D2.2 - First Transnational Access summary report

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ABSTRACT:

This document is the first report on the HPC-Europa3 Transnational Access activity. It covers the first reporting period (Months 1-18, i.e. 1 May 2017 – 31 October 2018). In this report, we provide statistics relating to the number of applications received, users who were given access, and computing time used. There is also information about the outreach and dissemination activities, selection procedure, and the first HPC-Europa3 users' group meeting, the Transnational Access Meeting (TAM 2018).

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Executive summary

HPC-Europa3's Transnational Access programme offers researchers in Europe, working in any field of computational science, the opportunity to collaborate with a researcher working in a similar field in a participating country, while gaining access to some of the most powerful High Performance Computing (HPC) facilities in Europe.

Over its 4-year lifetime, HPC-Europa3 aims to support more than 1200 research visits, and provide more than 90 million CPU hours of access.

This document is the first report on the HPC-Europa3 Transnational Access activity. It covers the first reporting period (Months 1-18, i.e. 1 May 2017 – 31 October 2018). In this report, we provide statistics relating to the number of applications received, users who were given access, and computing time used. There is also information about the outreach and dissemination activities, selection procedure, and the first HPC-Europa3 users' group meeting, the Transnational Access Meeting (TAM 2018).

1 Introduction

HPC-Europa3 is an EC-funded pan-European consortium of 10 High Performance Computing (HPC) centres and centres of excellence.

The central activity of HPC-Europa3 is the Transnational Access research visit programme, which is supported by the associated Networking Activities and Joint Research Activities. The programme funds collaborative research visits of up to 3 months' duration for computational scientists working in any discipline which can benefit from access to some of the most powerful computing facilities in Europe.

Nine of the ten consortium partners participate in the Transnational Access activity:

- Cineca (Bologna, Italy)
- EPCC (Edinburgh, UK)
- BSC (Barcelona, Spain)
- HLRS (Stuttgart, Germany)
- SURFsara (Amsterdam, the Netherlands)
- CSC (Helsinki, Finland)
- GRNET (Athens, Greece)
- KTH-PDC (Stockholm, Sweden)
- ICHEC (Dublin, Ireland)

Visits can be made to any research group in any of the countries in which the Transnational Access partners are based, with the exception of research groups within the same country where the visitor is currently working.

The programme is open to researchers of any level, from postgraduate to full professor, from research groups in the EU countries and Associated States. A small amount of the access is also available for researchers from outside Europe.

Visitors should be motivated by two factors:

- A need for access to some of Europe's most powerful HPC systems to improve their research activities;
- An identified likelihood of a successful collaboration – either via the forging of new collaborative links, or via the strengthening of one which already exists between the researchers involved or members of their groups.

During their visits, researchers and hosts are encouraged to work closely together, with the visitor integrated as closely as possible into the host research group. Meanwhile, the relevant HPC centre provides access to HPC resources, as well as consultancy and support to help the visitors make the most efficient use of these resources.

This report gives an overview of the organisation of the Transnational Access programme, and provides statistics on the applications received and visits carried out during the first 18 months of the programme.

The sections of the report are organised based on the timeline of an application, starting with outreach and publicity and then the application and selection process, then looking at application and visitor statistics, before moving to visit feedback, an overview of some initial project successes, and the first user group meeting, which is due to be held at the end of the reporting period.

2 Outreach and publicity

HPC-Europa3 Calls for Applications are issued 4 times per year, in February, May, September and November. The reason for choosing these dates (rather than having each closing date 3 months after the last) is based on previous experience and takes into account various factors such as avoiding having closing dates at problematic times (e.g. a closing date at the end of August typically results in many requests for late submission from people returning from holidays at the start of September), as well as ensuring decisions can be sent to applicants by important dates in the calendar (e.g. the November closing date must be early enough for the selection process to be complete and applicants informed of the decisions before the Christmas holidays begin, and similarly with the May closing date and the summer holiday period).

Outreach and publicity for the programme is co-ordinated by a Communication and Marketing Team, led by UEDIN and including members from each partner centre. All partners are expected to play an active role in publicising the programme, including CNRS, which is the only partner which does not offer Transnational Access.

