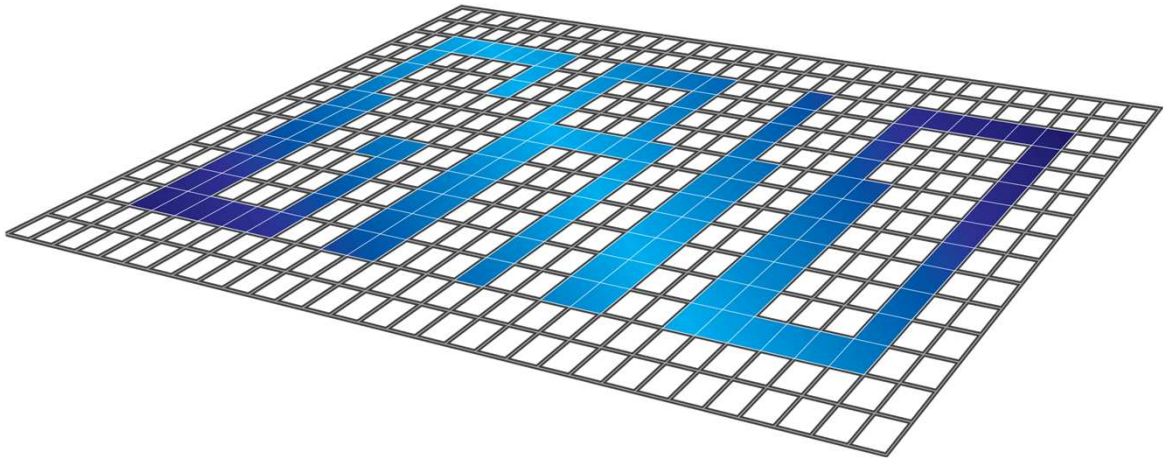
User Experience.
An emerging user community :

/O=dutchgrid
/O=users
/O=universiteit-utrecht
/OU=chem
/CN=Nuno Loureiro Ferreira @

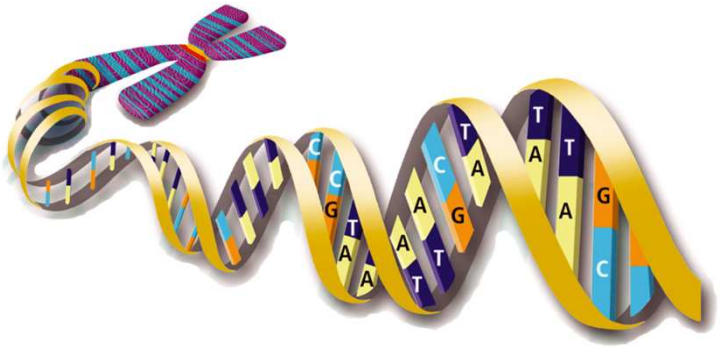
EGI Technical Forum 2010

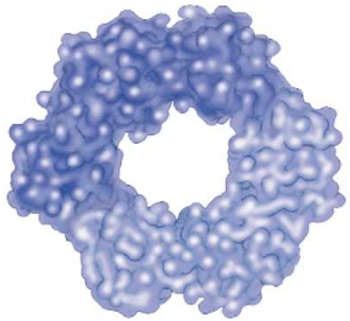
Outline

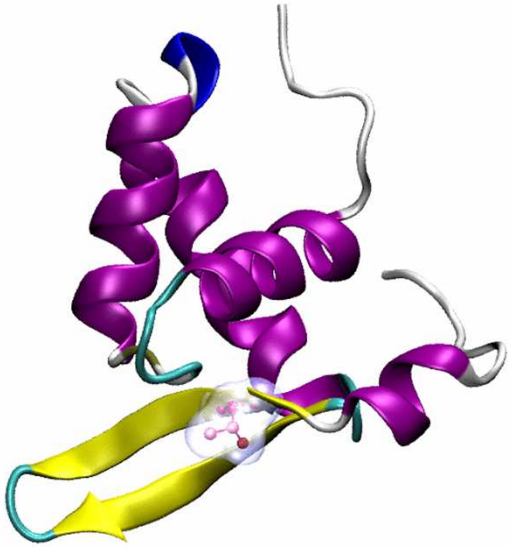
- Introduction & Scientific context
- The e-NMR project
- e-NMR Web portal
- Final remarks



Biomolecular structure … why?

