Academy of Finland

COMPUTATIONAL SCIENCE

RESEARCH PROGRAMME

– models and applications from social to natural sciences

LASTU

2010–2014

Programme memorandum

1 Foreword

At its meeting on 2 October 2007, the Board of the Academy of Finland granted a negotiation mandate to launch preparations for a research programme in the field of computational science.

The working group taking charge of preparations was appointed in March 2008. Representing the Academy's Research Councils on the preparatory group were Professor Jaakko Astola (Research Council for Natural Sciences and Engineering; Tampere University of Technology, chair); Professor Jaana Bamford (Research Council for Biosciences and Environment; University of Jyväskylä); Professor Pia Vuorela (Research Council for Health; Åbo Akademi University); and Professor Jaakko Pehkonen (Research Council for Culture and Society; University of Jyväskylä). In addition, the following experts were invited to contribute: Professor Christer Carlsson (Åbo Akademi University); Professor Mats Gyllenberg (University of Helsinki); Academy Professor Risto Nieminen (Helsinki University of Technology); Professor Pekka Neittaanmäki (University of Jyväskylä); and Professor Marjo Yliperttula (University of Helsinki). The scientific secretary for the preparatory group was Juha Fagerholm, Doctor of Science in Technology (CSC – IT Center for Science). Also contributing to the preparatory group from the Academy were Science Adviser Tiina Forsman, Senior Science Adviser Pentti Pulkkinen and Programme Managers Anssi Mälkki and Merja Kärkkäinen.

Round table discussions were held on Wednesday 4 June 2008 at the premises of the CSC – IT Center for Science, where the following experts were heard: prof. Raimo Hämäläinen (Helsinki University of Technology), programme manager Arto Kotipelto (Finnish Funding Agency for Technology and Innovation, Tekes), Academy prof. Hannu Oja (University of Tampere), prof. Kari Rummukainen (University of Oulu),prof. Keijo Ruotsalainen (University of Oulu), prof. Outi Savolainen (University of Oulu) and prof.Arto Urtti (University of Helsinki).

An exploratory workshop in preparation of the Computational Science Research Programme was held on Thursday, 21 August 2008 at Hotel Presidentti in Helsinki. The working groups were chaired by prof. Risto Nieminen, prof. Pia Vuorela, prof.Jaana Bamford and prof. Christer Carlsson. The workshop attracted an attendance of 110 participants.

All of the Academy four Research Councils will be participating in the Research Programme, which is scheduled to run for a period of five years: the Research Councils for Biosciences and Environment; Culture and Society; Natural Sciences and Engineering; and the Research Council for Health.

2 Background of the Research Programme

The information technology revolution has profoundly changed the ways of doing science. Computational science has emerged as the third pillar of scientific inquiry to accompany experiment and theory. The development of computational methods and tools is advancing at a strong pace in all disciplines.

Computational science is a field that uses numeric models instead of or together with direct experimental measurements or mathematical and theoretical analysis to investigate complex problems or phenomena. The main differences compared to traditional computer-assisted research lie in the intensity of computations, the large data volumes involved and often in the interactive nature of computation. The computational approach can yield considerable savings, allowing for the use of computer simulations instead of expensive and time-consuming experiments. Indeed there are many increasingly complex problems and phenomena where computational science offers the only viable way forward: examples include the sequencing of the human genome, forecasting the weather and resolving complex problems faced by modern society.

Advances in science have now made it possible to measure and influence the state of increasingly complex systems. Computational science allows researchers to get to grips with the laws that control and govern systems, even when they are so complex that traditional modelling is not feasible. This may eventually help to resolve some of the greatest challenges facing humankind, such as climate regulation, health promotion, understanding social networks, etc.

The tools of computational science are already being applied in a large number of disciplines to tackle challenging research problems. The application of computational methods requires not only methodological skills, but also an in-depth understanding of each field of application. Close multidisciplinary and interdisciplinary collaboration among experts in different fields is one of the typical characteristics of computational science. Another distinctive feature is the close interplay between and simultaneous evolution of the field of research and the computational methods applied in that field.