The team aims to publicise the programme to the highest number of relevant research groups in all of the 44 eligible countries[1]. An online meeting is held approximately 10-12 weeks before each closing date in order to review activities undertaken in the previous period and plan actions to publicise the upcoming closing date. It should be emphasised, however, that publicity for the programme is an ongoing effort which carries on during all stages of the call cycle.

Deliverable 2.1, Marketing Plan[2] describes the actions planned to publicise the programme, both to potential visitors and to potential hosts. The rest of this section describes what has been done so far.

2.1 Webpage and other marketing materials

The most important source of information for applicants is the webpage, which can be found at http://www.hpc-europa.org.

This contains all the information about the programme. It also contains the secure online portal for applicants, hosts, reviewers, and HPC-Europa3 consortium members, with each category of user having a different view when they log in.

- **Applicants** can fill in an application, download their decision letter, fill in their visit questionnaire, and upload their final reports and details of any resulting publications;
- **Hosts** can view the applications assigned to them for review and complete the associated evaluations, and fill in their questionnaire at the end of each visit;
- **Scientific Users Selection Panel members** can view the applications assigned to them for review, along with the associated documents, and submit their reviews;
- **HPC-Europa3 partners** can view applications to their centre, log information relating to visits (e.g. visit dates and computing time used), and monitor the status of their visitors' final paperwork.

The webpage was put together quickly at the start of the programme in order for all the necessary information to be available for the first Call for Applications; however, a full revision of both the content and the structure is currently underway, and an improved version of the website will be available within the next couple of months.

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[1] All 28 EU member countries plus Albania, Armenia, Bosnia-Herzegovina, Faroe Islands, Georgia, Iceland, Israel, FYR Macedonia, Moldova, Montenegro, Norway, Serbia, Switzerland, Tunisia, Turkey and Ukraine.
[2] https://b2drop.eudat.eu/s/jQuMD1KUOUpH6FM

Other marketing material has been publicised for distribution at events such as conferences, workshops and courses. This material is also available for download so that anyone can print their own copies – for example, a former visitor attending an event might want to take some promotional material with them to help publicise the programme.

- Flyer: https://b2drop.eudat.eu/s/2wW7piZrwLLkP3j
- Poster: https://b2drop.eudat.eu/s/3rZ7NKPeQ4o2yk5
- Pull-up: https://b2drop.eudat.eu/s/MG5mCSedDH7LrHY

A two-slide PowerPoint presentation has been created, giving an overview of the programme and how to apply. This can be incorporated into any presentation given to an audience which might include potential applicants, for example at a conference or during a course.

The first HPC-Europa3 newsletters were published in July and October 2018, and these will continue to be produced quarterly throughout the project. These were distributed to the subscription email list (which currently has more than 1900 subscribers), and are also available to download from the website, at http://www.hpc-europa.eu/public-documents. The link to each newsletter has also been publicised via social media.

The first newsletter contained an overview of the programme, a visitor success story, testimonials from some recent visitors, a focus on GRNET, and an overview of the NOMAD Centre of Excellence, with whom HPC-Europa has signed a Memorandum of Understanding which includes mutual project publicity as an objective.

With the first HPC-Europa3 SME workshop due to take place in November, the second newsletter focuses on how HPC-Europa3 can benefit SMEs. It includes a success story from a visitor who was hosted by an SME. HLRS, as the co-ordinator of the SME workshop, is the featured partner centre, while the external collaborative partner described is ETP4HPC, which is of relevance to SMEs as its membership includes European technology vendors.

For the first Transnational Access Meeting (TAM 2018) – see section 7 of this report – a water bottle with the HPC-Europa3 logo was produced as a promotional giveaway. It is hoped that this reaches the same level of popularity and ongoing use as the mugs produced under the first HPC-Europa programme (2004-2007), as more than a decade later people still ask if any more of those are still available.