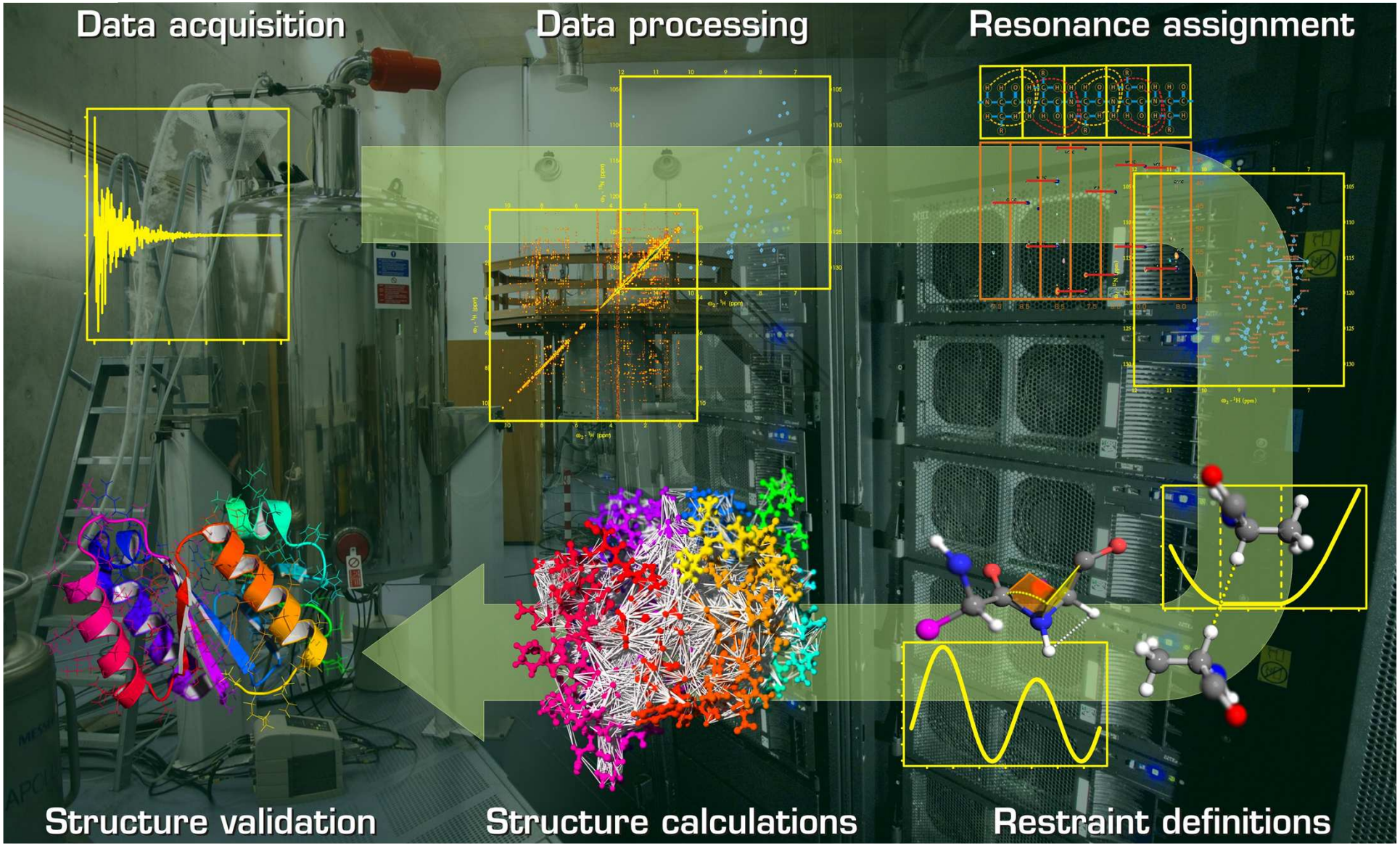




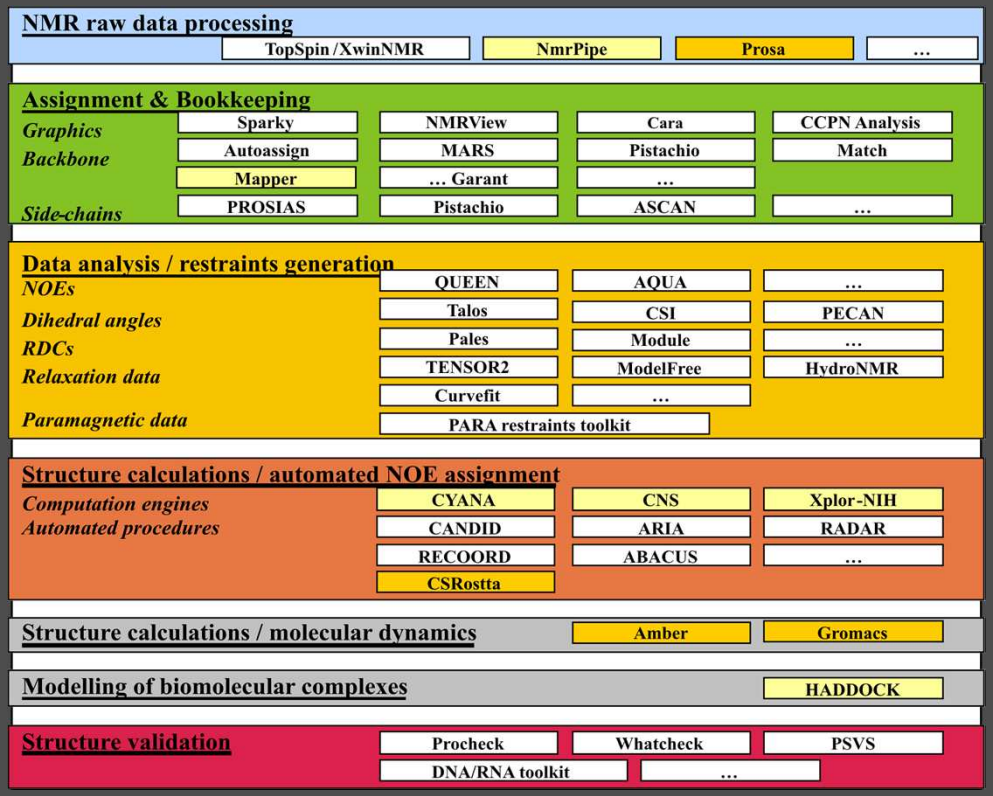


- **Function an mechanism of action**
- **Design of Experiments**