Key factors contributing to the breakthrough of computational science have included the rapid development of information technology, and particularly the phenomenal growth of computation and information management capacities, the growth and expansion of methodological expertise in different fields of research, and the explosion of data volumes produced by ever faster and more accurate measurement tools. Indeed computational science and technology are heading towards ever more complex systems that combine many traditional disciplines and that often have non-linear, multi-scale multi-objectives or highly data-intensive characteristics.

During the winter of 2006–2007, the Ministry of Education hosted a working group charged with drafting a proposal for the national development of computational science. In its memorandum (MoE working group memoranda and reports 2007:23) the working group suggested that the Ministry of Education and other public sector agencies provide funding for interdisciplinary computational science projects in both methodological and applications

research in 2009–2012. The Finnish Funding Agency for Technology and Innovation Tekes and the Academy of Finland were urged to step up their funding for research in computational science and to strengthen their expertise in this field. Furthermore, the Grid strategy working group suggested in its report (MoE working group memoranda and reports 2007:7) that an eScience programme be set up in Finland. As part of this programme it was proposed that the Academy and Tekes prepare and finance a research programme in computational science in 2009–2012 with a view to developing and applying the methods of computational science in new disciplines and to strengthening expertise in computational science. The Research Programme in Computational Science is a concrete step in the implementation of the Finnish eScience programme.

2.1 Computational science

Computational science is defined in different ways in different sources. In the United States, computational science is understood in somewhat narrower terms than is traditionally the case in Europe. The influential PITAC report offers the following definition:

Computational science is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems. Computational science fuses three distinct elements:

1. *Algorithms (numerical and non-numerical) and modeling and simulation software developed to solve science (e.g., biological, physical, and social), engineering, and humanities problems.*

2. *Computer and information science that develops and optimizes the advanced system hardware, software, networking, and data management components needed to solve computationally demanding problems.*

3. *The computing infrastructure that supports both the science and engineering problem solving and the developmental computer and information science.*

This definition places heavy emphasis on *integration* and *interaction* between the three component areas. In particular, close interaction between the first and second element is a crucial success factor in the search for the optimal solution.

A closely allied term that is often understood as synonymous with computational science is that of eScience. For instance, the definition of eScience outlined in the Action plan for the Norwegian eVITA programme comes close to the definition proposed here.

2.2 Links with other research programmes

Tekes has a closely related ongoing research programme in this field under the heading of Modeling and Simulation (MASI 2005–2009). Key areas of focus in the MASI programme include multiphenomena/multiscale modelling, modelling methods and tools, the development of services and business processes, and practical applications of modelling. The Academy's Research Programme on Mathematical Methods and Modelling in the Sciences in 2000–2003 (MaDaMe) can also be considered to have been an important precursor.

Computational research, modelling and simulation appear as either specific themes or generic activities in all Strategic Centres for Science, Technology and Innovation (CSTIs). Through its research projects, therefore, the programme will be well placed to support the research work carried out at these strategic centres.

There is growing international recognition of the great strategic importance of computational science to national competitiveness; prominent examples include the innovation systems in the US, China, India, Japan and the EU. Indeed most EU Member States, particularly the UK, Germany and recently France, have invested heavily in the development of computational science. Significant joint projects have also been launched at the Nordic level. There are ongoing multidisciplinary research programmes, among other countries, in the US, China, the UK and Norway, all of which are potential partners for programme cooperation.

The Computational Science Research Programme has several points of contact with the Capacities component of FP7, which is specifically designed to support the optimal use of existing European infrastructures and the development of new infrastructures. The Research Programme will facilitate the participation of Finnish research teams in these European projects, even though its main focus of interest lies in areas other than infrastructure.

The Research Programme will have links with the Nordforsk NORIA-net programme (2008–2009); with the Academy's Nanoscience Research Programme (FinNano); with the Academy's Research Programme on Photonics and Modern Imaging Techniques that is scheduled to start up at the same time; and with the ERASysBio ERA-Net programme.

