

User Experience.

An emerging user community :



/O=dutchgrid

/O=users

/O=universiteit-utrecht

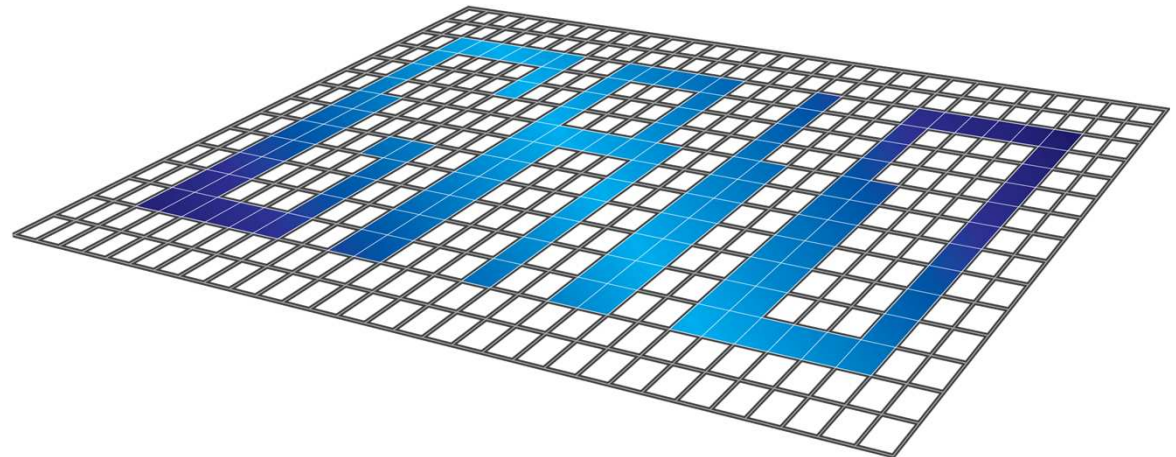
/OU=chem

/CN=Nuno Loureiro Ferreira @

