Collaboration agreement

Between

NeIC represented by NordForsk (NO ID: 971 274 255), Stensberggata 25, NO 0170 Oslo, Norway – hereafter referred to as the "Project owner",

CSC – IT Center for Science Ltd, (FI ID: 0920632-0), P.O.Box 405, FI 02101 Espoo, Finland,

SNIC – Swedish National Infrastructure for Computing represented by Uppsala University (SE202100293201), Box 337, 751 05 Uppsala, Sweden,

DeIC – Danish e-infrastructure cooperation, (CVR : 30 06 09 46, EAN: 5798000430723), DTU, Anker Engelunds Vej 1, DK 2800 Kgs. Lyngby,

UNINETT Sigma2 AS, (NO ID: 887 625 352) Abels gate 5 – Teknobyen, Trondheim, Norway.

These are hereafter referred to collectively as the "partners", or a "partner" (singular).

1 The agreement – scope and purpose

1.1 This collaboration agreement regulates the reciprocal rights and obligations of the various partners taking part in the project **"Collaborative Infrastructure for Scientific Software"**, hereafter referred to as the "project".

1.2 The following attached documents shall also be part of the collaboration agreement between the partners:

Appendix 1: A description of the project in form of a project directive.
Appendix 2: The partners' interest in and competence relative to the project.
Appendix 3: Project budget
Appendix 4: Terms of reference for the steering group

1.3 Each of the partners are required to contribute resources to the implementation of the project pursuant to the duties and obligations specified in this collaboration agreement and the project directive. With regard to one another, the consortium participants bear joint responsibility for implementation of the project and for achieving the results outlined in the project description.

1.4 The Project period will be from 1.10.2015 to 30.09.2017.

1.5 The collaboration agreement includes this signed agreement document with four appendices, cf. section 1.2.

2 Governance and Management

2.1 The project will have a steering group and a project manager.

2.2 The steering group approves the project plan and monitors the project's progress in relation to the project plan and responds to problems as needed. The terms of reference for the steering group are given in appendix 4.

2.3 Each of the partners are entitled to appoint one member to the steering group. The partners may unanimously agree to appoint additional members of the steering group. Partners are free to replace steering group members, but are required to keep the project manager apprised of who is representing the partner. The chair of the steering group is assigned by the project owner.

2.4 The project manager will be appointed by the project owner. The project manager reports to the steering group. The project manager is responsible for managing the project and its resources in accordance with this agreement and the guidelines given by the steering group. When appropriate, the project owner enters into a separate agreement with the employer of the project manager in a way that does not violate the terms of this agreement.

2.5 The project manager will summon the steering group to meetings with reasonable notice, usually no less than two weeks prior to the meeting date. The convening letter should be accompanied by an agenda and the documentation needed to deal with the items on the agenda. Decisions, recommendations and discussions of the meetings are recorded in proceedings that are made available to the partners.

2.6 The steering group has a quorum when more than half the members are present or participate in the steering group's deliberations. The steering group's decisions will normally be agreed on unanimously among the members that are present or participate in the steering group's deliberations. In ongoing matters that do not affect any of the partners' individual rights under the collaboration agreement, the steering group may take decisions by majority. When an unanimous decision or consensus is not possible, the meeting proceedings will reflect the diversity of opinions.

3 Partners' activities and/or financial support

3.1 The interests and competencies of the partners constitute the basis for their participation in the project. These interests and competencies are described in more detail in appendix 2.

3.2 Each of the partners shall perform the R&D activity, if any, that the partner in question has undertaken pursuant to the project directive, and/or provide the financial support specified in appendix 3.

3.3 With the approval of the steering group, a partner may assign parts of the R&D activity for which it is responsible to an appropriate subcontractor. This does not release a partner from its obligations to the other partners.

