minirosetta_pcs_file/DATA/1NKU/FRAG_CS-ROSETTA/
frag9.t000.rosetta.tab.gz -abinitio::stage1_patch /Volumes/Home/Users/christophe/Dropbox/
minirosetta_pcs_file/SCORE/score0_pcs1.wts_patch -abinitio::stage2_patch /Volumes/Home/Users/christophe/
Dropbox/minirosetta_pcs_file/SCORE/score1_pcs1.wts_patch -abinitio::stage3a_patch /Volumes/Home/Users/
christophe/Dropbox/minirosetta_pcs_file/SCORE/score2_pcs1.wts_patch -abinitio::stage3b_patch /Volumes/
Home/Users/christophe/Dropbox/minirosetta_pcs_file/SCORE/score5_pcs1.wts_patch -abinitio::stage4_patch /
Volumes/Home/Users/christophe/Dropbox/minirosetta_pcs_file/SCORE/score3_pcs1.wts_patch -native /
Volumes/Home/Users/christophe/Dropbox/minirosetta_pcs_file/DATA/1NKU/idealized_1NKU.pdb -
out:file:silent /Volumes/Home/Users/christophe/PCS_ROSETTA_RESULT/ABINITIO//
1NKU_exact_N1_PCS1.silent -out:file:scorefile /Volumes/Home/Users/christophe/PCS_ROSETTA_RESULT/
ABINITIO//1NKU_exact_N1_PCS1.sc -abinitio::rg_reweight 0.5 -abinitio::rsd_wt_helix 0.5 -abinitio::rsd_wt_loop
0.5 -abinitio::use_filters false -broker::setup /Volumes/Home/Users/christophe/Dropbox/minirosetta_pcs_file/
RUN/./1NKU_exact/setup_pcs1.txt -run:protocol broker -overwrite -PCS:normalization_id 1 -
in::file::native_exclude_res 1 2 3 4 5 6 7 8 9 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 -
mute core.scoring.methods.PCS.PcsEnergy -mute core.optimization.LineMinimizer
```



CS-ROSETTA web portal



home >> CS-ROSETTA

CS-ROSETTA

WeNMR GRID-enabled web portal

WeNMR home NMR services SAXS services WeNMR Support Center

WELCOME TO THE WENMR WEB PORTAL >>>

CS ROSETTA is a protocol which generates 3D models of proteins, using only the 13CA, 13CB, 13C', 15N, 1HA and 1HN NMR chemical shifts as input. Based on these parameters, CS ROSETTA uses a SPARTA-based selection procedure to select a set of fragments from a fragment-library (where the chemical shifts and the 3D structure of the fragments are known). The fragments are assembled using the ROSETTA protocol. The generated models are rescored based on the difference between the back-calculated chemical shifts of the generated models and the input chemical shifts. For more information see our online web portal [manual and tutorial](#) and/or consult the CS-Rosetta home page at: <http://spin.niddk.nih.gov/bax/software/CSROSETTA/index.html>.

WEBSERVER USER MANUAL AND TUTORIAL

CS ROSETTA WEBSERVER

To use the CS ROSETTA webserver you must have registered for an account. If you do not have a account yet you can [register here](#)

IMPORTANT: Before submitting any run to the CS-Rosetta web server it is strongly advised to remove any flexible tail and check the chemical shifts for outliers using TALOS+.

Setup your CS-Rosetta run

Give your run a name:

TALOS file to submit: [Browse...](#)

Number of models to generate:

RCSB PDBids to exclude from calculation:

[Exclude flexible parts?](#) ☒

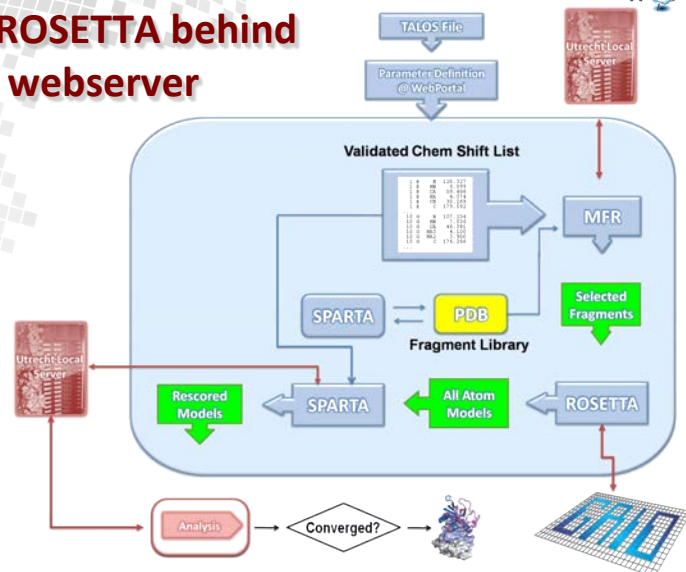
Username and password

Username:

Password:

[Submit Query](#)

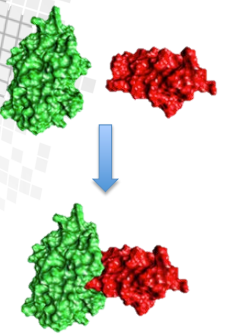
CS-ROSETTA behind the webserver



HADDOCK: Shedding light on biomolecular interactions



Haddock web portal



home >> HADDOCK

HADDOCK

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WeNMR home NMR services SAXS services HADDOCK tutorials WeNMR Support Center

WELCOME TO THE WENMR WEB PORTAL >>

HADDOCK (High Ambiguity Driven protein-protein DOCKing) is an information-driven flexible docking approach for the modeling of biomolecular complexes. HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. HADDOCK can deal with a large class of modeling problems including protein-protein, protein-nucleic acids and protein-ligand complexes.