2.3 References

1. Computational Science: Ensuring America's Competitiveness, Report to the President, President's Information Technology Advisory Committee, June 2005.

2. eScience – Infrastructure, Theory and Application (eVITA), Action Plan, The Research Council of Norway, January 2007.

3 Aims of the Research Programme

The aims of the Research Programme can be briefly summarized as follows:

Promoting the use of computational methods

One of the main aims of the Computational Science Research Programme is to promote the use of computational methods throughout society. In view of this objective, the programme will be working to develop computational methods and the necessary statistical, mathematical and computer science solutions; to promote the efficient and appropriate use of infrastructures; to support computational science research; and to develop computational applications for different disciplines and for interdisciplinary research on various scientific and social problems and phenomena.

Improving methodological skills and competencies

This objective involves raising levels of mathematical and computer knowledge in the research community and improving methodological skills and competencies. One of the key aims is to foster interaction between mathematics, computer science, information technology and research applying computational methods. The diverse range of problems covered means that the programme has points of contact with all of the Academy's fields of research.

Increasing interdisciplinary interaction and collaboration

Through the two objectives described above, the Research Programme will aim to facilitate interaction and exchange between research teams and different research disciplines. Computational science is fundamentally characterized by interdisciplinary collaboration and exchange between the substance sciences and algorithm and methods development. Significant scientific results, therefore, can only be achieved if there is good communication. As far as possible the projects in the programme should involve experts of different disciplines or methodologies. At the same time, individual focused projects can have great significance. The research efforts pursued in the programme are aimed at finding cutting-edge solutions that will point the way forward for future research practices.

Closer and more frequent interaction between research communities and individual research teams will facilitate the formation of new consortia, which in turn will help to achieve the critical mass that is necessary to reach the international forefront. The Research Programme may be a crucial factor in turning abstract ideas of collaboration into concrete joint activities.

Enhancing the application of good practices

A further objective of the Research Programme is to promote good practices in research that uses computational methods. Good practices refer among other things to information on data sources and utility and careful documentation in general. Additionally, the projects taking part in the Research Programme will be required to submit information management plans.

International networking

The final objective of the Research Programme is to promote the international networking of researchers. This will be achieved by means of programme coordination and through the researchers' own international contacts. Plans for cooperation between Nordic and other international funding agencies are outlined later in this memorandum.

4 Programme themes

Given the broad scope and coverage of the Research Programme, it is not feasible here to provide a definitive list but rather some selected examples of possible research themes. Many of the subject areas covered by the programme are inherently interdisciplinary and multidisciplinary by nature.

The Research Programme is focused on problem-driven computational research that aims at resolving problems by using computational methods. It comprises both computational and data-oriented lines of research in all disciplines, including biology, physics, chemistry, language research, health research, economics, engineering and the social sciences. Key criteria include the uniqueness and relevance of the research subject, the contribution of the research to methodological development and the comprehensiveness and relevance of the data.

Examples are provided by the new opportunities created in many disciplines by advances in information technology. One important area is represented by so-called Grand Challenges which address computationally intensive problems and fundamental issues in science and engineering; topical examples include climate change, energy issues, health and well-being, the security of global information networks, and management of the global economy. Models describing these problems involve several interconnected elements, and their resolution, verification and interpretation are both important to society and scientifically challenging.

Other typical examples include the modelling of disease mechanisms and the transfer and effects of medicines within the organism, the use of ultraefficient sequencing techniques, modelling natural language, the management of logistic networks, and understanding genetic regulation. In the fields of biology and social sciences it is crucial that researchers apply new and much larger datasets than they have done to date. Many of the fundamental problems of modern physics and chemistry are key areas of intensive computational research.

As one of the programme's main objectives is to improve methodological skills and competencies, the development of computational methods is obviously a high priority. Problem-solving algorithms and methods as well as simulation and modelling methods are also central to the Research Programme. One of the most common themes of computational science methods is multiscale modelling.

