



SEVENTH FRAMEWORK
PROGRAMME

Research Infrastructures

Deliverable 2.3

Reports on sustainability measures at each of the four production sites



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Prospects of WeNMR continuation

As described in D2.2 and reproduced below, WeNMR makes efforts to ensure continuation of the project results in the future. Each core partner site (Frankfurt, Florence, Utrecht, Padua) endeavors to **ensure that the WeNMR services will keep running**. Note that the sustainability plans for the Grid computational infrastructure of the different sites was also previously addressed in D2.1

- **Maintaining the hardware will continue** since NMR has always been associated with computing and running large facilities and laboratories will always require local computation resources. This was not funded by WeNMR.
- More problematic without future funding will be to maintain our middleware infrastructure since this requires quite some expertise and man power. For this **we anticipate that we will rely on National Grid Infrastructure for most of the grid services**. In principle, the only service required at a partner site in order to keep our web portals active is a User Interface (UI), in combination with robot certificates. We will however strive to keep all our grid services active after the end of the project, to bridge the gap until hopefully a follow-up project under the 2020 EU programme.
- **Software is expected to be kept updated**, as the software which is developed at the partner sites (e.g. HADDOCK in Utrecht, MaxOcc in Florence and CYANA in Frankfurt) will be updated and further developed through national or European research funding obtained by these partners. New services might be added on the request of external developers and such portals will be offered for the time they are being used or supported by the developer.
- For the **user community**, the **VRC and WeNMR website will keep operating** after the end of the project, provided that users, developers and ourselves keep using it by adding contents and answering requests. This is a standard task of software developers in general and the VRC site and its help center should facilitate this task. Costs for its operation and maintenance (i.e. mainly adding new features and dealing with Drupal issues) could be covered by including advertisements on the website or through the NMR marketplace that was introduced. Since most portals have a developer linked to the WeNMR help center, we expect that support will still be provided by the developers. Furthermore, with a "single sign on mechanism", we will be able to allow users without certificates to use our services in the future. This facilitation should lower the hesitation barrier for potential new users to using our services.
- **Future workshops on the tools offered are expected** to be offered either (semi-) commercially, or in joint efforts with other projects and organizations, like EMBO or national scientific communities. We intend to ensure the user community keeps growing as usage is the key to sustainability. To reach that goal, we intend to keep participating in conferences and workshops to promote the services offered by WeNMR.

Sustainability plan – Partner 1 – BCBR

Maintaining the hardware

The Utrecht site (BCBR) has currently one cluster integrated into the grid and several virtual machines hosting the various services. Another local cluster with over 700 cores is in production and could take over in case of hardware failure of the grid cluster. Further we are in the process of ordering a new cluster, which will ensure sufficient computing capacity for the coming years. All hardware currently integrated into the EGI grid is also used for the daily research of the group and hosts various web portals used by the worldwide community. As such maintenance of our hardware infrastructure is an intrinsic part of the group research.

Maintaining middleware with National Grid Infrastructures

The Utrecht site will keep operating its grid infrastructure and services as long as this is manageable from manpower perspective since no dedicated ICT support exists. All services are however running on virtual machines, which does facilitate the administration. Further we have discussed the option of having our grid infrastructure remotely managed by SURFSARA, something which is already in place in the Netherlands for the LifeScience distributed grid infrastructure. This will however only be considered if local support is no longer possible.

Maintaining software and portals

The Utrecht site will keep operating and maintaining the currently hosted web-portals, in particular:

- the HADDOCK web portal (both local version and grid-enabled version)
- the CS-Rosetta web portal
- the GROMACS web portal
- the UNIO web portal (in collaboration with Dr. T. Herrmann, ENS Lyon)
- the 3D-DART web portal

The Talos web-portal might be discontinued since the developers of this software are now offering their own web portal. We will therefore redirect traffic to their site. In that way users will be ensured of the most up-to-date software.

Maintaining VRC and WeNMR website

The VRC web site is hosted at the Utrecht site and will continue operating. The drupal systems allows for remote management by all involved partners. Basic support for the site's maintenance (drupal components) will be provided by the SpronkNMR partner. SpronkNMR will also aim at some commercial exploitation of the web site to generate some income to support the site maintenance. Further, another main developers of the web site, Dr. M. van

Dijk, will leave the university at the end of the project, starting his own company. We are currently discussing the possibility of some basic maintenance being offered by that new company after the end of the project.

The VRC site will remain the medium of choice for interaction with users, posting of tutorials, wiki entries and news and events. With the implementation of the SSO service, the portal also greatly facilitates the user administration for the various WeNMR web portals. Finally, the Utrecht group will keep providing support and expertise to the WeNMR help center for all issues related to services and software hosted in Utrecht.

Organization of future workshops

Next to the many WeNMR activities, the Utrecht group has and will continue to organize workshops covering various aspects of biomolecular NMR and in particular the HADDOCK software. WeNMR services and its VRC will be promoted at all conferences and workshops to ensure a high visibility of our services.

Sustainability plan – Partner 2 – BMRZ

Maintaining the hardware

The computer cluster used for the WeNMR services will be maintained. All essential grid services, beside the worker-nodes, are deployed as virtual machines and can easily be transferred when needed to maintain our services

Maintaining middleware with National Grid Infrastructures

We aim to maintain the essential grid middleware (currently EMI versions) up-to-date according to the requirements of the German NGI to anticipate on follow-up projects under the 2020 EU programme. We intend to keep the current setup in place, and for some services we may as well rely on the national and European infrastructure. In principle, the only service required to keep the BMRZ WeNMR web portals running on the grid is a User Interface (UI) in combination with a webserver and a robot certificate.