- **Understand Effects of Mutations**
- **Drug Design**

*N*uclear *M*agnetic *R*esonance

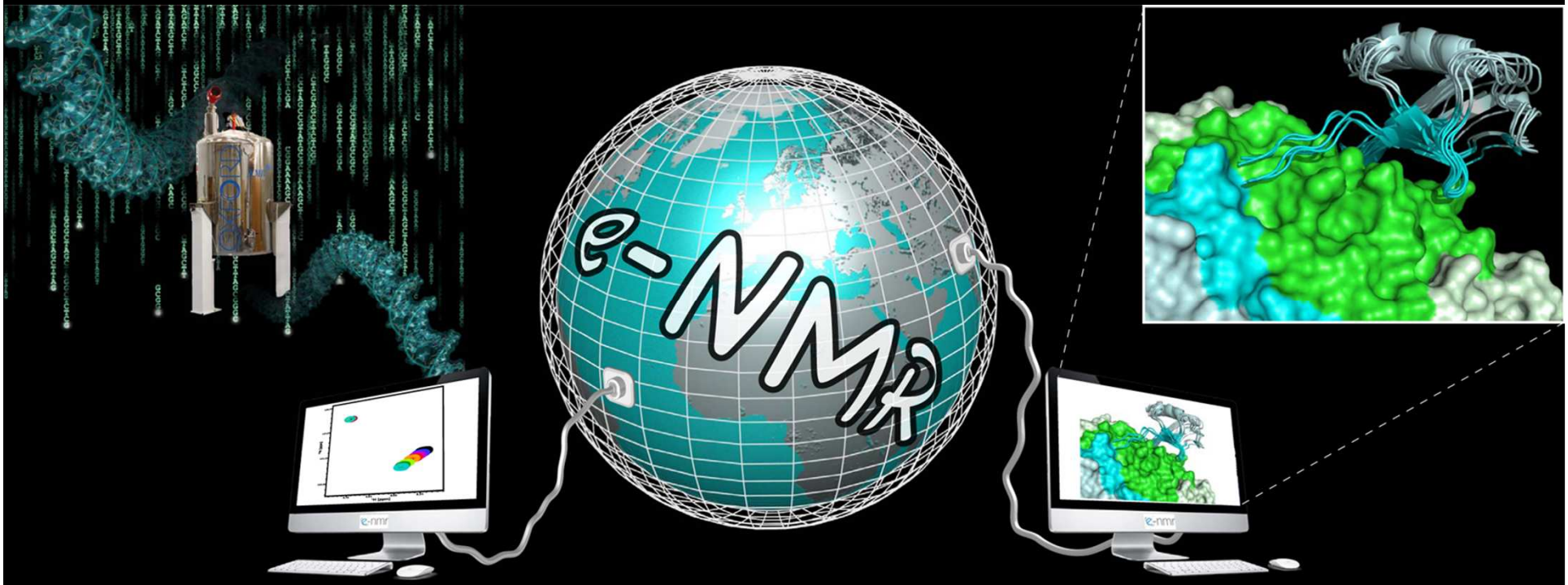


Practical issues ...