2.2   Social media

The following social media accounts have been set up:

- **Twitter:** https://twitter.com/HPCEuropa3
    - To date we have issued 180 tweets and have 244 followers.
    - The account is used for announcements about closing dates, new visits starting, success stories from visitors, and other relevant project news. Each tweet about a new visit "mentions" the visitor, their home research group and/or institute, the host, and the host's research group and/or institute, where these Twitter accounts exist. Often these are retweeted from these accounts, leading us to reach new followers from outside our existing network.
- **Facebook:** https://www.facebook.com/hpceuropa/
    - The Facebook account is also used for these project announcements and currently has 109 followers.
- **LinkedIn:** https://www.linkedin.com/company/29022707/
    - This account has been set up more recently and has so far only been used to announce Calls for Applications. We are at an early stage of engagement with LinkedIn and are still investigating ways to exploit this environment more fully, including the possible use of LinkedIn Campaigns to publicise closing dates.
- **YouTube channel:**
  https://www.youtube.com/channel/UC9uOpFQGP9V0TQPXFUOgs_A/playlists
    - This channel has only recently been set up and only one video has been uploaded onto it so far. This is one of a series of videos which have already been made, featuring visitors telling us a little about themselves and the work they will be doing during their visit. More videos have been recorded but need some post-production work before being uploaded – for example, some visitors spoke in their native language and subtitles need to be applied.
    - The channel also includes a playlist with links to videos about HPC-Europa from other sources (e.g. webinars about the programme broadcast by partners at UEDIN and CSC, and an overview video from HPC-Europa2, which is still mostly relevant).
- **Webinars:** As mentioned above, the YouTube channel contains links to two webinars which were broadcast by project partners. In addition to offering attendees at the live webinars the opportunity to ask questions, the archived versions have achieved considerable impact (the EPCC ARCHER webinar has been viewed more than 300 times), but were quick and easy to record. We will continue to promote these and consider creating updated versions as the project progresses.
- **Blogs:** Visitors are encouraged to write blogs about their visits and these will be incorporated into the revised HPC-Europa3 website. Some examples can be found among the guest blogs on the EPCC blog site: https://www.epcc.ed.ac.uk/blogs/guest

2.3 *Methods of publicising the programming*

As mentioned above, the programme is publicised online via the HPC-Europa3 website and websites of partner centres and associated organisations, e.g. PRACE[3], as well as via social media and electronic newsletters.

The Call for Applications is also distributed electronically to all relevant contacts, always keeping in mind the data protection principles of the GDPR. This includes research councils, scientific networks, and individual researchers (e.g. colleagues, former visitors, host researchers).

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[3] www.prace-ri.eu

Face-to-face contact is also a very important way of publicising the programme, with both HPC-Europa partners and former visitors having a vital role to play here. Word of mouth has always been one of the most effective ways of publicising the programme, and as the number of past visitors increases, we should see an exponential increase in the number of people who hear about the programme in this way. Project partners look out for relevant events which their colleagues will be attending and ask them to publicise the programme in whichever way they can, whether by displaying a poster or pull-up, handing out flyers, incorporating the 2-page PowerPoint overview of the programme into their presentation, or simply mentioning the programme to potential applicants. We ask our visitors and hosts to help us in the same way.

2.4 Dissemination of project achievements

Now that visits have been taking place for nearly a year, we are beginning to have some project achievements and successes to publicise. These will be disseminated in various ways.

- The first project report directory, compiling all the project reports received so far, is currently in production; this will be distributed in electronic format to contributing authors and their hosts and other interested parties, and will be available to download from the HPC-Europa3 website; the reports will also be available via a searchable interface on the website;
- Project successes will be publicised via social media, and particularly successful projects will be featured in the HPC-Europa3 newsletters;
- All visitors attending the user group meeting, TAM (the Transnational Access Meeting), will present the work resulting from their visit as either a talk or a poster;
- Visitors are asked to include an official acknowledgement of HPC-Europa3 in journal publications and conference presentations.

Publicising the successful outcomes of HPC-Europa3 visits should have a powerful impact in terms of raising awareness of the programme and encouraging people to apply.

2.5 Reaching new user groups

In accordance with European Commission policy, HPC-Europa3 aims to give priority to researchers who have not previously used the infrastructures, and those who work in countries where no such research infrastructures exist.

Outreach and marketing activities are crucial in order to raise awareness of the programme among such research groups. However, the requirements and motivations of researchers from countries which lack significant HPC resources are often different from those who come from research groups which are part of well-established HPC user communities.

2.5.1 Regional Access Programme

The new Regional Access Programme within HPC-Europa3 already goes some way to addressing this, by giving priority to user groups in under-represented countries, focusing on two separate regions: the Baltic States[4], and South East European Countries[5]. Under this scheme, researchers from these two regions who have little or no previous HPC experience will be given priority when applying to GRNET in Greece and KTH-PDC in Sweden, where they will be able to gain access to smaller amounts of HPC resources on less powerful, although still significant, HPC resources.