Maintaining software and portals

The software will be maintained and upgraded when needed. Some of the web portals run in-house BMRZ software (e.g. CYANA, UPLABEL and MDD-NMR) and can be kept up-to date to the latest versions. For other web portals (such as MARS) we anticipate on the input of the software developers and/or requests by the users. The web portals will be offered for the time they are being used and supported. Some new web portals are being developed and will be maintained in the same way as mentioned above.

Maintaining VRC and WeNMR website

BMRZ will participate in the help center as long as it is being offered. Furthermore there is a local feedback form in-place, where the users of the BMRZ WeNMR web portals can directly contact the staff maintaining the services.

Organization of future workshops

Workshops will be offered mostly in combination with other projects (such as EMBO and German NMR). BMRZ will keep participating in national and international conferences and promote the WeNMR services.

Sustainability plan – Partner 3 – CIRMMP

Maintaining the hardware

The CIRMMP site has currently one cluster integrated into the grid and several virtual machines hosting the various services. The current cluster cumulatively holds 80 cores. This hardware is used also for the daily research of the group and hosts various web portals for biomolecular NMR applications that are available to the worldwide community. Additional portals and databases related to the bioinformatics research activities at CIRMMP in the field of bioinorganic chemistry are hosted on separate servers.

We recently secured funds for the Regional (Tuscan) government for a significant expansion of our computing capacity, including a new cluster with 500-1,000 cores (depending on the outcome of negotiation also with suppliers), a GPU cluster harboring 16 Fermi GPUs, and storage capacity (SAN NAS) up to 20 Tb. This will be the largest upgrade of the computational infrastructure at CIRMMP since its involvement in the eNMR and WeNMR projects, and will ensure sufficient computing capacity for the coming years.

Maintaining middleware with National Grid Infrastructures

CIRMMP is a member of the Italian Grid Infrastructure (<http://www.italiangrid.it/about/members>). As such it is committed to maintaining the essential grid middleware up-to-date. This will be useful in anticipation of future initiatives as well as to sustain the services provided to researchers in biomolecular NMR. CIRMMP has tight interactions with INFN (Partner 4 and also a member of IGI) and thus will be able to rely on its documented willingness to support a number of components. The majority of services are hosted on virtual machines, which allows them to be moved with relative ease.

Maintaining software and portals

The CIRMMP site will keep operating, maintaining and, when required by internal or external users and deemed feasible for the available human resources, the currently hosted web-portals, in particular:

- the AMPS-NMR web portal, for AMBER MD simulations and macromolecular structure refinement
- the Antechamber web portal
- the Xplor-NIH web portal including paramagnetic restraints
- the AnisoFit web portal, for fitting pseudocontact shift and residual dipolar coupling data
- the MaxOcc web portal
- the sedNMR web portal

The AnisoFit, MaxOcc and sedNMR portals provide access to software entirely developed by CIRMMP. The AMPS-NMR and Xplor-NIH portals provide access to software developed by

external teams, for which CIRMMP produced add-ons, specifically aimed at handling paramagnetic restraints.

Maintaining VRC and WeNMR website

CIRMMP will participate in the help center as long as it is being offered. We will also continue to use the VRC as a dissemination media and reference point for tutorials and practical instructions related to the portals provided, also for use in training workshops. In addition, we will typically provide access to new portals developed in the context of other research activities at CIRMMP via the WeNMR VRC.

Organization of future workshops

The Florence group has and will continue to organize workshops covering various aspects of biomolecular NMR. This will presumably be done in collaboration with or within the context of other projects such as the ESFRI Infrastructure Instruct, which co-sponsored a WeNMR workshop in January of 2013, or the infrastructure project Bio-NMR. Plans for continuation of CASD-NMR will be made on the occasion of the next evaluation meeting; the costs for this activity indeed involve only the organization of such meetings, for which it will be necessary to find a sponsor. WeNMR services and its VRC will be promoted at the conference and workshops in which CIRMMP members will participate to ensure a high visibility of our services.

Sustainability plan – Partner 4 – INFN

Maintaining the hardware

INFN's contribution in terms of computing and storage resources offered to WeNMR will be maintained. It is currently composed by 6 resource centers (BARI, CATANIA, LNL, PADOVA, ROMA3, TRIESTE) providing a total of 6800 CPU-cores and 23.5 TB of storage space shared with other VOs, coordinated by the Italian NGI. Central services which are crucial for the WeNMR grid operations and monitoring, i.e. VOMS, GStat, Nagios and WMSMonitor will also continue to be supported by INFN at Padova and at the CNAF computing center of Bologna, with the support of the Italian NGI.

Maintaining middleware with National Grid Infrastructures

After the end of EMI, in April 2013, every EMI partner has committed to support their middleware components at least until April 2014. INFN has therefore committed, in cooperation with the Italian NGI, that the support to the components under its responsibility, i.e. VOMS, CREAM-CE, WMS, WNoDeS and StoRM will be maintained. The implementation of new features, e.g. on CREAM-CE, will also be possible upon request from the user communities, under well defined National or European funding schemes to be activated in the future. In the longer term perspective, the EMI partners have proposed to continue their joint activity by setting up MeDIA, a Middleware Development and Innovation Alliance (<http://www.eu-emi.eu/events/2013/media-launch>), aiming at continuing the collaboration on roadmaps definition, common functionality, interoperability and standardization in a lightweight and open form.

Maintaining software and portals

INFN is not involved in the development and maintenance of structural biology application software and their fruition through the WeNMR portals.

Maintaining VRC and WeNMR website

INFN will participate in the help center as long as it is being offered, and keep updated the Grid Tutorial section of the WeNMR website.

Organization of future workshops

INFN will continue to promote WeNMR services at national and international e-Science, Grid and Cloud conferences and workshops, in partnership with the Italian NGI.