3.4 In the event a partner does not perform the agreed R&D activity in a satisfactory manner, as well as on request by a partner who expects to be unable to perform in such a way in the future, the steering group may decide to transfer responsibility for the work in whole or in part to one of the other partners, based on specified terms and conditions. Such a transfer does not release a partner from its other obligations pursuant to appendix 3.[1]

1

3.5 The project owner takes the main responsibility to oversee the economic aspects of the project and remind the partners about their funding obligations if so needed. In general, the funding will be requested by the project owner from the partners and channelled by the project owner. Money streams are following the budget (appendix 3) and eventual transferred responsibilities. Payments between the partners are made once per three months.

4 Location, responsibility for human resources and agreements with employees and other affiliated partners

4.1 The partners agree to establish by contract the location of the activities and the manner in which the employer's responsibility will be handled for staff affiliated with the project. Under normal circumstances, employer responsibility and employment shall not be changed for employees who participate in the project.

4.2 The partners will sign necessary agreements with owners, employees (including individuals with dual employment), partners, sub-contractors, and others that are required to fulfil the relevant partner's obligations under this agreement, including measures to ensure any necessary transfer of intellectual property rights.

5 Project plan, ownership, reporting and publication of results

5.1 In order to render more concrete and follow up the measures in the project directive, a project plan shall be adopted by the steering group within 6 months of project start-up. The project plan serves as a point of departure for the technical and financial implementation of the project and stipulates the obligations of the various partners, cf. section 4.2 and appendix 2. The revised annual project plan also forms the basis for reports to be submitted to the project owner.

5.2 Partners shall without undue delay submit all project results, reports, accounting documentation and other documents that the project owner requires to fulfil its obligations to its funding authorities.

5.3 Project deliverables, including reports and software, will be made openly available to the public. Intellectual property rights of the project results shall be owned by the party or parties carrying out the work generating that result. Unless otherwise agreed in writing, any equipment purchased for the purposes of the project will remain the property of the partner making the purchase.

5.4 The project manager will report quarterly to the project owner and steering group.

---

*It is presumed that the partners can agree on reasonable compensation for the research contributions from which the consortium participant in question has been relieved.

6 Limitation of liability

6.1 The parties have no liability towards each other for damages or losses of any kind related to this Collaboration Agreement, unless the damages were caused by wilful conduct or gross negligence. Each partner shall be solely liable for any loss, damage or injury to third parties resulting from its actions under this Collaboration Agreement or from its use of the project results.

6.2 In respect of any information or materials supplied by one partner to another under the project, no warranty of any kind is given as to the sufficiency or fitness for purpose, nor as to the absence of any infringement of any proprietary rights of third parties. The recipient party shall in all cases be solely liable for the use to which it puts such information and materials.

7 Reservations and Termination

7.1 The agreement may be terminated by either partner for any material breach by the other partners of the obligations set out in the agreement, by giving a written notice to the other partners of the intention to terminate. The notice shall include a detailed statement describing the nature of the breach. If the breach is remedied within a period of 30 – thirty – days after delivery of the notice, the termination shall not take effect.

7.2 The partners' compliance with funding requires that the partners receive the necessary funds from their respective authorities. A partner that cannot comply can terminate this agreement with a 3 –three- months' notice.

7.3 The project owner may terminate the agreement with a 3 –three- months' notice based on a recommendation of termination by the steering group.

8 Governing law and legal venue

8.1 The agreement is governed by and shall be interpreted in accordance with Norwegian law. Any disputes shall be settled by Oslo district court, unless otherwise agreed between the partners.

***

This agreement has been prepared in 6 counterparts, of which each partner keeps one (1).

For and on behalf of CSC:

Place/Date:_____

_____

Pekka Lehtovuori, Director, Services for research

For and on behalf of SNIC:

Place/Date:_____

_____

Jacko Koster, Director

For and on behalf of DeIC:

Place/Date:_____

_____

Steen Pedersen, CEO

For and on behalf of UNINETT Sigma2:

Place/Date:_____

_____

Gunnar Bøe, Managing Director

For and on behalf of NordForsk/NeIC:

Place/Date:_____

_____ _____

Gunnel Gustafsson, Director, NordForsk Gudmund Høst, Director, NeIC

Appendix 1: Project directive

Collaborative Infrastructure for Scientific Software Development

Project directive

This project is a part of NeIC Generic Area Activity for 2015, “Activity GEN-7 Nordic e-Infrastructure for scientific software” and it is in line with Action 10 “Nordic eInfrastructure for scientific software” from the Nordic eScience Action Plan.

