Summary report and final evaluation Computational Science

Academy Programme (Lastu)

ACADEMY OF FINLAND

Contents

1. Introduction

This document is the final report of the Academy of Finland's Computational Science Academy Programme (Lastu). The report comprises both statistics on and an evaluation of the programme.

1.1. Lastu programme and its objectives

The decision to start preparing the Lastu programme was made at the Academy of Finland in 2007. A programme memorandum (see www.aka.fi/en/research-and-science-policy/academy-programmes/completed-programmes/lastu) was written by the preparatory group of the programme, which consisted of members of the research councils of the Academy of Finland and external experts. The memorandum describes the contents and the objectives of the programme.

Two calls were organised during the programme. Seven projects were funded from the first call in 2009 and five projects from the second call in 2011. Three additional projects from a separate international (ERA-SysBio+) call were connected to the programme. Hence, the programme comprised 15 projects in total. The overall funding of the two calls was 10 million euros. The brochure of the programme (see www.aka.fi/en/research-and-science-policy/academy-programmes/completed-programmes/lastu) includes a listing of all project titles. The three ERA-SysBio+ projects were left out from this final evaluation due to the fact that they were not originally planned to be part of the programme, and the projects did not ultimately find to fit well to the programme. Figure 1 illustrates the division of funding among the research organisations from the 2009 and 2011 calls.
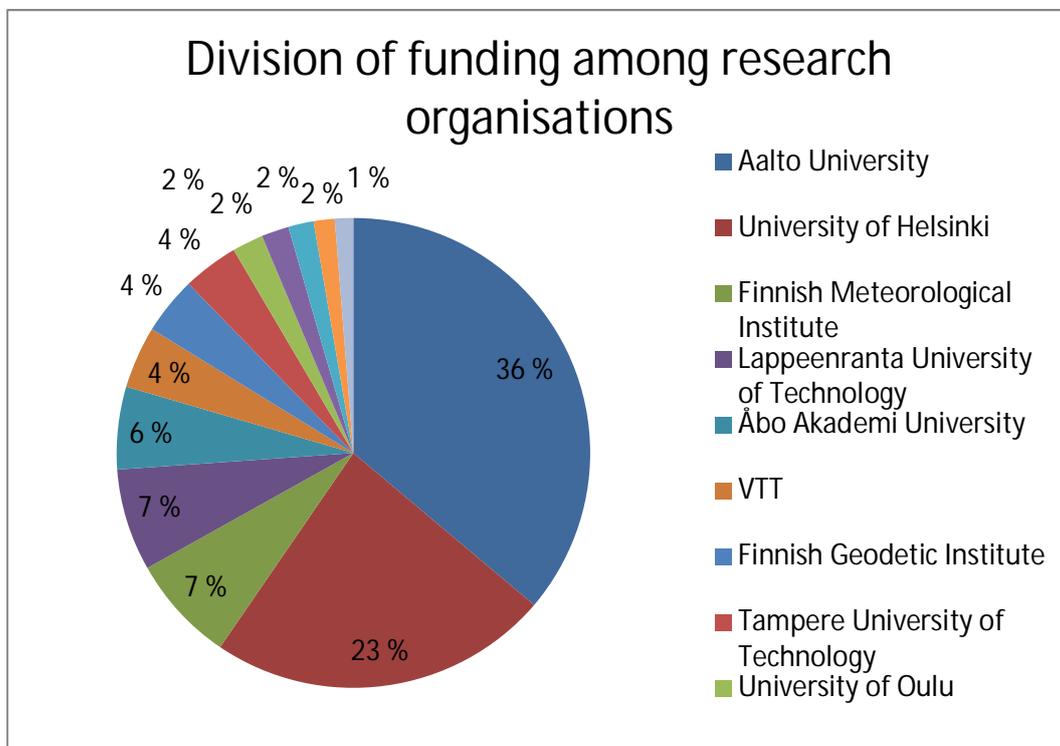

Figure 1. Division of funding among research organisations from 2009 and 2011 calls (12 projects in total).

1.2. Programme coordination and activities

Academy Programmes are thematic entities consisting of a set of individual projects. The programme is managed by a steering group with the help of programme managers employed by the Academy of Finland. The programme organises activities that support reaching the programme objectives. These activities generally consist of seminars, invited national and international seminar speakers, foresights and programme evaluation.

The opening seminar of the programme was organised in 2010. Programme seminars were organised annually from 2011 to 2014. The closing seminar was held in 2015. Examples of specific activities of the programme are the communications education seminar in 2012 and the dedicated seminar for young scientists in 2013. A foresight exercise on trends in computational science was organised in autumn 2015. The results from the foresight have been collected into a separate report (see www.aka.fi/en/research-and-science-policy/academy-programmes/completed-programmes/lastu). All these activities foster networking of researchers and dissemination of research results and ideas.

1.3. Programme evaluation

In line with common practice and to serve the needs of the research community, all Academy Programmes are evaluated. The focus of the evaluation is decided by the steering group of the programme.

It was decided that the programme evaluation would contain the following two parts:

> **part 1:** analysis of how the objectives of the programme were achieved
> **part 2**: multidisciplinarity (a cross-cutting theme and instrumental to the programme).

Part 1 of the evaluation was realised with a self-evaluation questionnaire, presented in Appendix I, sent to the principal investigators of the programme's projects. Part 2 was performed by an external expert, partly utilising the same questionnaire.

1.4. Contents of this document

Section 2 presents statistics from the final reports of seven individual projects (the projects funded from the first call). Section 3 presents **Part 1** of the evaluation of the programme. **Part 2** of the evaluation is presented in Appendix II.

2. Statistics

This section summarises statistics on the Lastu programme based on the final reports of the projects submitted in 2014. The statistics include only the seven consortia from the 2009 call. All of the statistics are based on the final reports of the 24 parties of the consortia. The five projects from the 2011 call were left outside this statistics because the collections of the statistics data for this report was started prior to the end of the funding periods of the projects of the 2011 call.

2.1. Research organisations of the programme

There were nine research organisations in the seven projects participating in the programme. Five of them were universities and four were other Finnish research organisations. The division of funding among them is illustrated in Figure 2.
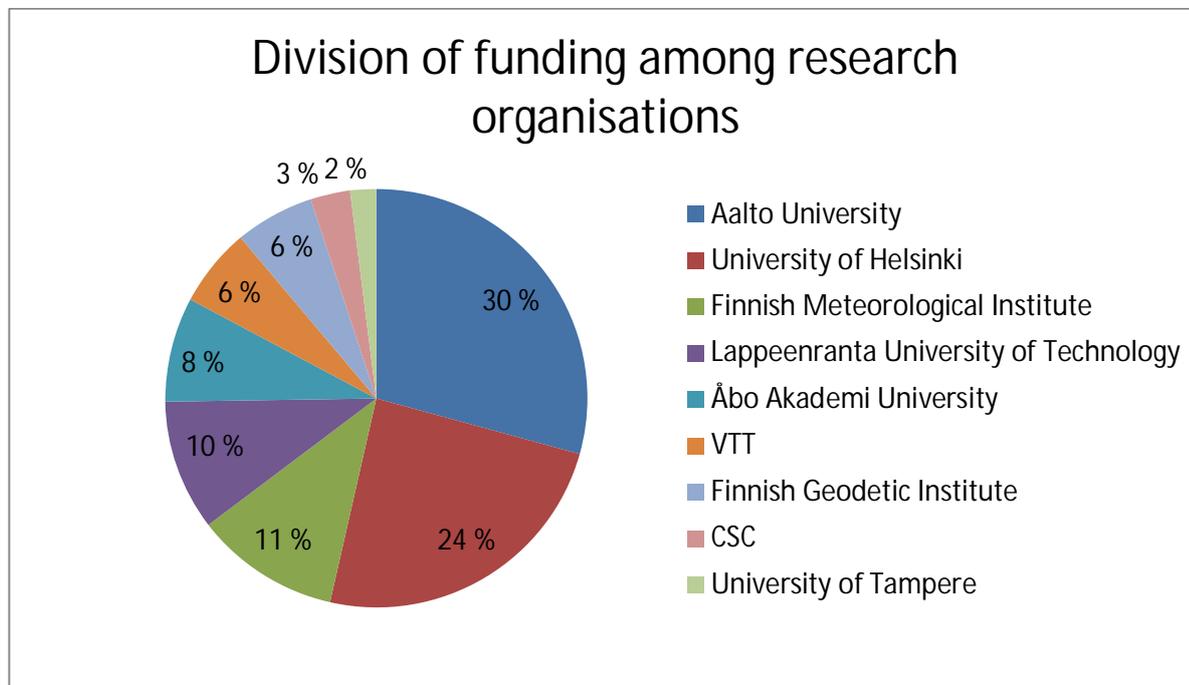
Figure 2. Division of funding between research organisations in the programme.

The largest funding proportions were granted to Aalto University and the University of Helsinki. Also, the number of subprojects was the greatest in those two: seven and five subprojects, respectively. The Finnish Meteorological Institute and Lappeenranta University of Technology had three subprojects. Åbo Akademi University and VTT Technical Research Centre of Finland had two subprojects each. The rest of the research organisations participated with one subproject each.

2.2. Personnel

According to the final reports, there were 161 people in total involved in the seven consortia (from the 2009 call) of the programme. In this section, the research personnel is examined from different viewpoints, including statistics on different personnel categories, the percentage of women, years of birth and the full-time equivalent (FTE) working time of the personnel.

2.2.1. Personnel categories

The personnel was divided into five categories: postgraduate students, postdoctoral researchers, researchers, assistant personnel and principal investigators. This division is used throughout the section. The largest category was postgraduate students, totalling 53. The second largest group consisted of assistant personnel (37). In addition, there were 26 postdoctoral researchers and 22 other researchers (incl. professors who were not principal investigators) involved in the programme.

Naturally, there were 24 principal investigators, one per consortium[1]. The relative personnel proportions in the different categories (in percentages) is shown in Figure 3.
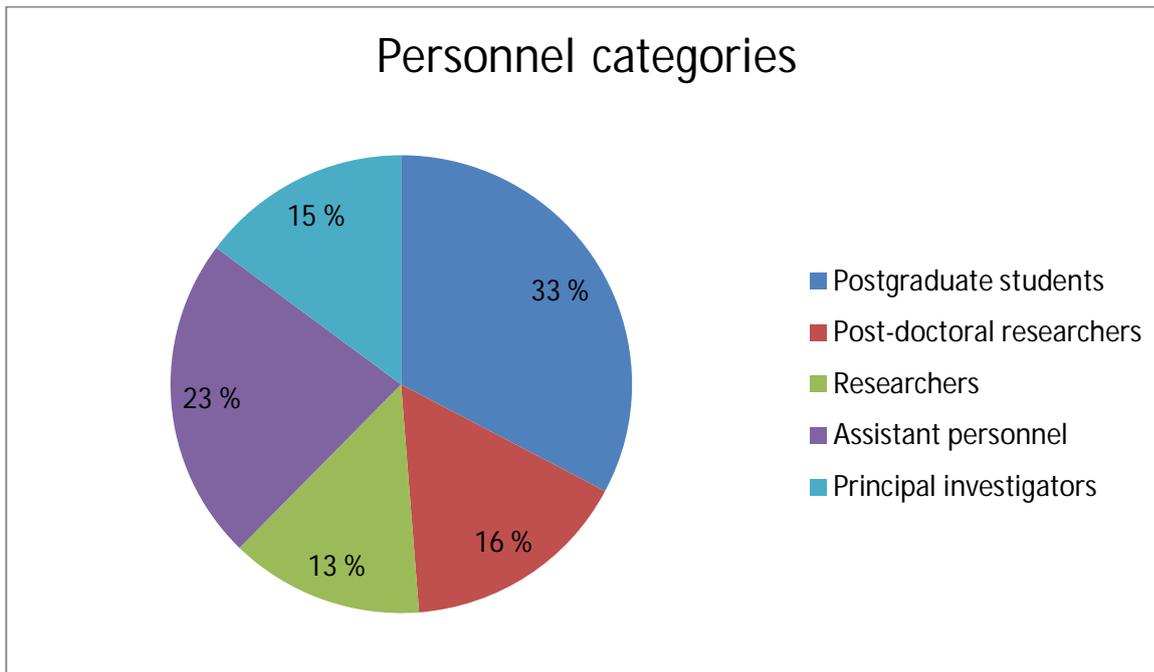
Figure 3. Relative proportion of personnel in the different categories.

2.2.2. Percentage of women

Out of the 161 people involved in the programme, 35 (approx. 22%) were women. This subsection presents some statistics on the percentage of women in the personnel. However, the category of assistant personnel has been excluded in order to put more focus on actual researchers (i.e. the other four personnel categories). The proportion of women among assistant personnel happened to be approx. 22 per cent though, so excluding them did not affect the average of 22 per cent mentioned above.

The proportion of women among the research personnel of each consortium is given in Figure 3. Consortium 5 had exactly the same amount of men and women in its personnel, and one of its final reports even brought up the importance of supporting the possibilities of women in science. According to these statistics, they did manage to show a good example in this respect. The rest of the consortia have clearly lower percentages of women. Consortia 1 and 3 still exceed the average with 31 per cent and 23 per cent, respectively, but the figures for consortia 2, 4, 6 and 7 remain clearly lower.

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[1] Some people were listed twice in the final reports, but they have been counted here only once. One person worked as a postgraduate student in one subproject and as a postdoctoral researcher in another. The person has been included in both categories and therefore the total number of people in the five categories seems to be 162, although there were only 161 people in reality.
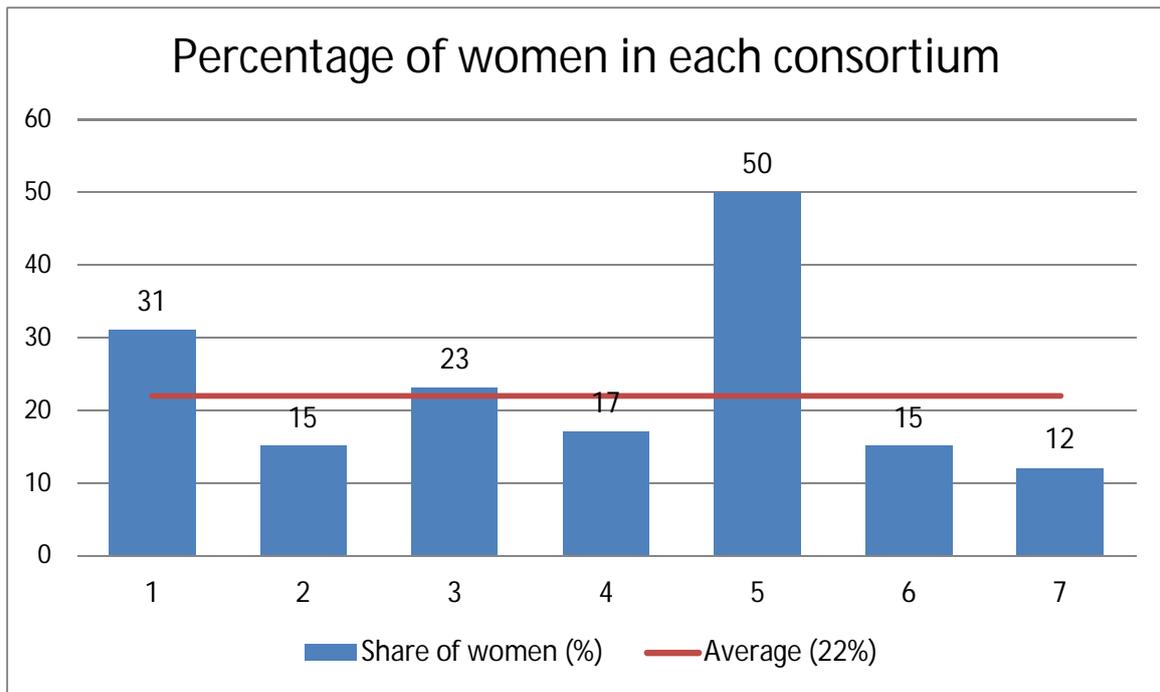
Figure 3. Percentage of women in the research personnel of each consortium (assistant personnel excluded).

The percentages of women in three out of four personnel categories are close to the average of 22 per cent. However, the category of researchers stands out with a percentage as high as 32. This is shown in Figure 4.
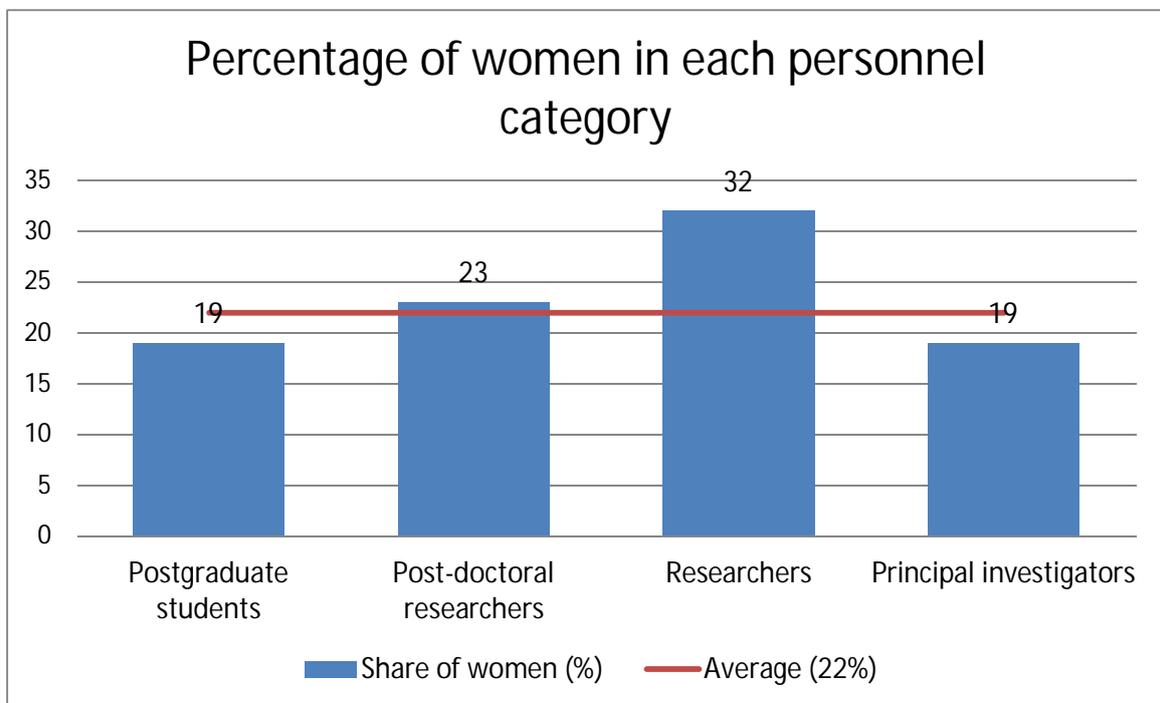
Figure 4. Percentage of women in the personnel categories (assistant personnel excluded).

