

Second Evaluation of NOTUR

Norwegian High Performance Computing Infrastructure

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To the Research Council of Norway.

The members of the Evaluation Committee reviewing the Norwegian national infrastructure submit the following report. The views presented in this report are the unanimous opinion of the members of the Evaluation Committee, and the members of the Evaluation Committee are fully in accord with regard to the assessments, recommendations and conclusions stated in the report.

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1. Objective and Background

This is the second international review of the NOTUR project focussing on the period from 2004. During this time there has been significant expansion in the HPC funding and the national infrastructure available to the research communities in Norway. The objective was therefore to evaluate the facilities according to the terms of reference given below, namely,

Based on the self-assessments provided by the institutions and site visits, the Evaluation Committee is to submit a report

- i) to evaluate the way in which the national eInfrastructure is organised and managed;
- ii) to assess its quality and relevance using the international state of the art, funding level and user needs as the frame of reference;
- iii) to produce a set of specific recommendations for the future development of the national eInfrastructure, including means of improvement.

The review took place during the week of June 9 to 13th 2008. The Evaluation Committee visited all the NOTUR sites and would like to express their thanks to all the staff that they met for their contributions to the discussion and for answering the many questions raised by the Evaluation Committee. Thanks are also due to Gudmund Host for the excellent organisation of the visit and the documentation provided.

2. Summary

The Evaluation Committee was impressed by the resources and the research activity taking place throughout Norway. It is clear that the investment in a national infrastructure is producing enhanced research activity throughout Norway, that existing areas of research are benefiting from the new facilities and that new areas of research are being pursued. Researchers in Norway now have facilities which compare favourably with other research groups throughout Europe and further afield. However, the investment and research benefits are dependent on a continued funding stream to ensure the facilities are updated in line with technology developments and applications requirements. The Evaluation Committee made a number of observations on how the infrastructure and its usage could be improved in particular

- i) more authority and leadership to coordinate the national infrastructure to develop a more national policy;
- (ii) a procedure for assembling and refining a stronger science-driven case for policies, procurements, etc;
- iii) a reorganisation of the existing committee structure to manage, promote and plan the national infrastructure.

3. Organisation of national eInfrastructure

i) Research Council of Norway

The Research Council has a number of funding initiatives reflecting the wide diversity in the funding of research in Norway such as Centres of Excellence, Centres for Research Based Innovation, and Large Scale Programmes, HPC infrastructure etc. which give long term funding opportunities to specific research topics; however, it is not clear how these initiatives are linked into the policy and co-ordinating structure within the Research Council. The Evaluation Committee *recommends* that more is done to ensure cross fertilisation of these initiatives to ensure that HPC and the national infrastructure is promoted across all funded activity in Norway.

The investment in 2007 by the Research Council is now beginning to bring new benefits in research opportunities, international collaboration and it is to the credit of the Research Council to have released and allocated the funding. However, given the large injection of funding in such a relatively short period of time it has also meant that new machines have appeared throughout Norway roughly at the same time and this, in turn, means that continuing the HPC investment and enhancement is all the more challenging. In a case of flat funding at the previous steady state level, it would mean that the current machines will be out of date within a few years. The Evaluation Committee *recommends* that a funding mechanism is put in place to smooth out the variations in funding and to ensure that an adequate funding stream is made available so that long term planning is possible and the current investments being made in research programmes and critical infrastructure are protected.

ii) Committees

The work to date should be considered successful at creating an initial instantiation of a national cyberinfrastructure. The first stages of an effective eInfrastructure have been put in place at the universities through NOTUR, collaborations are developing between the computing sites, researchers are using these systems and Sigma is operating as a national coordination centre. These developments are in accordance with the broad outlines of the Research Council and the sites and researchers have demonstrated a significant level of sophistication about the capabilities and potential of the eInfrastructure.

The next stages in the development of the eInfrastructure strategy will require careful evaluation of the continued utility of the current committee structure. The structure has a set of sub-committees that, as currently constituted, have drawn extensively upon the expertise of the existing technical leadership at the universities to create a technological “pull” for the scientific computational research community. As a result, the scientific users are successful nationally and internationally and have an increasingly sharp and pragmatic understanding of the capabilities of the eInfrastructure and are well prepared for creating the scientific “push” for the future.

The Evaluation Committee *recommends* the simplification of the current committee structure with the goal of creating an acquisition, support and evaluation strategy to address the long term computational, storage and visualisation requirements of the scientific researchers.

The Committee's observation was that the eVITA Committee was the primary committee for decision making in the development of HPC and the national infrastructure. The Evaluation Committee **recommends** that the eVITA committee has its terms of reference revised and that its membership reflect the wide diversity of Norwegian facilities both from a technical and a user point of view. There are essentially two areas which need to be developed, namely, operational and strategic, with the eVITA Committee providing the forum where these different aspects are reported and agreed.

The Committee believes that in general the overall responsibility for the national infrastructure should lie with the Research Council of Norway and within its committee structure. The relationship with UNINETT should be clearly defined - their role being more concerned with the networking provision and operations with the higher infrastructure activity being the responsibility of the Council's committee structure with Sigma involvement.

As a result the relationship with UNINETT Sigma needs to be clarified. The Evaluation Committee **recommends** that Sigma reports directly to eVITA and with operational responsibilities as agreed to by eVITA. Sigma should be able to act more directly and make decisions on the operation and co ordination of the resources, both hardware and human, at the sites.

In the future development and procurements the process should be grounded in better information and input from a range of stakeholders and end users. A recurring theme of the Evaluation Committee's observations across the sites visited is the lack of a process whereby the scientific case for the facilities is developed and refined. In practice this means the involvement of application scientists with their input being assembled and co ordinated to provide a forward look over a five year or longer period of time. The objective will be to construct a document - the scientific case - which records as far as is possible the requirements and future directions of Norwegian application scientists across a range of disciplines and which makes best estimate of future requirements while at the same time identifies new areas of HPC applications which could be encouraged into, for example, the HPC portfolio of applications. This document should be updated on a regular basis and subjected to the public comment of the research community through electronic means as well as public Town Hall meetings.

This scientific case can then be used as the cornerstone of the argument for the further funding of facilities in Norway. Essentially it is the precursor activity before a formal business case for the HPC procurements can be made. In this way the advancement and maintenance of facilities in Norway can be put on a more formal basis and can be justified and formalised within the current Research Council structure.