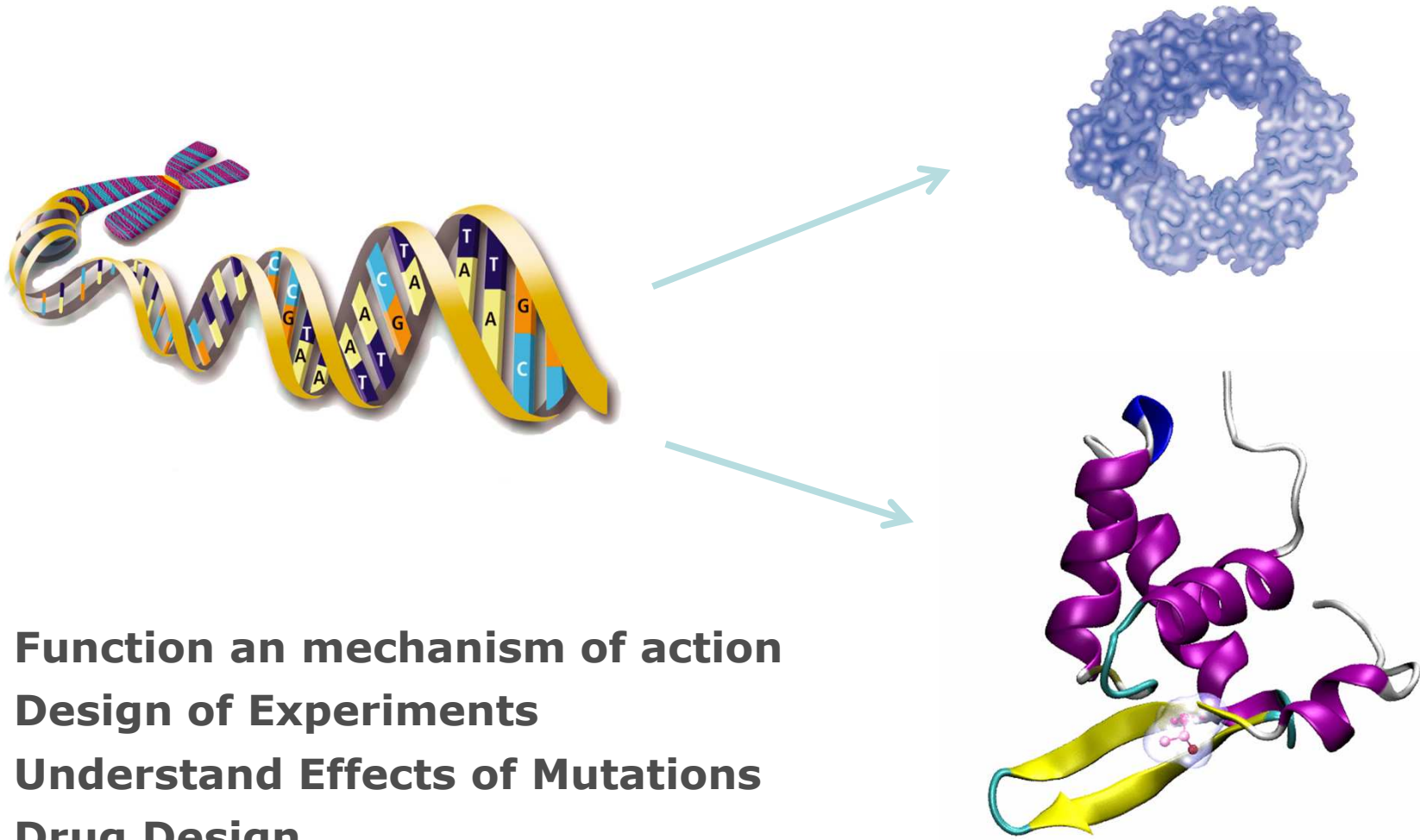
EGITechnical
Forum2010

Outline

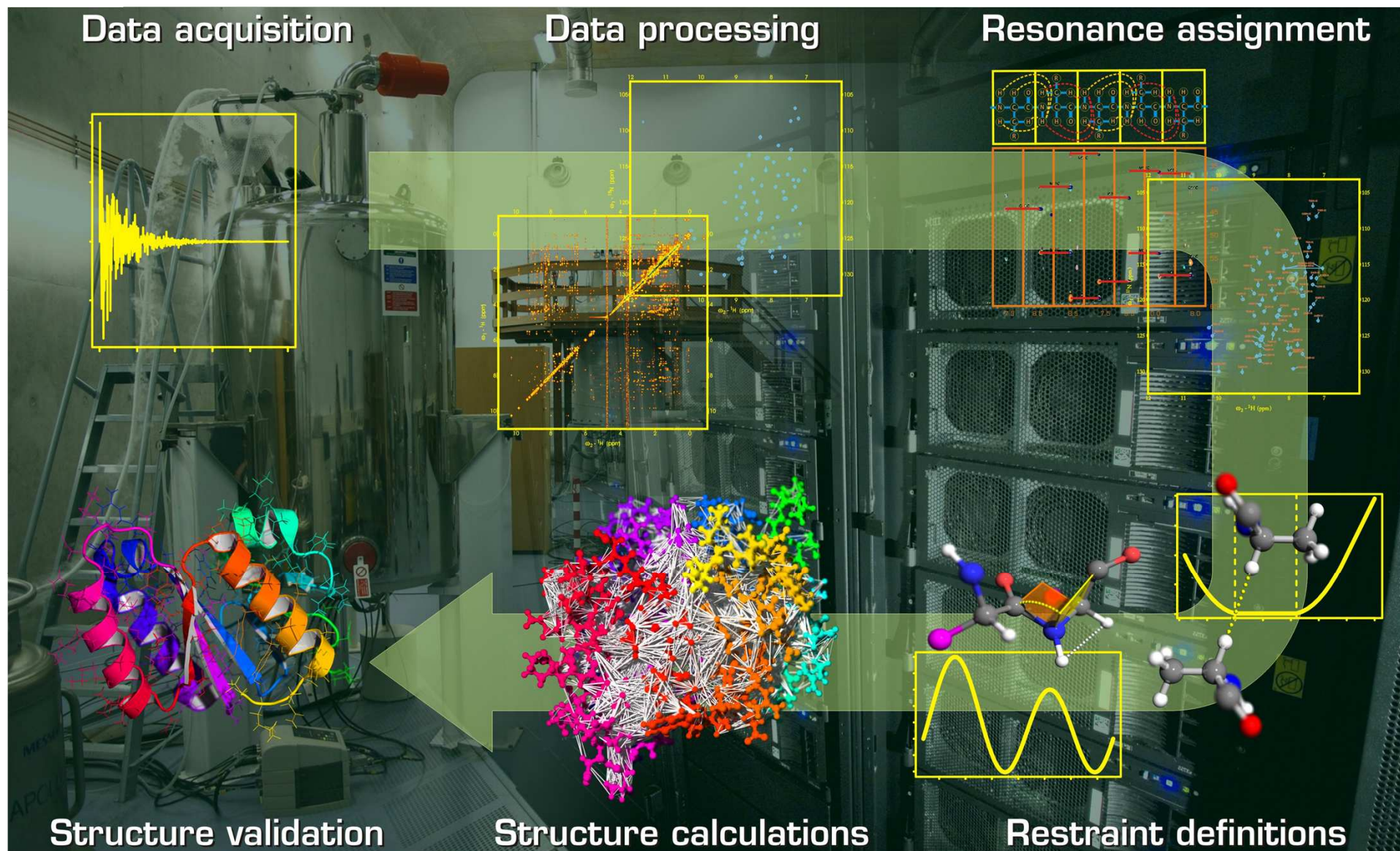
- Introduction & Scientific context
- The e-NMR project
- e-NMR Web portal
- Final remarks



