



Memorandum of Understanding between EGI.eu and WeNMR VRC

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BACKGROUND

The *Stichting European Grid Initiative* (hereafter referred to as "EGI.eu") is a foundation under the Dutch law which mission is to create and maintain a pan-European Grid Infrastructure in collaboration with National Grid Initiatives (NGIs) and associated participants (e.g. European International Research Organisations - EIROs) in order to guarantee the long-term availability of a generic e-infrastructure for all European research communities and their international collaborators. In its role of coordinating grid activities between European NGIs EGI.eu will: 1) operate a secure integrated production grid infrastructure that seamlessly federates resources from providers around Europe; 2) coordinate the support of the research communities using the European infrastructure coordinated by EGI.eu; 3) work with software providers within Europe and worldwide to provide high-quality innovative software solutions that deliver the capability required by our user communities; 4) ensure the development of EGI.eu through the coordination and participation in collaborative research projects that bring innovation to European Distributed Computing Infrastructures (DCIs). A summary of EGI.eu is attached as Annex 1.

The WeNMR VRC (hereafter referred to as "WeNMR") aims at bringing together complementary research teams in the structural biology and life science area into a virtual research community at a worldwide level, with a initial focus on the biomolecular Nuclear Magnetic Resonance (NMR) and Small Angle X-ray Scattering (SAXS) communities. Challenges in the post-genomic era, like the analysis of biomolecular interactions, call for European and worldwide interdisciplinary collaborations that are hardly imaginable without embracing the e-Science paradigms. This research needs virtual research platforms that provide the worldwide life science research community with user-friendly computation tools, platforms for data analysis and exchange, e-Science tools for conferencing, exchange of best practice and training, all supported by an underlying high performance e-Infrastructure. The WeNMR project (contract RI-261571), funded under the FP7 e-Infrastructure Virtual Research Community call, builds upon the established FP7 I3 eNMR 3 years e-Infrastructure project (grant no. 213010). Its steadily growing enmr.eu virtual organization (VO) is currently the second largest in the life science area with 235 member to date, over 10% of which outside Europe.

The main objective of WeNMR is to establish an e-Infrastructure-based global virtual research community for structural biology in the life sciences. To this end six objectives are defined: 1) to operate, maintain and further develop a user-friendly science gateway for the NMR and SAXS communities, 2) to establish a virtual research platform to serve as a digital knowledge repository, data exchange medium, and forum for (interaction with) the user community, 3) to provide support to software developers, users and other e-Infrastructure projects in an e-Science knowledge and training centre, 4) to foster the adoption and use of e-Infrastructure on a global scale by supporting a wide range of flanking disciplines within the life sciences, 5) to operate and consolidate the eNMR Grid infrastructure in line with NGIs and the EGI, and to extend it to interoperate with other worldwide Grid initiatives, 6) to develop a model to ensure sustainability of the project. The fact sheet of the WeNMR project is attached as Annex 2. The partners in the WeNMR project are represented indirectly in the EGI Council through their NGIs:

- Utrecht and Nijmegen: Dutch NGI via National Computing Facilities Foundation (NCF)
- Frankfurt, EMBL Hamburg (EGI Council member)
- INFN Padua, CERM Florence: Italian NGI
- Cambridge: UK NGI
- SpronkNMR: LitGrid via University of Vilnius

European Commission



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ARTICLE 1: PURPOSE

The purpose of this Memorandum of Understanding¹ (MoU) is to define a framework for collaboration between EGI.eu and WeNMR (hereafter also referred to as "the Party" or the "Parties").

The Parties recognise that through this MoU the opening of a wider and longer-term cooperation activities will bring significant benefits to both parties.

ARTICLE 2: DEFINITIONS

For the purpose of this MoU:

- (a) The term Virtual Organisation (VO) refers to a group of researchers with similar interests and requirements, who are able to work collaboratively with other members and/or share resources (e.g. data, software, expertise, CPU, storage space) regardless of geographical location.
- (b) The term Virtual Research Community (VRC) refers to an organisational grouping that brings together transient Virtual Organisations within a persistent and sustainable structure. A VRC is a self-organising group that collects and represents the interests of a focussed collection of researchers across a clear and well-defined field. Named contacts are agreed upon by the VRC to perform specific roles and these then form the communication channel between the VRC and EGI.eu
- (c) The term European Grid Infrastructure (EGI) refers to the production infrastructure the federated resources brought together by the participants within EGI.eu, or made accessible to the VRC through various MoUs that EGI.eu coordinates on behalf of the EGI community.
- (d) The term National Grid Initiative (NGI) refers to an entity as defined in the EGI.eu statute².