In practice this needs a sub committee to bring together the case for applications - a sub committee whose members are representative of the community and committed to the objectives advancing HPC in Norway. The Evaluation Committee **recommends** that such a sub committee - the Scientific sub committee - be introduced with clear terms of reference and reporting to eVITA. This sub committee should consist of members from the major applications groups across Norway and with a Chair person appointed from the academic community to lead the group for a 5 year period.

The Reinfra or Advisory Committee for Investment in eInfrastructure has a mandate for long term investment, international trends and need for computing resources. The Evaluation Committee **recommends** that the terms of reference and membership of Reinfra be enhanced

into a new subcommittee – the Technical sub committee reporting to eVITA- which in addition accumulates knowledge and information about the developments in the underlying technology, software and architectures being developed or proposed in the roadmap of many of the vendors and research groups. In this way the Norwegian research community will be better informed and up to date if and when money is available for new procurements and this will facilitate the purchase of new machines. One of the side benefits of such an approach could be the further and enhanced involvement of the computer science community in the national infrastructure.

The interactions between these two proposed sub committees of the hierarchy will be critical to the future growth and success of the Norwegian eInfrastructure.

4. Users

As part of the evaluation the Committee held a series of private meetings with users to ascertain their experiences, needs etc. as the main stakeholders in the national infrastructure. In general the feedback was positive - the users generally had very good experiences of the services that they were provided with and felt from their contacts with colleagues in the same discipline throughout Europe and further afield that they were well catered for. There was a wide range of usage patterns with cross submission of jobs between the machines which, with few exceptions, was efficiently facilitated by the network connections within the structure.

The level of user help for most queries of a general nature appears to be dealt with within a reasonable period of time, however, the way in which the more advanced user help requests are considered seems to be less well received. It is reasonable that such requests require more planning and detailed consideration – the regular submission deadline, that is, of 6 monthly intervals does not appear to be causing major problems at present. The range of software appears to be satisfying the user requirements and with few exceptions satisfying user demands – there was some comments on the consistency of the range of compilers and the software packages of a specialised nature being provided across the machines. The provision of software including commercial codes seems to be adequate and usefully co ordinated centrally through Sigma – it is therefore important that Sigma ensure adequate provision and consistency across all sites.

The users should be consulted on the nature and type of courses that are required and that such activities should be co ordinated centrally through Sigma. The outreach effort across the sites varied from very little to good activity; it is important that all sites engage in this activity and that they also engage, co operate and collaborate with the other sites in outreach activities and promote a sense of national co ordinated activity in this area. It is important that new potential users are targeted and identified – there is a substantial effort required to move users from the ‘workstation’ level onto the national infrastructure and that more effort is invested in hand holding these users etc. There was a good example of a University using the national infrastructure for the provision of its computing resources – there were little resources available locally – and the university researchers, as a result, were able to join in an international project of a significant nature. The Evaluation Committee were impressed by the range of projects some of significant international importance and many focussing on topics of prime and perhaps unique interest and benefit to Norway. The sites should try as far

as possible to make efforts to link up with other sites around the world which have the similar machines or applications portfolios in order to export and import best practice.

There were some examples of interaction with industry and cross fertilisation of ideas between users in the University and industry – for example, HPC had been the catalyst for projects. There have also been discussions of new facilities and degrees within the Universities at the highest level as a result of the Universities being part of the national infrastructure. This has been having an impact on the strategy of the Universities in some cases leading to multidisciplinary activity and is leading to the creation of possibly new degrees in areas such as computational science and engineering.

The split between local and national usage varies across sites and is related to users' requirements and disciplines. More effort should be expended in publicising the successful applications and their national and international impact as a result of the utilisation of the national infrastructure – many of the projects have the potential to be submitted as projects in some of the international HPC competitions with all the PR and benefits a successful submission can bring. There were some discussions on the publications emerging from the usage of the national infrastructure and how they are classified. The continued production of an annual report of all publications using the national infrastructure compiled as a true record of the impact of the national infrastructure and as part of the publicity of the investment is encouraged and felt to be an important aspect of the NOTUR initiative.

The Evaluation Committee was pleased to discover a high level of user satisfaction and hopes that this level is maintained. It is important that as mentioned previously the input of the users is formalised and that their requirements are regularly monitored. A sizeable community has been created and it is hoped this will expand as existing and new disciplines enlist the national infrastructure in its research progression. Given the high level of satisfaction the Committee *recommends* that the sites co operate and collaborate in areas of user service to ensure that the high level of satisfaction is maintained and enhanced.

One of the challenges for many countries is ensuring the engagement of application scientists and computer scientists in advanced computing facilities and activities. This requires finding a mechanism where both groups of scientists can find topics of mutual interest and benefit to their disciplines. The Evaluation Committee *recommends* that the Research Council fund a special programme of collaboration between application and computer scientists. Topics for such activities could be related to the major challenges in this area such as software for petaflop/s and involve the topics of programming models, compiler techniques, algorithms etc. for the new and exciting petaflop/s area which is about to unfold. This would also provide an opportunity for further European collaboration and international collaboration e.g. in the US Blue Waters project. This activity would best be organised as part of the eVITA programme.

European and international links and collaboration are important components in the advanced computing field as this requires technology which is of major interest to the most industrial and commercial countries. In the EU there are major activities taking place in the FP7 programme e.g. the PRACE initiative. Although it is not clear how these projects will turn out it is important that Norway perhaps as a single country or a part of the Nordic countries is fully engaged or at a minimum formally connected to the developments in European and international projects. This role is currently led by Sigma but needs to be enhanced with more academic involvement. There does not appear to be a mechanism in Norway where Norway's

input is co ordinated to maximise input in these activities. The Evaluation Committee *recommends* that a mechanism is put in place to ensure co ordination of Norwegian input to European and international initiatives; this could be through either one of the new sub committees or eVITA directly.