Examples of the methods used in computational science include the methods of discrete mathematics; the joint application of stochastic and deterministic methods; large-scale and complex optimization methods; metaheuristics; adaptive methods; physically or biologically inspired algorithms; and data-based methods. Many other algorithms and methods are also widely applied. Algorithmic and statistical data analyses and data intensive computing need to be supported by methods of data mining.

The resolution of a problem may require the development of facilitating techniques and tools: examples here include the parallelization of software for terascale computing, the

visualization of large datasets and research results, and the management and storage of large and, possibly, structured datasets. However the main focus in the Research Programme is on the problem at hand, not on the facilitating technology. The development of tools and technologies may be incorporated as part of the project in so far as it supports or is necessary for resolving the scientific issue in question.

Infrastructure development is not a priority concern for the Research Programme. Based on discussions with the CSC – IT Center for Science which is responsible for the allocation of scientific computing resources under the Ministry of Education, projects under the umbrella of the Research Programme will be given priority consideration in resourcing decisions. Fields that do not have the necessary IT infrastructure in place may require support in the form of IT services, software or databases, for instance, and funding for these purposes may be justified.

The Research Programme is specifically intended to support projects that will foster the creation of nationally significant research communities and that will be well placed to achieve significant breakthroughs by virtue of the international cooperation and knowhow of the people behind the project. In addition, research projects are encouraged that cut across the boundaries of the Academy's Research Councils.

5 Implementation of the Research Programme

5.1 Programme funding

The *Computational Science Research Programme* is funded by the Academy of Finland and is coordinated by a Programme Manager based at the Academy. The programme is scheduled to run for a period of five years, with research projects starting up during 2010 and 2011 for four-year terms in 2010–2015. The Board of the Academy of Finland has earmarked a total of 8.5 million euros for allocation under the first call for applications in 2009.

5.2 National cooperation

The Research Programme shares interests in common with the Tekes programme Modeling and Simulation (MASI 2005–2009), with the Academy's ongoing nanoscience programme (FinNano, 2007-2011) and with the Academy's forthcoming Research Programme on Photonics and Modern Imaging Techniques.

5.3 International cooperation

The Academy will seek opportunities for international funding cooperation in order to promote and support international collaboration through the programme. Over the next few years the Academy's major partners in cooperation will include India, Japan, China and Russia as well as Canada, the United States, Brazil and Chile, where steps will be taken to further intensify cooperation among the bodies funding this research. The Academy's Research Councils have submitted proposals for cooperation in the field of computational science with Brazil, India, Japan, China and Russia.

Preliminary talks have been held on the possibility of research programme cooperation with the US National Science Foundation (NSF). Together with the Research Programme on

Photonics and Modern Imaging Techniques, a joint call for applications with the National Natural Science Foundation of China (NSFC) will be opened in 2009.

In addition to any bilateral calls that are organized, all Finnish projects that are successful with their applications to the 2008 ERA-NET (ERA-SysBio) programme will be integrated as part of the Research Programme. Discussions have been held with the Norwegian eVITA programme and the joint Nordic eNORIA project on the possibility of collaboration through co-coordinated researcher seminars, for instance.

5.4 Timetable

Under the Research Programme funding will be provided to participating projects during 2010-2014. The projects selected in 2009 will start up no later than 1 January 2010; the projects selected in 2010 will start up no later than 1 January 2011. The latest possible project end dates are 31 December 2013 and 31 December 2014, respectively. The evaluation of the Research Programme will be carried out in 2015.

Programme Calls will be opened in 2009 and in 2010. Both calls will involve two stages. Decisions on any specific research themes for the 2010 call will be made by the Programme Steering Group during 2009.

Letters of intent (January 2009, dead-line 30 Jan; dates for 2010 will be decided later) shall be submitted in the form of relatively short plans of intent. The Programme Steering Group will submit its assessment to the Programme Committee regarding the applications it feels most closely meet the themes and criteria specified. The selected applicants will be requested to submit detailed research plans to the second stage (20 April – 15 May 2009). These projects will be announced on the Programme WWW pages and the applicants will be informed about the decision in writing.