Background

One of the main goals of NeIC is the provision of support to the e-Science research communities. For that it is required to facilitate collaborative work among different groups, provide of state-of-the-art e-Infrastructure services along with the necessary know-how for their utilisation.

Software development is at the core of e-Science research. Advances in hardware technology and computational algorithms put substantial pressure on software developers. Thus fast, efficient and reliable development cycles directly affect the speed and quality of e-Science work.

Yet our experience shows that a large number of academic research groups develop in-house software using very inefficient and outdated methodologies. The reason often being that many packages have started as one-person pet projects aimed at solving a specific problem at hand. But over the years the projects would grow with many new developers joining the team, and the codebase expanding considerably. The new functionality would make the software popular, widely used and important for whole research community. However, maintenance of such packages e.g. >10 year old ones, eventually creates substantial friction, which can be overcome with the adoption of proper software development methodologies.

Main reasons for the lack of adoption are unfamiliarity with existing solutions, and fear of potential steep learning curve, which will affect productivity. In fact, the opposite is true – sticking to old practices hurts very much the productivity in the long-term.

One initial step in direction of promotion of such best practices was the first academic course in software development tools at KTH in December 2014 (http://sese.nu/scientific-software-development-toolbox). It was organized by Radovan Bast (DALTON developer) and Rossen Apostolov (author of the current proposal and GROMACS developer) from Sweden, and Jonas Juselius (SYMBIOSES developer) from Norway. The teachers are developers of major software packages who have adopted and experienced the benefits of modern software development practices. The course was a very big success (the only negative feedback we had was that the students wished the course was longer!). It clearly showed the lack of expertise and pressing need for proper e-Infrastructure and tools.

SNIC has established a nation-wide network of application experts who acknowledge the need for provision of such infrastructure. During a provider forum meeting all national providers, i.e. SIGMA2, SNIC, CSC, DEIC, and RHNET, have also agreed on its benefits. Finally, the establishment of this infrastructure is in line with Action 10 “Nordic e-Infrastructure for scientific software” from the Nordic e-Science Action Plan.

Several software packages developed by Nordic research groups have large userbases worldwide and a big impact in their corresponding communities. Examples of such are ARC(http://www.nordugrid.org/arc), Gromacs (www.gromacs.org), Symbioses

(http://symbioses.no/doku.php), NordicESM, Dalton (daltonprogram.org), Chippster(http://chipster.csc.fi). Some of them (Gromacs, Dalton and Symbioses) are already using advanced workflows for development.

Project idea

This project proposes the establishment of software development e-Infrastructure, which is coupled with necessary technical expertise to address the growing needs of the computational communities.

The project includes three aspects.

First: Deployment of infrastructure. It will provide the necessary systems and tools, which could include:

- Distributed version control (DVC) repositories for scientific codes
  => allow for extremely easy collaborative code development
- Issue tracking systems
  => a necessity for any software project
- Code review systems
  => major improvement in the quality of the code, collaborative work, and skills of the programmers
- Code analyzers, debuggers and profilers framework
  => indispensable for catching errors or inefficiencies in the code
- Build systems, unit testing frameworks and report boards
  => automated testing before sharing of code
- Code Integration and benchmarking
  => automated software validation and performance monitoring

Depending on the available resources, the software e-Infrastructure can provide some or all of the above services. It could be extended with additional features, as needed.

Second: Extensive training activities. In order to quickly bring researchers up-to-speed, we will organise series of training events. The events will be organised as close to users as possible, e.g. at research institutions with large communities where we can achieve biggest impact.