2.2.3. Age breakdown of personnel

The personnel were divided into five categories based on their years of birth. The categories and their proportions are presented in Figure 5 (assistant personnel excluded). As Figure 5 shows, the research personnel was relatively young, over half of them were born between 1975 and 1984. The age breakdown of the different personnel categories is presented in Table 1.
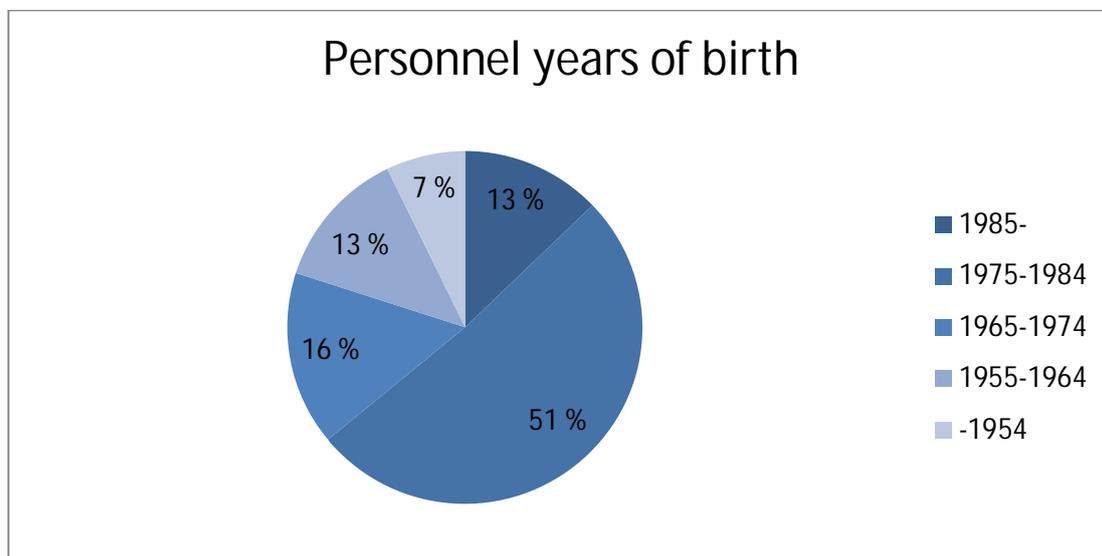
Figure 5. Years of birth of research personnel in the programme (assistant personnel excluded).

Table 1. Age breakdown of personnel.

	−1954	1955–1964	1965–1974	1975–1984	1985–	TOTAL
Postgraduate students			4	34	15	53
Assistant personnel	1	4	2	10	20	37
Postdoctoral researchers		2	3	20	1	26
Researchers	2	4	7	9		22
Principal investigators	7	10	6	1		24
TOTAL	**10**	**20**	**22**	**74**[2]	**36**	**162**[3]

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[2] One person worked as a postgraduate student in one consortium and as a postdoctoral researcher in another. However, the person has been included in both categories as a full person, and not as a 0.5 postgraduate student and 0.5 postdoctoral researcher. The person was born between 1975 and 1984, and hence, the correct number of people in that category would be 73.

[3] The number here is one bigger than the number given at the beginning of this section, where it was stated that there were 161 people involved in the programme. This is because one person worked as a postgraduate student in one consortium and as a postdoctoral researcher in another (see also previous footnote). However, the person has been included in both categories as a full person, and not as a 0.5 postgraduate student and 0.5 postdoctoral researcher.

2.2.4. FTE working time

The personnel in the seven consortia reportedly worked for 91.5 FTE (full-time equivalent) years during the programme. The proportions of total FTE working time for the five personnel categories are shown in Figure 6. The postgraduate students account for the biggest proportion: in absolute terms for 35.7 years of research. Postdoctoral researchers, researchers, assistant personnel and principal investigators account for 18.6, 19.3, 15.8 and 2.1 FTE years, respectively.

Division of FTE working time
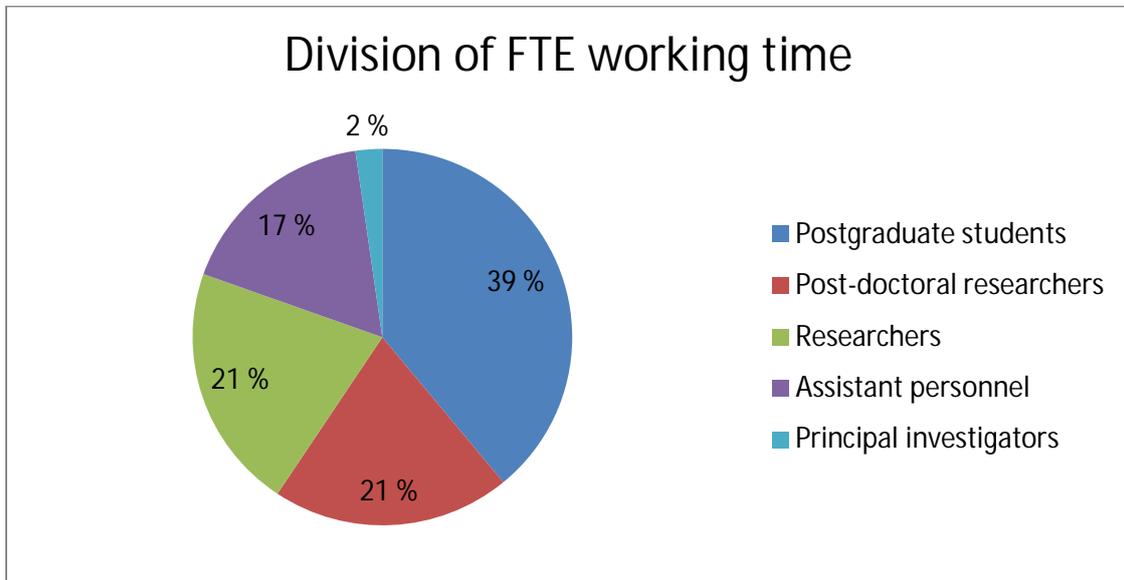
Figure 6. Division of FTE working time among the personnel categories.

The average FTE months per person in different personnel categories are shown in Figure 7. Postgraduate students, postdoctoral researchers and researchers have clearly higher FTEs compared to those of the assistant personnel and the principal investigators. For the latter, the explanation lies in the fact that according to the funding rules of the Academy of Finland, the workload of the principal investigators is generally limited to a maximum of six FTE months per project.

Average FTE months per person
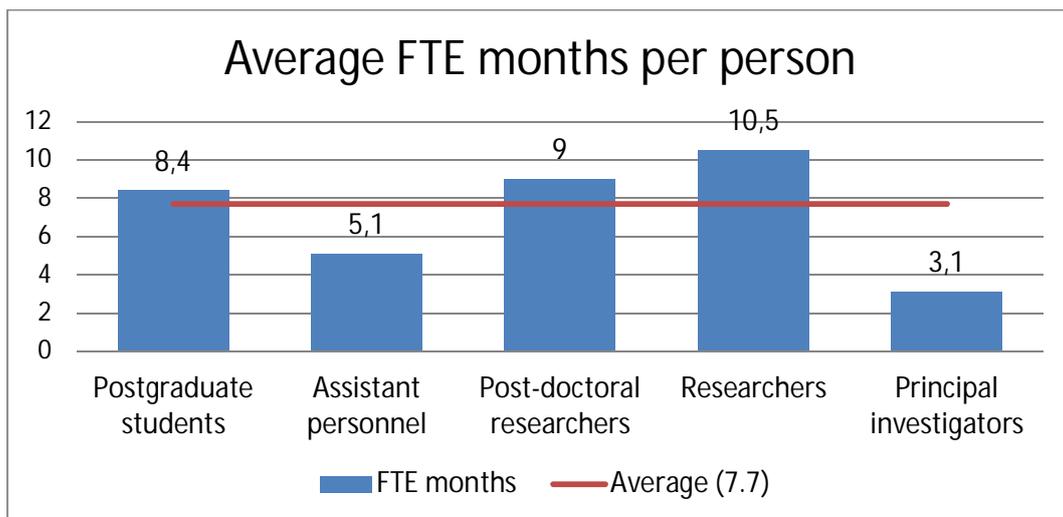
Figure 7. Average FTE months of a person in a personnel category and the average for all personnel.

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The lengths of the work periods for three of the personnel categories are presented in more detail in Figures 8, 9, 10, 11 and 12. Every reported work period (of a person) has been counted separately. If a person was mentioned two times in the list of the research personnel's FTE months, it was interpreted to mean that they had two separate work periods in the project in question.

Figures 8, 9 and 10 present the proportions of the lengths of work periods of postgraduate students, postdoctoral researchers and researchers, respectively. The variation is great in all personnel categories: the longest periods exceed 35 months, and the shortest ones are less than a month. For example, approximately 60 per cent of the postgraduate and postdoctoral work periods are shorter than six months. Researchers differ clearly in this respect: only 35 per cent of their work periods lasted less than six months.
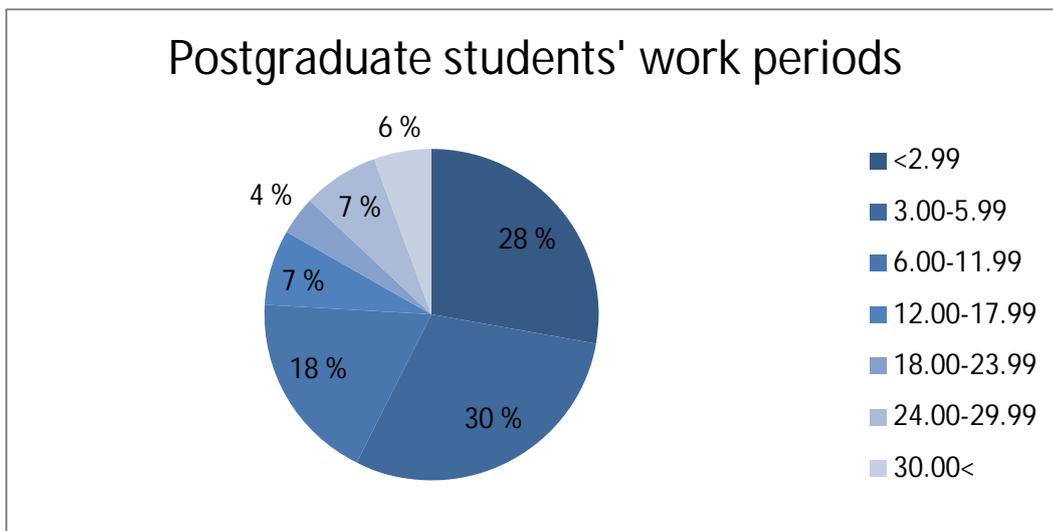
Figure 8. Proportions of the lengths (FTE months) of work periods.
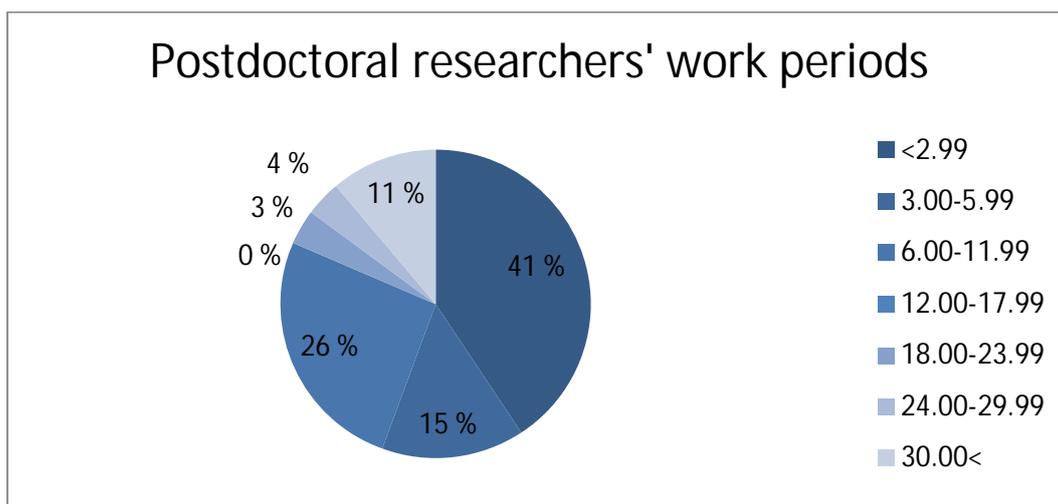
Figure 9. Proportions of the lengths (FTE months) of work periods.
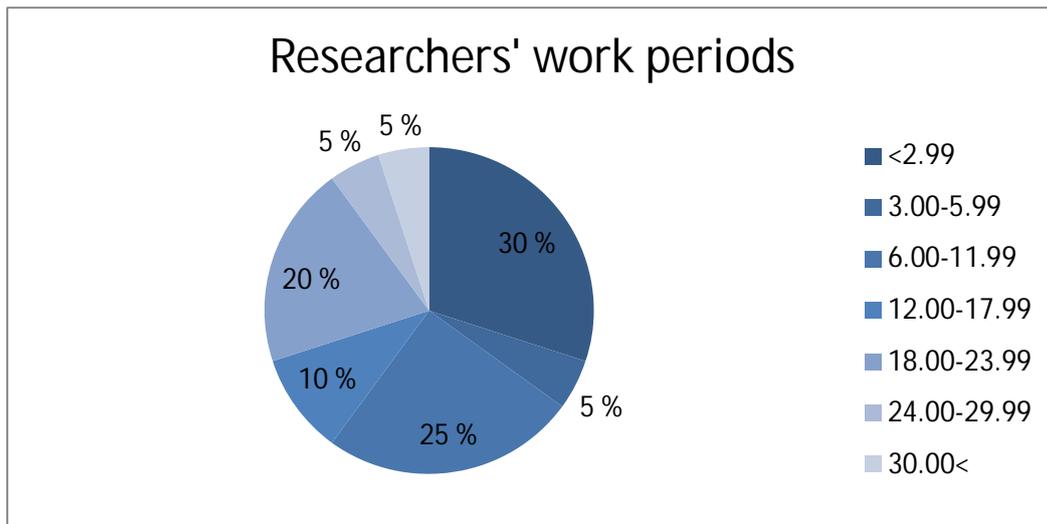
Figure 10. Proportions of the lengths (FTE months) of work periods.

The information presented in Figures 8, 9 and 10 is presented in a different form in Figure 11. Here, all personnel categories are in one column, separated by different colours. The numbers are absolute instances of the work periods in question, and not percentages as in the three previous figures. The most common length of a work period was less than three months. Work periods of 3–6 months and 6–12 months were also common.
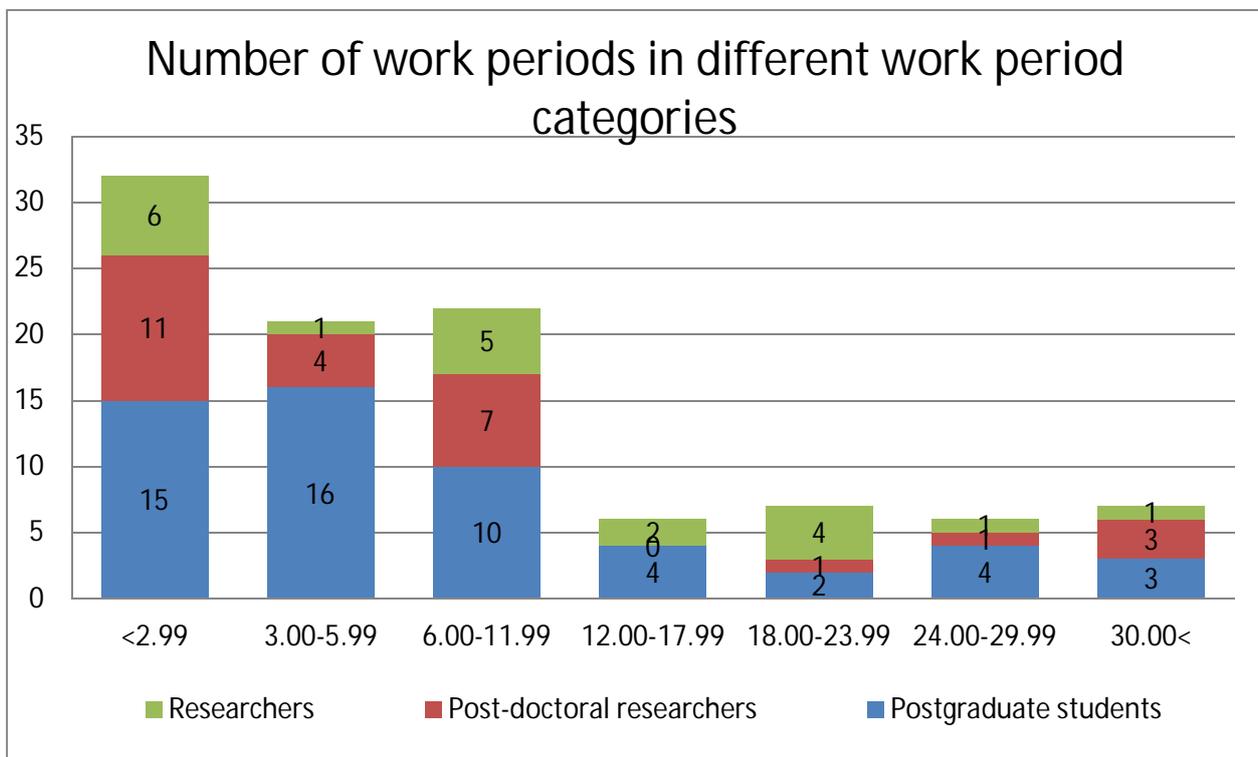
Figure 11. Number of individual work periods in different work period categories.

Figure 12 shows the amount of FTE months performed in the different work period categories. Despite the low number of work periods of more than a year (see Fig. 11), the absolute amount of FTE months is relatively high (see Fig. 12), approximately 66 per cent.
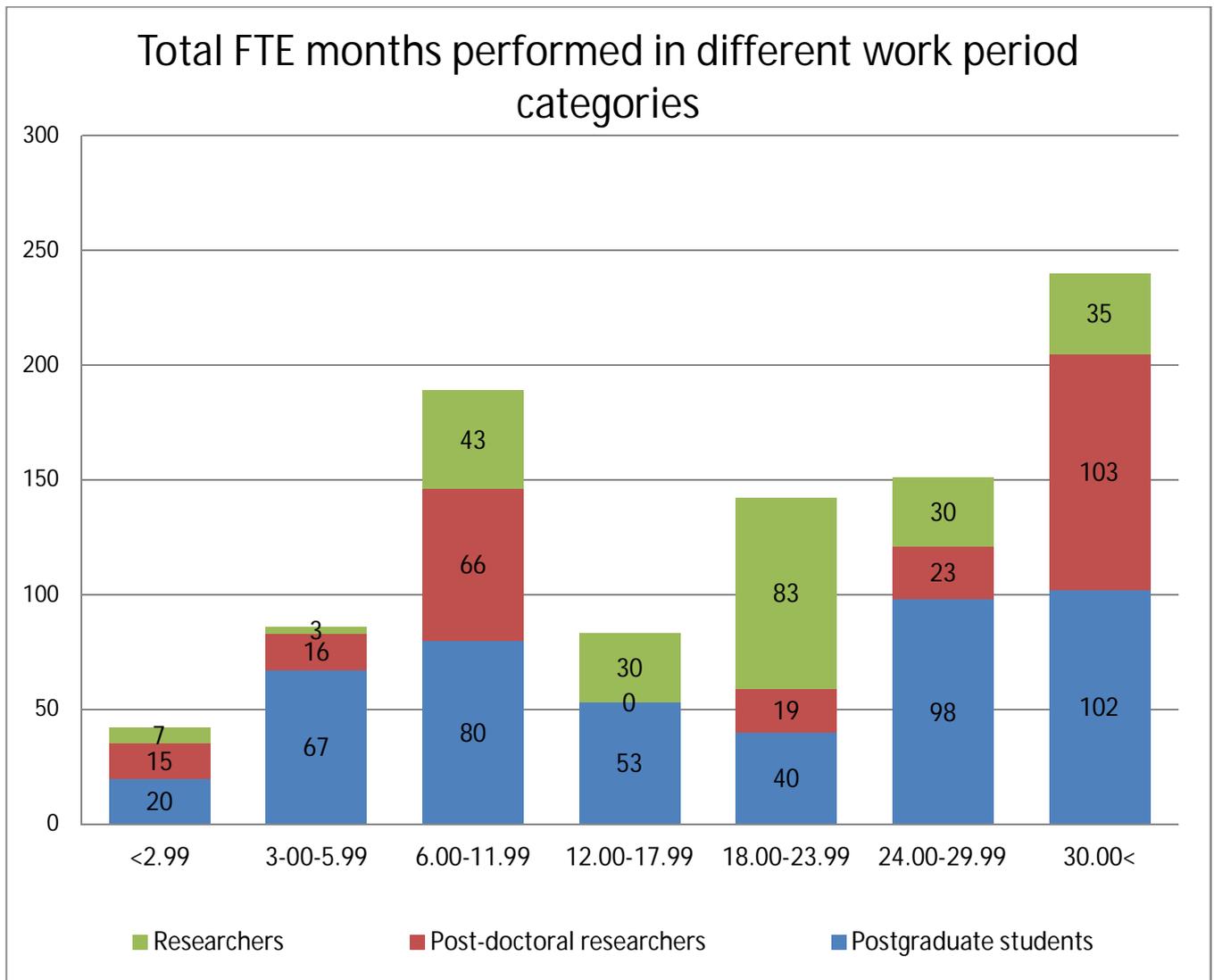
Figure 12. Total FTE months performed in the work period categories. The numbers inside the bars represent the total FTE months in the personnel categories in absolute terms.