On the wider front of the uptake and promotion of HPC there are several possible activities that would be beneficial in order to sustain the long term future of HPC in Norway. The Evaluation Committee *recommends* the creation of a number of targeted studentships. For example, there is a need for targeted PhD and MSc studentships in HPC to sustain a healthy skill-base. These studentships would be specifically for HPC activities across all disciplines and could be attached to other initiatives such as the Centres of Excellence. A possibility is to attach them to the existing HPC centres to ensure that as much synergy and interaction is possible both with researchers and centre operations. Each studentship would include a period committed to training at one of Norway's leading HPC centres; the balance of time would be spent working on a research project at their host institution

5. Management, staff and operations

The Evaluation Committee met with the leadership of Sigma, reviewed the self-evaluation for Sigma, discussed the interactions of each of the four sites with Sigma with the Sigma leadership, with each of the four sites and with individual users in the context of their scientific programmes.

The national eInfrastructure is embodied as a Metacenter. The Metacenter is composed of the set of university-based resources with the operational responsibilities at least partially under Sigma, which is several layers removed from eVITA. The universities make significant contributions to the acquisition and support of the computing centre resources and have developed areas of expertise and depths of knowledge in key areas. The universities have a very high level of autonomy in their daily operations and in their strategies for acquisitions, user support and policies. In some discussions with representatives of the university computing organisations, it was evident that the priorities of the national eInfrastructure were not as heavily weighted as the needs of the local user community but a spirit of cooperation and willingness to collaborate was present.

The process by which decisions on goals, implementation plans, acquisitions and evaluations are made under the current structure with Sigma is not well structured. Sigma has operational responsibility for NOTUR, NorStore and NorGrid and relies on Service Level Agreements with the sites to meet these responsibilities, which has usually, but not always, been sufficient. As the infrastructure increases in sophistication in response to the requirements of the computational scientists and Norway's roles in the EU grid and computing environment, the current processes and agreements will be limiting.

Sigma has an Advisory Committee made up of the IT/HPC management of the consortium partners to provide advice on the long term plans for the national eInfrastructure and a Board made up of six members who are primarily researchers who use the national eInfrastructure, which may serve to balance the technical depth and emphasis of the Advisory Committee. The integration of these two viewpoints into an effective strategy is the responsibility of Sigma and the magnitude of the task has been noted by the management of Sigma. Sigma has an appropriate level of understanding of importance of the scientific requirements as the

justification for the eInfrastructure. This understanding is evident in the Sigma self assessment document and in the discussions with the Managing Director of Sigma. The mechanisms to implement this understanding should be carefully considered by eVITA and the Research Council of Norway to ensure the success of the eInfrastructure. This relates directly to one of our principal *recommendations*, namely, that Sigma reports directly to eVITA and assumes operational responsibilities as agreed by eVITA. Sigma should be able to act more directly and make decisions on the operation and co ordination of the resources, both hardware and human, at the sites.

The management structure relies on Service Level Agreements (SLA) between Sigma and the individual sites that are part of the Metacenter. Each site manager is responsible for reporting progress and status to Sigma towards meeting the requirements of the SLA but is not required to break out the levels of effort for specific aspects of the SLA. This may allow a significant level of opacity in terms of the management of the funding provided from Sigma. This may be acceptable if there are well-thought out and structured SLAs in place. Given the increasing levels of understanding of the requirements for an effective eInfrastructure by all participants in the Metacenter and a goal for stronger emphasis on meeting the national scientific programme requirements, the Evaluation Committee *recommends* that Sigma and the sites put in place SLAs that are transparent and contain specific performance metrics. This is particularly timely as a Metacenter reference document is in preparation.

Sigma is responsible for the grid and storage components as well as the HPC aspects of the eInfrastructure. The discussions with the users yielded a significant level of satisfaction and usage of the HPC systems but few uses of the grid and storage components. These are both challenging technical areas and researchers require clearly defined, stable and sustainable environments in which to work. The Activity Plans for 2008 and, by inference, for future years for NOTUR, NorGrid and NorStore could be considerably strengthened with detailed descriptions of the services to be put in place, the timelines for these services and the scientific benefits of the services. This type of information should be developed by Sigma with the collaboration of the sites in the context of the Metacenter reference document and the SLAs.

6. Site assessment

The Metacenter provides a virtual HPC centered infrastructure. The intention is that the Metacenter provides a national resource allocation procedure, a unified management system for user accounts, accounting, reporting and software licenses and a standardised file organisation system. This requires the co operation and collaboration of the sites and Sigma in the achievement of these services. There are currently four sites operating across Norway as part of a Metacenter concept involving Bergen, Trondheim, Tromso and Oslo. The facilities at each site differ but a rough division is a focus on capability computing at Bergen and Trondheim and a focus on capacity computing at Tromso and Oslo.

The Committee *recommends* that the Metacenter concept should be better defined with clear responsibilities assigned, agreed and accepted by the participating partners, particularly for Sigma.

i) Bergen

The University has a well-established record in parallel and distributed computing going back many years. It is therefore an appropriate site for an HPC Centre and its associated activities.

The environment of the Centre is well supported and encouraged by the University and this has resulted in extra funding and incorporation within the University's management and strategy committees.

The Centre is a free standing unit with minimal interaction with the rest of the University's IT unit – this does not appear to have caused any problems but closer co operation is a model which could yield mutual benefits to all parties and the University.

The most recent procurement is the Cray XT4 with a peak performance of 51 teraflop/s. There is a sizeable staff in the area of computational science both in academic disciplines and support activities. The Centre and its staff are well engaged in HPC and grid computing and its application. There are strong internationally recognised application groups using the facilities and wide use of the range of machines available. In particular, climate research, oceanography, computational chemistry and computational physics.

The Centre favours the Metacenter model and believes in autonomy in the procurement process and would like to see a simplification of the Committee structure dealing with national co ordination of HPC resources.

The users' applications that were presented displayed a community which is benefiting greatly from the resources and the support. There have been some significant results produced and substantial international collaboration and presence which further underline the need for continuity in the provision of resources. Data preservation and maintenance is a facility which is directly needed and needs further rationalisation e.g. as to whether the scientists need to be directly involved or whether the support staff could provide such data facilities. It does appear that NorStore could be more involved in this activity. The split of resources between those provided locally and nationally was not clear e.g. which activities were the responsibility of the differently funded positions.

ii) Trondheim

The University is currently discussing a strategy for Computational Science and Visualisation as a multidisciplinary initiative involving application scientists, computer scientists and mathematicians. This Initiative has the support of the management of the University. This is highly commended by the Committee as a significant and appropriate development. However there are a number of obstacles which can frustrate such an interdisciplinary initiative for example, promotions for staff etc. which need to be carefully considered and agreed to ensure a successful outcome.