Biomolecular structure ... why?



Nuclear Magnetic Resonance



Practical issues ...

<u>NMR raw data processing</u>				
	TopSpin /XwinNMR	NmrPipe	Prosa	...
<u>Assignment & Bookkeeping</u>				
Graphics	Sparky	NMRView	Cara	CCPN Analysis
Backbone	Autoassign	MARS	Pistachio	Match
	Mapper	... Garant	...	
Side-chains	PROSIAS	Pistachio	ASCAN	...
<u>Data analysis / restraints generation</u>				
NOEs	QUEEN	AQUA	...	
Dihedral angles	Talos	CSI	PECAN	
RDCs	Pales	Module	...	
Relaxation data	TENSOR2	ModelFree	HydroNMR	
	Curvefit	...		
Paramagnetic data	PARA restraints toolkit			
<u>Structure calculations / automated NOE assignment</u>				
Computation engines	CYANA	CNS	Xplor-NIH	
Automated procedures	CANDID	ARIA	RADAR	
	RECOORD	ABACUS	...	
	CSRostta			
<u>Structure calculations / molecular dynamics</u>				
	Amber	Gromacs		
<u>Modelling of biomolecular complexes</u>				
	HADDOCK			
<u>Structure validation</u>				
	Procheck	Whatcheck	PSVS	
	DNA/RNA toolkit	...		

- # Applications
 - File formats
- Expertise
 - Installation
 - Software usage
 - NMR structure calc.
- Resources
 - CPU power
 - storage space
- Standards?
 - Comparison
 - Good practices

e-NMR objectives



- Integrated protocols of NMR applications
- Easy access to web interfaces
- Exploit GRID technology
- Lower the access level to GRID technology in life sciences

Crash course : Hello Grid!

```
[nuno@ui-enmr bcbr]$ ll ~/.globus
total 16
-rw-r--r--  1 nuno users 4947 Nov 14 17:19 usercert.pem
-rw-----  1 nuno users  963 Nov 14 17:20 userkey.pem

[nuno@ui-enmr bcbr]$ voms-proxy-init --voms enmr.eu
Enter GRID pass phrase:
Your identity: /O=dutchgrid/O=users/O=universiteit utrecht/OU=chem/CN=Nuno Loureiro F
Creating temporary proxy ..... Done
Contacting voms-02.pd.infn.it:15014 [/C=IT/O=INFN/OU=Host/L=Padova/CN=voms-02.pd.inf
Creating proxy ..... Done
Your proxy is valid until Wed Jan 27 03:44:48 2010

[nuno@ui-enmr bcbr]$ cat hello.jdl
Executable      = "script.sh";
StdOutput       = "hello.out";
StdError        = "hello.err";
InputSandbox    = {"script.sh"};
OutputSandbox   = {"hello.err","hello.out"};

[nuno@ui-enmr bcbr]$ glite-wms-job-submit -a -o jid hello.jdl
[nuno@ui-enmr bcbr]$ glite-wms-job-status -i jid
[nuno@ui-enmr bcbr]$ glite-wms-job-output -i jid --dir ./out
[nuno@ui-enmr bcbr]$ more ./out/hello.out
Hello Grid! I was here : wn3-enmr.cerm.unifi.it
```