2.3. Mobility

All seven consortia reported mobility. There were 58 individual visits realised in total. The lengths varied from 0.5 to 23 months, the average being 2.3 months. Most visits (42) lasted less than a month, eleven lasted 2–6 months and four lasted 7–12 months. One visit exceeded a year in length. The proportions of the lengths of the visits are shown in Figure 13.
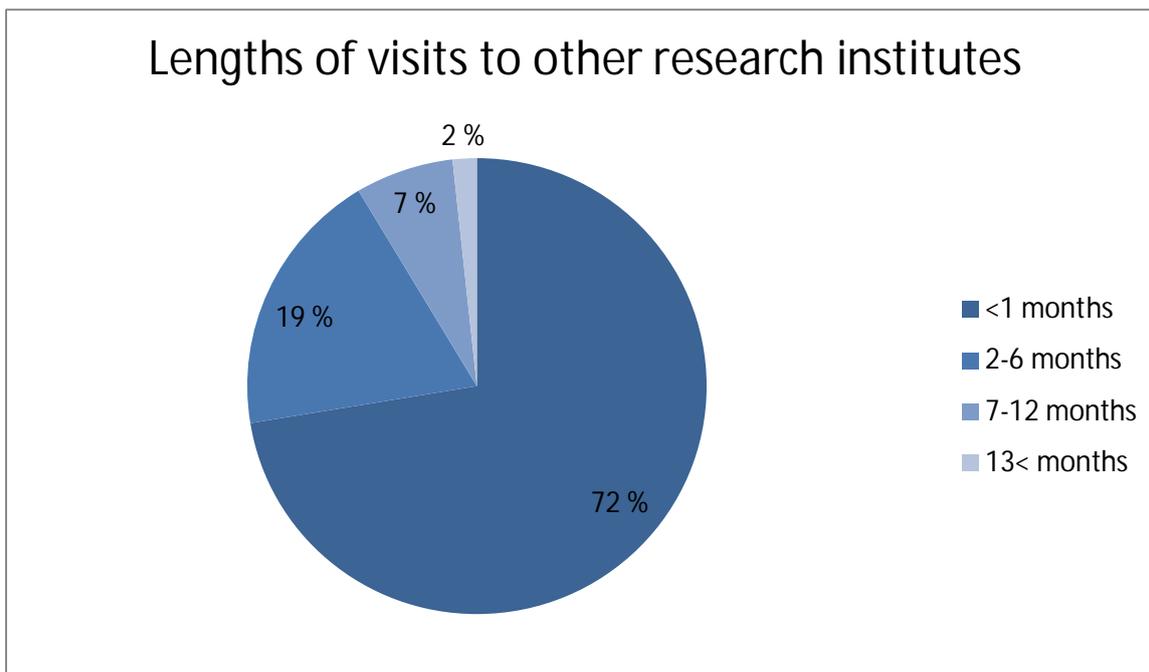
Figure 13. Proportions of lengths of individual visits to other research organisations.

Almost all of the reported mobility was outward from Finland. There was no inward mobility from abroad to Finland and only one within Finland. The most frequently visited countries were the United Kingdom (21 visits), Germany (16) and the United States (12). Austria, Belgium, Brazil, Cyprus, Finland, France, Japan, Slovenia and Sweden were visited once. Table 2 examines the three most popular destinations in greater detail.

Table 2. Three most popular destinations in the programme.

	Individual visits	Total length of all visits in months	Average length of stay in months	Different re-search organisa-tions visited
Germany	16	35.8	2.2	2
United Kingdom	21	20	1.0	5
United States	12	52	4.3	10

On average, there were 19 months of mobility per consortium. The mobility in months per each consortium is presented in Table 3. As the consortia differ in size, there is also information on the amount of mobility compared to the granted funding and to the FTE months. Based on the figures, consortia 3 and 4 seem to have been significantly more active in mobility than the other consortia.

In total, 36 people from the consortia took part in the mobility, which equals 22.5 per cent of the whole research personnel. Each of them spent on average approximately 3.7 months working in another university or research organisation. In Table 3, on the row 'Mobility in months per FTE

months', the amount of mobility in months is divided with total FTE months, giving the percentage of FTE months done outside the home research organisation. The result was that about 12 per cent of the total amount of work in the programme was carried out somewhere else than in an organisation directly participating in the programme.

Table 3. Mobility compared to granted funding and FTE months.

Consortium number	1	2	3[4]	4	5	6	7	Average
Mobility in months	12.0	13.0	55.3	22.0	12.5	8.5	9.0	**19.0**
Mobility in months per funding of 0.1 million euros	1.1	1.1	3.7	2.2	1.2	0.7	0.7	**1.6**
Mobility in months per FTE months	0.08	0.08	0.22	0.20	0.08	0.05	0.07	**0.12**

2.4. Project collaborators

Each of the seven consortia collaborated with some universities, research organisations or companies in addition to the ones who were officially part of the consortium. The collaboration included, for example, joint experiments and publications, exchange of data, joint PhD supervision, researcher exchanges and other research collaboration. The final reports listed 61 instances of this type of collaboration.

The collaborator organisations were divided into five different types listed in Table 4 together with the number of individual instances of collaboration and the number of different research organisations involved.

Table 4. Types of collaborator organisations.

Type of collaborator organisation	Instances of collaboration	Number of different research organisations involved
Universities	29	25
Research organisations	25	21
Companies	3	3
University hospitals	2	2
Other organisations	2	2
TOTAL	**61**	**53**

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[4] The Academy of Finland did not receive the final report from one of the six sub-projects of the consortium 3. The figures in 'Mobility in months per funding of 0.1 million euros' and 'Mobility in months per FTE months' are therefore based on total granted funding of the consortium from which the budget of the unreported sub-project has been left out.

A clear majority of the collaboration was carried out with foreign organisations: only four Finnish collaborators were mentioned. There were 19 different foreign countries in total. The countries and the number of reported instances of collaboration are listed in Table 5.

Table 5. Projects collaborators by country.

Country	Instances of collabora-tion	Number of different research organisations involved
United States	11	9
Germany	10	6
United Kingdom	8	8
Finland	4	4
Austria	3	3
Italy	3	3
Spain	3	3
Sweden	3	2
Czech Republic	2	2
Denmark	2	1
France	2	2
Netherlands	2	2
Belgium	1	1
Brazil	1	1
China	1	1
Estonia	1	1
Ireland	1	1
Japan	1	1
Norway	1	1
Switzerland	1	1
TOTAL	**61**	**53**

2.5. Publications

The total number of reported scientific publications was 347. Most of them, altogether 220 articles (approx. 63%), were original scientific articles (type A1); 74 (approx. 21%) were articles in conference publications (A4) and 31 (approx. 9%) were articles in conference proceedings (B3). Type A publications are peer-reviewed scientific articles, while type B publications are non-refereed articles. The other publication categories include, for example, book sections, reviews and theses, but their numbers remained much smaller than those of the three largest categories. The number of all published articles and their division into different categories are shown in greater detail in Table 6. The classification is based on the Ministry of Education, Science and Culture's publication type classification.

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Table 6. Number of publications in different categories.

Type of publication	Number of publications
A1 Journal article, original research	220
A2 Review article, literature review, systematic review	3
A3 Book section, chapters in research books	2
A4 Conference proceedings	74
B1 Non-refereed journal article	2
B3 Non-refereed conference proceedings	31
C1 Published scientific monograph	1
C2 Edited book, compilation, conference proceeding or special issue of journal	1
D3 Article in professional conference proceedings	2
F4 Model or plan taken into production/exploited	1
G1 Thesis for higher vocational diploma, bachelor's thesis	1
G2 Master's thesis, diploma work, upper higher vocational diploma	1
G4 Doctoral thesis, monograph	4
G5 Doctoral thesis, articles	4
TOTAL	**347**

Table 7 presents the number of publications and the number of publications per granted funding. The results show great variation between the consortia. The publication numbers vary from 11 to 108, the average being 49.6. Consortia 2 and 3 seem to have been very active in publishing.

Table 7. Publications and publications per funding of 0.1 million euros.

Consortium number	1	2	3	4	5	6	7	Average
Publications	11	90	108	27	35	50	26	**49.6**
Publications per funding of 0.1 million euros	1.0	7.4	7.2[5]	2.7	3.5	4.0	2.0	**4.1**

2.6. Degrees

The total number of degrees reported was 29: 20 doctoral degrees, eight master's degrees and one licentiate degree. One consortium funded both the master's and the doctoral degree for one person. Each consortium generated at least one degree.

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[5] The Academy of Finland did not receive the final report from one of the six subprojects of consortium 3. 'Publications per funding of 0.1 million euros' is therefore based on total granted funding of the consortium from which the budget of the unreported subproject has been left out. In addition, one of the final reports did not report any publications. Leaving also that out would of course result in an even higher number for consortium 3.

Only six degrees were fully funded by the project it was part of: two doctoral degrees and four master's degrees. For 17 degrees, the reported funding percentage was 50 per cent or below. The average funding percentage of the doctoral degrees was 42.8, so the programme can be said to have produced 7.7 full doctoral degrees. The average funding percentage of the master's degrees was 66.3, translating into 5.3 full degrees.

2.7. Inventions and patents

The number of invention notifications and patent notifications was low. Only one project reported three invention notifications and no project reported any patent notifications.

2.8. Fields of research

The seven consortia covered a wide range of different research topics. There were altogether 22 fields of research named in the final reports. All of them are listed in Table 8 together with the information on how many different subprojects and, on the other hand, different consortia mentioned each of them. Every consortium listed 1–5 fields relevant for their research. Figure 14 illustrates the number of fields of research and the number of subprojects in each consortium.

Table 8. Fields of research and number of times they were mentioned by different subprojects and consortia.

Field of research	Consortia	Subprojects
Applied mathematics	4	8
Computer science	4	4
Computational science	3	6
Physics	3	6
Meteorology and atmospheric sciences, climate research	2	6
Materials science and technology	2	3
Physical chemistry	2	3
Computational data analysis	2	2
Chemistry	1	4
Process technology	1	4
Signal processing	1	3
Geosciences	1	2
Nuclear engineering: fission and fusion	1	2
Systemic and cognitive neuroscience	1	2
Astronomy	1	1
Atomic and molecular physics	1	1
Fluid and plasma physics	1	1
Medical engineering	1	1
Neuroscience	1	1
Phonetics	1	1
Public health research	1	1
Statistics	1	1

Number of fields of research and subprojects by consortium
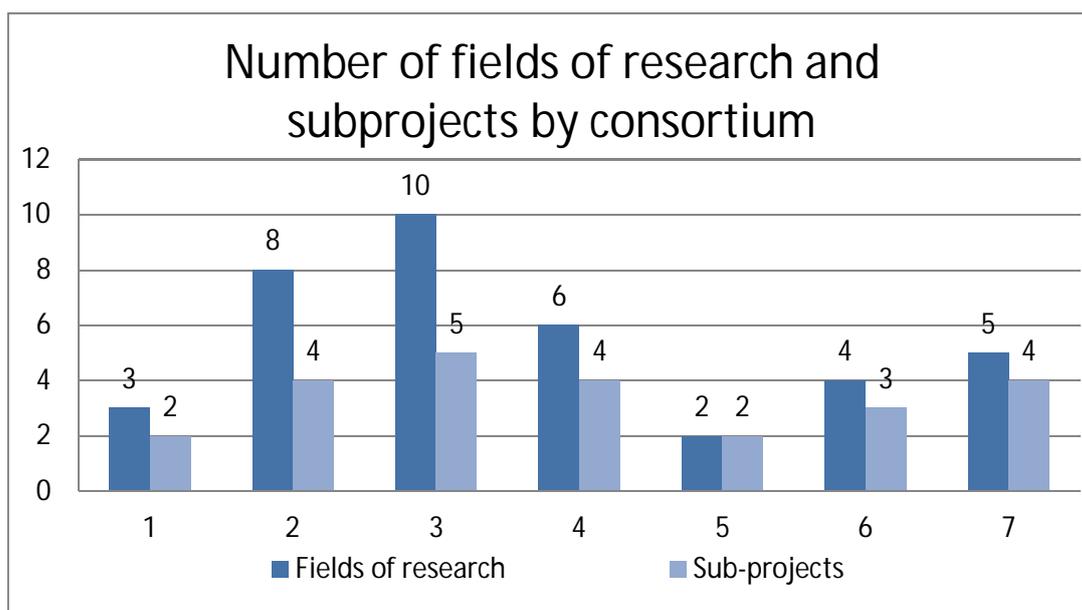
Figure 14. Number of different fields of research mentioned by each consortium and total number of subprojects in each of them.

2.9. Media

The programme was not very visible in the media aimed at a wider audience. Only one consortium was of significant interest to journalists, and it was featured in several newspaper, radio and television interviews mainly in Finland but also abroad. The consortium organised a few open lectures and workshops and was consulted for a new textbook for Finnish schoolchildren. In addition, the Academy of Finland organised a "science breakfast" for one subproject of the consortium. Some of the consortia did not report any communication outside the scientific community. Yet, most of them did mention interviews and articles in the media or some use of social media as well as other communication activity.

3. Programme-specific issues

This section presents the results of Part 1 of the evaluation (see Section 1.3) realised with a self-evaluation questionnaire (Appendix I) sent to the principal investigators of the programme in spring 2015. The questionnaire was sent to all 44 subproject leaders. The response rate was 68 per cent (30 people responded).

A web-based questionnaire (Webropol^{TM}) was used for the self-evaluation, and it consisted of the following six categories of questions:

1. General questions
2. Multidisciplinarity and its impacts

3. Programme effects in the field of computational science
4. National and international collaboration
5. Programme effects on the researcher career

4. Feedback

Part 1 of the evaluation (this section) utilises all these categories of questions excluding Category 2, which is used in Part 2 of the evaluation (Appendix II). There were overall 40 questions ranging from closed-ended questions to ordinal-scale and open-ended questions. The open-ended responses were classified into categories to be able to present generalised information or trends that occurred in the answers. This was done by using content analysis and textual analysis, with the focus on the text itself. Thus, analysing the context or the respondents' positions or purposes is minimised. However, it is good to bear in mind that some interpretation has been necessary in creating the categories[6].

The questionnaire was designed to provide information on how well the objectives of the Lastu programme were achieved. It should be noted that two of the respondents, whose projects were merged into the programme later, were funded under the ERA-Sysbio call, and the questionnaire did not consider the special nature of these international projects.

4.1. General Questions

4.1.1. How the consortia were formed

According to the questionnaire, the consortia were strongly based on existing contacts and collaborations (Question 1.2), see Figure 15. Scientific interests were mentioned as the primary basis for forming the consortium in 14 per cent of the cases. For many respondents, the programme was a driving motive for ideas about, for instance, unlocking important research problems together. Reputation was also an important factor in forming the consortium: "Consortium partners were known to perform high-level complementary research and to supplement each other".

It could be seen in the answers that the question was understood in two different ways. Some responded on behalf of the whole consortium, whereas the others responded on their own behalf. Three respondents said they had been invited by the consortium leader or principal investigator. One person in turn ended up in the consortium by contacting the consortium leader, whereas another had designed the consortium for themselves.

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[6] Anu Pynnönen (2013). *Diskurssianalyysi: Tapa tutkia ja olla kriittinen*

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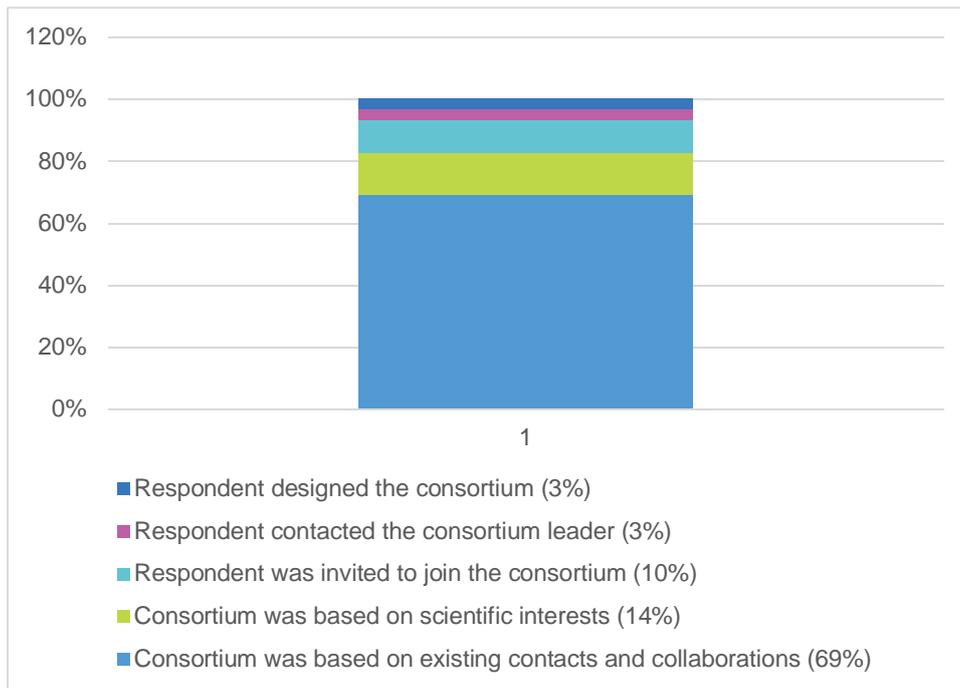
Figure 15: How did you end up in the consortium you formed? (Question 1.2)

Consortium leaders were asked whether they would have found a similar consortium if the Lastu programme had never existed (Question 1.3), see Figure 16. Despite the fact that most of the consortia were based on existing collaboration (Question 1.2), only two respondents were certain that they would have founded a similar consortium, and six respondents were certain that a similar consortium would not have existed. Figure 16, which includes all 29 responses, clearly indicates that the launching of the programme was crucial for establishing the consortia.
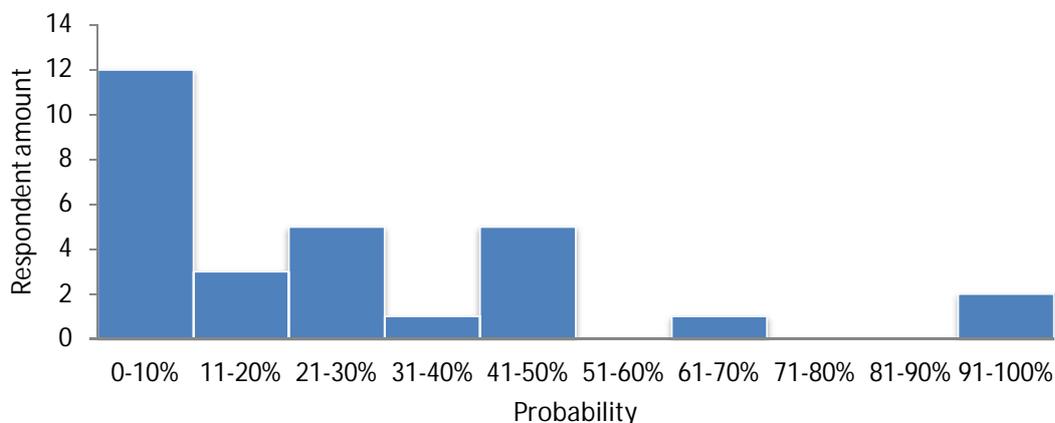
Figure 16: How likely is it that you would have founded a similar consortium if the Lastu programme had never existed? (Question 1.3)

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4.1.2. Added value of the programme

The added value of the Lastu programme was asked in Question 1.5 (see Fig. 17). The answers in this open-ended question were divided into seven categories shown in Figure 17. Since the categories were created by means of textual analysis (what is said), they may overlap by some of their parts (what is meant). For example, if the respondent said that the most significant added value was "a bigger team", they might have meant that a bigger team brings expertise from many areas of competence, or that it helps in creating new contacts (which were both categories of their own). Also, if one respondent mentioned several things, they were all coded into their own categories.