Third: Nordic-wide network of application experts. Building on the experience of e.g. the SNIC application experts' initiative, the project can create the nucleus of a wider communication

environment for exchange of expertise. This will be achieved naturally through jointly developing and the infrastructure and running the training activities.

Expected benefit

Adoption of modern tools and best practices for software development will bring considerably benefits to researchers by increasing:

- productivity of the researchers,
- quality of their codes,
- skills of the developers.

National providers will benefit from 1) the increased competence among their users, which will lead to 2) improved utilisation of their resources through development of better software, as well as 3) the long-term maintainability of locally developed software.

The Nordic region as a whole will benefit from the nucleation of a community and increased interactions between application experts from different countries, as well as with the corresponding user groups.

Basis

This project is a part of NeIC Generic Area Activity for 2015, “Activity GEN-7 Nordic e-Infrastructure for scientific software” and it is in line with Action 10 “Nordic eInfrastructure for scientific software” from the Nordic eScience Action Plan 2.0.

- Establishing a software development e-Infrastructure
- Coupling it with necessary technical expertise
- Extensive training and on-boarding activities

Contact persons

This is the list of persons that have knowledge on subject and have helped in the preparation phase.

Name	Email	Role
Rossen Apostolov	rossen@kth.se	**Author of the proposal** and SNIC Application expert in Molecular Simulations at PDC. He is a developer of one of the major Nordic codes, Gromacs, which has a sophisticated development infrastructure.
Dejan Vitlacil	vitlacil@kth.se	NeIC Generic Area Coordinator and **main contact** with NeIC
Jonas Juselius	jonas.juselius@uit.no	Jonas (University of Tromso) has expert knowledge in the domain of the proposal and is leading activities in line with the suggested activities. We have discussed the project and he is very interested in participating.
Radovan Bast	radovan.bast@gmail.com	Radovan (PDC) was the main organizer and leader of the “Scientific Software Toolbox”. He is a SNIC Application Expert in Electronic Structure, core developer of Dalton and Dirac, and has expert knowledge in the domain.
Andreas Jaunsen	andreas.jaunsen@uninett.no	Technical Provider Forum member (NO)
Jura Tarus	jura.tarus@csc.fi	Technical Provider Forum member (FI)
Ann-Charlotte Sonnhammer	ann-charlotte.sonnhammer@it.uu.se	Technical Provider Forum member (SE)
Torben Rasmussen	torbenr@nsc.liu.se	SNIC Application Experts Coordinator
Jon Kerr Nilsen	j.k.nilsen@usit.uio.no	Senior Engineer and ARC lead developer

Other

Nordic Cloud steering group will be chaired initially by Dejan Vitlacil, and later by Michaela Barth, representing NeIC as the project owner.

The funding partners as defined in the corresponding Collaboration Agreement are asked to appoint members for the steering group.

Expected funding partners are:

- CSC,
- SNIC,
- DeIC,
- UNINETT Sigma2.

Appendix 2: The partners' interest in and competence relative to the project

The partners are described in the following:

NeIC (the Nordic e-Infrastructure Collaboration) is funded by national research funding organisations in Denmark, Finland, Iceland, Norway and Sweden. The vision of NeIC is to facilitate the development and operation of high quality e-infrastructure solutions in areas of joint Nordic interest. The legal representative of and hosting organisation of NeIC is NordForsk, which is an organisation under the Nordic Council of Ministers.

CSC — IT Center for Science Ltd is administered by the Ministry of Education, Science and Culture. CSC is a non-profit company providing IT support and resources for academia, research institutes and companies: modeling, computing and information services. CSC provides Finland's widest selection of scientific software and databases and Finland's most powerful supercomputing environment that researchers can use via the Funet network. CSC is currently actively maintaining and developing several Cloud environments.

DeIC (Danish e-Infrastructure Cooperation) was established under the Ministry for Higher Education and Science by Act 70 of April 19 2012 with the purpose to support Denmark as an e-Science nation through delivery of e-infrastructures (computing, storage and network) to research and research-based teaching. Organizationally, DeIC belongs to the Danish Agency for Science, Technology and Innovation and is not an independent legal entity. DeIC is a virtual organisation, which means that all staff are employed in other organisations. Primarily at the Danish Technical University and to some extend at Aarhus University, Aalborg University, University of Southern Denmark and University of Copenhagen.