e-NMR web portal @ www.enmr.eu



The screenshot shows the e-NMR web portal homepage. The header features the text "home >>" and a large banner with the "e-NMR" logo and the text "NMR computational infrastructure". Below the banner is a navigation menu with links: Home, HADDOCK, Xplor-NIH, CYANA, CS-ROSETTA, FormatConverter, eNMR-database, eNMR-Grid, RSS, Software, and eNMR Wiki. The main content area is divided into two columns. The left column, titled "WELCOME TO THE E-NMR WEB PORTAL >>", contains two paragraphs of text. The right column, titled "PROFILE >>", contains two logos: the "e-nmr" logo and the "e-infrastructure" logo.

home >>

e-NMR

NMR computational infrastructure

[Home](#) [HADDOCK](#) [Xplor-NIH](#) [CYANA](#) [CS-ROSETTA](#) [FormatConverter](#) [eNMR-database](#) [eNMR-Grid](#) [RSS](#)

[Software](#) [eNMR Wiki](#)

WELCOME TO THE E-NMR WEB PORTAL >>

e-NMR aims at deploying and unifying the NMR computational infrastructure in system biology, a project funded under the 7th framework program of the European Union (Contract no. 213010 - e-NMR).

NMR plays an important role in life sciences (biomolecular NMR), and structural biology in particular, at both European and international levels. Our main objective is to optimize and extend the use of the NMR Research Infrastructures of EU-NMR through the implementation of an e-Infrastructure in order to provide the biomolecular NMR user community with a platform integrating and streamlining the computational approaches necessary for NMR data analysis and structural modelling (e-NMR).

PROFILE >>



User friendly interface

The screenshot shows the CS-ROSETTA web portal. At the top is a blue header with the logo and navigation links: Home, HADDOCK, Xplor-NIH, CYANA, FormatConverter, eNMR-database, eNMR-Grid, Software, and eNMR Wiki. Below the header is a welcome message and a paragraph describing the CS-ROSETTA protocol. The main section is titled 'CS ROSETTA WEBSERVER' and includes a registration notice. Below this is a 'Setup your CS-Rosetta run' form with fields for 'Give your run a name', 'TALOS file to submit' (with a 'Browse...' button), 'Number of models to generate' (set to 10000), 'RCSB PDBIds to exclude from calculation', and a checkbox for 'Exclude flexible parts? - Not recommended.'. There is also a 'help' link. Below the form is a login section titled 'Username and password' with fields for 'Username' (containing 'abonvin') and 'Password' (masked with dots), and a 'Submit Query' button. At the bottom, there is a section for 'Example of CS ROSETTA webservice output' and 'CS-ROSETTA WEBSERVER STATISTICS' showing server statistics generated on 2009-06-01 23:13:29, with 6 running requests and 0 queued requests.

CS-ROSETTA
e-NMR GRID-enabled web portal

Home HADDOCK Xplor-NIH CYANA FormatConverter eNMR-database eNMR-Grid Software eNMR Wiki

WELCOME TO THE E-NMR WEB PORTAL >>

CS ROSETTA is a protocol which generates 3D models of proteins, using only the ^{13}CA , ^{13}CB , $^{13}\text{C}'$, ^{15}N , ^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 spin.niddk.nih.gov/bax/software/CSROSETTA/index.html.