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

e-NMR objectives



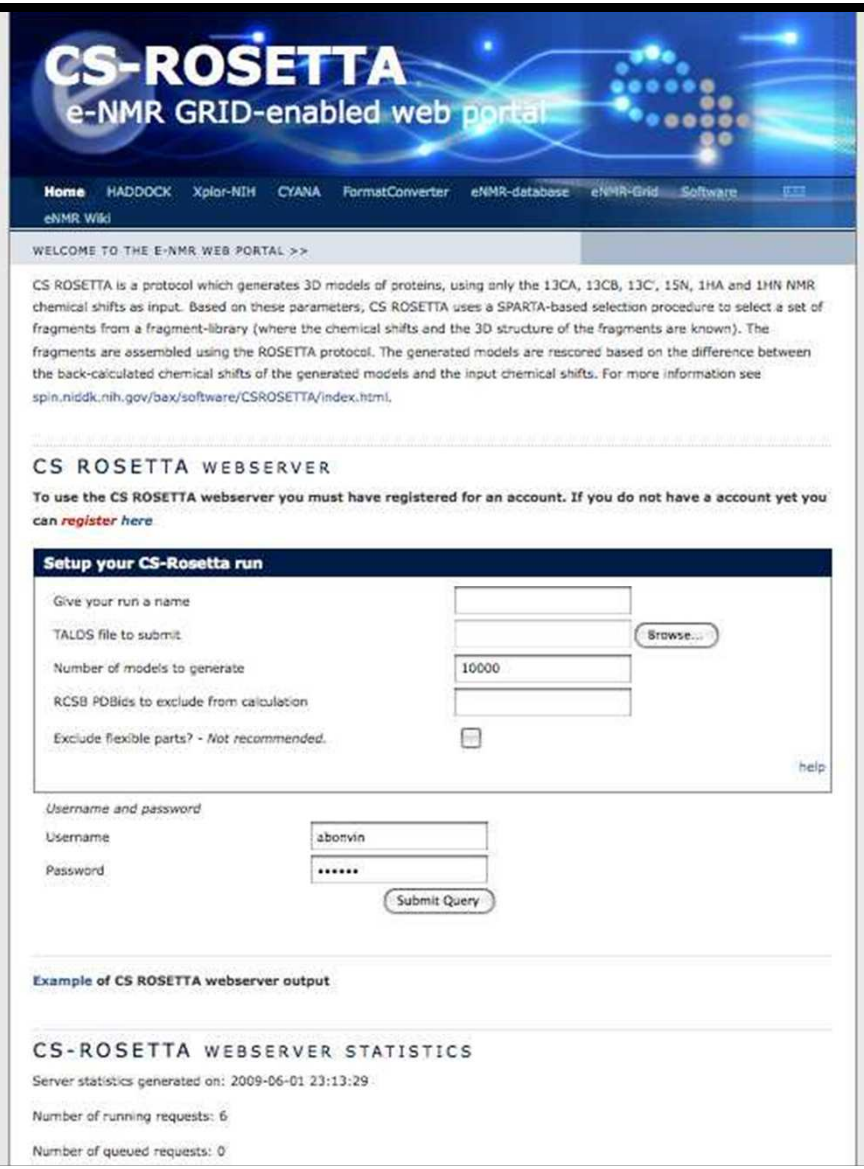
- Integrated protocols of NMR applications
- Easy access to web interfaces
- Exploit GRID technology
- Lower the access level to GRID technology in life sciences