NTNU has a long history of involvement with HPC and its applications. This started with the installation of a Cray X-MP/2 in 1986 and was the predecessor to a long line of different systems. The University is therefore well experienced in installing systems and providing a user service. The available system, Njord, which is shared 50/50 between the University and the Research Council; the University has invested heavily in a supporting infrastructure for the HPC machine. As a result of the resource allocation system with the ability to allocate resources locally some significant research work which may not have been possible through the national allocation system has been carried out.

NTNU has been in collaboration with one of the oldest research Institutes in Norway, SINTEF, for many years and has been able to expand their co operation as a result of the HPC system.

There is a support group currently of seven persons, five of which are covered by the national agreement. Support is supplied for local users as well as number of NTNU users who need the machines at Tromso.

In general the University is concentrating on HPC, providing advanced computing facilities and waiting to see if grid technology matures.

iii) Tromso

The University is proud to be the world's most northerly University and hence to house the world's most northerly supercomputer center. They can trace their supercomputing roots back to 1978 with a CDC Cyber system. The current system, Stallo, is a HP cluster installed in November 2007 and using the ROCKS cluster distribution operating system which gives a link to San Diego Supercomputing Center and other international partners. The connection to HP has led to other collaborations, for example, the Gelato Federation. There is close collaboration with the Norwegian Polar Institute for simulations in fields like oceanography and polar research and this has led to direct funding by the Institute. One of the major users is the Norwegian Meteorological Institute in a project known as EMEP based on pollution simulations. This, in turn, has led to the 50% funding of a position at the center to work on this model. Another significant user is the Center of Excellence in Theoretical and Computational Chemistry with a significant increase in performance of the Dalton code through staff efforts.

UIT has been hosting a central site for user documentation for sites in Norway which has been well received and hopefully can be maintained and developed further. The Stallo cluster is a node in NorGrid and receiving production job runs. They have a total staff complement of 6 for HPC, three of the post being guaranteed. They have had difficulty recruiting staff and maintaining a full staff complement. UIT has provided office and machine room space and the center is part of the University's IT department.

The HPC service is fully engaged in the national initiative and providing a well used and appreciated HPC service both locally and nationally. They have built up good expertise and links in cluster computing which is of benefit nationally.

iv) Oslo

The participation in the national eInfrastructure is provided by the Research Computing Services (RCS) group which is part of Center for Information Technology (USIT). UIO is the largest user of the national eInfrastructure with a wide range of users who utilise both local and national facilities at the other NOTUR sites. UIO is fully supportive of the diversity of machines within the national infrastructure and with the consequent benefits that allows in application development. Their machine provision is based on the teraflop/s Titan cluster. The HPC group is well qualified and well experienced and has been providing help and assistance in the traditional HPC disciplines as well as developing new HPC applications in areas including psychology, economics etc. This service is much appreciated in surveys of the users. UIO has been one of the main Norwegian sites to offer storage services and is well

engaged with the NorStore project and international projects ALICE and Atlas connected to CERN. The University is well engaged in international projects as well as with industrial partners who pay for part of the operational costs but get user support for free.

UIO will continue to focus on PC cluster technology and storage and grid services for both national and international users. The University provides 3 1/3 person years to complement the Sigma hosted posts.

The University feels dependent on NOTUR to satisfy user demand but also points out that some of its users have to go abroad to perform larger simulations; UIO would like to see this external usage reciprocated by international users accessing Norwegian machines. UIO also feels that the current system of large systems at the sites with small support groups is not optimal and that the Metacenter vision where competence flows easily between NOTUR sites should be significantly enhanced. There is also concern about the extension of advanced user support in that the university feels if this type of support becomes extended - greater than the current 6 months - then it will be directly related to the research project and research priorities and that the national allocation model conflicts with the University's research plans and objectives. This type of support should be funded by the local university. There is also concern about the decision making structure being too complex and to where the role of Sigma extends – essentially Sigma extends to a two year window with long term strategies being decided elsewhere.

7. Usage of resources

The Evaluation Committee met with users at all sites, with representatives of the Resource Allocations Committee, and with members of the staff who support users from all sites. Users were generally very satisfied with most aspects of the facilities, including the availability of facilities, their allocation, and the user support they received. The allocations process apparently works well, and the same group responsible for allocating time on facilities also assigns advanced user support. When asked how their support and access to computing facilities compares with that of their colleagues in other countries, most felt they are in better shape than others.

A wide variety of disciplines is represented in the user base, which utilises the systems across Norway according to suitability for the application, or in some cases simply on the basis of familiarity with the system. The Committee found a good mix of jobs at each site from groups at other sites, and there was no evidence of hesitation to support groups from remote sites. The Committee noted that there are relatively few users of the systems in biology, which is one of the major growth areas in computation. The groups working in this area did say they were very satisfied with the systems and support they received.

Although different disciplines were represented, the Committee did not see much evidence of multidisciplinary work in the computing projects represented in the users. Perhaps the most important of these interactions we found lacking was between computer science and science/engineering disciplines. The Evaluation Committee emphasises its earlier *recommendation* that programmes be developed to strengthen interactions between computer science and disciplinary research groups specifically and multidisciplinary research generally. The Evaluation Committee also *recommends* that special attention be paid to applications in the biological sciences to see if additional support is needed in that area.

The Committee also noted in particular that there appeared to be relatively strong efforts in fluid dynamics at different sites, some with advanced, multiscale, adaptive mesh applications. Yet these efforts appeared to be carried out in relative isolation from each other. While some of these groups had strong international collaborations, interactions among the groups within Norway were weaker than we might expect. To the Committee, this was representative of a lack of communication across the computing community. Although we noted that there were yearly meetings of users, e.g., the meeting in Tromsø the week before our review, the Evaluation Committee *recommends* that special attention be paid in the future to mechanisms to promote development of the computational science community, with more opportunities for all-hands user meetings, creation of topical user groups, for example, in CFD, biology, and so on. This is important for both novice and advanced groups alike, where for example, emerging areas like computational biology can be accelerated and advanced groups in fluid dynamics may be willing to share advanced software libraries with other groups in Norway to attack more advanced scientific problems.