CS ROSETTA WEBSERVER

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

Setup your CS-Rosetta run

Give your run a name

TALOS file to submit

Number of models to generate

RCSB PDBIds to exclude from calculation

Exclude flexible parts? - Not recommended. ☐

[help](#)

Username and password

Username

Password

Example of CS ROSETTA webservice output

CS-ROSETTA WEBSERVER STATISTICS

Server statistics generated on: 2009-06-01 23:13:29

Number of running requests: 6

Number of queued requests: 0

www.enmr.eu/webportal

Web portal to chemical shift-based structure calculations with Rosetta

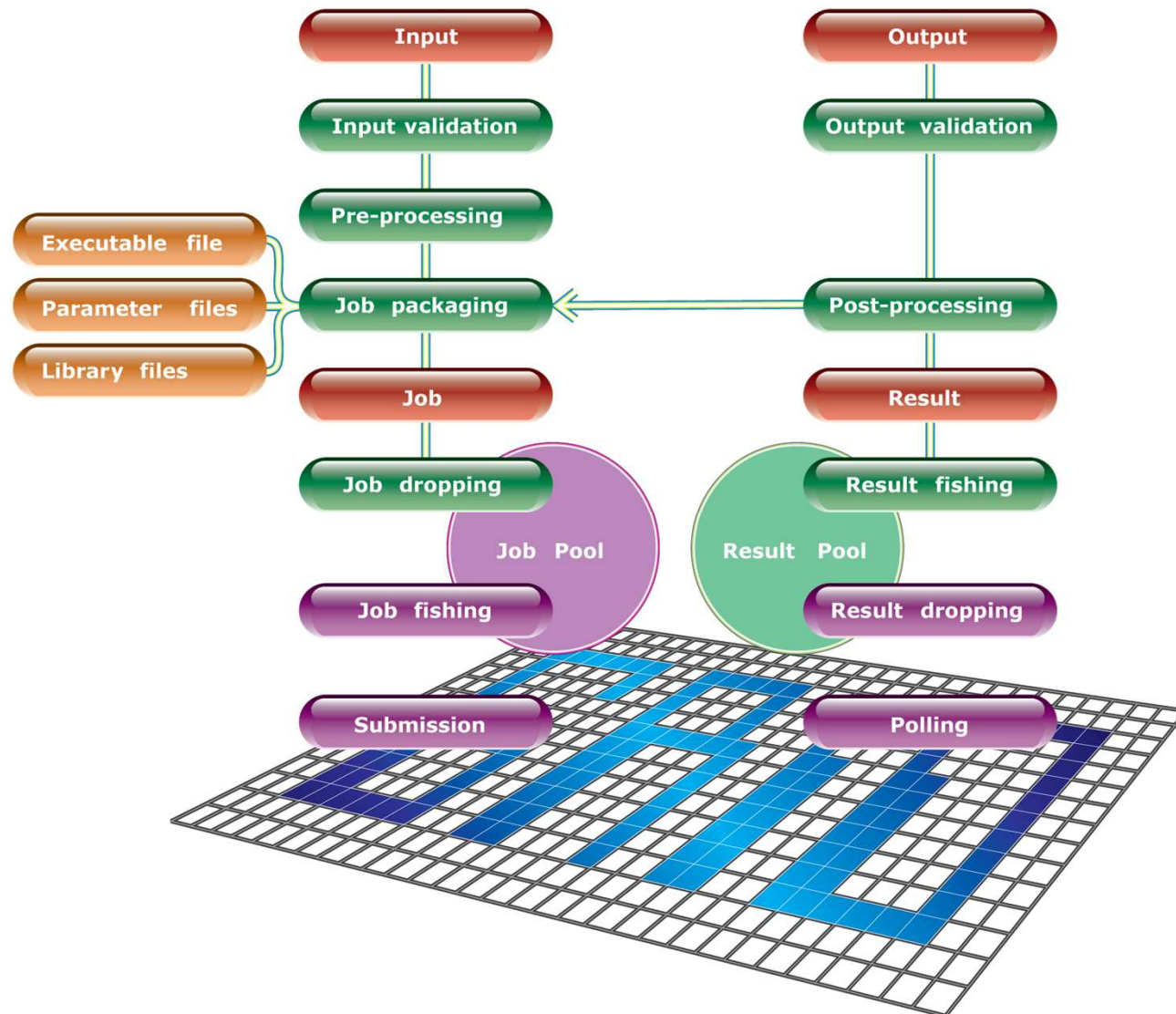
Rosetta is extremely CPU intensive and can perfectly make use of the GRID resources

One typical run would require between 1000 and 5000 CPU hours on a single processor!