ARTICLE 3: JOINT WORK PLAN

The goal of the collaboration defined by this MoU is to establish a formal relationship between WeNMR and EGI.eu. The WeNMR resource centres will be integrated to EGI through the respective National Grid Initiatives once they reach EGI production-quality. EGI and the relevant NGIs will jointly deliver the operational and user support services needed to make the WeNMR resources seamlessly, reliably and securely accessible to the relevant user communities.

As regards the user community around WeNMR, the project will bring them together as an emerging VRC in the area of structural biology and life sciences. The objectives of the collaboration are:

- 1. User support
- 2. Application integration
- 3. User Community policy and procedures
- 4. Requirements gathering
- 5. Sustainability
- 6. Dissemination

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¹ An MoU is a written agreement that clarifies relationships and responsibilities between two or more parties that share services, clients,

² See EGI.eu Statute: http://www.egi.eu/about/governance/





The specific activities to be carried out within the framework of the collaboration are $\frac{3}{2}$:

Activity: A.1 - User Support

Parties Involved: EGI.eu Chief Community Officer (Stephen Brewer), WeNMR VRC platform leader (Chris Spronk), *WeNMR* Project Coordinator (Alexandre Bonvin)

Description of work: This activity requires that the communication channels and contact points are agreed, the support services are defined and help desk integration is established. The activity will also involve compiling details of areas of specialisation where the VRC can contribute back to the wider EGI community. This could include for example: training material, application details, documentation and presentations that can be contributed to EGI.eu to be made accessible to all VRC members. Therefore, these items will be provided where applicable and drawn upon where needed. EGI.eu will act as a matchmaker in identifying needs from the community and encouraging relevant experts to share their knowledge and experience with the wider community. EGI.eu will also offer a consultancy service, which will provide specific assistance to a community where applicable and where resources permit.

Expected outcomes:

- Contact points: these will be defined within this MoU and updated when required
- Help desk integration: the relevant parts of the VRC help desk system will be integrated with EGI.eu
- Areas of expertise: VRC will provide a concise report detailing areas of expertise from within their community
- Reporting: all actions will be written as part of the standard formal EGI-InSPIRE and WeNMR deliverables; EGI.eu and WeNMR will both contribute to the respective reports
- Meetings: the quarterly UCB (User Community Board) meetings should be attended by a representative of WeNMR, with a minimum of two meetings per year attended in person. A representative may be required for the USAG (User Services Advisory Group) meeting. Similarly, the EGI will upon request attend meeting organized by the VRC (minimum of one per year)
- VRC contributions: the VRC will make available to EGI.eu training material, application details, documentation and presentations, either directly from the VRC web portal or by depositing it within the relevant training and application databases provided by EGI.eu
- EGI.eu consultancy support will be made available where applicable and where resources permit

Activity: A.2 – Support tools and services

Parties Involved: EGI.eu Chief Operations Officer (Tiziana Ferrari), EGI.eu Chief Community Officer (Stephen Brewer), WeNMR GRID operation leader (Marco Verlato), WeNMR Project Coordinator (Alexandre Bonvin)

Description of work: This activity covers both tools and services required from Operations as well as integration with those provided by User Community Support Team (UCST) Technical Services. It can also include applications and services that the VRC could provide for EGI.eu. Therefore, an early task will involve compiling detailed description of areas of specialisation where the VRC can contribute back to the Community.

Expected outcomes:

- Reporting: all actions will be written as part of the standard formal EGI-InSPIRE and WeNMR deliverables; EGI.eu and WeNMR will both contribute to the respective reports,
- A set of tools and services from EGI after agreement between the parties

³ Party leading the activity is underlined.

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- A set of tools and services from WeNMR after agreement between the parties
- Consultancy: hands on assistance and specific advice may be offered, from both parties, as a consultancy service if the need and the availability of resources permit

Activity: A.3 Formulation of User Community Policy and Procedures

Parties Involved: EGI.eu Chief Community Officer (Stephen Brewer), WeNMR Project Coordinator (Alexandre Bonvin)

Description of work: WeNMR will have influence through participation in User Community Board (UCB) and other formal bodies to the policies, procedures, services and tools relating to the WeNMR support process and infrastructure operation. Participation in the UCB is obligatory with a minimum of two physical meetings per year. EGI.eu will also consider attending formal meetings that the VRC may call.