The experience level of the users varied considerably from very advanced to beginning. Generally, the groups seemed to be able to take advantage of the systems to produce serious scientific results that seem to be competitive at the international level. However, this observation is based primarily on interviews conducted with users and not on a systematic assessment of the quality of the scientific papers produced. We were not presented with systematic scientific quality assessments in the form of publications resulting from the time allocations, except at Tromsø. The Evaluation Committee *recommends* that a systematic accounting of the scientific output across all sites be carried out, with complete lists of publications and analysis of their impact. This should be done at a national level, with data collected for the usage at all sites.

While users were always very positive about the quality of the facilities and support, when pressed the following issues came up consistently at every site:

- *Bandwidth.* Users complained that bandwidth to remote sites was often lacking, with perhaps the strongest complaints heard regarding the connection to Tromsø. We note that in principle the sites are all connected by high speed networks, with a bandwidth between sites of typically 10 Gbit/s (theoretical). This is not an unusual situation for supercomputing sites but there are clearly problems, perhaps at the local campus infrastructure, perhaps at the network interfaces to the machines themselves. When we brought this up at the various sites, we were assured that the problems did not originate with them! The Evaluation Committee *recommends* that the overall, end-to-end connectivity be monitored nationally, by Sigma, which should coordinate efforts to address any issues that are discovered.
- *Storage.* Users at virtually all sites mentioned there was not enough storage, and that considerable time was spent managing output and transferring it to places where they could analyze or archive it. The Evaluation Committee *recommends* that the issues of storage be analyzed for effectiveness for the national user base.
- *Support for extended visits to the sites.* It was noted by some users that it would be very desirable to visit a remote site where computing was being carried out for advanced code development, working with advanced user services groups, etc. The Evaluation Committee *recommends* that support for extended visits for periods from a few days to weeks be investigated for feasibility. This would

facilitate both the development of more advanced application codes and stronger ties between members of the community at the different sites.

- *Advanced visualisation.* It was noted by users and administrators at most sites that there is relatively little effort in scientific visualisation, and no national effort for advanced visualisation support. While we did find advanced groups working in the area, e.g., at NTNU, they did not appear to be closely connected to the national HPC efforts. The Evaluation Committee *recommends* that support for advanced scientific visualisation at a national level, with appropriate connections to the HPC environment, be investigated.
- *Documentation and training.* While users were satisfied with help they received, they noted that it was difficult to find documentation for software and services provided at the various sites (we did not investigate this ourselves, and do not know if this relates to one site or another in particular). It was also noted that very little attention is paid to hands-on training sessions for users to learn how to use the various systems, software libraries, message passing techniques, etc. The Evaluation Committee *recommends* that, at a national level, special attention is given to ensuring that adequate documentation for usage of systems is provided, and that a series of hand-on workshops be given on a regular basis for all systems operated at a national level.

Also, in regard to bandwidth, we note that as such high bandwidth is available in principle between the sites, it is possible to consider deploying HD video conferencing between sites for many purposes, including training, advanced user support, topical meetings devoted to applications in specific areas (e.g., CFD, computational biology, etc), and development of specialised courses in computational science. For the latter, the barriers of “low critical mass” against offering a specialised course in, e.g., computational materials science, can be overcome by team teaching such a class to all sites, collecting interested students from all universities, so that reasonable class sized may be achieved. This would also act to promote development of discipline-oriented communities that would accelerate the development of the computational sciences in Norway.

The Meteorological Institute (MI) is one of the major users of the national facilities, especially at NTNU for production forecasting, and requires special comment. The Meteorological Institute was generally satisfied in their ability today to get sufficient cycles on the IBM system for forecasting. On the other hand, they were very concerned that they do not have a strong enough voice in the future development of the computing environment, and also that they need more support from advanced user services than they are able to get. We find these to be legitimate concerns. The Evaluation Committee recognises the special needs of, and strategic role played by, the Meteorological Institute, and *recommends* that the Meteorological Institute be given a strong role in the scientific steering committee, which should be responsible for developing the future roadmap for eInfrastructure in Norway, including procurement and deployment of systems, policies on their use, and the user support models appropriate for the various constituents.

In our assessment of the user support, in addition to the above points we also found several issues in our discussions with users that require special comment.

- *User Input.* Although we stress again that users felt generally satisfied, we noted repeatedly that users do not have a satisfactory process to provide input into the operation of the systems, their selection, the services needed, and so on. Input

may be possible through annual user surveys, but this is not sufficient to support the development of the scientific community. This relates directly to one of our principal recommendations, namely, that a strategic scientific committee be developed to steer the development of the national computing infrastructure.

- *Queuing systems and national coordination.* The systems at each site appear to be well-managed, and with the recent expansion of facilities users are generally happy with availability of cycles provided to them. We did have at least one comment that more flexibility in queuing structures and allocations be provided, so that users have more ability to dynamically adjust their usage from site to site as their science develops in unpredictable ways. This issue is one reflection of the fact that there seems to be rather limited coordination at a national level of the queuing and operations of the facilities; rather, each site has a great deal of autonomy and seems to operate independently. This relates to another one of our principal recommendations, that Sigma take a stronger role in coordinating national eScience development and policies, including operation of facilities at each site, but at a national level.
- *Advanced User Support.* Although we applaud the efforts of advanced user services, and find this group to be very important for the development of the advanced scientific applications that run on the facilities, the funding model, as we understood it, is problematic. Funding for staff in Advanced User Support seems to be allocated on per-project basis, making continuity of staff support, and therefore attraction and retention of advanced staff, very difficult. A more productive model would be to provide long-term funding to staff at the various sites, and then allocate their *time* on a per-project basis. This way staff would be more secure, for longer periods, and users can be assured that there is a stable, expert staff available to help them develop their applications as needed, and allocated, by the Resource Advisory Committee. The Evaluation Committee *recommends* that the issues of staff support for Advanced User Support be investigated and adjusted if appropriate.

8. Collaboration and outreach

The Evaluation Committee found evidence of various levels of collaboration and outreach activities. To cite a few examples among many that were presented, the group at Tromsø appears to be active in development of Rocks, and has ongoing collaborations with San Diego Supercomputer Center; and the climate group has been deeply involved in the IPCC report on climate change; the groups in Oslo and Bergen are very active in the Nordic grid activities, and Sigma is involved in PRACE at the European level.