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

User friendly interface



www.enmr.eu/webportal

Web portal to chemical shift-based structure calculations with Rosetta

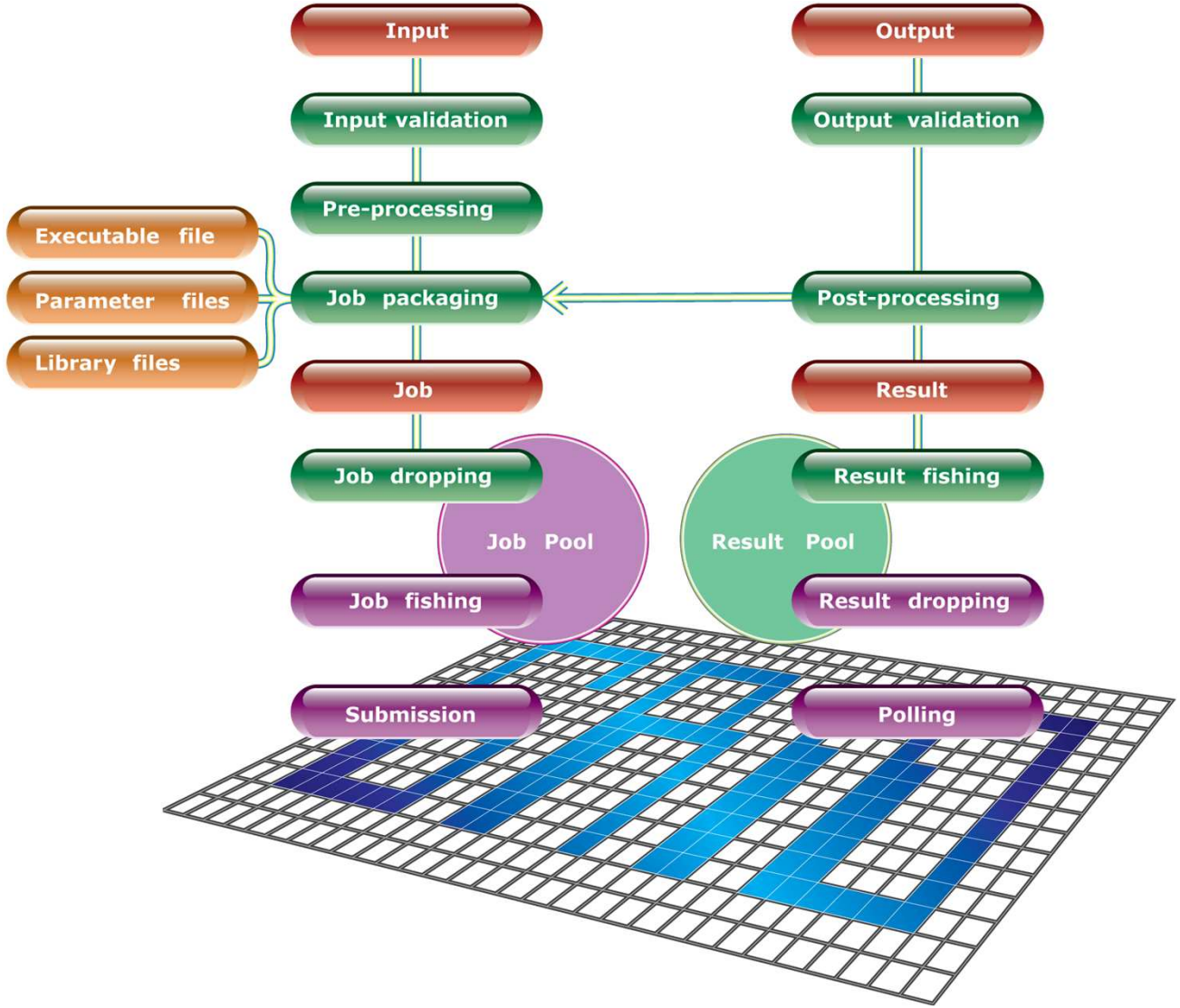
Rosetta is extremly CPU intensive and can perfectly make use of the GRID resources