More information about HADDOCK can be found on the HADDOCK website

PROFILE >>

we-nmr

e-infrastructure

SERVICES

The WeNMR web portal is an easy gateway for you to use many of the powerful software packages ported by the WeNMR consortium to the GRID.

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THE PARTNERS >>

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HADDOCK WEBSERVER

To use the HADDOCK eNMR GRID-enabled docking server you must:

- have registered for a GRID-enabled HADDOCK account
- have registered with the eNMR grid infrastructure.

Note: registration does require a valid grid certificate!!!

- HADDOCK server: the easy interface
- HADDOCK server: the prediction interface
- HADDOCK server: the expert interface
- HADDOCK server: the guru interface
- HADDOCK server: the multi-body interface
- HADDOCK server: the refinement interface
- HADDOCK server: the file upload interface
- HADDOCK server tool: generate AIR files for multibody docking

Logos: European Union, WeNMR, e-infrastructure, EGI

User friendly easy interface

we-nmr

HADDOCK

WeNMR (GRID-enabled) web portal

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WELCOME TO THE WENMR WEB PORTAL >>

This is the easy interface to the HADDOCK docking program. Please define the structure for each molecule you want to dock as well as the residues belonging to the interaction interface. Docking is performed with default settings that work well for average complexes. If you do not have any special wishes for the system you want to have docked, this is the way to go. Unfold the menus by clicking on the double arrows. Submit your job by providing your username and password and press submit.

You may supply a name for your docking run (one word)
Name:

First molecule

Structure definition

Where is the structure provided?

Which chain of the structure must be used?

PDB structure to submit

or: PDB code to download

Restraint definition

Data to drive the docking

Please supply residues as comma-separated lists of residue numbers

Active residues (directly involved in the interaction)

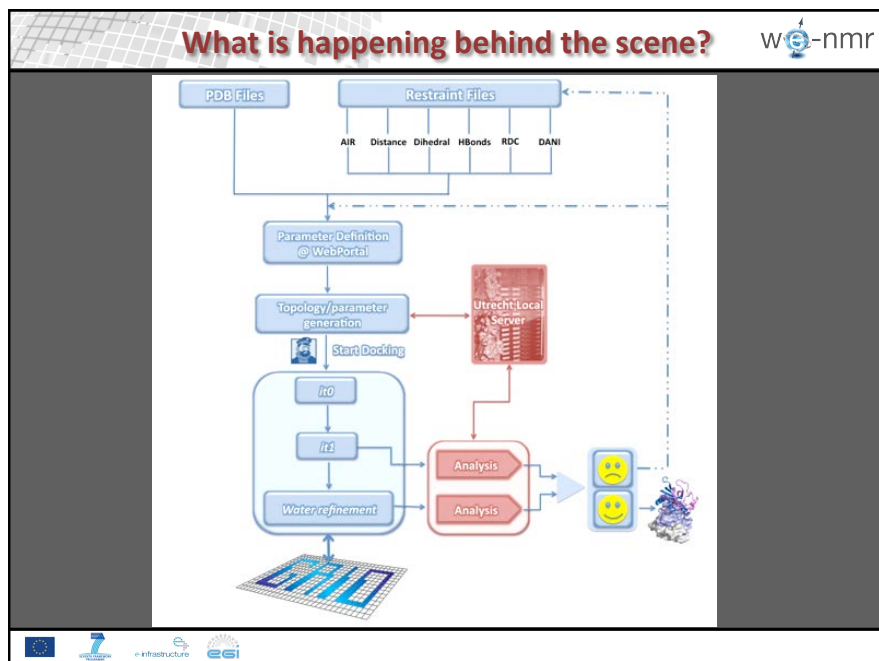
Passive residues (surrounding surface residues)

Define passive residues automatically around the active residues ☐

What kind of molecule are you docking?