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[4] Estonia, Latvia, Lithuania

[5] Albania, Armenia, Bosnia-Herzegovina, Bulgaria, Croatia, Cyprus, Georgia, Hungary, Israel, FYR of Macedonia, Moldova, Montenegro, Romania and Serbia

Drawing on the extensive networks of contacts which GRNET and KTH-PDC already have in these regions, we can reach researchers in these areas more effectively than we have done in the past. Further, by offering smaller allocations of time on less powerful machines, we hope to provide a vital stepping stone for inexperienced users to get started with HPC, and avoid the situation seen in the past where some applications from researchers in priority countries were turned down due to them requesting an insufficient amount of resources.

GRNET and KTH-PDC have embarked on a number of initiatives to publicise the "Regional Access Programme" to research groups in the target countries and encourage new users to apply via this initiative, which has a lower threshold for acceptance in terms of existing experience, and a broader view that the benefits to the applicant and their research group are greater than simply the scientific research output of the visit.

Although it is still early in the programme and the numbers are low, the initial results seem encouraging. Of 32 applications made from researchers working in the target countries for the Regional Access Programme, 9 were from researchers who did not have previous experience of access to similar HPC facilities, and 7 of these were accepted. Although this is in line with the general acceptance rate for HPC-Europa3 as a whole (see section 3 for more details), this is clearly a much higher rate of acceptance for this particular demographic than has been seen in previous programmes.

It is essential to identify emerging communities and new individuals and research groups who might be able to benefit from the programme, and this is an area where considerable effort must be invested in the coming months in order to boost application numbers. It is a time-consuming process, but must become a priority for the programme. The following methods will be employed:

- Partners will identify new contacts in their own countries, as well as in the countries assigned to them (usually on the basis of shared language or other pre-existing link), as detailed in D2.1 Marketing Plan;
- Visitors and hosts will be asked to provide a list of the leading European research groups in their fields;
- Operators of Tier-1 and Tier-2 facilities will be encouraged to publicise the programme to their users, some of whom may be ready to progress to larger platforms.