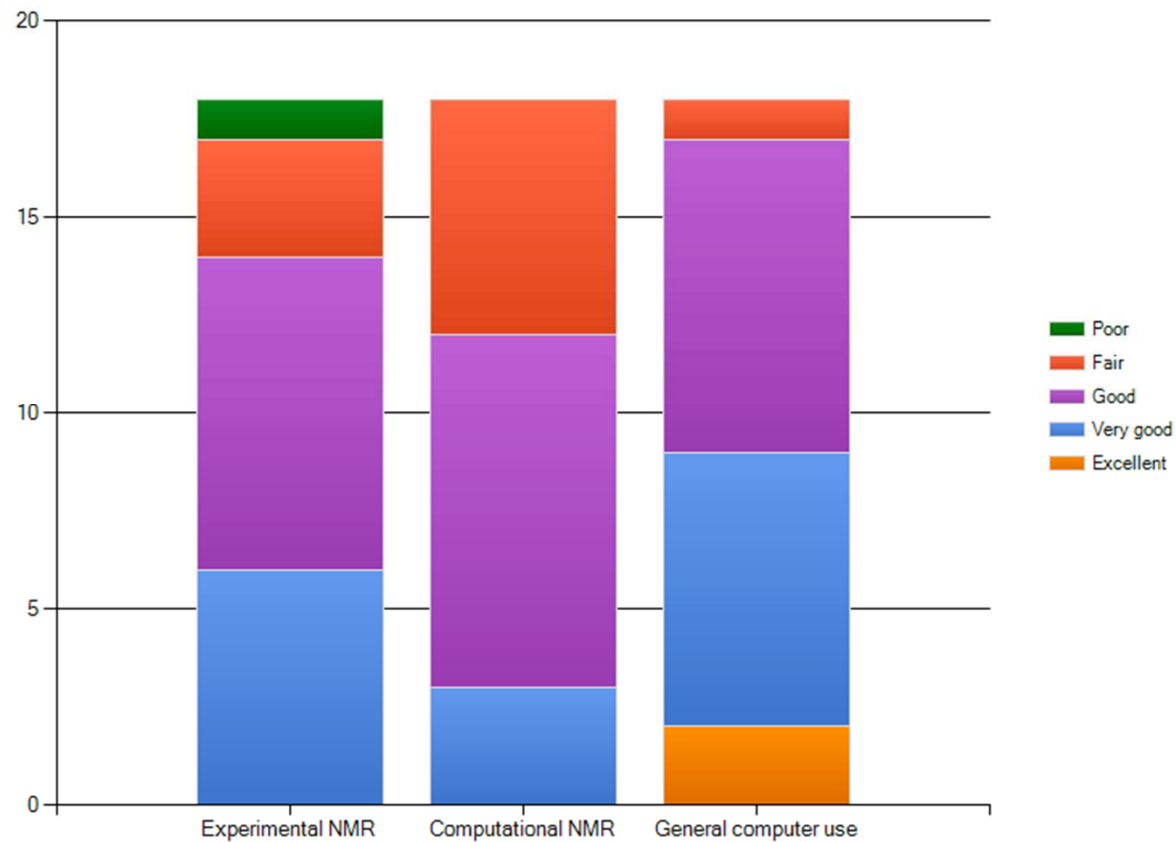
Only a few days on the GRID depending on the load

GRID daemon beyond a portal

(e-Token based robot certificate)