Second molecule

Logos: European Union, WeNMR, e-infrastructure, EGI



we-nmr

we-nmr

A few examples: GROMACS

Logos: European Union, WeNMR, e-infrastructure, EGI

GROMACS web portal

Runs in parallel on the Grid using GROMACS multithreading capability

Currently for efficiency runs on 6 processors

CREAM-CE features used for parallel job submission

GROMACS

WeNMR GRID-enabled web portal

Return to the WeNMR website

WELCOME TO THE WENMR WEB PORTAL >>

SETTING UP A GROMACS MD RUN STARTING FROM A STRUCTURE FILE

Welcome to the GROMACS web server your entry point for molecular dynamics on the GRID. New molecular dynamics simulations are started by filling out the form below. One submitted you will be redirected to the results page for your run where you will be informed on its progress and will be able to retrieve the results when the job is finished.

Required parameters

PDB file
Please upload a PDB file or GROMACS .gro file

Optional parameters

Simulation time
Please specify the simulation time in ns
1.0

Output resolution ns
0.05

Forcefield
Please specify the forcefield to use
GROMOS96 53af

Solvent model
Please specify the solvent model to use
default

Treatment of electrostatic interactions
Please choose how to treat electrostatics
Cut-off/Reaction Field

Advanced parameters

Salt concentration
Please specify the salt concentration (mol/l)
0.1539976

Temperature and Pressure
Specify temperature (K)
300.0

Specify pressure (Bar)
1.0



Involving software developers and pushing new developments: CASD-NMR

CORRESPONDENCE

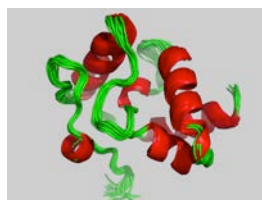
Nature Methods 6, 625 - 626 (2009)
doi:10.1038/nmeth0909-625

CASD-NMR: critical assessment of automated structure determination by NMR

Antonio Rosato^{1,2}, Anurag Bagaria^{3,4}, David Baker⁵, Benjamin Bardiaux⁶, Andrea Cavalli⁷, Jurgen F Doreleijers⁸, Andrea Giachetti¹, Paul Guerry⁹, Peter Güntert^{3,4}, Torsten Herrmann⁹, Yuanpeng J Huang¹⁰, Hendrik R A Jonker^{4,11}, Binchen Mao¹⁰, Thérèse E Malliavin⁶, Gaetano T Montelione¹⁰, Michael Nilges⁶, Srivatsan Raman⁵, Gijs van der Schot¹², Wim F Vranken¹³, Geerten W Vuister⁸ & Alexandre M J J Bonvin¹²

- 10 blind targets (structures to be determined by fully automated methods)
- 15 teams worldwide involved with their respective developer teams
- Assessment of results by independent team
- Impact: WeNMR & EU as drivers of innovation, leading to new software developments, increased trust in automated methods and improved services for end users

nature methods
Techniques for life scientists and chemists



CASD-NMR

Structure
Ways & Means
Structure 20, 227–236, 2012

Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data

Antonio Rosato,^{1,2} James M. Aramini,¹ Cheryl Arrowsmith,⁴ Anurag Bagaria,^{5,6} David Baker,^{5,6} Andres Cavalieri,⁷ Doreleijers,⁸ Alexander Eletsky,¹¹ Andrea Giachetti,¹ Paul Guerry,⁹ Aleksandras Gutmanas,⁶ Peter Yurken He,¹⁰ Torsten Herrmann,¹² Yuanpeng J. Huang,¹⁰ Victor Jaravine,^{6,11} Hendrik R.A. Jonker,^{6,11} Michael A. Oliver,¹ Longqi Gao,¹⁰ Guoshu Liu,¹⁰ Thérèse E. Malliavin,⁶ Rajeev Mari,¹ Binchen Mao,¹⁰ Gaetano T. Montelione,¹⁰ Michael Nilges,⁶ Paolo Rossi,⁹ Gijs van der Schot,¹² Harald Schwabe,^{6,11} Thomas A. Szyperski,¹¹ Michele Ver Robert Vernon,¹⁰ Wim F. Vranken,^{6,11} Sjoerd de Vries,^{10,11} Geerten W. Vuister,^{10,11} Bin Wu,¹⁰ Yunhuang Yang and Alexandre M.J.J. Bonvin¹²

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European Grid Infrastructure towards a sustainable infrastructure

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Want to know what a molecule looks like? Challenge a computer!

The first results have been published from a public challenge to automate the process of determining the shape and structure of a molecule from NMR data. Three of the teams who took up the challenge have now posted their work to the grid.

NMR (Nuclear Magnetic Resonance) is a technique used by many researchers to investigate how the constituents of a molecule interact and the shapes they form. It does this by exploiting a technique where one can 'listen' to atoms if one puts them into a very strong magnetic field. However, the music they play is complex and it requires a lot of work to interpret the NMR raw data obtained from a molecule before one can figure out its exact shape.

13 April 2012
Newman O'Neill

