A success story....

A worldwide e-Infrastructure for NMR and structural biology

Toward full automation of structure determination by NMR

10th e-Infrastructure Concertation meeting, Brussels March 6-7 2013

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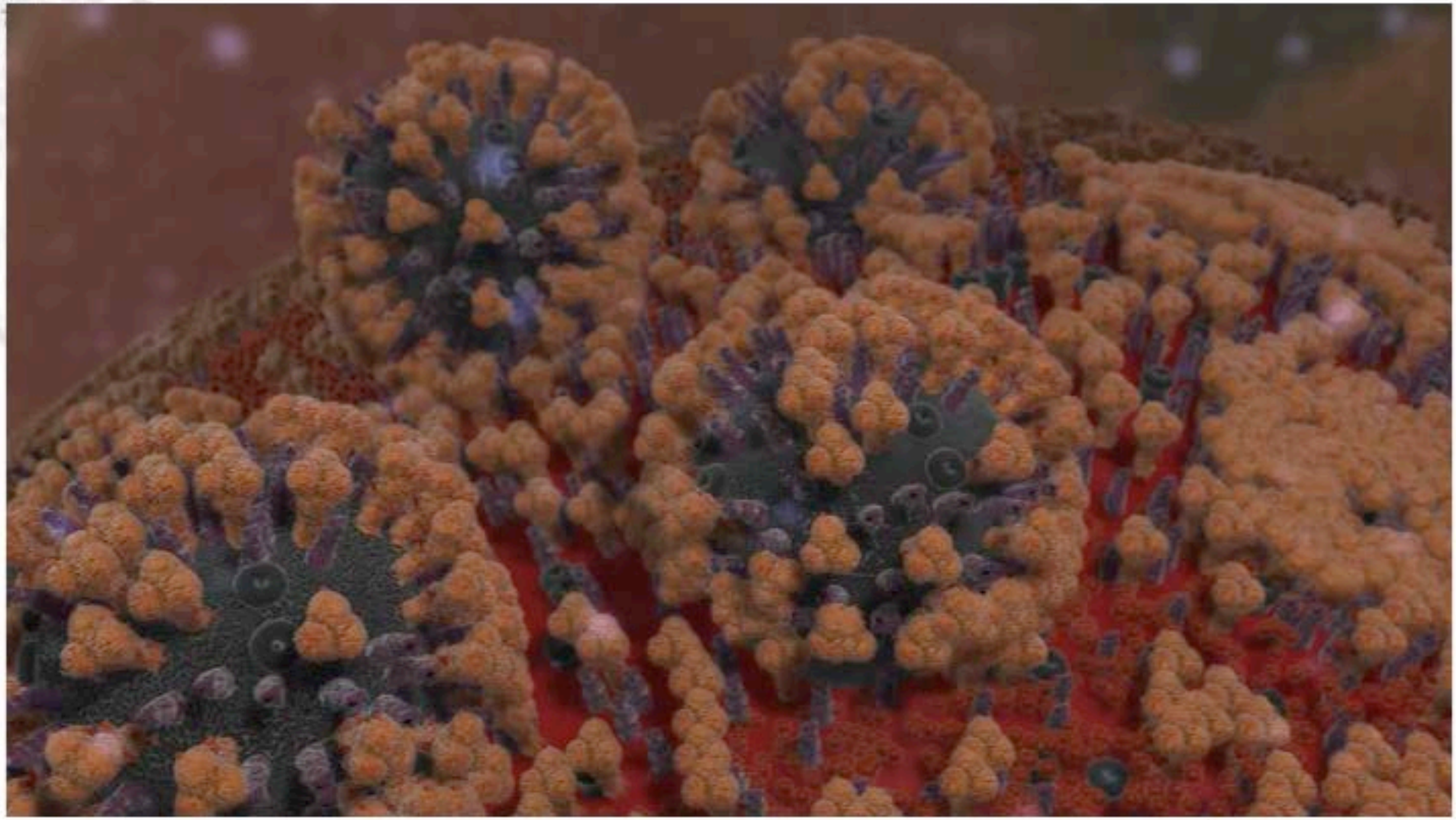
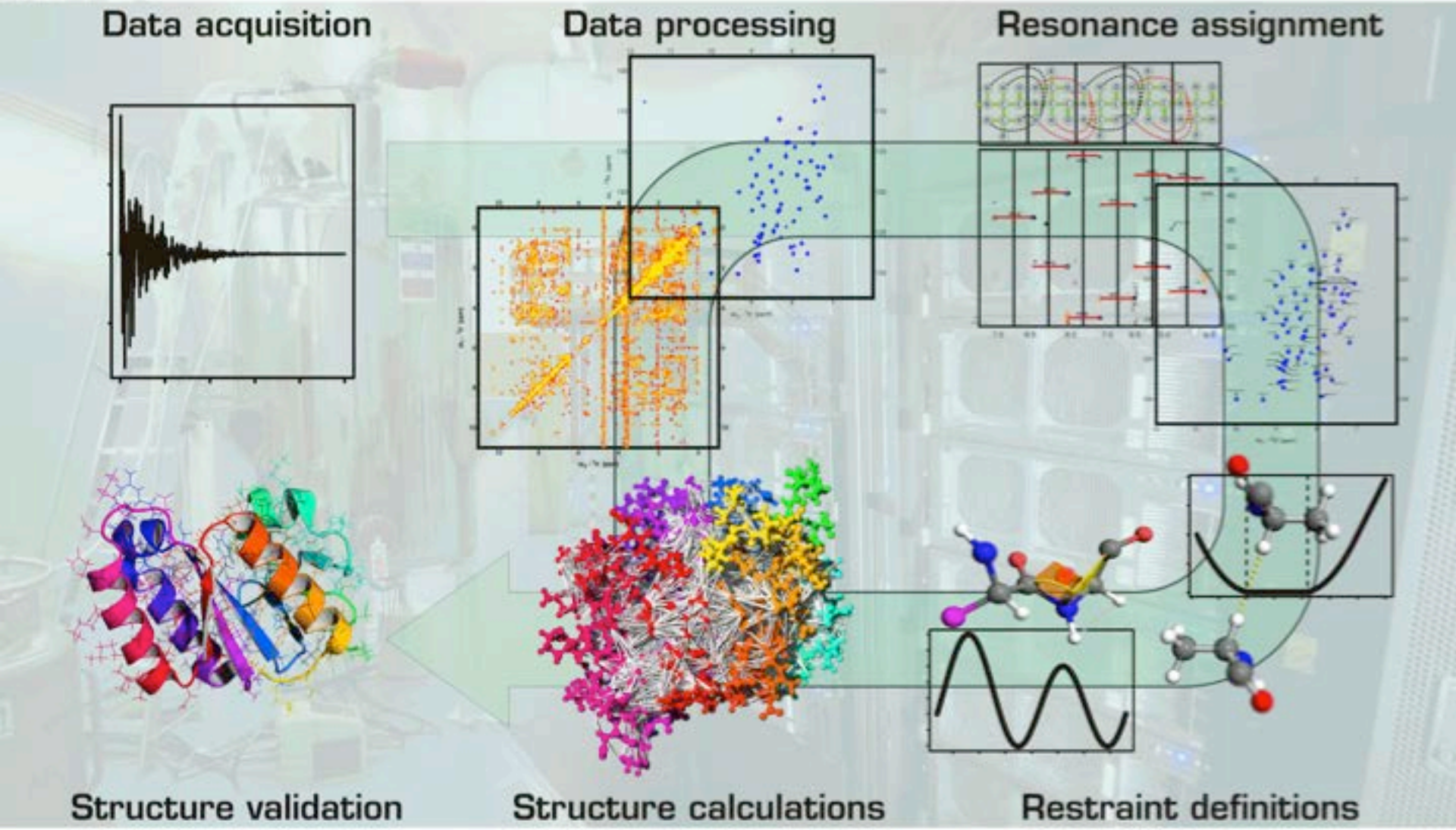
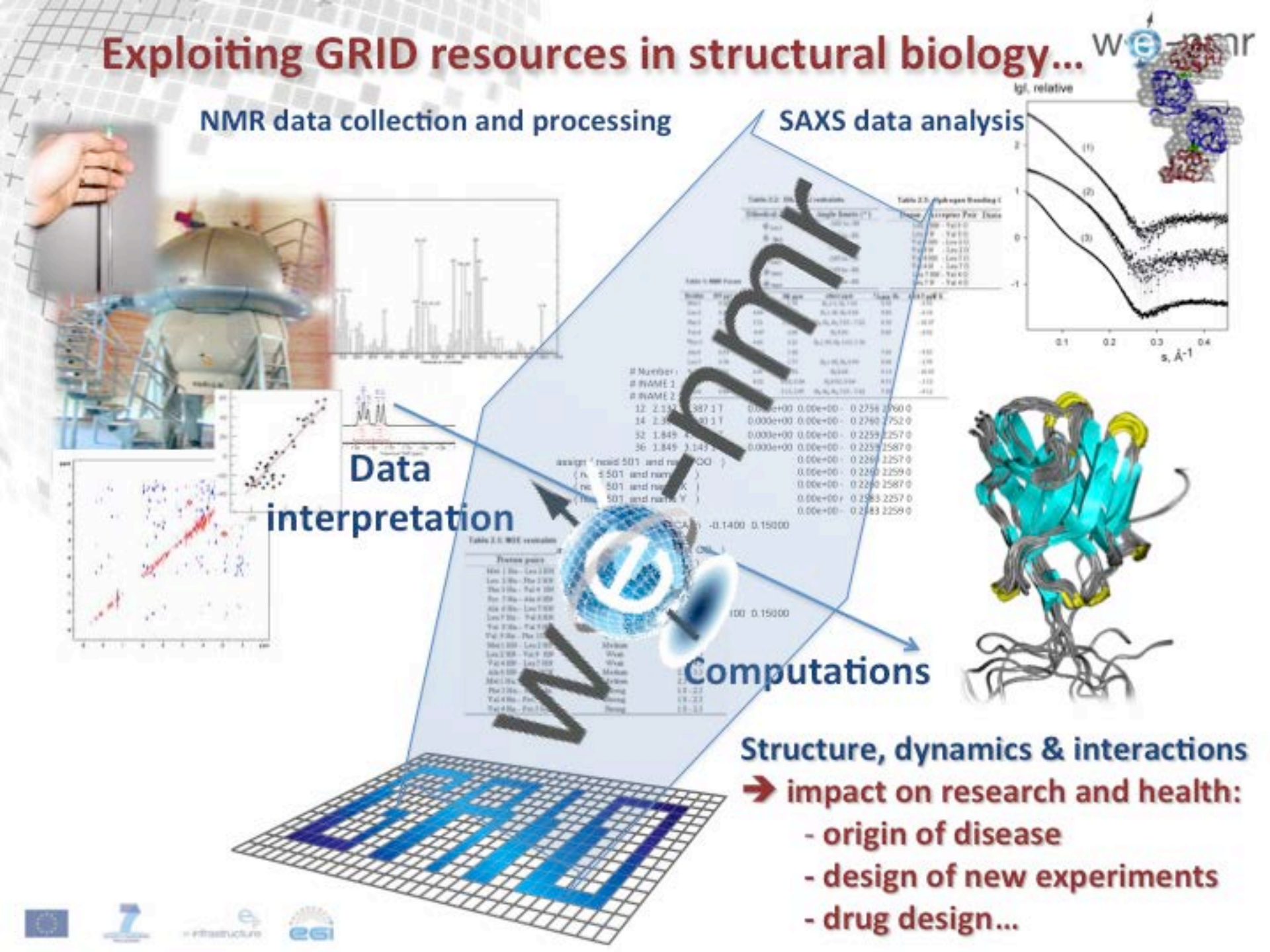
NMR and structural biology