In 13 responses, the added value was considered to be the multi- or interdisciplinarity and unlimited collaboration. This was said to bring research spin-offs, changing of ideas and support from a wider network of scientists.

The distinction between Categories 1 and 2 is not unambiguous. The answers in Category 2 was also related to the collaboration of multiple fields of science, but they highlighted things such as the experimental nature of the scientific work and the possibility to take risks. It was said that the programme brought together wider expertise and also a possibility to develop new methodology or areas of research. Benefits from a large team or consortium (Category 3) were mentioned four times. The category "Other" includes things such as a faster start to scientific research, larger funding and an emphasis on computational methods. Two respondents were unable to apply for funding for their project as an ordinary Academy Project due to the limitations set by the Academy of Finland (Category 7). Altogether 29 respondents answered this question.
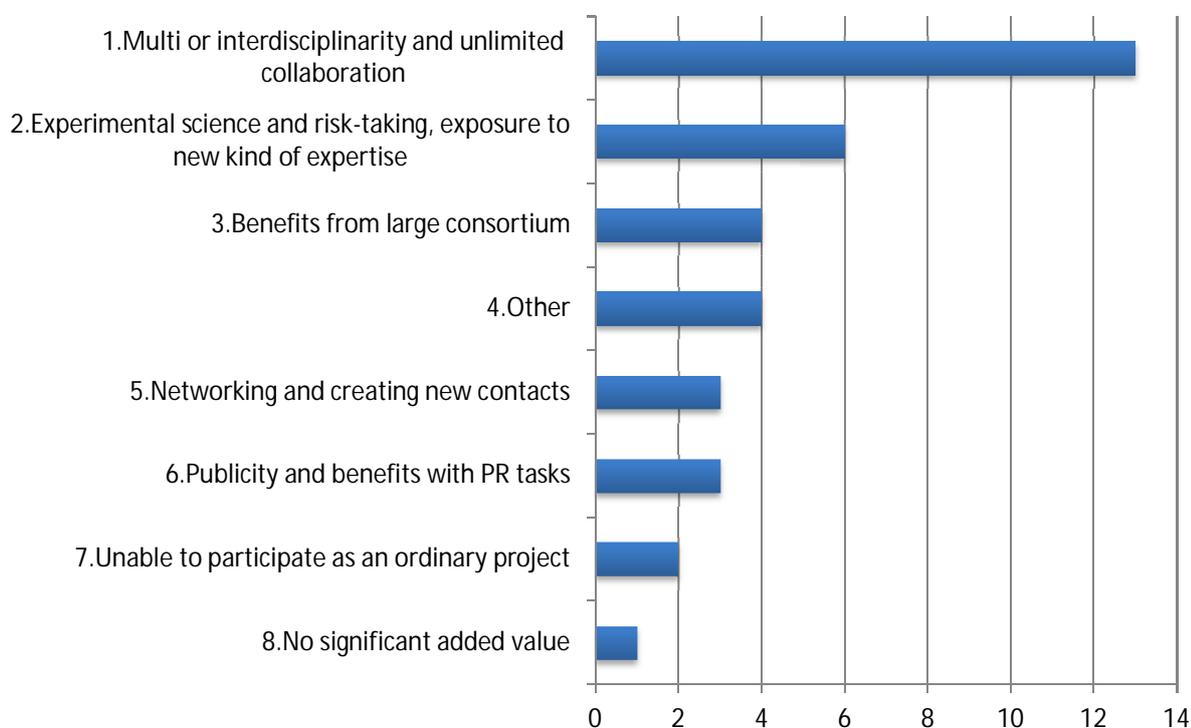
Figure 17. What was the most significant added value that participating in the programme brought to you compared to having been funded as an ordinary Academy Project (Question 1.5)?

4.1.3. Significant outcomes of the programme

The project leaders were asked what they considered to be the most significant outcome of their project (Question 1.6); see Figure 18. Altogether 29 responded to this question, but some respondents gave two or three different explanations. Most respondents stated that the most significant outcomes were their scientific outputs: new models, theories or methodology (see Category 1 in Figure 18).
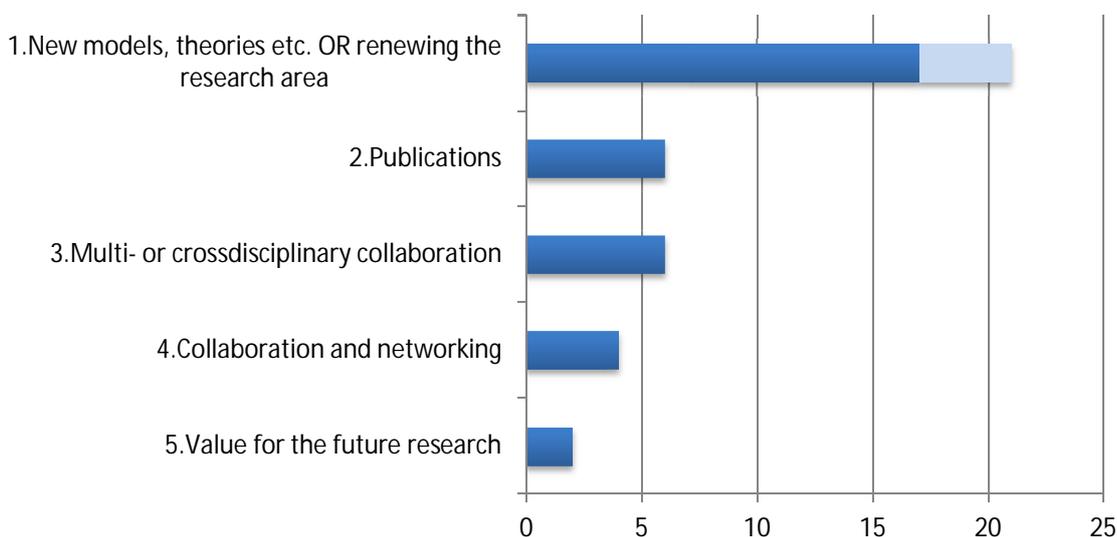
Figure 18. What do you consider to be the most significant outcome(s) of your project? The light blue part of the uppermost bar represents answers that suggested that the research area was renewed or redefined (Question 1.6).

Due to the highly detailed and project-specific answers, some of the answers are represented below as quotes.

> *"Improvement of electrical image tomography by applying the method to a very challenging object, the small and complicated laryngeal structures"*

> *"Paradigm for analysing the solvation effects on NMR chemical shifts based on photophysical concepts, such as magnetic absorption spectra and solvation-induced changes of excitation energies, as well as the differently signed solvation effects at different parts of the molecule depending on the localisation of excitations in the molecule."*

> *"We have performed extensive calculations on chromophore molecules at ab initio levels of theory. The calculations demonstrate the feasibility and accuracy of such an approach, whereas alternative methods often fail. We learned how to build cluster models for the simulations. We also developed an approach to consider solvent effect when studying magnetic properties."*

What was worth noting with the answers in Category 1 in Figure 18 was that some projects had clearly resulted in the renewing or redefining of the research area. These arguments are presumably

related to the encounter of different scientific cultures (Category 1), but they are separated in the uppermost bar with a light blue colour. Examples of these responses:

> *"A start of new research direction: the energetics, thermodynamics and dynamics of large water clusters. Dynamics studies of chemical reactions on ice."*

> *"In this type of multidisciplinary work, much effort is needed in merging the different research cultures and distilling the most relevant questions and approaches. I feel we have done a good job in that regard."*

> *"Initiative to re-design one of our main computational tools completely"*

Publications were said to be the most important outcomes by six respondents (Category 2). Similarly, six respondents mentioned multidisciplinary collaboration as one of the most important outcomes of their project (Category 3). Throughout the questionnaire, many stressed that the programme was a good start for well-working collaboration that will continue in the future. Examples of responses in Category 3:

> *"Consortium: established strong ties between computational and physics groups, leading to higher international visibility"*

> *"Cross disciplinary collaboration"*

Normal collaboration and networking were also mentioned as important outcomes (Category 4). Finally, two respondents felt that they had built something (strategic know-how, ideas) that has an impact on future research (Category 5).

4.1.4. Important publications

Project leaders were asked to list their most significant publications. The following references to articles were given.

> J.-P. Kauppi, L. Parkkonen, R. Hari, and A. Hyvärinen. Decoding MEG rhythmic activity using spectrospatial information. *NeuroImage*, 83:921–936, 2013.

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> Kujala J, Sudre G, Vartiainen J, Liljeström M, Mitchell T, Salmelin R. Multivariate analysis of correlation between electrophysiological and hemodynamic responses during cognitive processing. *Neuroimage*, 92: 207–216, 2014.

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> Almeida, J., Schobesberger, S., Kürten, A., Ortega, I.K., Kupiainen-Määttä, O., Praplan, A.P., Adamov, A., Amorim, A., Bianchi, F., Breitenlechner, M., David, A., Dommen, J., Donahue, N.M.,

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Downard, A., Dunne, E., Duplissy, J., Ehrhart, S., Flagan, R.C., Franchin, A., Guida, R., Hakala, J., Hansel, A., Heinritzi, M., Henschel, H., Jokinen, T., Junninen, H., Kajos, M., Kangasluoma, J., Keskinen, H., Kupc, A., Kurtén, T., Kvashin, A.N., Laaksonen, A., Lehtipalo, K., Leiminger, M., Leppä, J., Loukonen, V., Makhmutov, V., Mathot, S., McGrath, M.J., Nieminen, T., Olenius, T., Onnela, A., Petäjä, T., Riccobono, F., Riipinen, I., Rissanen, M., Rondo, L., Ruuskanen, T., Santos, F.D., Sarnela, N., Schallhart, S., Schnitzhofer, R., Seinfeld, J.H., Simon, M., Sipilä, M., Stozhkov, Y., Stratmann, F., Tomé, A., Tröstl, J., Tsagkogeorgas, G., Vaattovaara, P., Viisanen, Y., Virtanen, A., Vrtala, A., Wagner, P.E., Weingartner, E., Wex, H., Williamson, C., Wimmer, D., Ye, P., Yli-Juuti, T., Carslaw, K.S., Kulmala, M., Curtius, J., Baltensperger, U., Worsnop, D.R., Vehkamäki, H., & Kirkby, J.: Molecular understanding of sulphuric acid-amine particle nucleation in the atmosphere. *Nature*, Vol 502, pp. 359–363, 2013.

L. Aho-mantila et al., *Nuclear Fusion* 52, 103006–103007 (2012)

N. Özcan, J. Mareš, D. Sundholm, and J. Vaara: Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations, *Physical Chemistry Chemical Physics* 16, 22309–22320 (2014).

Schiestl-Aalto, P., Kulmala, L., Mäkinen, H., Nikinmaa, E. & Mäkelä, A. 2015. CASSIA – a dynamic model for predicting intra-annual sink demand and inter-annual growth variation in Scots pine. *New Phytol.*

Auvinen H, Raitio T, Siltanen S, Story B and Alku P 2014, "Automatic Glottal Inverse Filtering with Markov Chain Monte Carlo Method." *Computer Speech and Language* 28.

P. Ollinaho, H. Järvinen, P. Bauer, M. Laine, P. Bechtold, J. Susiluoto, and H. Haario: Optimization of NWP model closure parameters using total energy norm of forecast error as a target. *Geosci. Model Dev.*, 7, 1889–1900, 2014

Koukkari, P., Pajarre, R.: A Gibbs energy minimization method for constrained and partial equilibria, *Pure App. Chem.* Vol. 83, 2011, No. 6, pp. 1243–1254.

S. Leerink, et al., "Multi-Scale Investigations of Drift Wave Turbulence and Plasma Flows: Measurements and Total-Distribution-Function Gyrokinetic Simulations", *Physical Review Letters* 109 (2012) 165001; S. Leerink, PhD thesis, Aalto University

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H. Järvinen, P. Räisänen, M. Laine, J. Tamminen, A. Ilin, E. Oja, A. Solo- nen, and H. Haario. Estimation of ECHAM5 climate model closure param- eters with adaptive MCMC. *Atmospheric Chemistry and Physics*, 10(20): 9993-10002, 2010. doi: 10.5194/acp-10-9993-2010.

E. Hirvijoki, O. Asunta, T. Koskela, T. Kurki-Suonio, J. Miettunen; S. Sipilä, A. Snicker; S. Äkäslompolo, "ASCOT: solving the kinetic equation of minority particle species in tokamak plasmas", *Computer Physics Communications* 185 (2014) 1310–1321

Sahu B, Laakso M, Pihlajamaa P, Ovaska K, Sinielnikov I, Hautaniemi S, Jänne O. FoxA1 specifies unique androgen and glucocorticoid receptor binding events in prostate cancer cells, *Cancer Research*, 2013 Mar 1;73(5):1570-80.

4.1.5. Promotion of good practices

Project leaders were asked how their projects promoted the application of good practices in the field of computational science (Question 1.8). The practices were shortly discussed in the programme memorandum, and the promotion of good practices was also one of the main goals of the programme.

The answers roughly fell into two groups: those who mainly followed good practices and those who really tried to promote good practices. Many respondents followed good practices by stating that their group had carefully documented or shared data during the process. Following good practices also included the compiling of large datasets, publishing main results, maintaining analysis packages, using common platforms and building trust between partners. In some cases, the developed methods intrinsically included the improvement of good practices in the field. There were also a few respondents who did not particularly focus on promoting good practices in their projects. Some of the answers are quoted below.

> *"The project has matured our practices for project documentation, management of critical data for long-term storage, and maintenance of analysis packages. It has also resulted in ways to better take care of open access principles."*

> *"ASCOT-4, the totally re-written suite of codes, is now written using the good practices both algorithmically and in facilitating future enhancements, debugging and mastering the code. E.g., it uses Doxygen for automatic documentation!"*

4.1.6. Relevance of hypotheses, themes and objectives in the Lastu programme memorandum (as seen today)

Project leaders were asked how relevant they regarded the programme's hypotheses, themes and objectives today as compared to how they were written in the programme memorandum in 2008 (Question 1.9). This question was asked with a view to assessing the significance and weight of the results of the programme.

The hypotheses, themes and objectives of the programme defined in the programme memorandum from 2008 were considered to be appropriate by approximately 70 per cent of the respondents. Four respondents had some ideas about what could be added today. According to one respondent, the computational facilities and services of CSC – the IT Centre for Science (www.csc.fi) should have been more strongly involved in the programme. There was also an opinion that the research in computational science should be more strategic. One respondent called for more emphasis on mathematical modelling and methodology development. Altogether 21 out of 30 respondents answered the question.

4.2. Programme impacts on computational methods research

One of the objectives of the programme was to increase mathematical and computational knowledge and methodological skills in the research community. The questions related to these objectives were targeted at those who consider themselves more as developers of computational methods than as users or appliers of computational methods. Altogether 18 out of 30 respondents considered themselves to be developers or both developers and users of computational methods.

4.2.1. Contribution to increasing mathematical and computational knowledge and methodological skills in the research community

One of the questions concerned how the projects have contributed to increasing mathematical and computational knowledge and methodological skills in the research community (Question 3.2). According to the answers, innovations, new expertise, methods, solutions and collaborations, among other things, have emerged. There were answers from altogether 18 respondents, and some of the answers are presented below.

> *"We developed new machine learning methods for analysing brain imaging data"*

> *"We have made an unexpected discovery that ice cannot be ferrolectric. The referee of our article said that this is a statement of brave men. There have been contacts with us on this issue"*

> *"Very much, due to MANY talks I have given around the world for both technical and general audiences about the CSI Speech results"*

> *"The scope of our new method's applicability ranges from functional behaviour of nanosize particles to features of dynamic superequilibria in large scale industrial and environmental processes. Thus the method gives a large array of potential uses in the fields of materials and process chemistry as well as in the development of sustainable technology"*

> *"Developing robust Principal Component Analysis in cases of missing data"*

4.2.2. Types of solutions developed

To assess the realisation of certain specific objectives of the programme, the project leaders were asked what other kinds of solutions they have developed in addition to the computational methods (Question 3.3). The results are shown in Figure 20. The results show that both computer science solutions, mathematical solutions and statistical solutions have been developed relatively equally. Sixteen project leaders responded to this question.
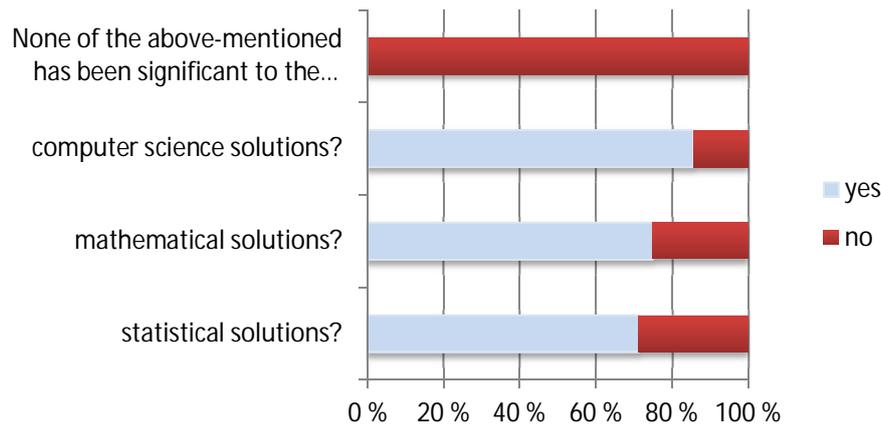
Figure 20. While developing new computational methods, have you also developed any related and necessary …
(Question 3.3).

4.2.3. Extent of application of developed techniques

The project leaders were asked whether the methods developed in the projects have been applied also outside the Lastu projects (Question 3.4). This question was answered by 17 respondents. Eleven of them answered that their method is used or has been used outside their project. In the rest of the cases, the methods had either not been applied in other contexts or had been used partially or not as such. Some quotes are presented below:

> *"Yes, the approach has been adopted and implemented at ECMWF into their Integrated Forecasting System (which is developed by joint-funding of its over 20 European member states)"*

> *"Yes, seems to be increasing, the applications ranging from surface energies of (nanosize) alloys to thermochemical reactions in supercritical fluid."*

> *"Not yet but one graduate student is now looking for other datasets that would be used for testing the feasibility of the methods"*

4.3. National and international collaboration

The questionnaire also aimed at finding out how important international collaboration had been to the projects, to what extent there had been international recruiting and whether the new collaborations will continue. These issues are discussed in this subsection.