Expected outcome:

- EGI.eu and WeNMR will participate in UCB and other meetings subject to agreement
- EGI.eu policy and procedures that reflect a consensus across all VRCs and EGI.eu
- Reporting: all actions will be written as part of the standard formal EGI-InSPIRE and WeNMR deliverables; EGI.eu and WeNMR will both contribute to the respective reports

Activity: A.4 Requirements gathering

Parties Involved: Chief Community Officer (Stephen Brewer), Technical Manager (Michel Drescher), WeNMR GRID operation leader (Marco Verlato), WeNMR VRC platform leader (Chris Spronk), WeNMR Project Coordinator (Alexandre Bonvin)

Description of work: This activity is an opportunity for the VRC to feed their requirements into EGI.eu and hence influence the evolution of the infrastructure and the support services. EGI.eu will accept requirements in various formats from Use Cases to User Stories depending on what works for the VRC. The UCST will process and normalise the requirements in order to compare and combine them with others from across all of the communities. The combined prioritised requirements will be presented to UCB for ratification before submission to Technical Coordination Board (TCB). The UCST will provide support to *VRC* in the form of guidelines, services and workshops to help them capture and prioritise their own requirements.

EGI.eu

Expected outcome:

- Prioritised and well defined requirements from the VRC submitted on a periodic cycle to be agreed with EGI.eu
- Feedback: EGI.eu will provide regular feedback on the status of the requirements supplied by the VRC
- Reporting: all actions will be written as part of the standard formal EGI-InSPIRE and WeNMR deliverables; EGI.eu and WeNMR will both contribute to the respective reports

Activity: A.5 Sustainability

Parties Involved: EGI.eu Chief Community Officer (Stephen Brewer), Policy Development Manager (Sergio Andreozzi), WeNMR Sustainabily WorkPackage leader (Harald Schwalbe), WeNMR Project Coordinator (Alexandre Bonvin)

Description of work: There is an expectation that both EGI.eu and VRC will last beyond any specific projects; mutually beneficial initiatives to help achieve this should be defined as part of this activity. EGI.eu will provide advice and support to *VRC* in order to help it produce a compelling sustainability plan appropriate for their needs. The activities will be embedded as much as possible within the Sustainability WorkPackage of the WeNMR project.

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Expected outcome:

- Establish sustainability plan for the VRC including organisational structure and governance model, this plan should include details of how the representative for the VRC will communicate with the community and maintain a position of trust within this community
- Increased support for VOs falling under the WeNMR VRC by NGIs with mediation by EGI.eu when possible
- Reporting: all actions will be written as part of the standard formal EGI-InSPIRE and WeNMR deliverables; EGI.eu and WeNMR will both contribute to the respective reports
- Annual report: WeNMR will make available to EGI.eu its annual progress report (following EU reporting directives) describing the status of the project and its associated VRC

A.6 Dissemination

Parties Involved: EGI.eu Dissemination Manager (Catherine Gater), WeNMR Outreach WorkPackage leaders (Gert Vriend/Geerten Vuister), WeNMR Project Coordinator (Alexandre Bonvin)

Description of work: The objective of this activity is to maximise the impact of both WeNMR and EGI.eu through the efficient coordination of dissemination. This will involve establishing contact points for communication channels, publications as well as sharing timing constraints relating to both parties. WeNMR and EGI.eu will collaborate and help each other in the production of dissemination material and also disseminate the progress and results from the collaboration within the EGI.eu community and WeNMR.

Expected outcome:

- Reporting: all actions will be written as part of the standard formal EGI-InSPIRE and WeNMR deliverables; EGI.eu and WeNMR will both contribute to the respective reports
 - Launch: advertise the start of the collaboration in each party website with a dedicated static page, article and press releases (within 1 month)
 - Events: joint sessions at EGI.eu and WeNMR events will be planned in order to disseminate the progress and results of the collaboration
 - Publications: Inform EGI.eu on any scientific/academic publications published issued by the WeNMR
 - Presentations: Inform WeNMR on any e-Science or related presentations of EGI.eu in which WeNMR is explicitly mentioned

ARTICLE 4: TIMELINE AND REPORTING

The EGI.eu Policy Development Team (PDT) will coordinate the periodic review of the progress of the activities defined in Article 3 (Joint Work Plan), follow-up the milestones defined below and distribute reports to both Parties. Special meetings between the points of contact designated under Article 5 (Communication) shall be held, as often as necessary, to examine the progress in the implementing of this Agreement. Dates related to time elapsed from the signing of the MoU.