However, the Committee felt that more could be done in all areas of outreach and collaboration, and that these activities could be better coordinated at the national level. The efforts described above seem to be left to individuals at each site (and this is also good), whereas a more comprehensive approach with clearer lines of responsibility for various international collaborations could be very beneficial. Accompanying our recommendations for a stronger national effort to create a strategic roadmap of Norwegian eScience, the Committee also *recommends* that this include a discussion of how to better coordinate international collaborations that are in the national interest. This is especially true for projects at a regional (e.g., Nordic Grid activities) and European (e.g., PRACE) level. Such activities

could include designating a spokesperson representing Norway for such projects, who then represent the national interests of Norway in a more systematic way, and considering exchange programmes from staff from Norwegian centres to their counterparts in Europe, the USA, etc.

On the issue of industrial cooperation, the Committee found some activity and would certainly encourage more. This could be extremely advantageous in areas of the national interest, e.g., in the oil and gas area. We would encourage exploration of partner programmes with industrial partners, where for example Advanced User Services time could be provided for research partnerships with companies who need to advance their industry through use of advanced computing facilities. It is also very common for companies to work with universities through graduate student internships, which could be formally organised at the national level. Developing industrial programmes to advance the use of HPC in industry is important not only for the competitiveness of industry, but also to help advance university-industry partnerships that provide better training for students, and generally help create a more healthy and robust computational ecosystem. The Committee *recommends* that industrial partnerships in HPC be explored and developed at a national level if possible.

In terms of a strategy for building eScience competence across Norway, the Committee has a number of recommendations. Although we found a high degree of expertise and competence among the staff of all centres and the among the user groups with whom we met, we also feel that much more can be done both locally and on a national level to advance the state of the art, and for Norway to take better advantage of the significant recent investments that have been made in developing national eScience activities. In short, the Committee *recommends* the following (which also applies to outreach for new users within universities, research institutes, and industry):

- A competitively awarded programme of fellowships in eScience to support graduate students in computational science applications.
- A series of planning grants awarded to encourage science and computer science groups to work together to examine next generation applications for eScience, for all relevant disciplines, but specifically in terms of petascale computing, grids, networks, visualisation, etc. These could pick up on the Grand Challenge document which stopped short of projecting with any serious detail what the next generation science problems demand in terms of computing facilities, algorithms, software environments, networks, and so on. The results of these studies could be taken as input to the strategic Scientific planning sub committee we are also recommending be put in place.
- As mentioned above, we believe a more proactive series of hands on workshops should be carried out at a national level, which should occur regularly, some of which should have a disciplinary focus. For example, in addition to MPI, OpenMP, parallel I/O, visualisation, etc, we also recommend specific workshops for computational chemistry, biology, materials, CFD, etc, where outside experts are also invited to showcase international state of the art as well as that nationally. Such workshops will also facilitate the building of a stronger Norwegian eScience community.
- As also mentioned above, we would encourage the universities associated with the HPC sites to consider developing national, collaborative courses in eScience applications, utilizing the high bandwidth available at all sites to carry out HD video conferencing. This would be useful not only for training but also for semester-long courses in, for example, computational fluid dynamics, biology, climate modelling,

etc, which can be team taught by the collective faculty, available for credit locally, and complete with hands-on exercises on the systems available.

- Another strategy to investigate is international exchanges, where students may spend a term at a national lab or site such as NCSA, and where a local student from those sites may spend a term at one the Norwegian sites.

Lastly, we comment on the development of interdisciplinary research programmes, which are becoming increasingly important for scientific programmes. We saw evidence of different programmes specifically along these lines at both NTNU and in Bergen, and commend these activities. We would encourage a broader national programme of interdisciplinary collaborations, specifically between computer and discipline scientists. This can be encouraged with funding mechanisms that require teams of researchers from different disciplines to work together to attack important problems. At the local level, we resonated with the goals of programmes like those described to us at NTNU, and only wish to point out that incentives and rewards for interdisciplinary collaborations are tricky and need to be very carefully considered. To give one example, promotion criteria for faculty in traditional departments are often at odds with the goals of interdisciplinary collaboration, and therefore such interdisciplinary programmes need to be supported carefully, and at the highest levels of university administrations.

9. Financial support and funding

The Norwegian eInfrastructure efforts have clearly demonstrated their usefulness to the scientific community and these efforts have enabled the users of the resources to conduct research on par with their collaborators and competitors across Europe. This is a highly laudable accomplishment on the part of the providers of the resources and demonstrates the technical talent that is available in the Norwegian university system in the area of HPC and the readiness of the Norwegian researchers to push their research programmes ahead.

The capability and range of computational resources that exists today is a result of early investment by the Norwegian Research Council and the universities in the concepts and expertise associated with HPC and related topics, such as grid computing, coupled with a significant short term increase in funding in 2007 for out of cycle system acquisitions, NorStore and NorGrid. The universities that successfully upgraded their systems in 2007 demonstrated a depth of experience and a commitment that has been fostered by a unique partnership with the Research Council of Norway. This partnership has notable strengths and is strongly commended by the Committee.

The universities derive local benefits from their contributions to the acquisition and operation of a system on their campus. These contributions are on the order of half of the total cost of ownership for the system and include providing appropriate facilities to house a system, the utilities necessary to run the system and some of the support staff to operate the system. The benefits include developing local computational expertise using the fraction of the system resources that are allocated by the university in recognition of the contributions. It is worth noting that the universities are themselves primarily funded by the government of Norway.

The Research Council of Norway, through Sigma, provides the majority of the funding for the acquisition of the systems, support for on-site personnel to operate the system and for

personnel to work with applications scientists as advanced user support. The responsibility for coordinating the acquisitions and advanced user support lies with Sigma.

The base funding reported for NOTUR for the 2005-2014 period is 21.7M NOK with one time funding provided in 2007 of 52M NOK for out of cycle system acquisitions, 11.2M NOK for NorStore and 6.8M NOK for NorGrid. As a result of this funding increase, the support and maintenance costs have increased or are projected to increase from the 2007 levels. The number of personnel associated with the advanced user support is currently three FTEs across the Metacenter, which provides a minimal level of support given the presence of the new systems.

The additional funding in 2007 is providing the opportunity for Norwegian researchers to have access to resources that are competitive within Europe. The consequence of the nearly simultaneous recent acquisitions is that the systems will all become less competitive at the same time. Maintaining a level of competitiveness will require continued investments in HPC and associated resources. The base funding level will only permit minimal upgrades to the HPC systems while efforts on NorGrid and NorStore are currently underfunded.