The NMR structure determination workflow



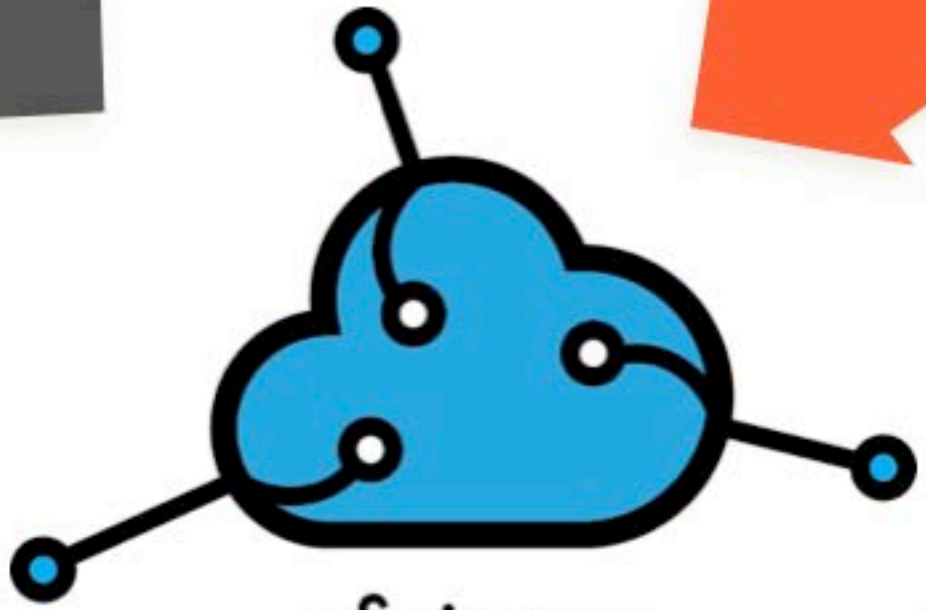
Exploiting GRID resources in structural biology…