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Date	Activity	Achievement	
04/2011	A.6	Both parties to announce the collaboration agreement on their web sites	
05/2011	A.1	Outline VRC's areas of expertise	
05/2011	A.1	Help desk integration (VRC & EGI)	
05/2011	A.2	List of applications and services needed by the VRC	
05/2011	A.2	List of applications and services that the VRC can offer	
January, annually	All	Summary of the main achievements, open issues and future plans related to the collaboration between the VRC and EGI.eu. The input must cover all of the activities that are defined in the Joint Work Plan section of the signed MoU.	
Every 3 months	A.3	Participation in UCB – with a minimum of two physical meetings per year	
Every year	A.4	Updated and prioritised requirements for the community	
Every 3 months	A.4	Feedback from EGI on progress on requirements progress	
Month 6	A.5	VRC sustainability plan – description of the Sustainability work package of WeNMR	

ARTICLE 5: COMMUNICATION

The Parties shall keep each other informed on all their respective activities and on their progress and shall consult regularly on areas that offer the potential for cooperation through the agreed channels.

Joint working groups may be established to examine in detail proposals in areas assigned to them by the Parties referred to in Article 3 (Joint Work Plan) and to make recommendations to the Parties.

Each Party shall designate a "points of contact" that will be responsible for monitoring the implementation of this MoU and for taking measures to assist in the further development of cooperative activities. Such points of contact shall be the ordinary channel for the Parties' communication of proposals for cooperation.⁴

The primary point of contact for each Party is:

EGI.eu: Sergio Andreozzi, Policy Development Manager

EGI.eu – Science Park 105 – 1098 XG Amsterdam, the Netherlands

Tel: +31 (0)20 592 2285 E-mail: sergio.andreozzi@egi.eu

⁴ For the full and detailed contact list of VRC required by the accreditation procedure see Annex 5.

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WeNMR: Prof. Alexandre M.J.J. Bonvin – Coordinator

Bijvoet Center for Biomolecular Research, Utrecht University

Padualaan 8, 3584 CH Utrecht, the Netherlands

Tel.: +31-30-2533859 Fax: +31-30-2537623 Email: a.m.j.j.bonvin@uu.nl

Questions of principle or problems that cannot be solved at primary contact level will be taken to the EGI.eu Director and the WeNMR project Coordinator.

ARTICLE 6: PARTICIPATION IN EGI.EU GROUPS

WeNMR agrees to name a technical representative (with deputy) for the EGI User Community Board (UCB). UCB terms of reference are available on request.

WeNMR may be asked to nominate representatives to serve on other advisory groups as appropriate. For example, this might include the User Services Advisory Group (USAG). USAG terms of reference are available on request.

The VRC will accept and comply with EGI.eu's policies and procedures relating to the use of EGI's production infrastructure.

ARTICLE 7: RIGHTS AND RESPONSIBILITIES

The procedure is set out in Annex 3.

ARTICLE 8: FUNDING

Each Party shall bear the costs of discharging its respective responsibilities under this MoU, including travel and subsistence of its own personnel and transportation of goods and equipment and associated documentation, unless otherwise agreed in this MoU.

Each Party shall make available free of charge to the other Party any office/meeting space needed for the joint activities.

The Parties' obligations hereunder are subject to their respective funding procedures and the availability of appropriated funds. Should either Party encounter budgetary problems in the course of its respective internal procedures that may affect the activities carried out under this MoU, that Party shall notify and consult with the other Party in a timely manner in order to minimise the negative impact of such problems on the cooperation. The Parties shall jointly look for mutually agreeable solutions.

ARTICLE 9: ENTRY INTO FORCE, DURATION AND TERMINATION

This MoU will enter into force when signed by the authorized representatives of the Parties and shall remain in force until completion of the activities identified in Article 3 (Joint Work Plan), or upon termination of the projects in which the Parties participate, or upon three (3) months prior written notice by one Party to the other. In the event of termination, the parties shall endeavour to reach agreement on terms and conditions to minimise negative impacts on the other Party. In the event of the continuation of the present cooperation, the Agreement may be extended and/or amended by mutual agreement in writing.

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ARTICLE 10: AMENDMENTS

The MoU may be amended by written agreement of the Parties. Amendments shall be valid only if signed by the authorized representatives of the Parties.

ARTICLE 11: ANNEXES

Annexes 1, 2, 3 and 4 attached hereto have the same validity as this MoU and together constitute the entire understanding and rights and obligations covering the cooperation accepted by the Parties under this MoU. Annexes may be amended following the provisions of Article 9 (Amendments).

ARTICLE 12: LANGUAGE

The language for this MoU, its interpretation and all cooperative activities foreseen for its implementation, is English.