4.3.1. Influence of the programme on creating new national and international collaborations

The Lastu programme was considered to be an important factor in generating new national and international research collaboration (Question 4.1), as 50 per cent of the respondents viewed its influence as "very important" and 30 per cent thought it had been "important" (see Fig. 21). Only two people mentioned that the programme had not been important in terms of creating new contacts. All 30 respondents answered this question.
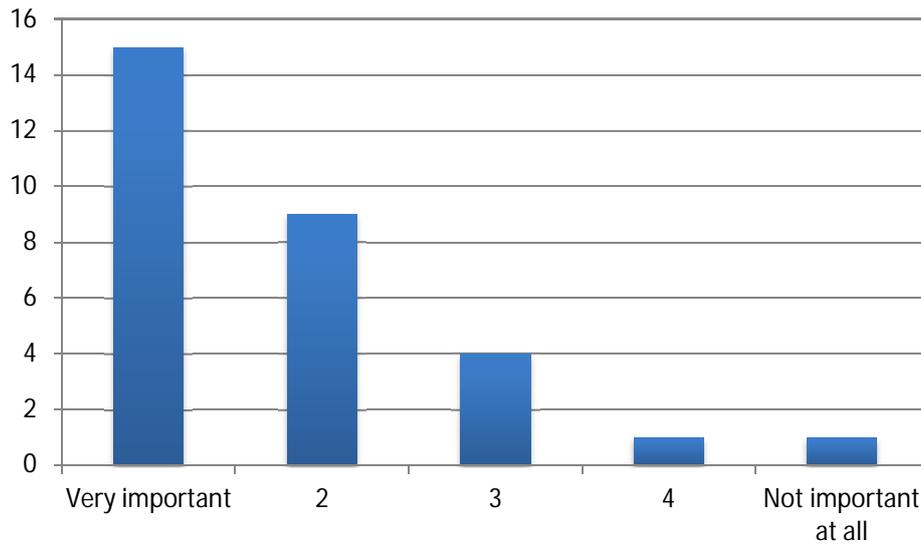
Figure 21. How important a factor did you feel that being part of this programme was in generating new national and/or international research collaboration (Question 4.1)?

4.3.2. Influence and consequences of new national and international contacts

It was also of interest to know whether there the collaboration with new contacts has continued (Question 4.2). More than 90 per cent of the respondents had had discussions about putting up a new research project (see Fig. 22). Approximately 80 per cent had discussed applying for funding for a new project, whereas some 55 per cent had already submitted their new application. Finally, surprisingly many respondents (21%) had already received funding. It is likely that these figures will increase with time.The response rate varied in this four-part question between 80 and 93 per cent.
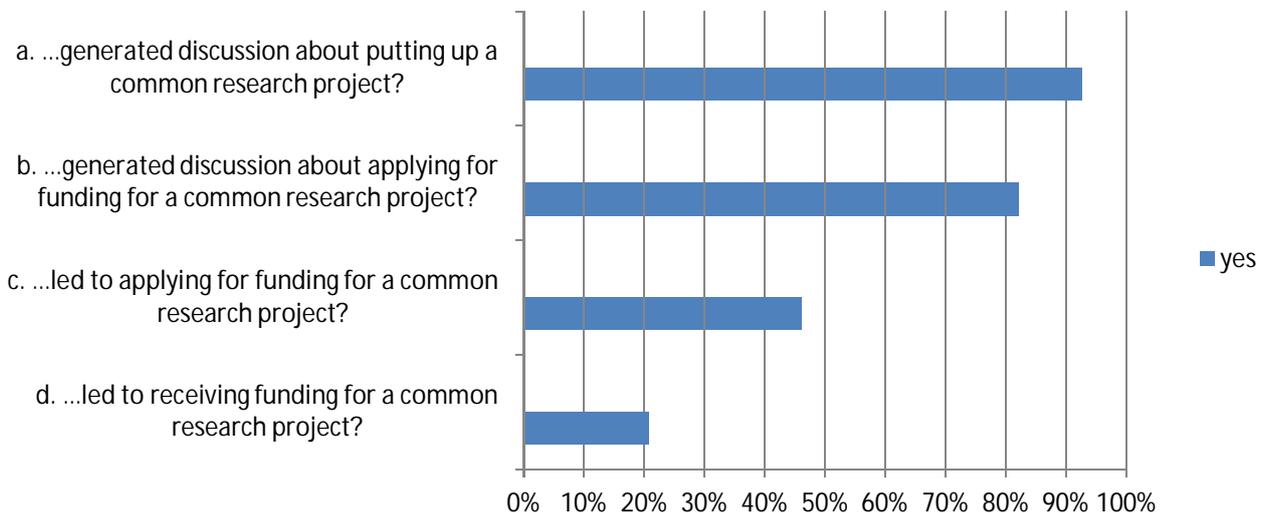
Figure 22. Has the programme succeeded in establishing new national or international contacts for you that have … (Question 4.2).

4.3.3. International recruiting

Question 4.3 asked if there had been international recruiting in the projects. 15 out of 27 answered that there had been some international recruitment. In eight cases, the recruits were postdoctoral researchers (e.g. Czech and French researchers), and in five cases they were doctoral students (e.g. Chinese and Turkish researchers). Other countries mentioned included Brazil, the United States and Pakistan.

4.3.4. Programme's influence on the quality of international collaboration

Most project leaders found that the programme had supported or deepened their projects international collaboration in a qualitative manner (Question 4.4). The rest felt that the programme had not deepened the collaboration or that it was difficult to assess the role of the programme. Some of the comments are cited below.

> " It opened up new collaboration with scientists representing the field of impedance tomography field and inverse mathematics"

> "Yes, new collaborations, new thinking, tentative and concrete openings towards new top-level research groups in Europe."

> "Getting to know international groups and their level of computation and understanding of the physical problem."

> "It opened connections to ECMWF as mentioned above, and partly to MIT."

> "Yes, our Lastu partners have entered the European fusion programme and received funding from it."

> "Our PhD student is now a post-doc researcher at ECMWF"

4.3.5. International research collaboration (SWOT analysis)

The respondents were asked to briefly describe the international research collaboration of their project through a SWOT analysis (Question 4.5). There were some misunderstanding concerning this question. Some respondents understood the question to cover the whole project and not particularly the international collaboration aspect of the project.

> ***Strenghts***

> "Strong collaborators with very good experimental infrastructure and resources"

> "We have established our position in the emerging field of machine learning in atmospheric modeling"

> "We have built a very good knowledge of large scale time dependent electron transfer simulations and that is a strength of future collaborations."

"Finding strong partners abroad."

"To wider our thinking and views, and to get familiar with other research practices."

Weaknesses

"Distance, largely different time zones, hard to organize as much interaction as we would have liked."

"Weak follow up opportunities."

"Senior level scientists have high admin load and cannot focus on the research"

"Too few international collaborations contacts"

"New research area no quick ways to collaborate internationally"

Opportunities

"Very good new possibilities that can be utilized at any future step, and all this benefits Finnish science."

"Common interests, highly complementary approaches and knowhow --> great possibilities for innovation."

"International financial support, benchmarking with other group"

"Novel analysis possibilities will lead to enhanced collaboration"

"Large networks of the participating groups provide visibility for the project."

"To apply funding from European Comission""Having bright minds together has potential to lead excellent results"

Threats

"It is very difficult to plan long-term due to funding challenges"

"To reach critical mass on international level."

"International competition is strong, we need to choose carefully our research projects"

"Larger groups could in principle pass us in our field of expertise. However, at the moment we are clearly ahead of others."

"In high risk/high gain projects, it is always possible that the final outcome is close to zero (only incremental results instead of finding breakthroughs)."

4.4. Programme impact on research careers

A part of the questionnaire concerned the programme's impacts on research careers. Question 5.1 was: "This question concerns those who were employed in your subproject as doctoral candidates and who have since finalised their theses. For how many of these theses did this programme have a significant impact?" The result was that the programme had had a significant impact on 36 theses in total.

The follow-up question (Question 5.2) was: "How have the research careers of these newly graduated doctors continued after the project?" In total, seven newly graduated doctors are now researchers abroad. In total, 16 doctors have continued working in the original group, one of whom has received a three-year Postdoctoral Researcher's grant from the Academy of Finland. In total, five doctors have moved to another research group in Finland, and two have moved to work with a consortium partner. Six doctors have moved to work in the business sector. None of the newly graduated doctors have moved to non-researcher positions in the public sector. This data is depicted in Figure 23 below.
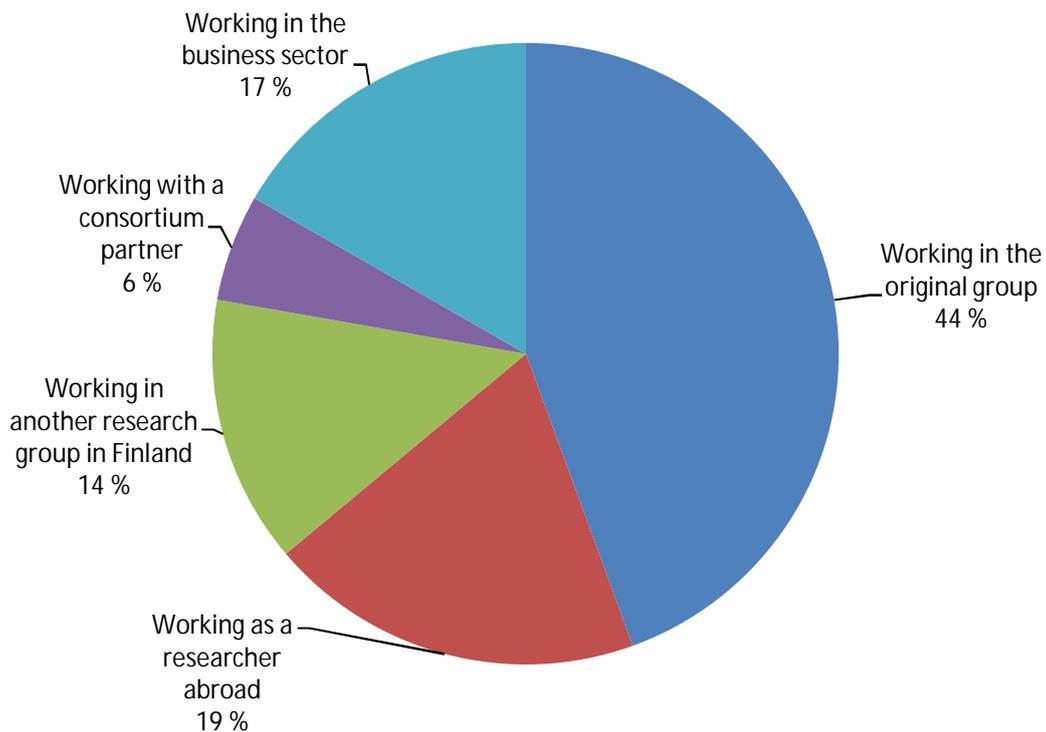
Figure 23. How have the research careers of the newly graduated doctors continued after the project (Question 5.2)?

4.5. Feedback on the programme

The feedback received from the project leaders via the questionnaire was mainly positive. It was much appreciated that a computational science programme was funded as such, because often they are seen more like by-products. Some respondents hoped that the programme would continue in some way. Respondents called for a well planned strategy for computational science.

The programme was regarded as having had a lot of both visible and invisible impacts on Finnish science. It built skills and innovativeness among the researchers and research groups. The media relations training, for instance, was seen beneficial and as something that could be further developed.

Two respondents mentioned that the projects in the programme were quite different from each other, and therefore the collaboration with other projects was scarce. On the other hand, there were also many respondents who particularly appreciated the interaction of the consortia and who learned a lot from this collaboration.

4.6. Observations by the programme managers

The steering group of the programme decided that the programme managers would express their own perceptions about the important issues related to the results of the evaluation. These perceptions are presented topic-wise below.

Formation of consortia: A majority of the project leaders considered that the Lastu programme was a very important factor in the formation of their consortia, although most consortia were based on existing contacts and collaborations.

Added value of the programme: Multi- and interdisciplinary collaboration and exposure to new kind of expertise were regarded as significant elements in terms of the added value of the programme. Especially the interdisciplinarity had a great impact on researchers' professional capabilities, researcher training, partnership and networking.

Outcomes: Most of the respondents stated that the most significant outcomes were their scientific outputs, that is, new models, theories or methodology. Some even considered having renewed their research area. The new methods developed have also been put to good use outside the projects.

Creation of new collaborations: The programme was very successful in establishing new national and international collaborations. Almost all PIs had discussed putting up a new research project, and as many as one-fifth of them had succeeded in receiving funding.

Research career: A majority of the newly graduated doctors of the programme have continued their career outside their original research group after the project.

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APPENDIX I: The self-evaluation questionnaire

Category 1: General questions

1.1 Through which call were you funded? (If you were funded through multiple calls, please, mark 'Call 2011', and answer to all the questions from the perspective of the project funded through 2011 call.)

1.2 How did you end up with the consortium you formed?

1.3 How likely is it that you would have founded a similar consortium if the Lastu programme never existed?

1.4 Were you the consortium leader?

1.5 What was the most significant added value that participating in the programme brought to you compared to having been funded as an ordinary academy project (max. 2 sentences)?

1.6 What do you consider to be the most significant outcome(s) of your project?

1.7 Which one of your project's publications do you consider the most significant? Why? (max. 3 sentences)

1.8 How has your project enhanced the application of good practices in the field of computational science research? (As indicated in the programme memorandum, good practices mean, for example, information on data sources and utility and careful documentation. The programme memorandum is available at http://www.aka.fi/en/research-and-science-policy/academy-programmes/current-programmes/lastu/)

1.9 How appropriate do you find the hypotheses, themes and objectives written in 2008 in the Lastu programme memorandum? What would you add or remove?

Category 2: The impacts of the multidisciplinary character of the programme

2.1 What kind of disciplines/fields did the consortium aim at bringing together? If you select more than one option, please prioritise your selections (1=most important, 2=second most important, etc).

2.2 Which disciplines/fields were involved in the consortium, and in what roles? You can draw on your own understanding of disciplinary classifications.

2.3 How established was the interdisciplinarity of the consortium? Please select one option.

2.4 At which 'level' of research activity did interdisciplinarity manifest itself most strongly? If you se-

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lect more than one option, please prioritise your selections (1=most important, 2=second most important, etc). However, answer the following two questions (2.4 and 2.5) by using the strongest 'level' as your reference point.

2.5 Please describe shortly the nature and significance of interdisciplinarity at the selected level(s). Mention the participating disciplines/fields as you perceive them.

2.6 Which 'element(s)' of research did your interdisciplinary activities center around? If you select more than one option, please prioritise your selections (1=most important, 2=second most important, etc).

2.7 Please describe shortly your interdisciplinary activities around the selected element(s).

2.8 What kind of challenges did interdisciplinarity bring about? If you select more than one option, please prioritize your selections (1=most important, 2=second most important, etc).

2.9 Please describe shortly the challenges of the selected kind(s).

2.10 Please assess the impacts of the project's interdisciplinarity on the following areas both verbally (what kind of difference did interdisciplinarity make?) and numerically (how important was the given impact?). Use a scale 1-3 (1=very important, 2=somewhat important, 3=not important) for the numerical assessment. If the given area was outside of the project's activities, leave the item empty.

2.11 Have you continued collaboration with your consortium partner(s) after the Lastu programme?

2.12 Please describe the collaboration

Category 3: The influence of the programme in computational methods

3.1 Which of the following best represents your role in the Lastu consortium you were part of?

3.2 Please explain shortly your selection.

3.3 Please, describe briefly (max. 3 sentences) how your project has contributed to the increase of mathematical and computational knowledge and methodological skills in your research community.

3.4 While developing new computational methods, have you also developed any related and necessary

3.5 Has the computational method that you have developed been applied outside your own project?

Category 4: National and international collaboration

4.1 How important a factor did you feel that being part of this programme was in generating new national and/or international research collaboration?

4.2 Has the programme succeeded in establishing new national or international contacts for you that have

4.3 Was there any international recruitment in your sub-project? Please describe briefly.

4.4 Did participating in the programme support or deepen the international collaboration of your project in a qualitative manner? Please, justify briefly.

4.5 Describe briefly the international research collaboration of your project through SWOT analysis.

Category 5: The impacts of the programme in scholar career

5.1 This question concerns those who were employed in your sub-project as doctoral candidates and who have since finalised their theses. For how many of these theses did this programme have a significant impact?

5.2 Related to the question 5.1, how have the research careers of these newly graduated doctors continued after the project? How many of them

5.3 Complementary comments on the above.

5.4 This question concerns those who were employed in your sub-project as doctoral candidates and who have since finalised their theses. For how many of these theses this programme did not have a significant impact?

5.5 Related to the question 5.3, how have the research careers of these newly graduated doctors continued after the project? How many of them

5.6 Complementary comments on the above.

Category 6: Feedback

6.1 Which question in this questionnaire did you find good/apt? Please, justify briefly.

6.2 What other questions would you have found relevant/useful in this questionnaire? How would you have answered them?

6.3 What else would you like to tell about the programme?

APPENDIX II: A closer look at multidiciplinarity aspects of Lastu programme

Author: Katri Huutoniemi

Executive summary

Given the stated goals of the program, **interdisciplinarity was a norm** rather than exception in the funded projects. The projects successfully applied computational methods to understand and solve complex problems in various domains of science and society, including domains that had not yet fully exploited the advanced computing capabilities. Besides the 'vertical' integration of methods and substance fields, the program also facilitated interaction in a 'horizontal' direction, i.e. between fields that traditionally operate within their own experimental and theoretical settings. Almost all projects have also continued the interdisciplinary collaboration established in the LASTU program.

The program has mainly strengthened existing networks of collaboration rather than created completely new contacts. The **interdisciplinary scope** of many projects was modest, covering research fields that interact with each other on a more or less regular basis. Moreover, while computational methods are becoming more frequent in the social sciences and humanities, too, these domains were less represented in the program. A few projects did cover humanities issues, such as the human aspects of cognition, language, speech or health, but especially the involvement of social sciences was low.

While the rationale of interdisciplinary collaboration in most projects was to better understand a real-world phenomenon, the **organization of interaction** between disciplines depended on the specific goals of each consortium. Interdisciplinarity served one or more of five general functions: problem solving, conceptual bridging, exploration, method development, and technology development. Interdisciplinarity was instrumental especially for the first three functions. Interdisciplinary collaborations aiming at *problem solving* started with a real world issue, such as climate uncertainty, problems in spoken language, or forest management, and designed their interaction for finding an appropriate problem formulation and its solution. Attempts to *conceptual bridging* took place among two or more theoretically oriented partners, with a view to investigate links between different disciplinary approaches (e.g. physical and chemical scales) to the same phenomenon. Interdisciplinary collaboration also served the *exploration* of unknown scientific territories (e.g. two-person neuroscience) by combining intellectual resources in a new way. While these functions organize interdisciplinary interactions in many domains of research, computational science may be salient by virtue of boosting these functions by advanced computing capabilities.