The scale of the systems is rapidly growing along with the power density within the systems. An additional factor that must be considered is that the costs associated with operating advanced computing systems are increasing due to the need for more robust infrastructure to provide additional power, cooling and networking capabilities.

The Committee noted that there is an unmet need to support efforts directed towards the education of the next generation of researchers, post doctoral positions in computational sciences and ongoing faculty development and training.

It is the conclusion of the Committee that previously established base funding level with the one time increase has served Norwegian researchers well to date. However, the factors noted above all lead to a **recommendation** by the Committee that the strategic plan for the national eInfrastructure be formulated that is based on the requirements of the scientific priorities for the Norwegian computational researchers including clearly defined funding priorities for the eInfrastructure that allow these scientific goals to be met.

A final comment. The Evaluation Committee has been presented with a large of amount of information, talked with many people and visited many sites and has gained a substantial overview of the NOTUR Initiative throughout Norway. As a result it has made a large number of comments and compiled a list of many recommendations. The Committee has not taken into account the costs of the recommendations and realises that they may be difficult to achieve within current funding levels but present their findings based on the terms of reference. The Committee hopes that their report is helpful to both the research communities and the funding bodies in Norway in progressing and enhancing what is an impressive national infrastructure.

Appendix 1: Terms of Reference for the Evaluation

The Research Council of Norway: Evaluation of national eInfrastructure

Terms of reference

I. Introduction

The national high performance computing project NOTUR (I) was established in 2000 with NTNU as leading partner. The project was carried out by NTNU in collaboration with the universities in Bergen, Oslo and Tromsø, the Meteorological Institute, Statoil, SINTEF, and some other partners. The project was financed in part by the Research Council of Norway (RCN) with 22 MNOK per year, and in part by the consortium.

In October 2004, a 10-year agreement (for the period 2005-2014) was signed between UNINETT AS (operator of the national research and education network) and RCN for the future responsibility for the development of a Norwegian infrastructure for computational science. On December 2., 2004, UNINETT Sigma AS (Sigma), a subsidiary of UNINETT AS, was created with a board of directors and a set of bylaws that regulate the operations of the board. The agreement with UNINETT requires that the enterprise be evaluated under the auspices of the Research Council of Norway within 3-4 years after startup.

The collaborative model and project activity of the NOTUR project was carried over into the new NOTUR II project (2005-2014). Sigma is project manager and the universities in Bergen, Oslo and Tromsø, NTNU and the Meteorological Institute are consortium participants. Also the NOTUR II project is financed in part by the RCN and in part by the consortium participants.

NOTUR II is currently a project under the research programme eScience, Infrastructure, Theory, and Applications (eVITA) that was established by the RCN's Board of Science Division (BSD) for the period 2006-2015. A strategic committee for eInfrastructure investments that advises the eVITA Programme Board was established in December 2005. Furthermore, the allocation of CPU-hours, storage and advanced user support is done by a separate resource allocation committee.

Presently the Norwegian infrastructure for computational science is a distributed infrastructure that encompasses four high performance computing (HPC) centers. The NOTUR II project builds on the (local) HPC centers of the four university partners, each of which has its own profile of expertise, strategies, and interests. The HPC centers are the main executors within NOTUR II and operate supercomputer facilities and provide user support services.

Later, Sigma has been given the responsibility to manage both a national Grid initiative (NorGrid) and a national storage project (NorStore), building on the NOTUR consortium model. In addition to the three projects described above, the Research Council's eInfrastructure funding also covers a share of the Nordic Data Grid Facility together with Denmark, Finland and Sweden. The national research network is funded directly by the Ministry of Research.

The objective of the evaluation

The objective of this evaluation is to review the overall state of eInfrastructure for Norwegian research with a particular emphasis on the resources under the auspices of the RCN and in the NOTUR system; including HPC, Grid, storage and support services. The main target for the evaluation is the activity organized through and around Sigma. However, it is also of interest to receive comments on relevant boundary conditions and interfacing activities. These include the national research network, as well as Nordic and international compatibility and collaborations. The evaluation should provide a critical review and a recommendation which can aid the RCN in further development of the organization and scope of the national eInfrastructure. The Research Council's Board of Science will take the final decision on further action. .

Methods

An international Evaluation Committee will be appointed. Self-assessments provided by Sigma and the consortium participants will contribute to the basis for the evaluation. The committee will perform site visits to the parties. Interviews will be undertaken with Sigma, consortium participants, eVITA programme committee and its subcommittees, resource providers, university leaders, user groups, Ministry, the Research Council and other stakeholders that the committee may find relevant. The Committee is requested to write a report with a set of specific recommendations. The Committee's written report is expected to be based on the elements and questions given below. The assessments and recommendations should be at consortium participant, project management and national governance/organisational level. The Committee's final report will be submitted to BSD.

II. Mandate for the Evaluation Committee

Based on the self-assessments provided by the institutions and site visits, the Evaluation Committee is expected to present the evaluation in a written report with a set of specific recommendations for the future development of the national eInfrastructure, including means of improvement. The Committee is requested to evaluate the way in which the national eInfrastructure is organised and managed and assess its quality and relevance using the international state of the art, funding level and user needs as the frame of reference. Some specific points are given below.

Organisation of national eInfrastructure

Give an assessment of the organisation of eInfrastructure in Norway, addressing:

- The environment for national strategy development
- The organizational hierarchy and sharing of responsibilities between various committees
- Processes for goal-setting and decision-making
- Interaction with stakeholders
- Pros and cons of the consortium model
- Pros and cons of organizing Sigma as a subsidiary of UNINETT
- Sustainability and long-term perspectives
- Are there aspects of the organization that should be strengthened or changed in order to meet the requirements of Norwegian scientists and the Meteorological Institute?

Quality and relevance of national infrastructure

Give an assessment of the quality and relevance of the eInfrastructure, including a comparison with other countries in the Nordic region, EU and the industrialized world, including:

- Specific aspects of HPC, Grid, storage and support services
- Is the infrastructure oriented towards the needs from Norwegian scientists and Research Council priorities?
- Does the infrastructure meet the operational needs from the Meteorological Institute?
- Does the infrastructure practise an open access data policy?

Management, staff and operations

Give an assessment of Sigma as an enterprise, covering project management and details of the project operations.