ARTICLE 13: GOVERNING LAW - DISPUTE RESOLUTION

The terms of this MoU shall be interpreted in accordance with their true meaning and effect independently of national and local law. Provided that if and insofar as this MoU does not stipulate, or any of its terms are ambiguous or unclear reference shall be made to the substantive laws of Belgium. Disputes shall be resolved by amicable settlement or failing which by arbitration in accordance with the procedure set out in Annex 4.

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Memorandum of Understanding between EGI.eu and WeNMR

IN WITNESS WHEREOF, the Parties have caused their duly authorised representatives to sign two originals of this Memorandum of Understanding, in the English language.

The following agree to the terms and conditions of this MoU:

Dr. Steven Newhouse

EGI.eu Director

Prof. Alexandre M.J.J. Bonvin WeNMR Project Coordinator

11-03-2011

Date





Annex 1 EGI.eu

Background to EGI.eu

To support science and innovation, a lasting operational model for e-Infrastructure is needed – both for coordinating the infrastructure and for delivering integrated services that cross national borders. The objective of EGI.eu (a foundation established under Dutch law) is to create and maintain a pan-European Grid Infrastructure in collaboration with National Grid Initiatives (NGIs) in order to guarantee the long-term availability of a generic e-infrastructure for all European research communities and their international collaborators.

In its role of coordinating grid activities between European NGIs, EGI.eu will:

- Operate a secure integrated production grid infrastructure that seamlessly federates resources from providers around Europe
- Coordinate the support of the research communities using the European infrastructure coordinated by EGI.eu
- Work with software providers within Europe and worldwide to provide high-quality innovative software solutions that deliver the capability required by our user communities
- Ensure the development of EGI.eu through the coordination and participation in collaborative research projects that bring innovation to European Distributed Computing Infrastructures (DCIs)

The EGI.eu is supporting 'grids' of high-performance computing (HPC) and high-throughput computing (HTC) resources. EGI.eu will also be ideally placed to integrate new Distributed Computing Infrastructures (DCIs) such as clouds, supercomputing networks and desktop grids, to benefit the user communities within the European Research Area.

EGI.eu will collect user requirements and provide support for the current and emerging user communities. Support will also be given to the current heavy users of the infrastructure, such as high energy physics, computational chemistry and life sciences, as they move their critical services and tools from a centralised support model to one driven by their own individual communities.

The EGI.eu community is a federation of independent national and community resource providers, whose resources support specific research communities and international collaborators both within Europe and worldwide. EGI.eu, coordinator of EGI.eu, brings together partner institutions established within the community to provide a set of essential human and technical services that enable secure integrated access to distributed resources on behalf of the community.

The production infrastructure supports Virtual Research Communities – structured international user communities – that are grouped into specific research domains. VRCs are formally represented within EGI.eu at both a technical and strategic level.

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Annex 2 WeNMR fact sheet

Summary: Structural biology and life sciences in general, and NMR in particular, have always been associated with advanced computing. The current challenges in the post-genomic era call for virtual research platforms that provide the worldwide research community with both user-friendly tools, platforms for data analysis and exchange, and an underlying e-infrastructure.

WeNMR groups different research teams into a worldwide virtual research community. It builds on the established eNMR e-Infrastructure and its steadily growing virtual organization, which is currently the second largest VO in the area of life sciences. WeNMR will consolidate the operation of the current services and provide an e-Infrastructure platform and Science Gateway for structural biology towards EGI for the users of existing infrastructures. It will involve researchers from around the world and will build bridges to other areas of structural biology. Integration with SAXS, a rapidly growing and highly complementary method, is directly included in WeNMR, but links will also be established to related initiatives. WeNMR will serve all relevant INSTRUCT communities in line with the ESFRI roadmap.

Objectives: The main objective of WeNMR is to establish an e-Infrastructure-based global virtual research community for structural biology in the life sciences. To this end six objectives are defined: 1) to operate, maintain and further develop a user-friendly science gateway for the NMR and SAXS communities, 2) to establish a virtual research platform to serve as a digital knowledge repository, data exchange medium, and forum for (interaction with) the user community, 3) to provide support to software developers, users and other e-Infrastructure projects in an e-Science

knowledge and training centre, 4) to foster the adoption and use of e-Infrastructure on a global scale by supporting a wide range of flanking disciplines within the life sciences, 5) to operate and consolidate the eNMR Grid infrastructure in line with NGIs and the EGI, and to extend it to interoperate with other worldwide Grid initiatives, 6) to develop a model to ensure sustainability of the project.