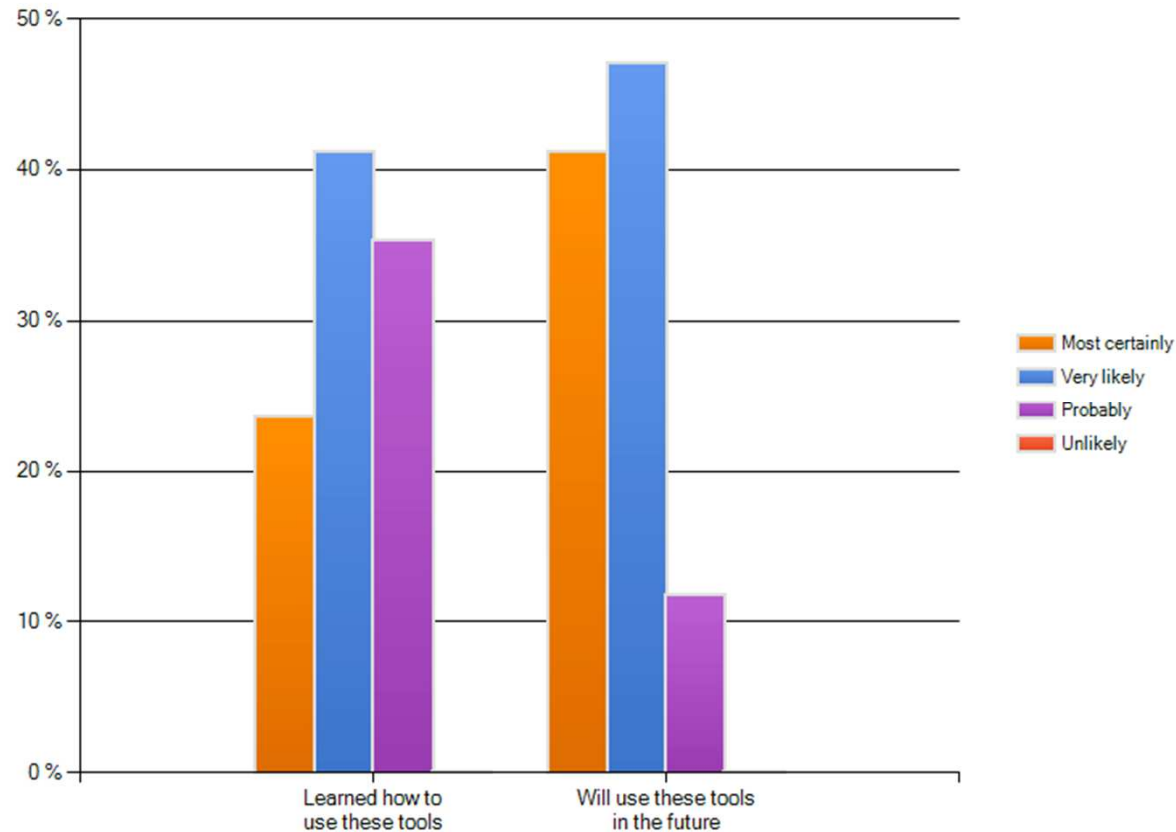


NMR User profile (I)