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

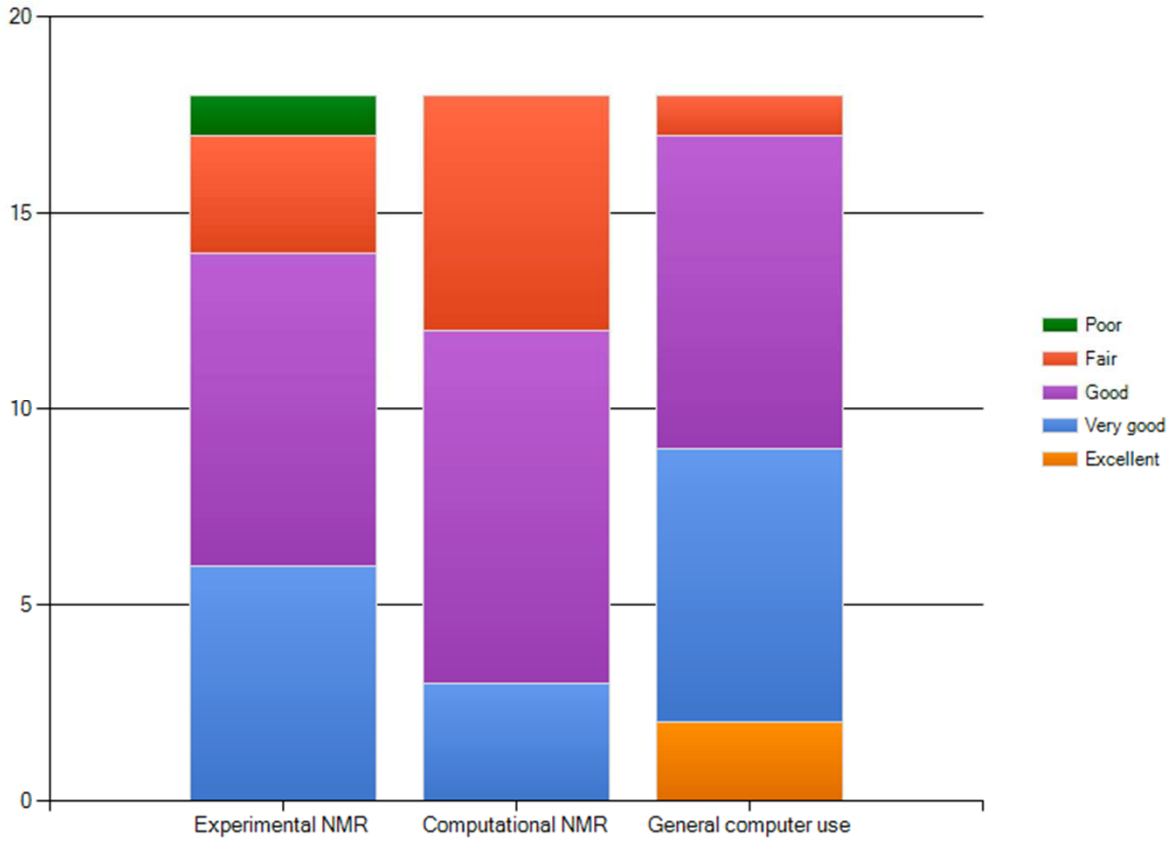
Only a few days on the GRID depending on the load

GRID daemon beyond a portal

(e-Token based robot certificate)

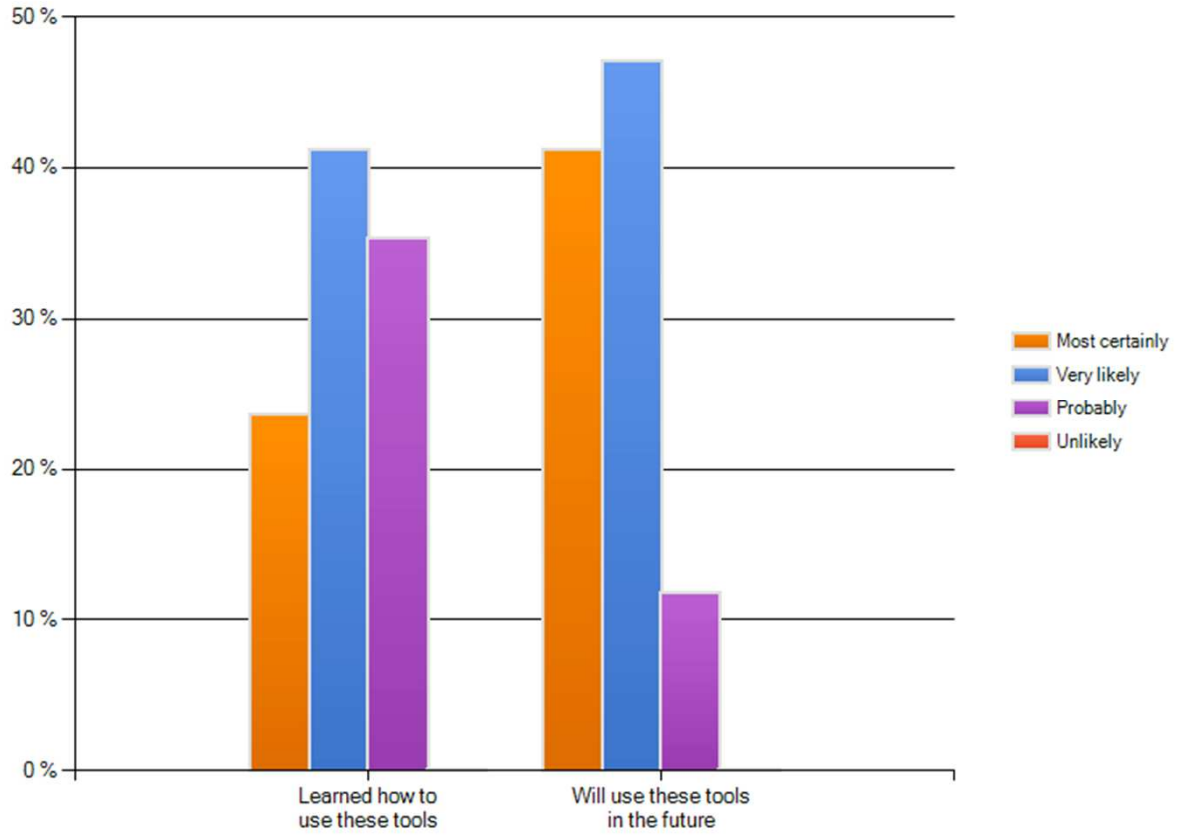


NMR User profile (I)