Action plan: WeNMR will

NMR data collection and processing

SAXS data analysis

Data

Interpretation

Structure, dynamics & interactions

Impact on research and health:

origin of disease

design of new experiments

drug design

.....

operate and further consolidate the e-Infrastructure deployed within the eNMR project. A virtual research community platform will be established in the first year to serve as the central entry point for all communities and the main dissemination portal of the project. WeNMR will strengthen the European ties with National Grid Initiatives, the new EGI and PRACE initiatives toward an effective sharing of the offered service. Collaborations will be established with the Asian, South-African, South- and North-American GRID initiatives, in close contact with existing EC projects, to extend and open the WeNMR Life-Science Gateway at a global level in

Contract n°: RI-261572

Project type: CP-CSA

Start date: 01/11/2010

Duration: 36 months

Total budget: 2′434′000 €

Funding from the EC: 2′150′000 €

Total funded effort in person-month: 264.5

Web site: www.wenmr.eu

Contact person:

Prof. Alexandre Bonvin email: a.m.j.j.bonvin@uu.nl tel.: +31 30 2533859 fax.: +31 30 2537623

Project participants:

, .	-
BCBR	NL
BMRZ	DE
CIRMMP	IT
INFN	IT
RUN	NL
UCAM	UK
EMBL	DE
SpronkNMR	LT

Keywords:

Nuclear Magnetic Resonance spectroscopy (NMR), Small Angle X-ray Scattering (SAXS), structural biology, life sciences, proteins, DNA, complexes, web portals

Collaboration with other EC

funded projects:

East-NMR, contract no. 228461

Bio-NMR, contract no. 261863

EU-IndiaGrid2, contract no. 246698

Gisela, contract no. 261487

CHAIN, contract no.





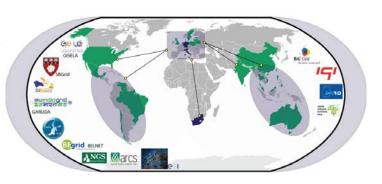
the second year of the project. WeNMR will further establish and promote best practices in life sciences and offers (virtual) training services to worldwide researchers throughout the entire duration of the project.

Networking activities: The Networking Activities (NA) build on the extensive human collaboration network successfully implemented within the e-NMR project. They aim at extending it 1) geographically, i.e. involving users and other stakeholders from many new countries, 2) in size, i.e. by increasing the number of users in all countries, and 3) scientifically, i.e. by involving new scientific communities that share an interest in structural biology in its broader sense. In addition to individual laboratories and research teams, a crucial role in this process will also be carried out by National and Regional Grid Initiatives, as well as by researchers in Industry. NA further aim at establishing sustainability measures for future operation, both in terms of continuous feedback and quality control as well as in financial form. A large variety of disseminative actions will target stakeholders including the e-Science, bio-NMR and SAXS communities, the more general structural biology and life sciences communities, industrial researchers, as well as the general public.

Service activities: The computational GRID infrastructure is central to the services offered by WeNMR; its operation, maintenance and consolidation are therefore core Service activities. The infrastructure will be expanded to worldwide Grid initiatives, which is an important factor to both increase the available computational resources and the user community. WeNMR will also operate a Virtual Research Community portal that will address the needs of the various user communities, from general public to experienced users and software developers. For each community, a number of services, information channels and communication tools will be deployed.

Joint Research activities: The WeNMR Joint Research activities (JRA) aim at improving the integrated services offered by the project in order to reflect the latest scientific developments. To enhance the possibilities for actual experimentation, the project will develop remote, secure access to experimental SAXS facility. Finally, to ensure an efficient usage of the WeNMR web portals and services, systematic attention will be paid to user-interaction with- and communication between the portals and the services. The JRA main three objectives are: 1) to provide a multidisciplinary approach (NMR/SAXS/validation) to the characterization of biomolecular interactions 2) to provide a secure remote access to SAXS instrumentation and 3) to provide web services and end user tools.

User communities: The **NMR** community in the Life Sciences is composed of a large number of research teams that tackle a vast portfolio of different biological problems. We estimate its size to around 1000 research groups worldwide; their size and expertise vary from a few researchers with access to limited instrumentation to large research units with extensive,



state-of-the art equipment (e.g. the European, North American and Japanese large-scale NMR research infrastructures). The SAXS community is similarly diverse: thousands of research groups worldwide employ SAXS as a method to obtain structural information of a wide variety of non-crystalline objects, including, but not limited to, biological macromolecules in solution. Only few dozens of these groups however maintain instruments, which range from small lab sources to full-

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scale third generation synchrotron radiation facilities themselves; most users visit the large synchrotron facilities with SAXS beamlines. The research teams making use of NMR and/or SAXS often collaborate with a large number of scientific groups that are skilled in molecular and cell biology and provide samples for the experimental measurements. The outcomes of these studies are of interest for an even wider community of scientists, because of the biological and biomedical implications of the results attained.

