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Three years of WeNMR: successes and challenges

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Structural biology is concerned with the determination of the three-dimensional structures of bio-macromolecules and their complexes. The field contributes to society by supporting a wide range of applications that include drug design, crop improvement, and engineering of enzymes of industrial significance. Its present challenges include the integration of data from various methods, gaining access to sufficient computational resources, developing off-the-shelves solutions for non-expert and dealing with large data sets.
The three-year FP7 project WeNMR (Wassenaar et al., J. Grid. Comp. 2012) aimed and succeeded to optimise and extend the use of Nuclear Magnetic Resonance (NMR) and Small-Angle X-ray Scattering (SAXS) to determine the structure and properties of proteins and other medically important molecules. For this, a Virtual Research Community (VRC) scientific gateway was established (www.wenmr.eu), offering training material, a support center, standard workflows, services through easy-to-use web interfaces and a single-sign-on mechanism. After three years of operations, the WeNMR VRC has grown to over 900 users and its VO (enmr.eu) over 575 users from 42 countries worldwide (36% outside Europe). Software applications often used for NMR, and, more recently, SAXS have been made available through web application portals (39 to date), making efficient use of the European Grid Infrastructure (EGI).

Wider impact and conclusions

In summary, WeNMR has successfully built a vibrant, worldwide and highly active Virtual Research Community promoting the use of e-Science solutions for excellent science in structural biology.

URL(s) for further info

www.wenmr.eu

Description of work

WeNMR brings together a diverse group of stakeholders and has tight connections with various European Research Infrastructure projects (e.g. BioNMR) and the ESFRI Instruct project. It is the user-friendly access to software solutions and the computational resources of the grid that attract users, together with the excellent support and training offered. More than 90 peer-reviewed articles have been published by consortium members and external users in high-ranking journals.

WeNMR is currently supported by 31 grid sites from various countries including in Europe the National Grid Initiatives (NGIs) of Belgium, France, Germany, Italy, the Netherlands, Poland, Portugal, UK, and outside Europe, Brazil, China, Malaysia, South Africa, Taiwan and US, for a total of over 82K CPU cores, all of this shared with others regional and global VOs. The dedicated computing and storage resources of WeNMR (located in Utrecht, Florence and Frankfurt) correspond to 320 CPU cores and 3.9 TB of disk space. Over 2M SI2K.years were consumed during the three years of the project corresponding to 5.4M grid jobs. It is the second most used VO in life sciences and the largest in terms of number of users.

WeNMR has actively promoted the use of e-Science solutions at national and international conferences and organized several workshops. Some of the lectures are available from the WeNMR YouTube channel. In addition, WeNMR has also reached out to e-Infrastructure resource providers at regional, national (NGIs) and European (EGI) levels and even worldwide levels (e.g. via connections to Open Science Grid and XSEDE in the US) and to researchers in industry. It has created several movies for the general public, including the highly viewed Stories from Grid and SAXS animation movies.

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