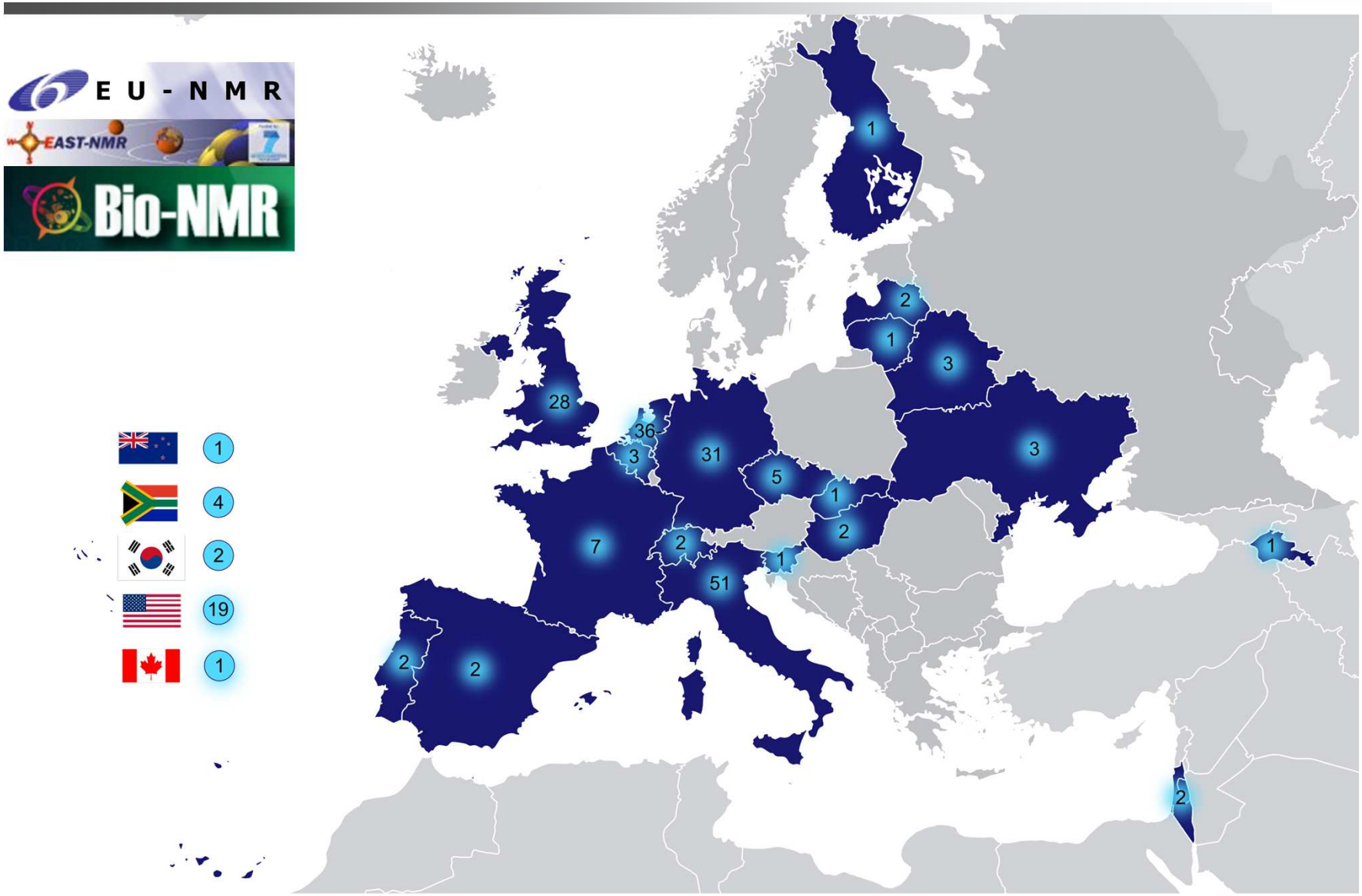
Knowledge level of participants in three key areas

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!