International aspects: As the title of the project states, WeNMR aims at providing a worldwide e-Infrastructure for NMR and structural biology. As such, it is a strongly internationally oriented project that reaches far outside Europe. International aspects are embedded in all activities of the project.

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Annex 3 Rights and Responsibilities

A. GENERAL

- 1. WeNMR agrees to adhere to applicable policies and procedures relating to the use of the production infrastructure.
- 2. A Party which makes material, equipment or components available to the other Party, for the purposes of activities under this MoU shall remain the proprietor of such material, equipment or components.
- 3. Each Party shall remain fully responsible for its own activities, including the fulfilment of its obligations under any grant agreement with the European Commission or under any consortium agreement related thereto.

B. PERSONNEL

- 1. Each Party shall be solely responsible for any personnel hired to carry out work under this MoU.
- 2. In case personnel employed by one Party temporarily carries out work under this MoU on the premises of another (hereafter referred to as "secondment"), the following provisions shall apply:
- (a) The persons seconded shall be subject to all regulations, including, in particular, safety regulations, applicable on the site of the Party they are seconded to.
- (b) The personnel seconded by a Party to another shall remain employees of the Party having seconded them and such Party, as employer, shall bear exclusive responsibility for the payment of salary and for the procurement of adequate social security and insurance, including third party liability insurance and health insurance.
- (c) Unless otherwise agreed by the Parties concerned, Intellectual Property Rights generated by personnel seconded by a Party to another shall be owned by the Party having seconded such personnel.

C. INTELECTUAL PROPERTY RIGHTS AND LICENSE

- 1. "Intellectual Property Rights" shall mean all intellectual creations including but not limited to inventions, know-how, layouts, drawings, designs, specifications, computer programs, reports, processes, protocols, calculations and any other matter and protected by intellectual property rights, whether registered or not, including patents, registered designs, copyrights, design rights and all similar proprietary rights and applications for protection thereof.
- 2. Intellectual property rights generated by a Party under this MoU shall be the property of that Party who shall be free to protect, transfer and use such Intellectual Property Rights as it deems fit.
- 3. Notwithstanding the foregoing each Party shall grant the other a non-exclusive royalty free, perpetual license to use the Intellectual Property Rights generated by it under this MoU for use within its project or for the exploitation the results thereof. Such license shall include the right to sublicense the entities involved in the project.

D. JOINTLY OWNED RESULTS

1. Results that were jointly generated by both Parties will be jointly owned by the Parties, hereinafter referred to as ("Jointly Owned Results") and each of the Parties shall be free to use these Jointly Owned Results as it sees fit without owing the other Party any compensation or requiring the consent of the other Party. Each Party, therefore, for example and without limitation, has the transferable right to grant non-exclusive, further transferable licenses under such Jointly Owned Results to third parties. Each Party shall be entitled to disclose such Jointly Owned Results without restrictions unless such Jointly Owned Results contain a Joint Invention in which case no disclosure must be made prior to the filing of a priority application.

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2. With respect to any joint invention resulting from this MoU (i.e. any invention jointly made by employees of both Parties), the features of which cannot be separately applied for as Intellectual Property Rights and which are eligible for statutory protection requiring an application or registration (herein referred to as "Joint Invention"), the Parties shall agree on which Party will carry out any filling as well as any further details with regard to persecuting and maintaining of relevant patent applications.

E. PUBLIC RELATIONS

- 1. Any publication by a Party resulting from the activities carried out under this MoU shall be subject to prior agreement of the other Party not be unreasonably withheld.
- 2. EGI.eu and WeNMR may each release information to the public, provided it is related only to its own part of the activities under this MoU. In cases where the activities of the other Party are concerned prior consultation shall be sought. In all relevant public relations activities, the contribution of each Party related to activities covered by this MoU shall be duly acknowledged.

F. CONFIDENTIALITY OF INFORMATION

- 1. The Parties may disclose to each other information that the disclosing Party deems confidential and which is (i) in writing and marked "confidential", or (ii) disclosed orally, and identified as confidential when disclosed, and reduced in writing and marked "confidential" within fifteen (15) days of the oral disclosure (hereafter referred to as "Confidential Information"). Confidential Information shall be held in confidence and shall not be disclosed by the receiving Party to any third party without the prior written consent of the disclosing Party.
- 2. Notwithstanding the foregoing a Party is entitled to disclose Confidential Information which it is required by law to disclose or which, in a lawful manner, it has obtained from a third party without any obligation of confidentiality, or which it has developed independently from any Confidential Information received under this MoU, or which has become public knowledge other than as a result of a breach on its part of these confidentiality provisions.