- Staff, organisation, leadership and strategy of Sigma
- Project management of NOTUR II, NorGrid and NorStore: responsibility, authority and internal communication
- The project organisation and the meta-center
- Are issues of quality assurance and improvement handled adequately?

Site assessment

For each site in the project organisation please assess the organization and service provided addressing in particular:

- Does the site cater for specific user needs?
- Is the site managed according to project objectives?
- Quality of operations, user support and services provided
- Is the staffing adequate and is the competence profile reasonable?
- Does the site have dedicated project staff?
- Is there a clear division between project work and other work?
- University's long-term strategy for provision of eInfrastructure services
- University's financial support to the HPC center
- Active collaborations with external parties and industry, external funding

Usage of resources

Give an assessment of the allocation and use of resources, including

- The resource allocation policy and the work of the resource allocation committee.
- Queuing system, its implementation and national coordination
- The role of the Meteorological Institute's operational forecasts. Efficiency of operational codes, system reliability, and resource-sharing with other users.
- User satisfaction and mechanisms for communication with users
- Level of support activities, quality of regular and advanced user support

- Are the scientific results from eInfrastructure usage well-documented and does the scientific output seem reasonable?
- Is there a clear scientific added value of the eInfrastructures?
- Are some user groups absent, over- or underrepresented?

Collaboration and outreach

Evaluate the collaboration activities and the outreach efforts, including

- International relations, including Nordic collaboration
- What is the extent of industrial collaboration, both at project management level and at the site level? Should this be expanded? If so why and in what directions?
- Strategy for competence building and activity within education in the use of eInfrastructures
- Outreach towards new users within universities, research institutes and industry

Interaction with stakeholders

This aspect of the evaluation should include the interaction with

- the consortium participants at the institutional level, such as the university leadership
- user groups, such as
 - Centres of Excellence, research institutes, major disciplinary groups (e.g. high energy physics, chemistry, geosciences, ...)
- The Norwegian Meteorological Institute
- funding agencies, such as
 - The Research Council
 - Ministries
- industry, research institutes

Financial support and funding

Please assess the general financial situation for eInfrastructure.

- Is the volume of current funding sufficient to cover user demands?
- Are the current funding mechanisms appropriate?
- The distribution of resources between high performance computing, Grid and data storage
- The distribution of resources between hardware investments, operations, user support

Future developments and needs

The plans for the development of the national eInfrastructure for the next five-year period will be evaluated.

Miscellaneous

- Have the recommendations and problems identified in the previous NOTUR evaluation been addressed? In what way?

- Are there any other important aspects of Norwegian eInfrastructure that ought to be given consideration?

Background material for the evaluation

The following written material will form the point of departure for the evaluation:

- Self-evaluations according to a standardised outline, from project manager and from each consortium participant
- Project descriptions for NOTUR II, NorGrid and NorStore
- Progress reports for 2007 for NOTUR II, NorGrid and NorStore
- Activity plans for 2008 for NOTUR II, NorGrid and NorStore
- Mandate for Resource Allocation Committee (translated from Norwegian). Policy for resource allocations
- Mandate for Advisory Committee on eInfrastructure Investments, with extensions
- NOTUR User Survey 2007
- National Strategy for eInfrastructure, ReInfra - The Committee for Investments in eInfrastructure, The Research Council of Norway, Oslo, 2008 (to appear)
- Investments in the Norwegian eInfrastructure for Computational Science - An investment plan for the period 2007-2016, ReInfra - The Committee for Investments in eInfrastructure, The Research Council of Norway, Oslo, March 2007. ISBN 978-82-12-02425-0 (printed version), ISBN 978-82-12-02426-7 (pdf)
- Agreement between UNINETT and Sigma (translated from Norwegian)
- eVITA Programme Plan
- Aerts P, Lüthi H P, Ynnerman A (2004) Evaluation of NOTUR. NOTUR – A Norwegian High Performance Computational Infrastructure. The Research Council of Norway. ISBN 82-12-01991-8
- The Future of High-Performance Computing in Norway, Risto Nieminen, Anne C. Elster, Knut Børve, Roar Skålin og Lina von Sydow, The Research Council of Norway, November 2003
- The Research Council of Norway, Oslo 2000 (English version)

Other documentation that the committee find relevant may be made available upon request.

Self-assessments

Self-assessments will be produced by project responsible (Sigma) of the three eInfrastructure projects and by each consortium participant. The self-assessment is a narrative description of accomplishments related to the project objectives and associated contributing factors identified in the project plan. The self-assessment should provide the evaluation committee with a clear picture of the participant's own performance and contributions.

The self-assessments should not exceed 20 pages (plus attachments) for Sigma and 5 pages for each consortium participant. These should contain:

- Information about the organisation and resources, including important user groups
- History, development, strategy and future plans of the site. Local funding and contribution to the national projects.
- Active collaborations with external parties and industry, external funding
- Restatement of objectives for project involvement
- Main contribution to reaching project goals
- Most significant achievements for the evaluation period

- Challenges faced and how these were dealt with
- List project personnel with % project employment

As attachments, CVs of core personnel should be included.

Additional material to be provided by Sigma includes

- An overview and justification for changes, if any, in the strategic plan
 - An overview of researcher training and outreach activities up to the midway evaluation
 - Key financial and administrative figures and factors associated with Sigma
- As attachment, CVs of core personnel and a list of major research results achieved up to the evaluation, supplemented by a list of publications and any bibliometric data that illustrates the scientific added value of using the national eInfrastructure

Time schedule for evaluation

The evaluation will be conducted according to the following approximate timeline:

December 2007	Evaluation framework discussed with Board of Sigma
January 2008	Stakeholders propose members of Evaluation Committee
February 2008	Terms of Reference and members of the Evaluation Committee appointed by BSD
4. April 2006	Deadline for self-assessments
May 2008	Evaluation Committee meets in Oslo, Bergen, Trondheim, Tromsø
June 2008	Scientific Committee submits evaluation report
September 2008	Approval of report and decision on prolongation by BSD
October 2008	Publishing and implementation of decision

The meeting of the committee will be organised during one week in May 2008 and include site visits to the project manager and consortium participants. In conjunction with this meeting, the committee will arrange individual hearings with the stakeholders. Apart from this meeting, communication between the committee members is expected to take place by e-mail or phone.