The WeNMR VRC

Community

Infrastructure



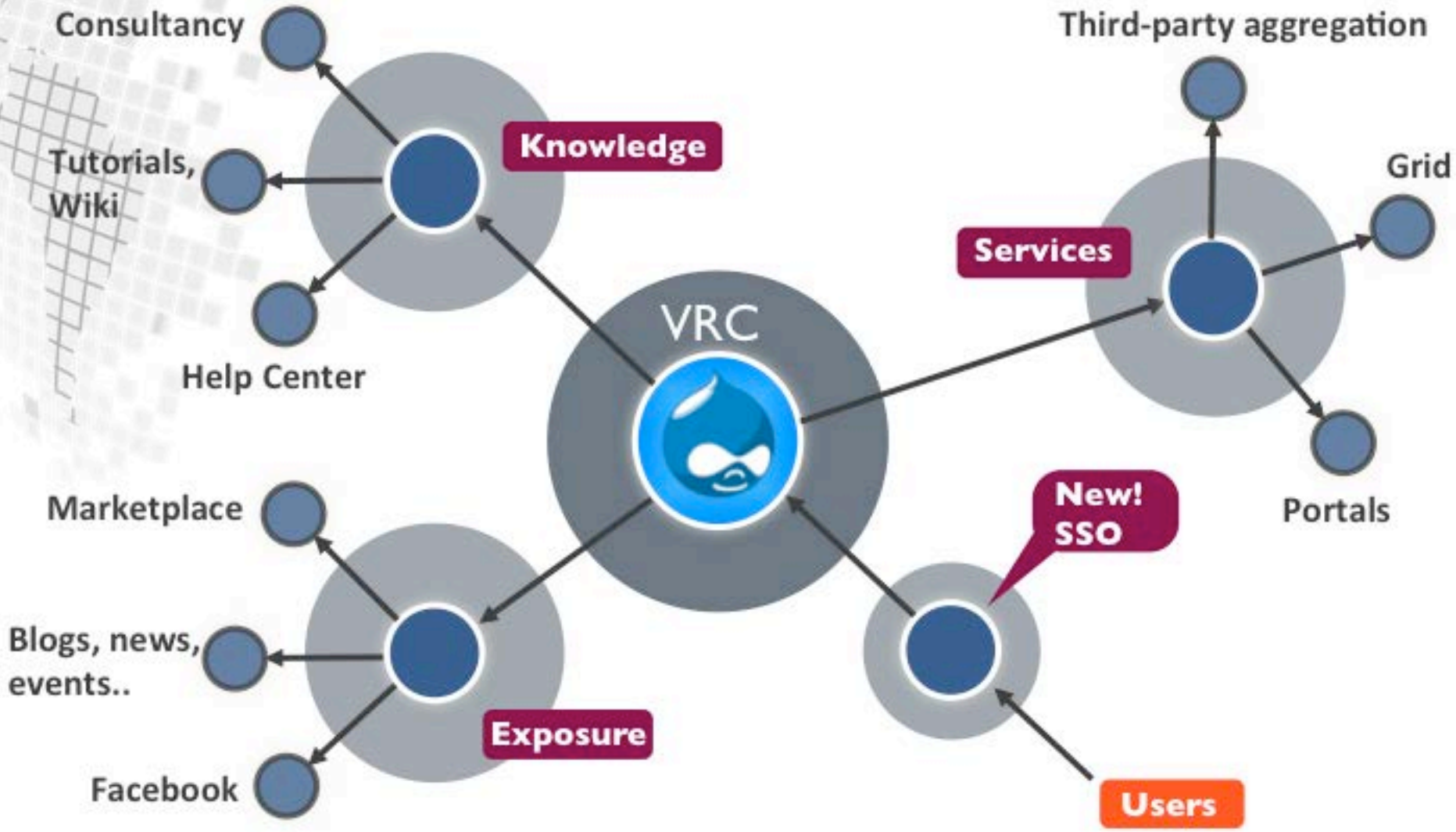
eScience
hub in the Cloud

Science

Knowledge

eScience hub for NMR and structural biology

The WeNMR VRC



www.wenmr.eu

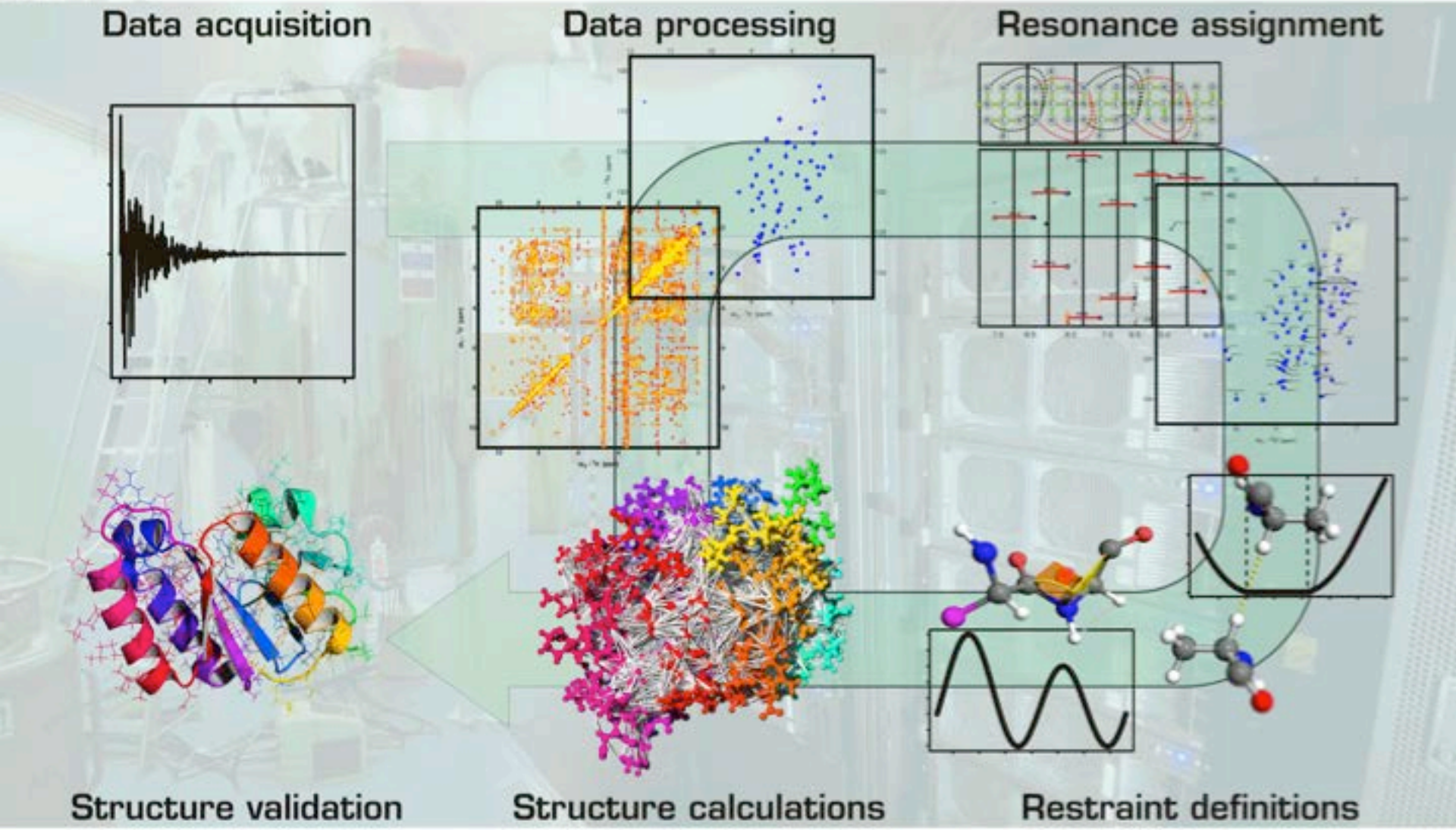
The WeNMR services portfolio

WeNMR platform (February 2013)

- Largest VO in the life sciences
- > 500 registered users (29% outside the EU)
- ~ 45 000 CPU cores
- > 330 CPU years over the last 12 months
- > 1.25 million jobs over the last 12 months
- User-friendly access to Grid via web portals

www.wenmr.eu

The NMR structure determination workflow



CORRESPONDENCE

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

nature methods
Techniques for life scientists and chemists

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

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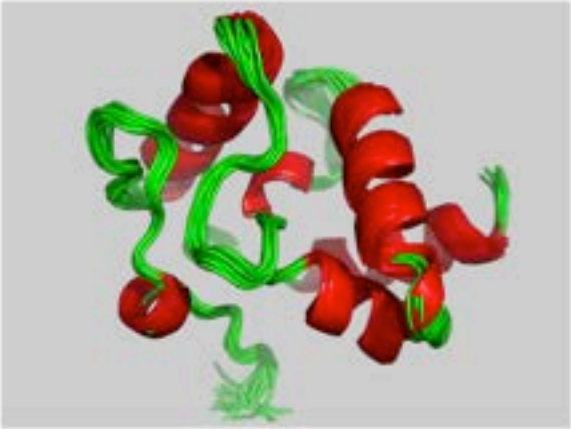

- **10 blind targets** (structures to be determined by fully automated methods
- **15 teams worldwide** involved with their respective developer teams
- Assessment of results by independent team

- **Impact: WeNMR & EU as drivers of innovation, leading to to new software developments, increased trust in automated methods and improved services for end users**

CASD-NMR

Structure

Ways & Means

Structure 20, 227–236, 2012

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

Antonio Rosato,[1,2,*] James M. Aramini,[3] Cheryl Arrowsmith,[4] Anurag Bagaria,[5,6] David Baker,[6] Andrea Caval
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research advances

April 2012 technical highlight

Protein Structure Initiative

Blind faith

SBKB [doi:10.1038/sbkb.2011.73]

A rigorous assessment of automated NMR structure determination demonstrates the reliability of the method.

Protein structure determination by NMR spectroscopy requires complete chemical shift assignments and manual analysis of thousands of atomic interactions known as nuclear Overhauser effects (NOEs). Recently developed algorithms use these data to calculate structures in automated, iterative NOE assignment protocols. Additional methods have emerged that rely on the intrinsic structural information encoded in the chemical shifts supplemented with NOE data.

Rosato and colleagues (PSI NESG) present the results of CASD-NMR, a blind assessment of how the available automated methods compare with the traditional manual approach. The authors stringently evaluated the results for ten structure determinations of monomeric proteins ranging in size from 60 to 150 amino acids. They assessed three groups of automated methods using either NOE or chemical shift data, or a combination of both. The accuracy and convergence of the automatically calculated structures was compared to manually solved reference structures using the root-mean-square deviation (RMSD) of structured backbone regions.

Setting a threshold for accuracy at an RMSD of 2 Å from

European Grid Infrastructure

towards a sustainable infrastructure

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

13 April 2012
Neasan O'Neill

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 ported 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.

Acknowledgments

The team

Alexandre M.J.J. Bonvin
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European Molecular Biology Laboratory, Hamburg, DE
Spronk NMR Consultancy, LT
Academia Sinica

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WeNMR
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