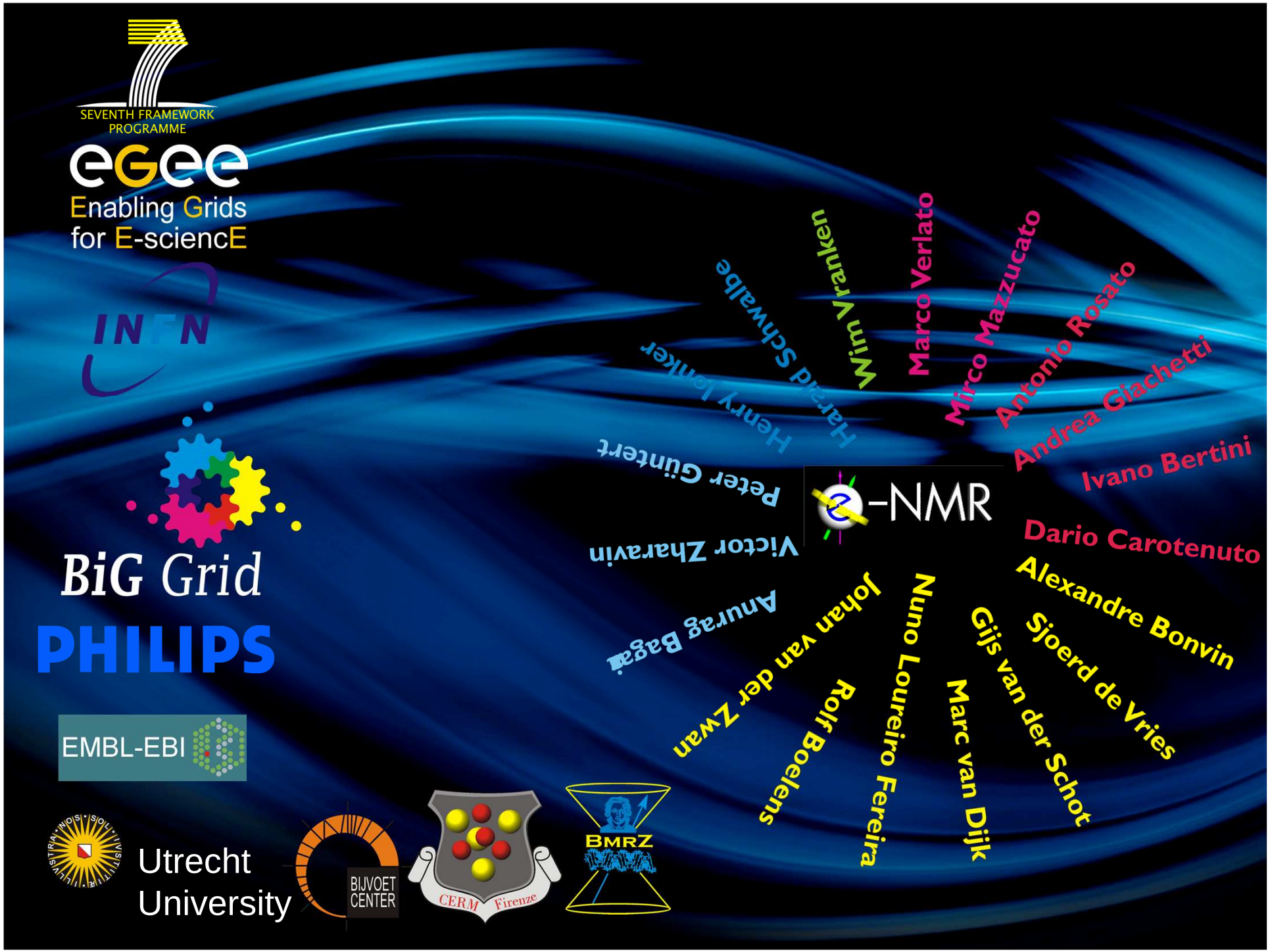
- Manuals for the e-NMR software and web-portals
- e-NMR use-cases for use with the User Interface
- PnP version of the gLite 3.1 UI (based on Gilda PnPUI)
- Virtual instances of UI with e-NMR enabled

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


SEVENTH FRAMEWORK PROGRAMME
eGee
Enabling Grids for E-sciencE
INFN
BiG Grid
PHILIPS
EMBL-EBI
Utrecht University
BIJVOET CENTER
CERM Firenze
BMRZ
e-NMR
Wim Vranken
Marco Verlato
Mirco Mazzucato
Antonio Rosato
Andrea Giachetti
Ivano Bertini
Harald Schwalbe
Henry Jonker
Peter Güntert
Victor Zharavin
Dario Carotenuto
Anurag Bagai
Johan van der Zwan
Nuno Loureiro Fereira
Alexandre Bonvin
Rolf Boelens
Marc van Dijk
Gijs van der Schot
Sjoerd de Vries