2.6   Where did applicants hear about HPC-Europa3?

The table below shows where our applicants heard about HPC-Europa3. The total numbers add up to more than the number of applications, as most visitors had heard about the programme from more than one source.
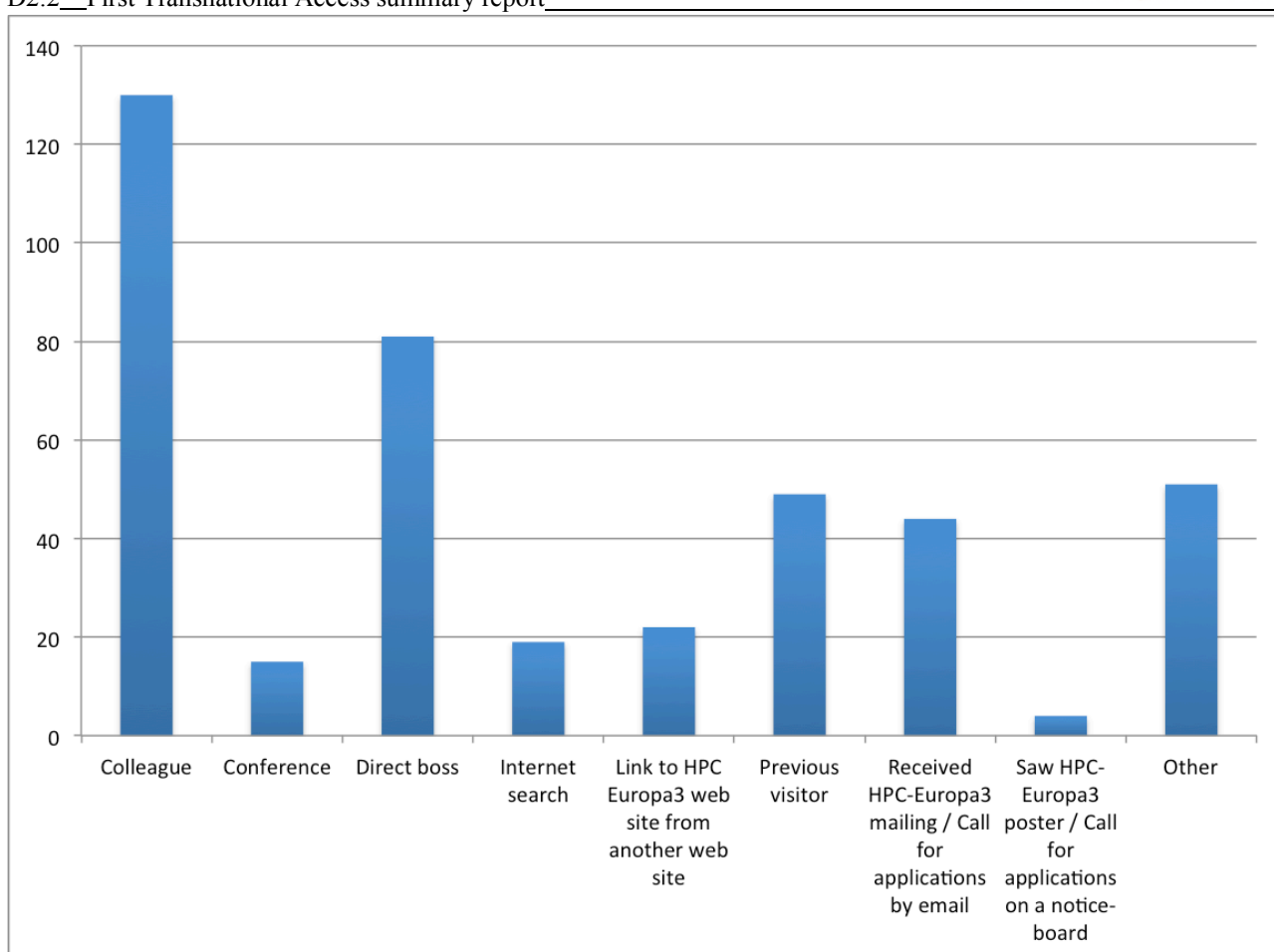
Figure 1: Where applicants heard about HPC-Europa3

3   Evaluation and Selection Process

The HPC-Europa3 selection process is based on the procedure used in the previous HPC-Europa programmes (2004-2012). This procedure was refined over the lifetime of those programmes, with the aim of giving all candidates a fair review, but at the same time keeping the review process reasonably lightweight.

3.1   Selection process for HPC-Europa3 applications

The evaluation and selection process is a two-stage procedure, each of which takes place over a period of approximately two weeks.

During the first stage, two independent evaluations are submitted:

- **Technical Evaluation Form** – carried out by a member of the HPC centre to which the application is made; this assesses the case made for requiring access to the HPC facilities at the centre, and comments on the suitability of the resources requested (both hardware and software). Evaluations are classed as **α** (accept), **β+** (probably accept), **β-** (probably reject) or **γ** (reject).
- **Host Evaluation Form** – carried out by the proposed host research collaborator (an expert in the domain); this comments on the scientific merit of the proposal and assesses the proposed

host's interest in collaborating with the visitor. Evaluations are defined as **very enthusiastic**, **enthusiastic**, **some interest** or **no interest**.

At the end of the first stage of the evaluation process, a Technical Evaluation Form and Host Support Form should have been submitted for each application.

The second stage of evaluation involves a further review of each application by two members of the Scientific Users Selection Panel (SUSP), who consider not only the information included in the application itself, but also the information provided in the Technical Evaluation Form and Host Support Form. SUSP reviews are classed as **α** (accept), **β+** (probably accept), **β-** (probably reject) or **γ** (reject).

Finally, the panel and consortium members come together for the selection meeting (SUSP meeting), at which the final decisions are taken.

To assist with this process and save time at the meeting, the online system automatically sorts the applications into 3 categories:

- **Fast-track accept** – all reviews are positive (Technical Evaluations and SUSP reviews are all either **α** or **β+**, Host Support Form is **very enthusiastic** or **enthusiastic**);
- **Fast-track reject** – all reviews are negative (Technical Evaluations and SUSP reviews are all either **β-** or **γ**, Host Support Form has only some interest, states no interest, or is missing altogether as no willing host has been identified);
- **To be discussed** – all applications with a mix of positive and negative evaluations, or for which any SUSP reviews are missing.