Interdisciplinarity was realized in the projects through concrete research activities that served as nexuses between disciplinary partners. Key **areas of interdisciplinary exchange** were the *definition of research problems* (e.g. how to operationalize climate uncertainty to improve weather forecasts), the selection and development of *theoretical concepts or models* (e.g. bridging models that cover different scales in time and space), and interpretation of *empirical evidence* (e.g. using new imaging methods for studying the vocal folds). Interdisciplinarity was thus an integral part of the

research process, rather than an addition to it. None of the projects, for example, performed inter-disciplinary activities around the application of results only.

The importance of specific interdisciplinary activities, however, was often perceived differently by different partners. 'Importers' of computational methods, for example, emphasized the role of inter-disciplinary collaboration in the interpretation of data, whereas 'exporters' put a premium on interdis-ciplinary exchanges around theoretical concepts. Divergent interests were rarely an obstacle for successful collaboration. Instead, they enabled an effective **division of cognitive labor**, as parties could pursue their specific goals in harmony while benefitting from the complementary expertise of each other.

Major challenges of interdisciplinary collaboration lay in *epistemic or cognitive* differences between the participating fields. Partners did not always understand each other's goals, concepts, methods, or language, which brought about problems in identifying the most relevant research questions, strik-ing an appropriate level of analysis, or agreeing upon a common vocabulary. *Cultural or operational* challenges relating to different ways of designing models, balancing between theory and data, or writing academic papers were also common. Challenges were overcome by trial-and-error in the course of collaboration, which often resulted in delays in the completion of research. Many project leaders, however, stated that the challenges of interdisciplinary research were *not much different* from those of conventional academic research.

The **scientific publications** of the seven already reported projects distributed across 21 out of 27 disciplinary categories listed in the Scopus journal database. While the most diverse set of publica-tions spanned across 13 disciplinary categories, the least diverse of them spanned only three cate-gories. Also the interdisciplinary balance of publications varied between the projects, and the overall balance of the program's publications was biased toward a single discipline, Physics and Astronomy. Based on the *disciplinary diversity* of publications, five of the seven reported projects were clearly interdisciplinary. At the same time, the degree of *co-authoring* between consortium partners was relatively low: only one project regularly integrated the contributions of different disciplines into joint publications. The emphasis the project leaders put on *interdisciplinary learning and capacity* building, however, suggests that some of the most important impacts of interdisciplinary research cannot be captured by quantitative performance measurement.

1.1. Interdisciplinarity

1.1.1. Introduction

Computational science is not an academic field of its own, in the traditional sense of having its own subject matter and institutional structures, but refers to the widespread use of advanced computing capabilities to understand and solve complex problems. The development of computational ap-proach is advancing knowledge production in many corners of science, including natural sciences, life sciences, social sciences, humanities, and especially in a growing number of technological and other applied fields. The LASTU Program Memorandum (p. 4) describes the state-of-the-art of com-putational science as follows:

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> *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.*

Against this backdrop, one of the main goals of the program was to facilitate interaction and exchange between research teams and different research disciplines, especially between the 'substance sciences' and algorithm and methods development. This goal is closely related to the other goals of the program, which include: promoting the use of computational methods; improving methodological skills and competencies; enhancing the application of good practices; and international networking.

Within the LASTU program, interdisciplinarity had an *instrumental role* in two senses: On the one hand, interdisciplinarity was not pursued for its own sake, i.e. in order to create intellectual and institutional coherence across a heterogeneous set of scientific activities, but as an instrument for achieving relevant ends. On the other hand, the role of interdisciplinarity in attaining those ends was deemed indispensable. The ends themselves, however, were not imposed from 'above', i.e. based on the science policy need to tackle a topical issue faced by society, but were left open to researchers' choices. The interdisciplinarity of the LASTU program was thus largely driven by the development of the research fields themselves.

The instrumental, yet open-ended, goals of interdisciplinarity in the program provide a starting point for this evaluation. First, given the internally-driven nature of interdisciplinary collaboration, the primary focus of attention here is on interdisciplinary activities within the funded research projects, rather than in the research program as a single entity. The unit of analysis is thus a *research project,* which is a research endeavor by a consortium of two or more research teams from different organizations, or by a single research team. The evaluation of the LASTU program comprises 15 research projects in total, but evaluation data from some projects is very limited.

Second, and related to the previous point, the constitution of interdisciplinarity is not taken for granted, but as part of the evaluation itself. The rationale behind this approach is that the interdisciplinarity of the LASTU research projects is of less distinctive character than, for example, of projects originating from a demand-driven initiative for interdisciplinary collaboration.[7] Seen as a 'bottom-up' phenomenon, i.e. as resulting from the self-organization of science itself, interdisciplinarity is more difficult to distinguish from ordinary disciplinary work.[8]

This evaluation aims at capturing the interdisciplinarity of the LASTU projects by combining different methods and data. It is based on the following set of empirical material:

(1) The *public description* of the funded research projects in the Academy of Finland archives (all 15 research projects). For the three projects funded through the ERA-SysBio call, public descriptions in the respective ERA-NET www-page were also consulted.

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[7] Indicators for this kind of interdisciplinarity are more established; see e.g. Bergmann et al. 2005, 2012.
[8] Preliminary indicators do exist, however. This evaluation draws partly on the typology and indicators of interdisciplinary research I have been developing; see e.g. Huutoniemi et al. 2010.

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(2) *Online survey* sent to the team leaders of the research projects in spring 2015 (the question-naire was sent to all 46 team leaders; the number of respondents was 30, and they repre-sented 11 out of 15 research projects). The questionnaire included six questions relating to interdisciplinarity, all of which contained two parts: a multi-choice question and an open-ended question that asks specification for the choice. The questionnaire is in Appendix I.

(3) *Semi-structured interviews* with selected team leaders (seven interviews from four research projects). The interviewees were selected from the already finished projects, and the aim was to include research projects in which the boundaries between the disciplines involved, as well as the interdisciplinary objectives, were obvious in the original research plan. Interview ques-tions expanded data from the questionnaire, allowing for opportunities for deeper probing and clarification.

(4) *Publication lists* of the finished and reported research projects (the seven research projects funded through the 2009 call). Publication data was acquired from the final reports of the projects, and it covers all the scientific papers mentioned in the reports (publication catego-ries A1, A2, A4 and D3. The data was analyzed with bibliometric methods described in Sec-tion 1.4.

In what follows, the interdisciplinarity of the LASTU research projects is analyzed in terms of three major dimensions. Section 1.2 addresses the interdisciplinary *composition* of the projects, focusing on the configuration of the disciplines or fields involved in each project and the division of cognitive labor between them. Section 1.3 addresses the *implementation* of interdisciplinary research in the projects, including the ways in which knowledge from different disciplines was brought together and the specific challenges and solutions that had arisen from it. Section 3.4 analyzes the *outcomes* of interdisciplinarity in terms of scientific publications, as well as the potential impacts on both research capabilities and the utilization of knowledge.

Each of the three dimensions of interdisciplinarity is evaluated by drawing on diverse empirical ma-terial. The public description of the projects (data item 1) and survey responses (data item 2) are used to get an overview of the interdisciplinary characteristics of the research projects. More specific insights of these characteristics are drawn from the interviews with selected team leaders (data item 3). The publication lists of the finished projects (data item 4) are used for a quantitative analysis of the interdisciplinarity of the projects' outcomes.

1.1.2. Interdisciplinary composition of the projects

In the LASTU program, interdisciplinarity seemed to be a norm rather than an exception. It was deemed 'fundamental to the project' or 'key to most that we did' by many survey respondents. One respondent stated that 'it is not possible to think of this research in non-interdisciplinary mode'.

Interdisciplinary collaboration in a majority of research projects was not new. Many consortium part-ners had collaborated with each other already before this LASTU project (n=13), or at least some of the consortium partners had previous experience of similar interdisciplinary collaboration (n=14).

Moreover, some of the interdisciplinary partnerships were continuation of collaboration between senior researchers and their previous students. Only few respondents stated that the interdisciplinary collaboration in the project was clearly different from the previous experience of the partners (n=3). The program has thus mainly strengthened existing networks of collaboration – including existing interdisciplinary connections – rather than created completely new ones. This is not surprising, though, given the small size of the academic community in Finland: Personal contacts across disciplinary boundaries are not rare, which makes interdisciplinarity a natural part of research.

As expected, the most significant form of interdisciplinarity took place *between* the consortium partners, but interdisciplinarity *within* a research team or an individual mind was also recognized by more than half of the respondents (see Figure 1.2-1). In several research projects, the composition of research teams was tailored to the specific interdisciplinary task at hand, and researchers from the 'partner's field' were sometimes hired into a research team. Many respondents also stated that meaningful collaboration would have been impossible without the interdisciplinary competence of individual researchers. Such competence was deemed extremely important when applying computational methods to new areas, i.e. when the research questions themselves were not entirely clear from the outset (see Section 1.3. on the implementation of interdisciplinary research). On the other hand, interdisciplinary collaboration was also perceived as a source of learning and new insight for individual researchers and research teams, often extending beyond the specific problem of the research project (see Section 1.4 on the outcomes of interdisciplinarity).

Figure 1.2-1. The distribution of responses to the question: 'At which "level" of research activity did interdisciplinarity manifest itself most strongly? If you select more than one option, please prioritize your selections.' N=30.
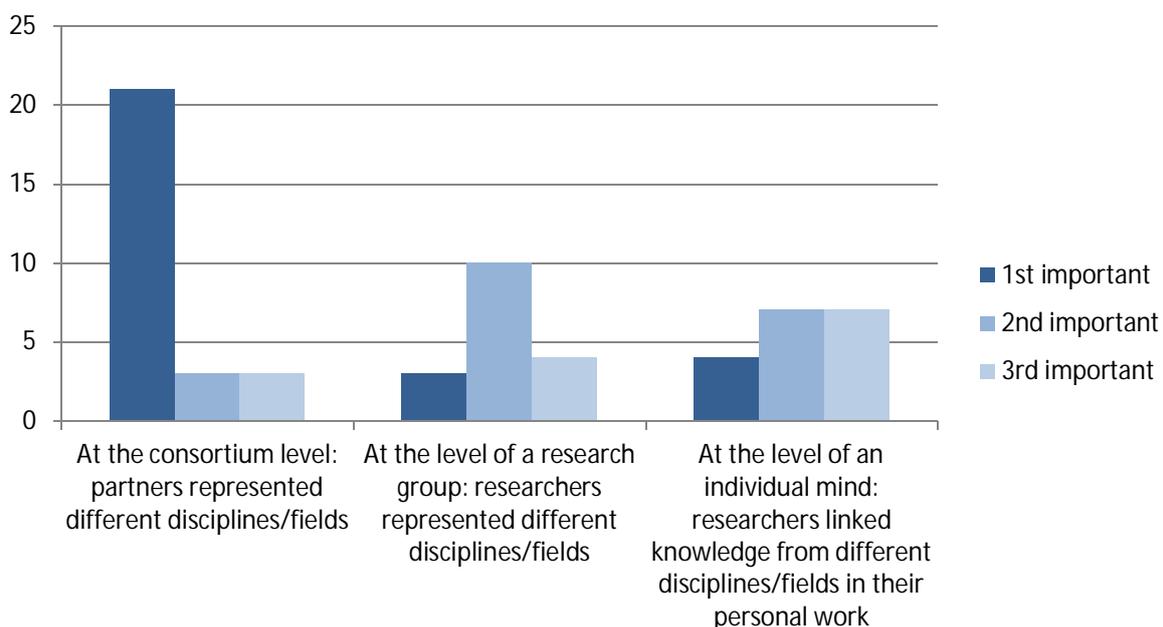
Research fields involved

The interdisciplinarity of the projects, documented in the self-evaluations, most frequently aimed at bringing together *computational methods and 'substance' fields*. Another frequently selected option was to bring together *different (theoretical or methodological) specialties within computational sciences* (see Figure 1.2-2). In the first category, interdisciplinary collaboration was based on a clear

division of tasks between 'methods' and 'substance' teams, whereas in the second category, the partners represented disciplines that typically investigate similar phenomena but operate at different scales, focus on different aspects, or rely on different methods. The difference between the two categories was not, however, always clear, and a significant number of respondents selected both categories as relevant for their research project.

Figure 1.2-2. The distribution of responses to the question: 'What kind of disciplines/fields did the consortium aim at bringing together? If you select more than one option, please prioritize your selections.' N=30.
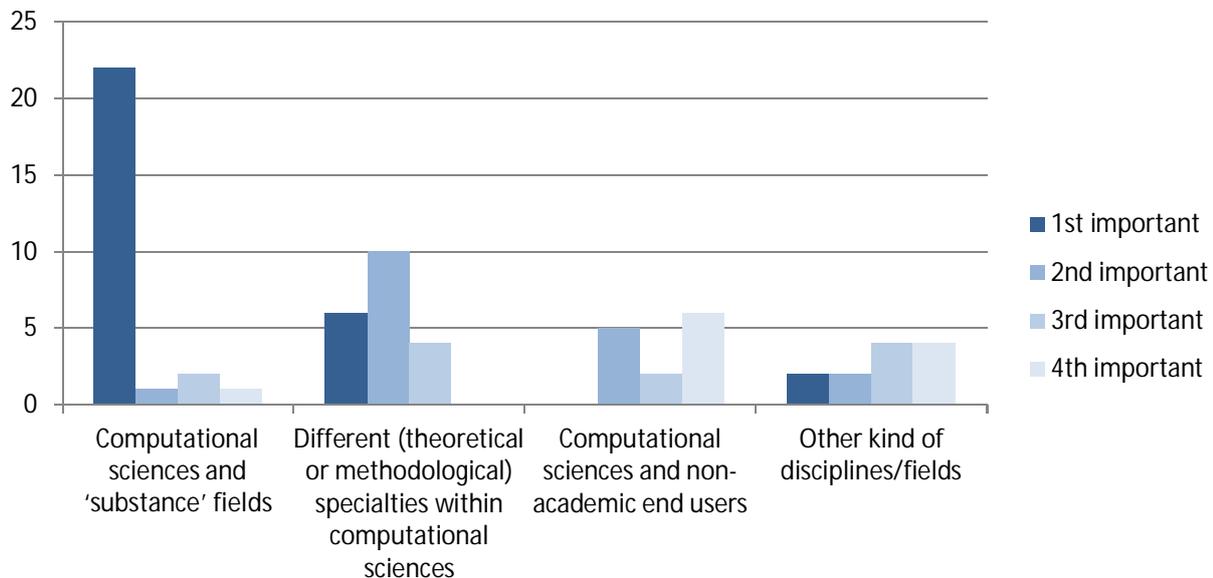
Most frequently mentioned research fields were applied mathematics, machine learning[9], advanced statistics, as well as specialized computational approaches in physics, chemistry, materials science, systems biology, bioinformatics, and various branches of engineering. The latter fields were considered by some respondents as computational sciences themselves, whereas for other respondents, they represented areas to which computational techniques are applied. Other fields in which computational methods were applied include climate research, meteorology, forest sciences, linguistics, neuroscience, neuroimaging, immunology, radio astronomy, health care, and speech research. The interdisciplinary composition of each project, including the function[10] of interdisciplinary collaboration, is summarized in Table 1.2.

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[9] 'Machine learning' is used here as a synonymous for 'computational data analysis', which is the term that appears in the Academy of Finland classification of research fields. The reason for selecting this term is the feedback from an interviewee acting in this field.

[10] Interdisciplinary activities around these functions are discussed in more detail in Section 3.3.

Table 1.2. The interdisciplinary composition of each project, including the division of cognitive labor between the consortium partners, the computational methods used, their specific areas of application, and the overall function of interdisciplinary collaboration.

Research project	Division of cognitive labor	Computational methods	Application area	Function of interdisciplinary collaboration	Call: LASTU 2009
Computational analysis of complex brain imaging data (BrIAn)**	Computational methods vis-à-vis a substance field	Machine learning	Neuroscience	Exploration	
Novel advanced mathematical and statistical methods for understanding climate (Novac) **	Computational methods vis-à-vis a substance field	Applied mathematics; advanced statistics	Climate research	Problem solving	
Computerized inversion for spoken language – An interdisciplinary consortium on inverse problems in the production and perception of speech (CSI Speech)**	Computational methods vis-à-vis several substance fields	Inverse mathematics	Spoken language; health care	Problem solving & exploration	
Computational research chain from quantum chemistry to climate change (ComQuaCC)**	Different spatio-temporal scales of atmospheric reactions	Atmospheric physics, chemistry	Atmospheric science	Conceptual bridging	
From ultrarapid data transfer into science - Near realtime VLBI application (eVLBI+GEO)	Computational methods vis-à-vis a substance field	Distributed data processing, transfer and storage of very-long-baseline interferometry	Geodesy	Technology development	
Multiscale modelling of chemical processes (MUMO)	Different scales of chemical processes	Computational fluid dynamics, molecular modeling etc.	Chemical technology; materials science	Conceptual bridging & technology development	

** The research project was selected for a closer examination through interviews.
No survey responses were received from the project; the only available data is the public description of the project.

Turning teraflops into megawatts (SimiTER)	Different technological specialties	Numerical simulations	Plasma physics; materials science	Problem solving & technology development	
Systems approach to gene regulation biology through nuclear receptors (SYNERGY)	Computational methods vis-à-vis a substance field	Machine learning, computational systems biology	Medicine; biochemistry	Exploration	Call: ERA-SysBio
Signalling pathways and gene regulator networks responsible for Th17 cell differentiation (Tcellnet)	?	Computational systems biology; bioinformatics	Immunology	Exploration	Call: ERA-SysBio
Integrative systems analysis of the shoot apical meristem (iSAM)	?	Systems biology	Plant development	Exploration	
Computational modelling of brain's language	Different methodological approaches	Computational linguistics, machine learning, neuroimaging	Cognitive neuroscience	Method development	Call: LASTU 2011
Quantum simulations of molecular optical properties in the condensed phase	Different aspects of the same class of molecules	Computational approaches combining electronic structure theory and molecular dynamics simulations	Light absorption (in e.g. human eye, chlorophylls, dye molecules)	Exploration	Call: LASTU 2011
Bridging atomistic biophysical simulations and computational systems biology for applications to type 1 diabetes (AtomSysBio)	Different types of models, covering different scales in time and space	Physics/ chemistry based simulations combined with computational systems biology	Diabetes research	Conceptual bridging & method development	

Multi-scale modeling of tree growth, forest ecosystems, and their environmental control	Computational methods vis-à-vis a substance field	Machine learning and data mining combined with field measurements	Forest sciences	Problem solving	
Computational and mathematical models for electromagnetic wave interaction with complex material structures	Computational methods vis-à-vis two substance fields	Applied mathematics; computer simulations	Electro-magnetism; material science	Conceptual bridging & exploration	

The division of cognitive labor

The rationale of interdisciplinary collaboration, and the roles of different disciplines in it, was further clarified in interviews with selected project leaders. These research projects made use of computational science to address phenomena pertaining to brain functions (*BrIAn*), spoken language (*CSI Speech*), climate variability (*Novac*), or atmospheric processes (*ComQuaCC*). While the overall rationale behind the projects was to better understand a real-world phenomenon, the scientific motivation for interdisciplinary collaboration was often different for different parties. Complementary interests provided a basis for an effective division of cognitive labor, as parties could pursue their specific goals in harmony while benefitting from the expertise of each other.

BrIAn consisted of two research teams, one in neuroscience and one in machine learning, and the goal of this consortium was to analyze human brain activity in resting state, during natural stimulation, and in social interaction. Better understanding of these situations is at the cutting edge of modern neuroscience, but the required neuroimaging data is too complex to be analyzed using conventional statistical methods. At the same time, it constitutes an interesting real-world case for machine learning. Research tasks and responsibilities were clear from the outset, and interdisciplinary collaboration was smooth and predictable.