Based on a scientific review of the applications and bearing in mind the objectives specified for the Research Programme, the Programme Steering Group will submit its proposal regarding the projects to be funded to the Subcommittee of the Programme, which will make the final funding decisions.

The final timetables and themes for joint international calls will be issued on the programme WWW pages.

5.5 Programme Steering Group

Direction and supervision of the Research Programme rests with the Programme Steering Group, which consists of members of the Academy's Research Councils, representatives of other organizations associated with the programme, and expert members. Other experts may also be invited to participate in the steering group.

The role of the Programme Steering Group is to:

- to steer and monitor the programme,
- to prepare the process for evaluating applications,

- to submit a proposal to the responsible funding bodies concerning the projects to be funded
- to submit proposals for supplementary calls for applications and/or additional funding to the Research Councils and other funding bodies if necessary,
- to submit proposals for projects to be added to the programme at a later date,
- to plan and organise the final evaluation of the programme,
- to steer and support programme coordination,
- to promote the utilisation of research results.

5.6 Programme coordination

The aim of the Research Programme is in every possible way to help the research projects develop into a coherent and cohesive structure through active exchange of information and cooperation. This requires coordination aimed at facilitating the achievement of the goals set for the programme. In this way it is hoped that the projects will reinforce one another and that the programme will generate new kinds of multidisciplinary research knowledge. The researchers in charge of the projects selected to take part in the programme will therefore be required to commit themselves to the goals of the programme and to support the goals of coordination throughout the programme and during its evaluation.

The responsible leaders of the projects involved in the programme will be expected to:

- assume responsibility for and report on the scientific progress of the project and its application of funds according to the instructions of the Programme Manager and funding bodies;
- make sure that the whole research team attends all meetings, seminars and workshops organized by the programme coordinator and facilitate exchange of information and cooperation between the research groups in the programme;
- take part in producing reviews, syntheses and information material around the Research Programme; and
- actively disseminate information about the programme's progress and results on public and scientific forums.

The programme manager will work closely with the projects and facilitate the achievement of programme objectives. The programme manager will coordinate information and communications around the programme, promote research cooperation between the projects as well as establish contacts with society, industry and foreign research bodies. Joint seminars, workshops, training courses and electronic communication will be used.

Responsibility for programme coordination rests with the Academy of Finland and Programme Manager Merja Kärkkäinen.

5.7 Final evaluation

The Research Programme will be evaluated upon its completion. The evaluation will consider the following aspects:

- achievement of the programme's objectives
- implementation of the programme (coordination, role of steering group, participation in the programme)
- scientific quality of the results achieved
- outcomes and impacts, integration of the results and preparation of synthesis at programme level
- evidence of scientific, social and economic impacts of the programme
- researcher training and the advancement of research careers
- national and international cooperation
- dissemination of information on the programme's work.

The research teams funded through the programme shall report annually on the progress of their work or as specified by the Programme Steering Group and upon completion of the project submit a final report to the Academy of Finland. The reports shall include lists of all scientific publications and all academic theses completed in the project.

6 Application procedures and project review criteria

The research programme has a two-stage call. Application deadlines are strict. The application and its appendices shall be drafted in English via the online services at www.aka.fi/eng > For researchers > Log in to online services. Then select *New application* > **Computational Science Research Programme**

The call for applications is open both to individual research teams and to consortia made up of several research teams. Funding applications submitted to the Academy are required to comply with:

1. The general guidelines applicable to all calls given in the Academy of Finland's January 2009 call
2. The detailed guidelines on submitting an application that are available under www.aka.fi/eng > For re-searchers > How to apply > Guidelines
3. The detailed information on the format and length of appendices that is available under www.aka.fi/eng > For researchers > How to apply > Appendices
4. This research programme memorandum

6.1 Letters of intent

Letters of intent shall be submitted via the Academy's online service no later than 30 January 2009 by 16:15. The application deadline is strict. **Only** the requested appendices are appended to the application. The appendices shall be drafted in accordance with the Academy's guidelines.