These lists are circulated before the meeting and each HPC-Europa3 partner is asked to check their own applications in case any applications on either of the fast-track lists should be discussed at the meeting – this might be an application on the fast-track accept list which should only be accepted if a certain condition is met, or an application on the fast-track reject list for which extra information has become available since the evaluations were submitted, for example.

The aim is to reach a final decision on every application by the end of the meeting. However, this is not always possible, for a variety of reasons, such as additional information being requested from either the applicant or the host, or a third SUSP review being carried out in the case where the two allocated SUSP reviewers did not manage to reach an agreement on the decision. Offers may be made unconditionally, or conditional on certain criteria, such as reduced or increased visit length, decreased request for HPC resources, or further information to be provided. Most rejected applicants are given a personalised explanation of why their application was unsuccessful, and if appropriate they are encouraged to reapply to the following closing date, with advice on which aspects of their application to improve and recommendations of any additional information which they should provide. The HPC-Europa team aims to communicate all decisions to applicants within 2 weeks of the meeting.

3.2 Closing dates and selection meetings in first reporting period

Five Calls for Applications were launched during this reporting period. Four of the corresponding selection meetings were held by online videoconference, with the final one held in person in Edinburgh, in conjunction with the first HPC-Europa3 user group meeting, TAM 2018 – the Transnational Access Meeting (see section 7).

There are three face-to-face meetings planned over the lifetime of the HPC-Europa3 project, each of which will be held in conjunction with one of the TAM user group events. This gives the selection panel members a valuable opportunity to meet the HPC-Europa3 team and other members of the

panel in person, as well as giving them the chance to see the outcomes of some of the visits which they have approved.

Call number	Closing date	Selection meeting	Type of meeting
1	07/09/2017	06/10/2017	Online videoconference
2	16/11/2017	12/12/2017	Online videoconference
3	28/02/2018	04/04/2018	Online videoconference
4	17/05/2018	18/06/2018	Online videoconference
5	13/09/2018	22/10/2018	Face-to-face meeting in Edinburgh in conjunction with TAM 2018.

Table 1: HPC-Europa3 closing dates and selection meetings, M1-18

3.3 Members of the Scientific Users Selection Panel

The HPC-Europa3 Scientific Users Selection Panel (SUSP) is currently composed of 22 members. However, in order to try to improve the match of reviewers' scientific backgrounds to the applications assigned to them, and also to spread the load of reviews more evenly, we are looking to increase the number of panel members for future calls. We have collated a list of possible new members and will be sending invitations to them following the selection meeting in October.

The current membership of the panel is given in Table 2.

Name	Institute	Country	Domain
Prof. Eduard Ayguadé	Department of Computer Architecture, UPC – BarcelonaTech	Spain	Informatics
Prof. Marco Bernasconi	Department of Materials Science, University of Milano-Bicocca	Italy	Physics
Prof. Stefano Borgani	Astronomical Observatory of Trieste, University of Trieste	Italy	Physics
Prof. dr. Ria Broer	Department of Theoretical Chemistry, Groningen University	The Netherlands	Chemistry
Prof. Andrea Cavalli	Department of Pharmacy and Biotechnology, University of Bologna	Italy	Chemistry
Dr. Mary Cryan	School of Informatics, University of Edinburgh	UK	Informatics
Dr. Zoe Cournia	Biomedical Research Foundation, Academy of Athens	Greece	Life Sciences
Dr. Berk Hess	ScilifeLab & KTH	Sweden	Life Sciences
Prof Karoliina Honkala	Department of Chemistry, University of Jyväskylä	Finland	Materials Science
Prof. Eleni Katragkou	Department of Meteorology and Climatology, Aristotle University of Thessaloniki	Greece	Earth Sciences
Dr. Timo Kiviniemi	Department of Applied Physics, Aalto University	Finland	Physics
Prof. Dr.-Ing. Eckart Laurien	Institute of Nuclear Technology and Energy Systems, University of Stuttgart	Germany	Engineering
Prof. Francisco Javier Luque	Faculty of Pharmacy, University of Barcelona	Spain	Chemistry
Dr. Carole Morrison	School of Chemistry, University of Edinburgh	UK	Chemistry
Prof. Dr. Wolfgang Nagel	Center of Information Services and High Performance Computing, TU-Dresden	Germany	Informatics
Dr. Zilvinas Rinkevicius	Theoretical Chemistry and Biology, KTH Royal Institute of Technology	Sweden	Chemistry
Prof. Kari Rummukainen	Department of Physics, University of Helsinki	Finland	Physics
Prof. Silvano Simula	Department of Mathematics and Physics, Roma Tre University	Italy	Physics
Prof. Dage Sundholm	Department of Chemistry, University of Helsinki	Finland	Chemistry
Dr. Prashant Valluri	School of Engineering, University of Edinburgh	UK	Engineering
Prof. dr. Jordi Vila	Department of Meteorology and Air Quality, Wageningen University	The Netherlands	Earth Sciences
Prof. Gustavo Yepes	Department of Theoretical Physics, Autonomous University of Madrid	Spain	Physics