The goal of *CSI Speech* was to develop novel computational inversion methods for the research, analysis and synthesis of spoken language. The problem setting, and the composition of participants, was more diverse than in *BrIAn*, for example, in that several overlapping research themes were identified at the crossroads of computerized inversion and speech-related research. The division of labor, however, was clear: one research team tailored inversion algorithms for spoken language (applied mathematics); another team developed inversion based technologies to model speech production, and to use these technologies in speech synthesis (speech technology); a third team combined experimental and computational methodology to model brain mechanisms relating to speech perception (biomedical engineering); and a fourth team developed inversion-based methods to investigate the mechanisms and effects of vocal overloading (vocology). Despite this initial division of tasks, disciplinary boundaries were occasionally dissolved[11] around common problem solving (see Section 1.3).

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[11] This implies a deeper form of interdisciplinarity than the division and coordination of disciplinary labor. It expresses 'interdisciplinary interpenetration', which refers to processes where disciplinary boundaries are reshaped as a result of constructive border engagements (e.g. Fuller 1993, Ch. 2).

More interactive responsibilities were needed especially when the definition of problems was at the center of collaboration. In *Novac,* the goal of interdisciplinary collaboration was to evaluate and improve the reliability of climate models. All four consortium parties had specialized expertise in computational methods, but two of them acted as method 'exporters' and the other two as method 'importers'. Applied mathematicians, machine learning specialists, atmospheric scientists, and climate modelers worked in close collaboration to develop an algorithm for improving the reliability of weather forecasts. According to their own account, the group of mathematicians served as 'doctors' for the climate modeling software, diagnosing possible problems and their solutions, with the help of machine learning specialists who recognized relevant structures from big data sets. Atmospheric scientists and climate modelers provided theoretical understanding of climate behavior as well as the technical infrastructure (supercomputers, models, data) for modeling.

As opposed to the other three projects, *ComQuaCC* did not divide its disciplinary labor between experts in methodology, on the one hand, and experts in substance, on the other hand, but between the *different scales* of modeling atmospheric processes: it aimed to develop a theoretical framework for modeling a computational research chain from quantum chemistry to climate change. The chemists provided detailed knowledge of small-scale phenomena occurring at the level of single molecules, which helped aerosol physicists to make their broader-scale models more accurate. Climate modelers, in turn, provided knowledge of the practical implementation of the models.

1.1.3. Implementation of interdisciplinary research

Interdisciplinarity, in contrast with multidisciplinarity, refers to the active co-production of knowledge among disciplinary parties. In order to evaluate the implementation of this co-production, project leaders were asked in the questionnaire to define the 'elements' of research that their interdisciplinary activities centered around. According to the responses, interdisciplinarity was realized most frequently in the *definition of research problems* (n=11), such as making choices between different approaches and distilling the most relevant questions, or seeking the right kind of operationalization of research problems (see Figure 1.3-1). Secondly, interdisciplinarity was realized in *theoretical concepts, models or hypotheses* (n=9), which played a more or less important role also in collaborations that focused primarily on other things, such as data analysis or application of results. Project leaders illustrated the importance of theoretical elements by e.g. noting that interdisciplinary collaboration had led to the discovery of a new method, model, or way of thinking. A third frequently selected nexus of interdisciplinary activities was *empirical objects, data or analyses.* Respondents prioritizing this category (n=6) were typically those who 'imported' computational methods to their fields, and thus gained new evidence of empirical phenomena with the help of methodological specialists. Method 'exporters', in turn, often recognized this category as the second or third important element of interdisciplinary research in their project.

Figure 1.3-1. The distribution of responses to the question: 'Which "element(s)" of research did your interdisciplinary activities center around? If you select more than one option, please prioritize your selections.' N=30.
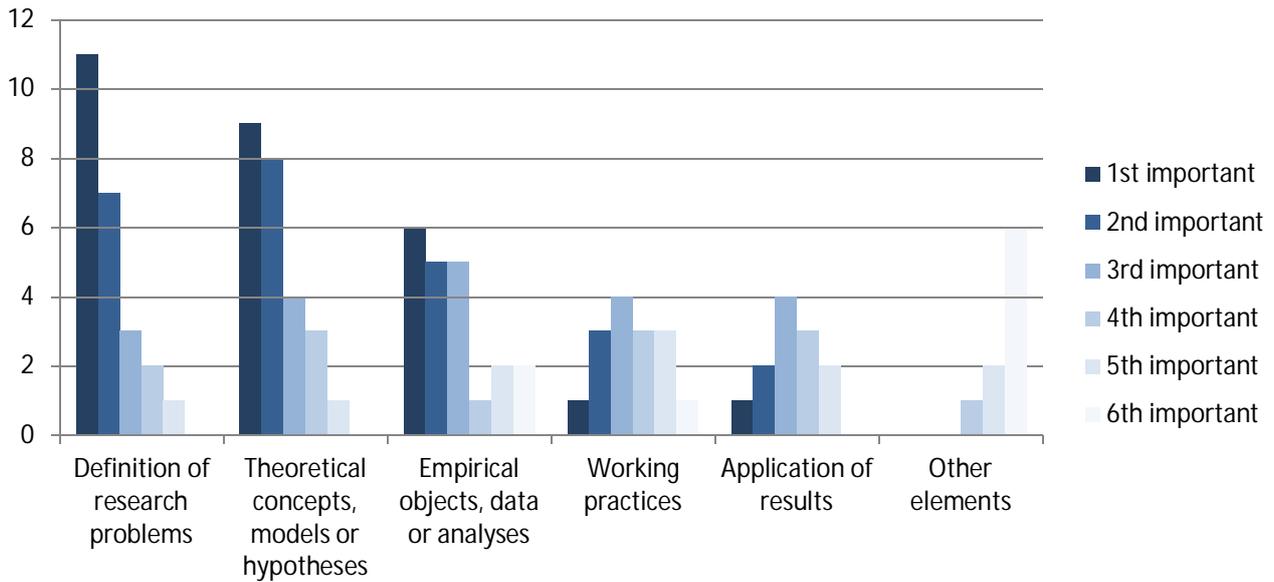
Despite the way in which interdisciplinarity was realized, the challenges reported by most project leaders were *epistemic or conceptual* by nature (of top priority, n=15; see Figure 1.3-2). Partners from different fields did not always understand each other's goals, concepts, methods, or language, or simply were not familiar with them. The presence of such cognitive differences brought about challenges in identifying the most relevant research questions, striking an appropriate level of analysis, agreeing upon a common vocabulary, etc.

Figure 1.3-2. The distribution of responses to the question: 'What kind of challenges did interdisciplinarity bring about? If you select more than one option, please prioritize your selections.' N=30.
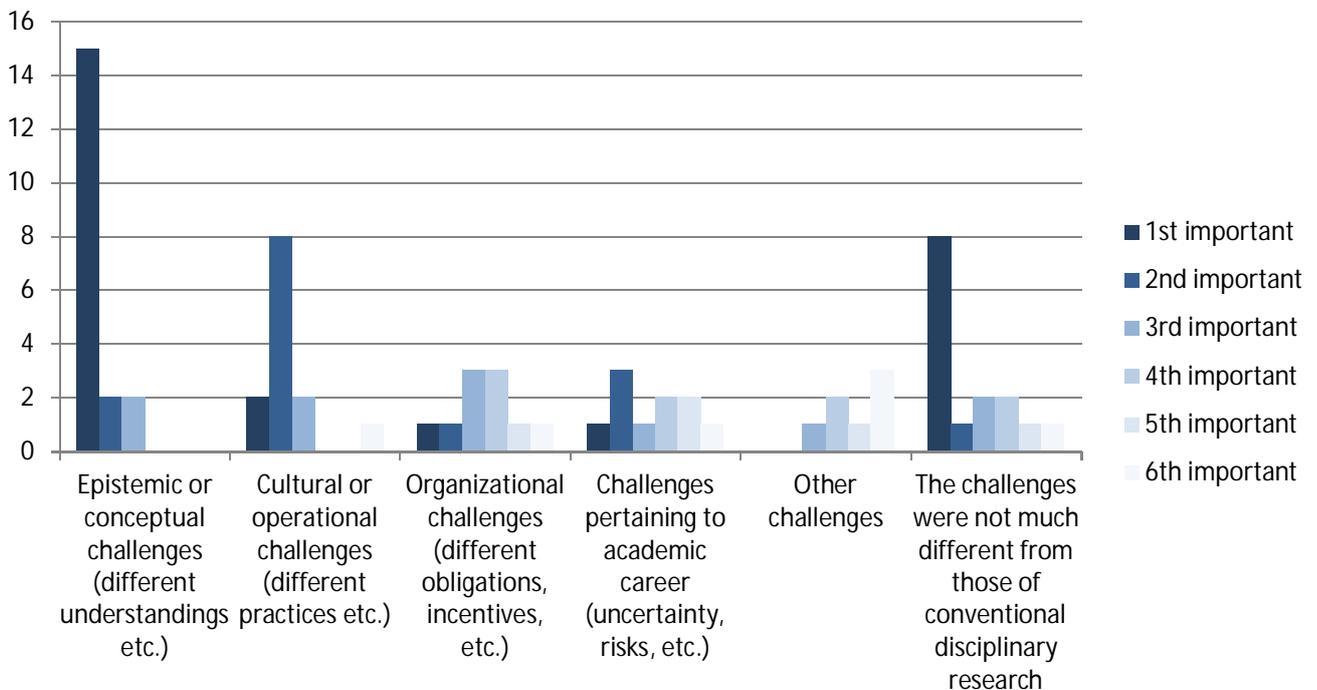
Cultural or operational challenges were also frequently recognized (n=13), though few respondents regarded them as being of top priority (n=2). These challenges related, for example, to different ways of designing models or different practices in writing academic papers. A common operational challenge pertaining to computational science, in particular, was described by a survey respondent as follows:

> *The usual procedure in computational inversion is to start with simulated and simple data, develop methods for that, and move step by step towards real data. The first algorithms can be slow; speeding them up is a 'priority two' goal. Speech signal researchers always work with real data and put great weight to the speed of computation. It took a while to learn how to work together.*

Similar experiences were reported by interviewees, too, especially by those who worked as method 'exporters' in their projects. When operating in their respective disciplinary settings, mathematicians and physicists, in particular, tend to develop models and methods at high level of abstraction, without paying too much attention to their relevance for particular purposes. When collaborating with the modelers of 'real-world' phenomena, however, their models often turn out to be inefficient with big data, focus on 'wrong' optimization functions, etc. Similar differences occur in publication practices. Whereas mathematicians, and to some extent physicists, usually publish 'ideas' and only use simple showcases to demonstrate their potential, engineers and other users of computational methods publish 'tools' accompanied by a full demonstration of their applicability in real-world situations.

In addition to the *epistemic/conceptual* and *cultural/operational* challenges, interdisciplinarity brought about some *organizational* and *career-related* challenges. Such challenges, however, were typically perceived as being of minor importance. When ranked number one (n=1 in both categories), they were related to more general tensions between competition and collaboration in international, multi-partner projects, or to the increasing funding difficulties in fundamental research, rather than to the interdisciplinary nature of research per se.

Interestingly, approximately every fourth respondent (n=8) thought that *the challenges of interdisciplinary research were not much different from those of conventional disciplinary research*, and every second respondent (n=15) recognized this statement as somewhat relevant for their project.

Further analysis of these findings, in combination with other evaluation material, can illustrate some general features of implementing interdisciplinarity in computational sciences. It seems that interdisciplinary research in the LASTU projects served especially three epistemic functions[12] – *problem solving*, *conceptual bridging*, and *exploration* – many of which could co-exist in a single project and even in the work of individual teams or researchers. The realization and challenges of interdisciplinarity can be characterized in relation to these functions.

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[12] Other functions – including method and technology development – did occur as well (see Table 1.2), but the role of interdisciplinarity in serving those functions was not always obvious in the public description of the projects, nor did it stand out in the interviews with project leaders. In the literature, similar characterizations of interdisciplinary functions exist (e.g. Boix Mansilla et al. 2006; Barry & Born 2013)

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Problem solving

The definition of *research problems* was key to interdisciplinary collaboration in *CSI Speech*, for example. The application of computational inversion methods to the research of spoken language required that inversion mathematicians went through basic problems in this domain together with the specialists, based on an initial hunch that new mathematical solutions should be available. Similar search of solvable problems occurred in *Novac* among applied mathematicians, machine learning specialists and climate modelers. While the goal of *Novac* was to reduce the uncertainty of climate predictions, especially weather forecasts, the exact nature of the problem was itself a problem which could have not been solved without interdisciplinary collaboration.

Interdisciplinarity in these projects was not simply about problem *solving* but as much about problem *setting*. A central operation was an open-ended exploration of problem areas with a view of finding a methodologically feasible problem formulation. The exact problem was thus specified and scoped out simultaneously with its possible mathematical solutions. At the same time, relatively clear understanding of the needs of the 'problem owners' – those whom the research is supposed to serve – was required. In *CSI Speech*, for example, mathematicians and engineers inquired each others' methods for (speech) signal processing in order to find out how to best solve problems of vocal folds, experienced by vocologists and speech therapists. Through intensive collaboration, they ended up developing a new way of speech signal processing that, among other things, significantly improves the standard inversion-based technology for synthesizing high voices typical of women and children. An important target group of the *Novac* research were those who do weather forecasts, and one the most significant outcomes of the project was indeed a new algorithm implemented by the European Centre for Medium-Range Weather Forecasts.

Conceptual bridging

Experiences from *ComQuaCC* illustrate a different kind of interdisciplinary inquiry, based on an explicit attempt at conceptual bridging and theoretical integration. Like *Novac*, *ComQuaCC* dealt with modeling and predicting atmospheric phenomena, but it focused on fundamental rather than applied issues: The driving force of interdisciplinary collaboration was the desire to improve the scientific understanding of atmospheric aerosols. While one consortium partner was specialized in applied issues, the interdisciplinary novelty – and challenge – was collaboration between two theoretically oriented research teams, one in chemistry and the other one in physics. At the center of this collaboration was search for theoretical links between systems of different spatio-temporal scales by using a computational approach. The specific research questions and computational objectives of different parties did not coincide as such, but were targeted to advance the construction of a shared modeling framework.

Conceptual-bridging was an important epistemic goal for the applied mathematicians in *CSI Speech*, too. While the overall goals of the project were directed toward applications of computerized inversion to spoken language, the motivation of mathematicians for such interdisciplinary work was based on the desire to generalize. In this project, abstract mathematical concepts were effectively implemented in new areas, which broadened the sphere of their application. The potential of generalization across specific problem areas was an important driver for interdisciplinary collaboration for the part of mathematicians and other method developers in all projects.

Purely theoretical incentives for interdisciplinary collaboration may not lead to optimal performance, however, since the collaboration may remain loose. In *ComQuaCC*, for example, despite related theoretical interests and regular bi-monthly research seminars, only few actual points of collaboration were established between the chemists and physicists, and few co-authored papers were produced by them (see Section 1.4). Interviews with the project leaders suggest that the institutional environment (mainly funding) may be more difficult for this kind of interdisciplinary basic research than for either interdisciplinary problem-solving or (mono)disciplinary basic research.

Exploration

In addition to providing new *solutions* to problems in many substance fields, as well as a means of bridging disciplinary *concepts*, computational science serves the *exploration* of unknown scientific territory. Its capacity to process complex data, create order to big data sets, and operate with virtual experiments makes it a powerful asset for such exploration. While all the four projects under closer scrutiny took advantage of this asset to some extent, *BrIAn* is a good example of interdisciplinary research organized around scientific exploration. At the center of interdisciplinary collaboration was complex brain imaging data, which contained new evidence of brain functions in specific situations. Part of the project funding was invested in creating laboratory infrastructure for neuroscientific experiments, which were designed for the production of data for computational analysis. The interdisciplinary innovation of this project was not so much in the identification of new problems or developing new theories or models than in the analysis of novel data, which enabled new insight on brain connectivity. The interaction between the consortium partners was organized around this aspect.

When taken as a principal goal of interdisciplinary research, exploration requires high expectation of scientific advancement, including state-of-the-art knowledge, methods and equipment. These conditions seemed to be present in *BrIAn*. However, investment in new areas of research is also risky. Given the temporary nature of LASTU funding, building new laboratory infrastructure in *BrIAn* did not completely pay off – as yet. After successful experiments, all interesting data could not be analyzed in the course of the remaining funding period.

Besides containing the risk of new investments, interdisciplinary exploration brings a fundamental cognitive challenge of recognizing relevant phenomena without knowing what exactly to look for. While machine learning is often deemed relatively independent of the problem areas to which it is applied, interdisciplinary exploration seems to require an overlapping problem space. This was, indeed, a critical aspect of *BrIAn*. Despite the general neuroscientific competence of the data analysis team, they did not necessarily know at the outset which features of the data were most interesting to neuroscientists.

Experiences of the four projects reveal that the implementation of interdisciplinary collaboration is rarely fully predictable in terms of any particular goal. Attempts to problem solving may end up with new problem formulation, for example, and theoretically oriented work may produce unexpected constructions. Exploration, by definition, confronts unknown phenomena. Essential features of interdisciplinary collaboration are thus balancing between intended goals and emerging findings, between interdisciplinary ambitions and their actual realization, etc. According to all interviewees, interdisciplinary research turned out to be more time-consuming than expected. The four-year funding period was considered too short for most projects. While this is the case in all research projects to some extent, interdisciplinary or not, interdisciplinarity brings about further delays due to the many

challenges pertaining to cognitive, cultural, and institutional boundaries between established disciplines.

1.2. Outcomes of interdisciplinarity

The diversity of publications

One way to evaluate the outcomes of interdisciplinary research is to look at the disciplinary diversity of publications produced by the research projects. In the present evaluation, the publication profile of the seven research projects funded through the first call of applications (2009) was examined. The disciplinary diversity of publications was measured by Shannon entropy[13], which is calculated on the basis of two indicators: variety and balance. 'Variety' refers to the number of disciplinary categories represented by the journals[14] (according to the *Scopus* journal classification system[15]) in which the project's results are published. 'Balance' reflects how evenly the papers are distributed across those categories. The results of this analysis are summarized in Table 3.4 and illustrated in more detail in Figures 1.4-1 and 1.4-2.

Table 3.4. The number, disciplinary variety, disciplinary diversity, and interdisciplinary co-authoring of scientific publications (papers in peer-reviewed journals and conference proceedings) reported by the projects funded through the LASTU 2009 call. Interdisciplinary co-authoring refers to the share of publications that involve authors from at least two different research teams of the consortium.

Project	Number of publications	Disciplinary variety of publications	Disciplinary diversity of publications	Interdisciplinary co-authoring of publications
BrIAn	11	7	1,7	18 %
ComQuaCC	50	11	1,8	10 %
CSI Speech	85	13	2,1	20 %
eVLBI+GEO	30	3	0,9 *	10 %
MUMO	21	10	2,0	0 %
Novac	24	9	1,9	71 %
SimITER	106	8	1,3	20 %
The projects as a whole	*327*	*21*	*2,5*	*20 %*

* Only 7 out of 30 publications could be classified; 23 publications reported by the project were not included in any of the available databases (*Scopus, Web of Science, Publication Forum Classification*).

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[13] $-\sum_i p_i \ln p_i$, where p_i is the proportion of papers in disciplinary category *i*.

[14] Many journals are associated with more than one disciplinary category. I took all those categories into account when calculating the disciplinary diversity of publications. As a result, the sum of the disciplinary categories of the publications equals more than 100% of the number of publications for each project. This is a common practice in measuring interdisciplinarity; see e.g. Porter et al. 2007.

[15] In case a journal or a proceeding was not included in the *Scopus* database, disciplinary categories were checked from the *Publication Forum Classification* that operates within the Federation of Finnish Learned Societies.