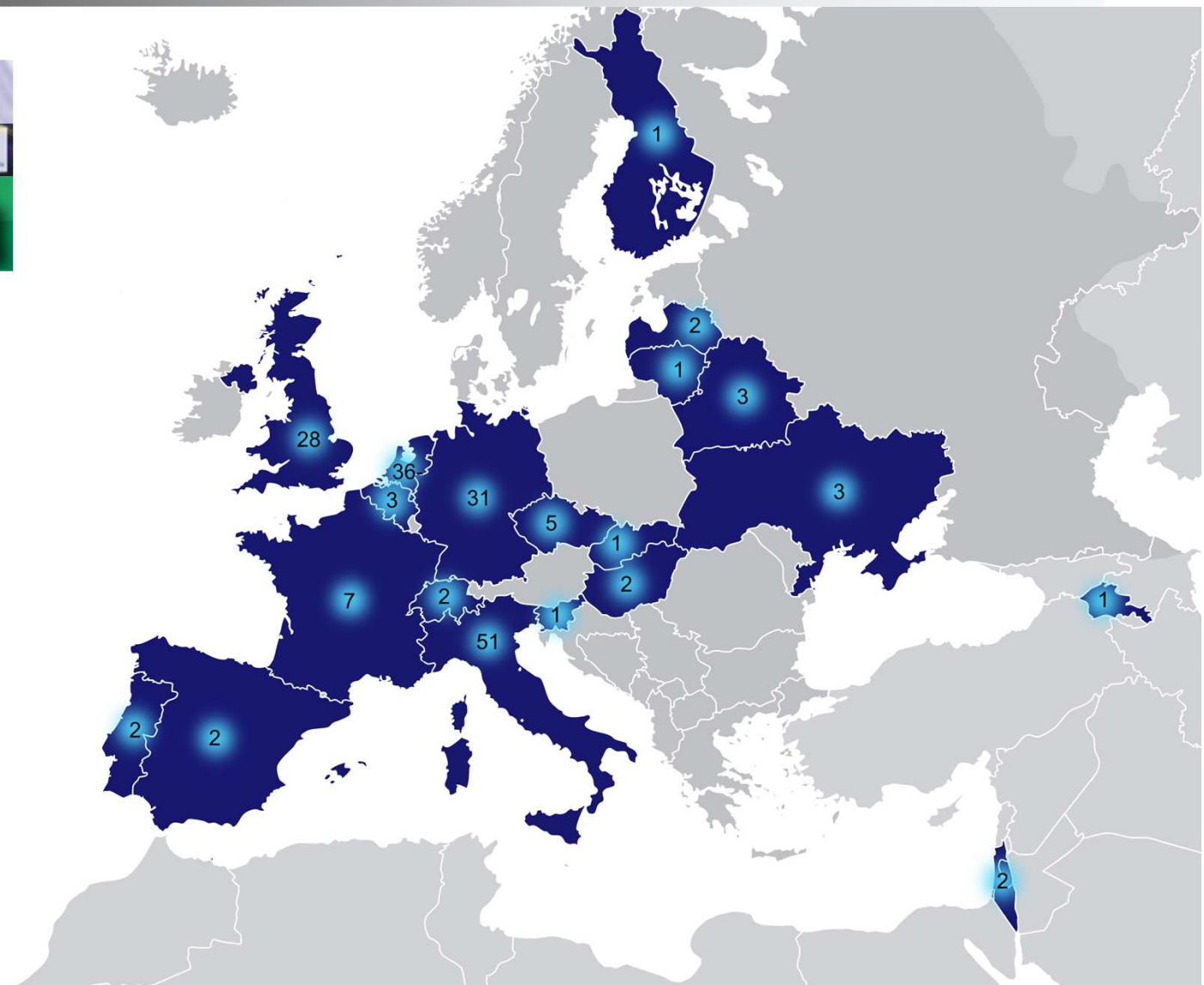
Knowledge level of participants in three key areas

NMR User profile (II)



Participant assessment of workshop tool elucidation, and future prospect for tool (web portals) usage

VO users distribution



Some facts to summarise ...

- **2nd largest VO in the life sciences**
- **210 registered users and growing**
- **> 13000 CPUs**
- **> 350 CPU years over the last 12 months**
- **20% of Life Sciences on the Grid**
- **User-friendly access to e-Infrastructure via web portals**

e-NMR platform operational and well used!

- **Manuals for the e-NMR software and web-portals**
- **e-NMR use-cases for use with the User Interface**
- **PnP version of the gLite 3.1 UI (based on Gilda PnPUI)**
- **Virtual instances of UI with e-NMR enabled**

Zwartkijken / Idées Noires

"Life cycle of a GRID computing job?
That's something like:

Conception ...,
Abortion ...,
Conception ...,
Birth ...,
Premature death ...,
Reanimation ..., etc?
:p
T."

20100127 – 11 AM



eGEE
Enabling Grids
for E-science



BiG Grid
PHILIPS



Utrecht
University



e-NMR

Victor Zharavin
Peter Güntert
Henry Jonker
Harald Schwalbe
Wim Van Ken
Marco Verlat
Mirco Mazzucato
Antonio Rosato
Andrea Giachetti
Ivano Bertini
Dario Carotenuto
Alexandre Bonvin
Sjoerd de Vries
Gijs van der Schot
Marc van Dijk
Nuno Loureiro Ferreira
Rolf Boelens
Johan van der Zwan
Anurag Bagai