Table 2: Membership of the Scientific Users Selection Panel (SUSP)

4 Application and Visit Statistics

4.1 Overview of applications received and approved in Months 1-18

During this first reporting period, there were 5 Calls for Applications, for which 266 applications were received in total.

Of these, 50 were received for the 5th call and will be reviewed at the selection meeting on 22nd October – after the date of writing this report.

Of the remaining 216 applications reviewed at the first 4 selection meetings, 166 were approved, giving an acceptance rate of 77%.

Due to the long period of time which had elapsed since the previous HPC-Europa programme had ended in December 2012, a considerable set-up period was necessary. Before the first call for applications was launched, the webpage and underlying applications database had to be set up from scratch, although the experience of the previous programmes certainly helped to inform the design of these. New partners needed considerable guidance in order to set up their local logistical and technical support, and with such a long gap between the programmes, there was also very little continuity of staff within the partner centres which had been part of HPC-Europa2. Further, a new selection panel had to be appointed.

The systems were put in place in time for the first call for applications to be launched towards the end of Month 2 (end of June 2017, just before the summer holiday period), with a closing date in Month 5 (September), allowing people time to complete their application form on their return from their holidays. The first selection meeting was therefore held in October (Month 6), and with the Christmas holiday period coming just two months later, most accepted applicants started their visits in January (Month 9) or later, with only 9 visits starting in 2017. Therefore, in Table 3: Applications per centre M1-18, the planned visits (M1-18) have been adjusted based on a linear allocation starting in M8 (December 2017), and covering a period of 41 months instead of 48.

However, despite this adjustment, it can be seen that the number of visits in M1-18 is well below the target number, even after adjusting for a 41-month period. Experience from previous projects suggests that application numbers always increase significantly over the lifetime of the project, in part due to the "word of mouth" effect which has always been a very significant factor in building awareness of the programme. As more people participate in the programme, they will inevitably tell others of their experiences, and the programme will naturally gain increased visibility. There will also be more results to publicise as more visitors take part, and this too will aid dissemination.

After a long period without an HPC-Europa programme running, there has been a natural loss of awareness of the programme – for example, an entire cohort of PhD students will have passed through Europe's universities without the opportunity to participate, and newer students will not have had peers who have taken part. Further, many people in our existing network of contacts had moved on since the last programme, and the GDPR has further implications in terms of sending unsolicited emails. All of these factors have contributed to a reduced impact of publicising the programme within existing networks, and due to the efforts required to set up a new programme being higher than anticipated, staff have not had as much available time as planned to identify new contacts.

With visits now having been taking place for almost a year, the processes are more fully embedded and centres know how to deal with most issues which arise. This should allow staff to dedicate more of their time in the coming year to a much more thorough and far-reaching publicity effort.