The evaluation criteria for letters of intent are how well the project ties in with the topic of the research programme, its contribution to realisation of the programme objectives and the project proposal's innovative value and applicability. The Academy will select the applicants that are invited to submit a full application during March 2009. The Academy will post information on the selection on its website and notify applicants of its decision in writing.

6.1.1 Letter of intent by one research team

- Online application form

Appendices to the application:

- a plan of intent, no more than four pages in length
- the CV of the responsible project leader, no more than four pages
- the list of publications of the applicant, the length of which is not limited. The applicant is requested to clearly indicate the ten key publications relevant in terms of the research plan.

6.1.2 Letter of intent by a consortium

Only the consortium leader submits a letter of intent.

- Online application form

Appendices to the application:

- the consortium's plan of intent, no more than six pages in length
- curricula vitae for the consortium leader and the responsible leaders of the sub-projects, combined as one document, no more than four pages for each researcher
- lists of publications of the consortium leader and the responsible leaders of the sub-projects, combined as one document, with the ten most important publications in terms of the research plan clearly indicated for each leader of a sub-project

6.2 Full applications

The Academy will select the applicants that are invited to submit a full application on the basis of the letters of intent during March 2009. The Academy's online services will open to applicants that have been invited to submit a full application about one month before the application deadline. **The application deadline for full applications is 15 May 2009 at 16:15.** The application deadline is strict.

Only the requested appendices are appended to the application. The appendices shall be drafted in accordance with the Academy's guidelines.

6.2.1 Full application by one research team

- Online application form

Appendices to the application:

- an abstract, no more than one page in length
- a research plan, no more than 12 pages
- the CV of the responsible project leader, no more than four pages
- the list of publications of the responsible project leader, with the ten most important publications in terms of the research plan clearly indicated
- statement by an ethics committee or the Committee on Animal Experimentation, if relevant
- a progress report for any research projects with Academy funding that the responsible project leader is involved in and for which no final report has yet been submitted
- an invitation from a foreign university or research institute if the research is conducted abroad.

6.2.2 Full application by a consortium leader

- Online application form, with which funding is applied for only for the consortium leader's own research team.

Appendices to the application:

- an abstract drafted in accordance with the consortium guidelines, no more than one page
- a research plan drafted in accordance with the consortium guidelines, no more than 15 pages
- curricula vitae for the consortium leader and the responsible leaders of the sub-projects, combined as one document, no more than four pages for each researcher
- lists of publications of the consortium leader and the responsible leaders of the sub-projects, combined as one document, with the ten most important publications in terms of the research plan clearly indicated for each leader of a sub-project
- statement by an ethics committee or the Committee on Animal Experimentation, if relevant
- a progress report by the consortium leader and the responsible leaders of the sub-projects on their Academy-funded research projects for which no final reports have been submitted, combined as one document
- invitation by a foreign university or research institute, if the research is conducted abroad.

6.2.3 Application by responsible leader of a sub-project of the consortium

- Online application with which funding is applied for only for the research team of the responsible leader of the sub-project
- **No** appendices are to be appended to the application of a sub-project. The consortium leader collects and combines all appendices of the consortium as part of his/her application.

6.3 Evaluation criteria

The scientific quality of the applications will be reviewed by an international panel of experts. The criteria applied include:

- project compatibility with the research programme,
- scientific quality and innovativeness of the research plan,
- feasibility of the research plan,
- national and international contact network of the applicant/research team/consortium,
- researcher training and advancement of the research environment,
- competence and expertise of the applicant/research team/consortium, and
- in the case of a consortium application, the added value generated by the consortium.

The detailed instructions for how to evaluate applications that are given to the experts on the panels are available on the Academy website at www.aka.fi/eng > For researchers > Reviewing applications. It is useful to read these before submitting an application.

7 Further information

Academy www-pages

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