G. LIABILITY

- 1. Each Party shall use reasonable endeavours to ensure the accuracy of any information or materials it supplies to the other Party and of any other contribution it makes hereunder and promptly to correct any error therein of which it is notified. The supplying Party shall be under no obligation or liability other than as stated above and no warranty or representation of any kind is made, given or to be implied as to the sufficiency, accuracy or fitness for a particular purpose of such information, materials or other contribution or as to the absence of any infringement of any proprietary rights of third parties through the possession or use of such information, materials or other contribution. The recipient Party shall be entirely responsible for its use of such information, materials or other contribution and shall hold the other Party free and harmless and indemnify it for any loss or damage with regard thereto.
- 2. Except in case of gross negligence or wilful misconduct, neither Party shall be liable for any indirect or consequential damages of the other Party, including loss of profit or interest, under any legal cause whatsoever and on account of whatsoever reason.

H. PARTICIPATION IN SIMILAR ACTIVITIES

1. Parties are not prevented by this MoU from participating and activities similar to those described in this MoU with third parties. There is no obligation to disclose any similar activity to the other party. However, when considered of mutual benefit, both parties are encouraged to involve the other party in similar activities to the goal of disseminating the knowledge about EGI.eu.

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Annex 4 Settlement of Disputes

- 1. All disputes or differences arising in connection with this MoU which cannot be settled amicably shall be finally settled by arbitration in accordance with the procedure specified below which shall be adapted in the light of the number of Parties involved.
- 2. Within thirty (30) calendar days of written notification by a Party to the other Party of its intention to resort to arbitration, the first Party shall appoint an arbitrator. The second Party shall appoint an arbitrator within three (3) months of the appointment of the first arbitrator. The two arbitrators shall, by joint agreement and within ninety (90) calendar days of the appointment of the second arbitrator, appoint a third arbitrator, who shall be the Chairman of the Arbitration Committee.
- 3. If the second Party fails to appoint an arbitrator or the two arbitrators fail to agree on the selection of a third arbitrator, the second or, as the case may be, the third arbitrator, shall be appointed by the President of the Court of Justice of the European Communities.
- 4. Unless otherwise agreed by the Parties concerned within thirty (30) calendar days of the provision of notice referred to in Article 12 above, the arbitration proceedings shall take place in Brussels and shall be conducted in English. The Parties shall within one month of the appointment of the third arbitrator agree on the terms of reference of the Arbitration Committee, including the procedure to be followed.
- 5. The Arbitration Committee shall faithfully apply the terms of this MoU. The Arbitration Committee shall set out in the award the detailed grounds for its decision.
- 6. The award shall be final and binding upon the Parties, who hereby expressly agree to renounce any form of appeal or revision.
- 7. The costs including all reasonable fees expended by the Parties to any arbitration hereunder shall be apportioned by the Arbitration Committee between these Parties.

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Annex 5 Full and Detailed Contact List

Role	EGI.eu	VRC
Coordinator	Chief Community Officer	WeNMR Coordinator
	(Steve Brewer) and Director of	(Alexandre Bonvin): providing
	EGI.eu (Steven Newhouse	strategic and managerial input
		on the <i>VRC</i> 's activity
User support and training	Chief Community Officer	WeNMR VRC portal leader
	(Steve Brewer)	(Chris Spronk)
Operational issues (GRID-	Chief Operations Officer	WeNMR GRID operation
related, operation, security)	(Tiziana Ferrari)	(Marco Verlato)
Dissemination	EGI.eu Dissemination Manager	WeNMR Outreach (Gert
	(Catherine Gater):	Vriend)

And as additional contacts depending on the issue I would suggest the WP-leaders of WeNMR:

- WP2 Sustainability Prof. Harald Schwalbe
- WP3 Outreach Prof. Gert Vriend
- WP4 Grid operation and maintenance Prof. Antonio Rosato
- WP5 Worldwide Grid extension Dr. Marco Verlato
- WP6 Virtual Research Community Dr. Chris Spronk
- WP7 Research Platform Dr. Dmitri Svergun

With WP 2&3 falling under Coordination/Networking, WP 4-6 under Services and WP7 Joint Research Activities.

These contact points may be the same person. These representatives (or additional people) may be invited to participate in other EGI.eu bodies depending on the interests of the *WeNMR* VRC will make sure to keep EGI.eu Chief Community Officer updated with any changes to the contact list.

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