The Swedish National Infrastructure for Computing (SNIC) is a national research infrastructure that provides a balanced and cost-efficient set of resources and user support for large scale computation and data storage to meet the needs of researchers from all scientific disciplines and from all Swedish universities and university colleges. The resources are made available through open application procedures such that the best Swedish research is supported. The SNIC infrastructure is funded by the Swedish Research Council (Vetenskapsrådet) and the university partners. SNIC is organised as a long-term project (2012-2016), with its own Board.

UNINETT Sigma2 AS manages the national infrastructure for computational science in Norway, and offers services in high performance computing and data storage. The services are organised in research infrastructure projects, financed by the Research Council of Norway and collaborators. The business is run non-commercially. UNINETT Sigma is a subsidiary of UNINETT and is headquartered in Trondheim.

Appendix 3: Budget and resources

NeIC partners (CSC, DeIC, Sigma2, SNIC) will provide resources as in-kind R&D activity. Of that committed R&D activity, NeIC funds maximum 50%. The remaining partner funding will be aligned with national and EU funding. The total number of FTEs for the duration of the project is estimated to reach 4,5 FTEs, or 2,25 FTE per year. The project also includes travel, workshop and some event costs; to be covered by NeIC. The budget proposal is as follows:

Partner	Annual effort, project year 1	Annual effort, project year 2	Total effort	NeIC share
CSC	0,5	0,5	1,0	50%
DeIC	0,5	0,5	1,0	50%
SNIC[2]	0,75	0,75	1,5	67%
UNINETT Sigma2	0,5	0,5	1,0	50%
Total	2,25	2,25	4,5	

NeIC funding includes 0,25 FTE to maintenance of the SGAS[2] system, previously co-funded by Sigma, SNIC and NeIC. The final budget, including integration of SGAS, will be defined in the project plan.

[2] https://wiki.neic.no/wiki/SGAS_maintenance_project

Appendix 4: Terms of Reference for the Project Steering Group

The project is governed by a steering group appointed by the partners, with the authority to make decisions on behalf of the partners within the project. The steering group is chaired by the NeIC representative. The steering group has the following responsibilities:

- Ensure the success of the project, by
- Understanding and communicating the expected benefit.
- Ensuring that the project results contribute to the expected benefit.
- Making decisions in steering group meetings.
- Actively supporting project management.
- Being the formal link between the project and operations.
- Making decisions regarding issues where project management has no authority.
- Approving the detailed project plan and any additional deliverables described therein.
- Monitoring the project and approving progress reports.
- Approving deliveries and transfers of deliverables to operations.
- Understanding the responsibilities associated with the task and reserve sufficient time to execute them.

Being the formal link between project and operations entails:

- Identifying changed prerequisites in operations.
- Taking care of effects in home organisations.
- Priorities and connections to other projects.
- Securing outer dependencies of the project, outer prerequisites outside the authority of project management.
- Ensuring formal personnel issues are handled.

Actively supporting project management entails:

- Marketing the project and acting as its ambassador.
- Being available, and acting as a “sounding board” between steering group meetings.
- Staying constantly informed about the project’s status.
- Ensure availability, competencies and quality for the resource categories concerned.

NeIC coordinates the project. Project coordination includes the responsibility to find an adequate project manager being able to carry out the agreed work. When appropriate, NeIC enters into a separate agreement with the employer of this project manager in a way that does not violate the terms of this agreement (c.f. Collaboration Agreement 2.4).

A full quorum is required for the steering group to take decisions. The steering group should strive for agreement, but may reach decisions by voting. In these cases, each partner gets a vote. The steering group may at their own discretion invite observers. With a uniform decision a major stakeholder (who agrees to deliver something to the project) may become a full member of steering group. With unanimous decision they may be given a voting right.