Alltogether, the publications of the seven consortia distribute across 21 out of 27 disciplinary categories listed in the *Scopus* journal database (see Figure 1.4-1). The disciplinary diversity of publications was highest in *CSI Speech* and *MUMO* consortia, and relatively high also in *Novac*, *ComQuaCC* and *BrIAn*. In *SimITER* and *eVLBI+GEO*, the diversity of publications was notably lower. The measure of diversity used here, however, does not take into account 'disparity', i.e. cognitive distance among disciplinary categories, which is a crucial aspect of disciplinary diversity[16] yet require more complex calculations than was possible to make for this evaluation. A qualitative assessment of disciplinary disparity[17] in different consortia suggests that there are obvious differences between the consortia in this respect. In *MUMO*, for example, disparity is much lower than in *CSI Speech*: While publications from *MUMO* distribute across natural sciences and engineering, and mostly among neighboring fields – chemical engineering, chemistry, and engineering – publications from *CSI Speech* distribute across a broader range of disciplines in natural sciences, engineering, humanities and social sciences. These and other similar differences are visible in Figure 1.4-2.

Figure 1.4-1. The disciplinary distribution of all scientific publications reported by the seven projects funded through the LASTU 2009 call.

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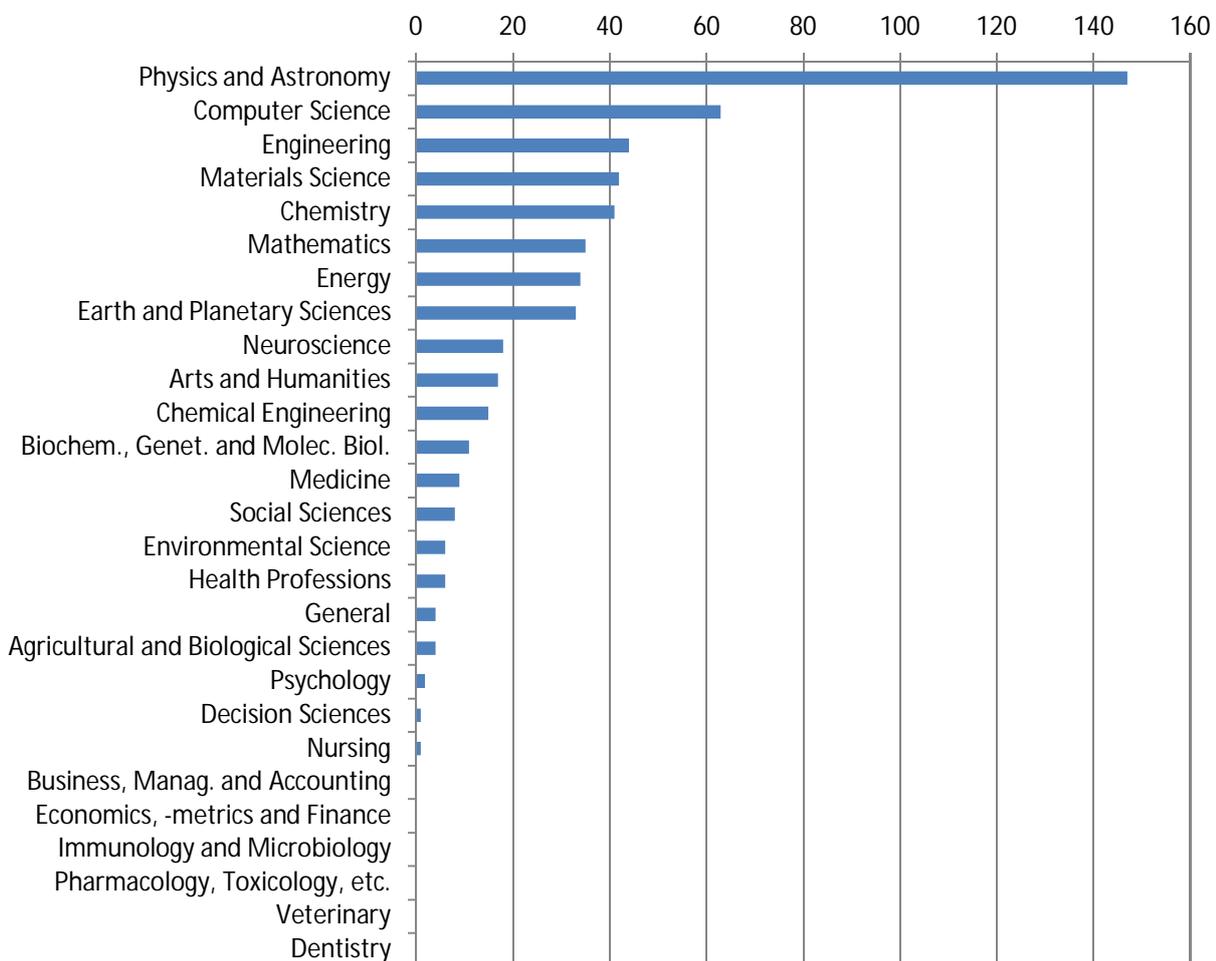
[16] See Rafols et al. 2012.
[17] A qualitative equivalent of 'disparity' is the 'scope' of interdisciplinarity; see Huutoniemi et al. 2010.

Figure 1.4-2. The disciplinary distribution of scientific publications reported by each of the seven projects funded through the LASTU 2009 call. The list of disciplinary categories contains all the 27 categories used in Scopus journal database.
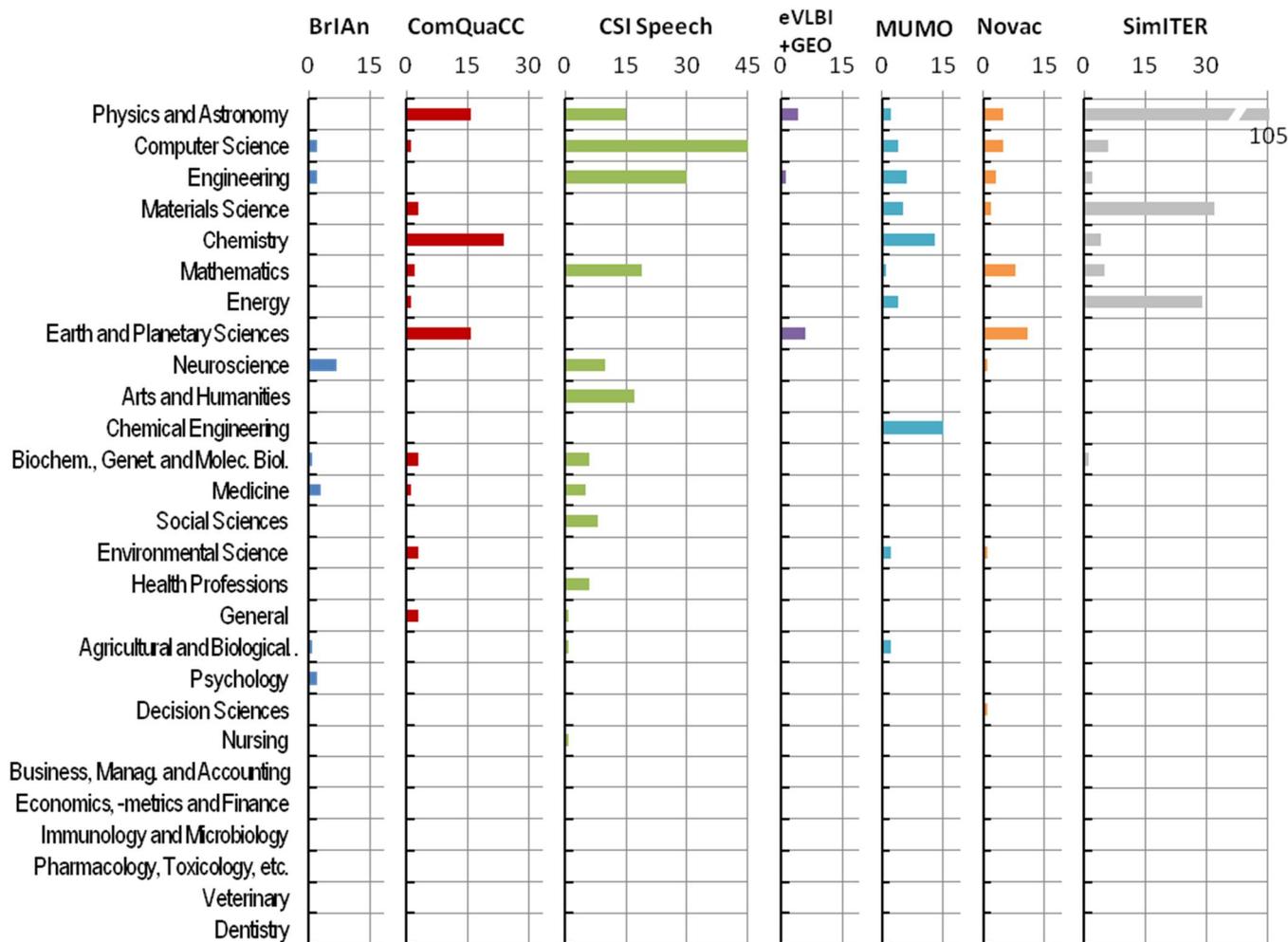
Interdisciplinary co-authoring

Interdisciplinarity is not only about disciplinary *diversity*, but also about making *connections* between the various bodies of knowledge drawn upon. The outcomes of interdisciplinarity in this respect were evaluated by looking at the degree of co-authoring between the consortium partners.

Interdisciplinary co-authoring was relatively low in all projects except *Novac* (see Table 3.4). On average, every fifth paper reported by the projects involved authors from at least two different research teams of the consortium (other kinds of interdisciplinary co-authoring were not evaluated). This is somewhat surprising, given that most consortia were built on previous collaborations. On the other hand, many publications reported by the projects were not solely the result of LASTU but relate to the work of the researchers more broadly. At the same time, some of the most important papers resulting from the interdisciplinary research done in LASTU were still in the pipeline, as such papers typically take longer than intra-team publications due to the many challenges involved – not least the differences in publication cultures (see Section 1.3).

Impacts on research capabilities

The potential impacts of the projects' interdisciplinarity were mapped in the questionnaire to project leaders. A large majority of respondents (n=27-30) noted that interdisciplinarity had either very important or somewhat important impact on their *professional capabilities as researchers*; on *researcher training*; and on *partnerships and networking* (see Figure 1.4-3). Frequently mentioned impacts on professional capabilities were the new things the respondents had learned from other fields, but also the 'enforcement to go outside the comfort zone' and the increased ability to communicate across disciplinary divides. Researcher training was reported to benefit from interdisciplinarity by exposing young researchers to a broader or complementary view of their research topic, and providing doctoral students, post docs and visiting scholars a better learning environment. Two respondents expressed also critical views on the impact of interdisciplinarity on researcher training; it was considered to be difficult, if not too demanding. The impacts of interdisciplinarity on partnerships and networking with other researchers or organizations, including international networking, were considered at least of some importance by all (n=30) respondents.

Figure 1.4-3. The distribution of responses to the question: 'Please assess the impacts of the project's interdisciplinarity on the following areas both verbally (what kind of difference did interdisciplinarity make?) and numerically (how important was the given impact?). Use a scale 1-3 (1=very important, 2=somewhat important, 3=not important) for the numerical assessment. If the given area was outside of the project's activities, leave the item empty.' N=30.
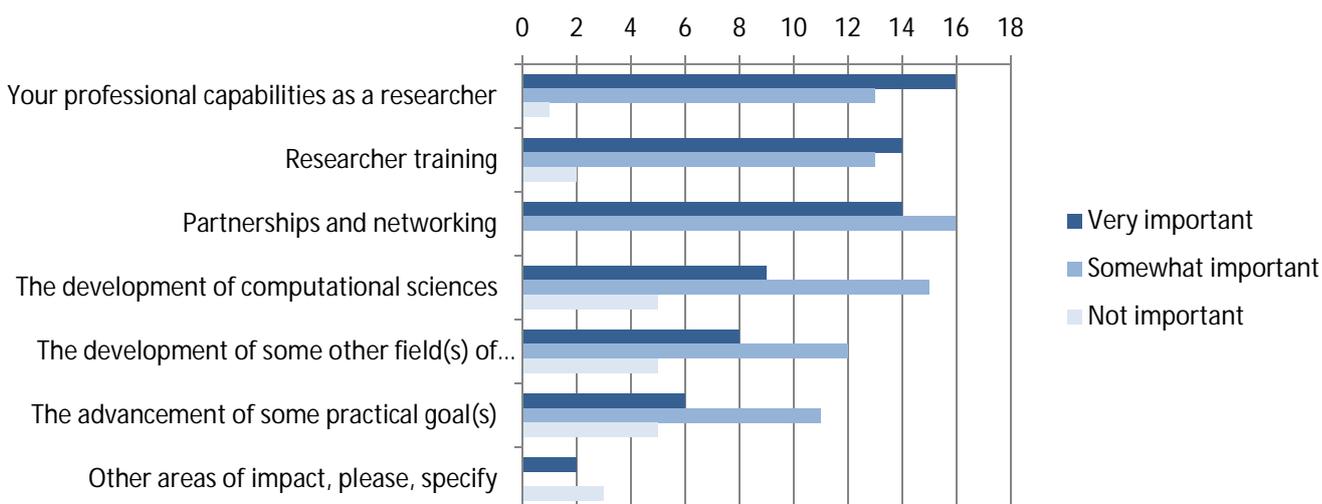
Somewhat more modest estimates were given about the impacts of interdisciplinarity on the *development of computational sciences,* as well as on the *development of some other field(s) of science.* Even so, many project leaders considered especially the former impacts as essential (n=9), and one respondent stated that 'interdisciplinarity is nearly mandatory to make real progress in computational science'. Developments in computational science were reported to result from using computational methods in new contexts and disseminating the state-of-the-art to other fields. Developments in other fields of science resulted from similar influences. The application of computational methods to specific fields was often perceived to advance the target field as well – this was the case, for example, in forest science, neuroscience, physics, materials science, and speech research. Evidence of such impacts is visible in the distribution of the projects' publications across these and other disciplinary categories (see the previous sub-section).

On the other hand, interdisciplinarity was perceived as *not important* to the development of science (either computational or other) by some respondents (n=5 in both cases). Moreover, the experiences reported in the open-ended question of impacts suggest that some of the positive influences did not result from interdisciplinarity per se. The LASTU program helped computational chemistry, for example, to strengthen its internal coherence and achieve some critical mass to sustain its existence. In this case, LASTU may have supported discipline formation rather than interdisciplinarity.

Given the complex nature of knowledge production, however, it is often impossible to distinguish the impacts of interdisciplinarity from other influences. This became evident in many interviews with project leaders. New insights into the ferroelectricity of ice in *ComQuaCC*, for example, would not have arisen without the collaboration of chemists with aerosol physicists around water molecules, even if the issue was outside the focus of collaboration. On the other hand, some of the developments in atmospheric modeling in the same project could have emerged even without the specific interdisciplinary consortium established in LASTU. Another difficulty in evaluating the impacts of interdisciplinarity is the slow pace at which new connections between research fields pay off. The emphasis the interviewees and survey respondents put on interdisciplinary learning and capacity building suggests that some of the most important impacts of interdisciplinary research cannot be captured by quantitative performance measurement.

One of the systemic effects of interdisciplinarity on scientific development can be the higher flexibility of academic labor markets and thus of academic career, which was experienced by some project leaders as more job opportunities for their students or easier access to different research institutes. In this respect, the LASTU program can be credited with lowering disciplinary boundaries in the domain of computational science in Finland. As explained by an interviewee, computational approach enables the operation of knowledge production in a 'virtual laboratory', independent of the physical laboratories of disciplinary science. He considered this a huge advancement of science in general and acknowledged the LASTU program for contributing to this goal. Another interviewee, however, was critical of the program because of such ambitions. He regarded 'computational sciences' as an artificial construction created for advancing a certain scientific agenda, rather than being a coherent research field. These contradictory opinions do not disregard, however, the observation that computational approaches are influencing the system of science at large, and in doing so, blurring the boundaries between established disciplines.

Impacts on utilization of knowledge
In addition to various scientific impacts, interdisciplinarity had a positive impact on the utilization of research-based knowledge in the advancement of technology, health, decision making, or other areas outside of science. More than half of the respondents perceived the impact of interdisciplinarity on the implementation of research findings into practice as either as very important or somewhat important (see Figure 1.4-3). Interdisciplinarity was reported to lead, for example, to 'a practical application that saves hugely researcher time in the future [as] trial-and-error is replaced with a universal algorithm'. Other examples of the advancement of practical goals were the development of new tools for speech therapists; the development of new simulation software for predicting the effects of environmental factors on tree growth; and the development of new ideas for solar cell material screening.

One the other hand, some respondents considered the impacts of interdisciplinarity on knowledge utilization unclear or unimportant. Both interviews and survey responses reveal that interdisciplinarity did not always go hand-in-hand with the advancement of practical goals. Investments in conceptual bridging or exploration, for example, sometimes required that research teams shift attention away from topics that are most attractive to the public or more likely to become commercialized in the near future. Even interdisciplinary problem solving sometimes meant that practical impacts were delayed, due to e.g. the 'disruptive' nature of suggested solutions. *CSI Speech*, for example, invented a new device for speech therapists, but faced difficulties in commercializing the device because it was not profitable enough in the eyes of potential funders.

Few respondents recognized other areas impacted by interdisciplinarity. One project leader reported a positive impact on public awareness: The application of computational science to a new field had aroused the interest of public media and helped bringing science to general audiences – even to children via school books.

3.5. Conclusions

In the LASTU program, interdisciplinarity seemed to be a norm rather than an exception. This is not surprising, given the 'inherently' interdisciplinary nature of computational sciences: in this domain, the boundaries between disciplines are less substantial than in some other contexts. For example, many researchers perceived themselves as both *developers* and *users* of computational methods, and new professional identities were created around specialized computational approaches, such as computational neuroscience, computational chemistry, climate modeling etc. The LASTU program has substantially contributed to the problem-driven, interdisciplinary development of the domain.

The instrumental goal of interdisciplinarity in the program, i.e. to facilitate interaction and exchange between algorithm and methods development, on the one hand, and 'substance sciences', on the other hand, has been largely achieved. The funded research projects have successfully applied computational methods to understanding and solving complex problems in various domains of science and society, including domains that have not as yet fully exploited the advanced computing capabilities. Interdisciplinary collaboration in a majority of research projects was not entirely new, however. All project leaders who responded to the questionnaire, except only one, have also continued the interdisciplinary collaboration established in the LASTU program.

Besides the 'vertical' integration of methods and substance fields, the program has also facilitated interaction in a 'horizontal' direction, i.e. between fields that have traditionally operated within their own experimental and theoretical settings. Working in a 'virtual laboratory', afforded by computational methods and equipment, has enabled new convergences between, for instance, physics and chemistry, chemistry and biology, and mathematics and electromagnetics. This development, however, is more difficult to evaluate due to its slow pace and systemic nature.

This said, the data gathered within this evaluation suggest that computational methods have strong interdisciplinary potential also for unifying science in a horizontal direction. In this respect, the LASTU program represents a modest effort. The interdisciplinary scope of most projects was relatively narrow, covering research fields that interact with each other on a more or less regular basis. Moreover,

while computational methods are becoming more frequent in the social sciences and humanities, too, these domains were less represented in the program. A few projects did cover humanities issues, such as the human aspects of cognition, language, speech or health, but especially the involvement of social sciences was low. In the future, stronger links with computational social science would enhance the potential of computational approach to unify science and take the whole scientific enterprise a step forward.

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