HPC-Europa3 centre	Applications received	Applications reviewed to date	Applications accepted	Acceptance rate[6]	Planned visits M1-48	Planned visits M1-18[7]	Visits started	Visits completed	Deviation from plan[8]	Average visit length (weeks)	Average requested visit length (weeks)
BSC	57	45	32	71%	210	56	28	24	-28	8.0	8.5
CINECA	30	22	17	77%	180	48	12	10	-36	6.4	7.1
CSC	18	15	16	106%[9]	190	51	16	16	-35	5.4	5.8
EPCC	73	54	34	63%	200	54	30	22	-24	8.0	9.0
GRNET	15	12	9	75%	40	11	5	4	-6	9.6	10.3
HLRS	25	25	21	84%	150	40	15	15	-25	8.0	8.0
ICHEC	5	5	4	80%	20	5	2	2	-3	7.0	7.0
KTH-PDC	22	19	16	84%	40	11	16	13	+5	6.6	7.8
SURFsara	21	19	17	89%	190	51	15	12	-36	8.1	8.8
Total	**266**	**216**	**166**	**77%**	**1220**	**327**	**141**	**120**	**-183**	**7.4**	**8.3**

Table 3: Applications per centre M1-18

The shortfall of visitors leaves a challenging reprofiling of visitors, for which the 6 centres with the most planned visits in particular will need to plan carefully, in terms of availability of computing resources as well as staff time to support more visitors at any given time.

HPC-Europa3 centre	Planned visits M1-48	Visits started	Visits remaining	Revised monthly target M19-48	Revised annual target M19-48
BSC	210	28	182	6.1	73
CINECA	180	12	168	5.6	67
CSC	190	16	174	5.8	70
EPCC	200	30	170	5.7	68
GRNET	40	5	35	1.2	14
HLRS	150	15	135	4.5	54
ICHEC	20	2	18	0.6	7.2
KTH-PDC	40	16	24	0.8	10
SURFsara	190	15	175	5.8	70
Total	**1220**	**139**	**1081**	**36.0**	**432**

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[6] Based on "Applications accepted" divided by "Applications reviewed to date"

[7] Based on linear allocation over 41 months (excluding the first 7 months for project set-up and first call / evaluation)

[8] Visits started minus planned visits M1-18

[9] Occasionally visitors are accepted for a host which was not their first choice, in a different country, making it possible for a centre to have an apparent acceptance rate >100%.

4.2 Access planned and delivered

The table below shows the access (i.e. computational resources) planned and delivered over the first reporting period. Figures are given in Allocation Units (AUs).

TA centre	Access planned (AU) – minimum quantity of access to be provided (M1-48)	Average quantity of access to be delivered per user (planned)	Total access delivered M1-18	Average access allocated per user-project M1-18[10]
BSC	8.400.000	40.000	1.179.514	49.146
CINECA	31.034.483	172.414	2.470.000	176.429
CSC	7.392.996	38.911	2.231.778	139.486
EPCC	27.027.027	135.135	1.714.009	57.133
GRNET	n/a	n/a	265.369	66.342
HLRS	4.213.483	28.090	78.764	5.251
ICHEC	1.503.759	75.188	10.810	5.405
KTH-PDC	4.000.000	100.000	1.236.840	95.142
SURFsara	9.500.000	50.000	416.537	37.867
Total	**93.071.748**	**76.288**	**9.603.621**	**75.619**

Table 4: Summary of access planned and access delivered, M1-18

This table shows that the amount of access delivered is significantly less than would be expected by M18 with linear allocation, even when profiled to take account of visits starting only in M8 of the programme. However, when comparing the average quantity of access planned per user at each centre to the average access actually allocated, it can be seen that most centres have provided close to their target average allocation per visitor.

However, CSC has provided more than 3.5 times the planned resources per visitor (in part due to one user making heavy use of GPUs, which are approximately 15 times more expensive in CPU time than normal cores. Meanwhile EPCC, HLRS, ICHEC and SURFsara have provided substantially less computing time per visitor than planned. In the case of HLRS and ICHEC this has partly been due to the HPC systems being unavailable for periods of time – where possible visits have been planned to take into account the downtime, although as upgrade timetables are prone to change, this has not always been possible.

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[10] Based on the number of users for whom access has been reported. Note that the final access allocated per visitor will be higher, as figures have been reported for visits which are still in progress, and visitors continue to have access to the HPC resources for up to 4 months after their visits are finished.

It should be noted, of course, that the final allocation per visitor will be higher than given here, as many of these users are still undertaking their visits or are within the period of time after their visit during which access to the machines is continued.

4.3 Applicant profiles

In this section we have analysed the applicants to the HPC-Europa3 programme with respect to:

- Country of research group
- Scientific discipline
- Demographic information (gender, age)
- Level of seniority

4.3.1 Country of Origin

Applications have been received from a wide variety of countries, including almost all of the EU member states, with the exception of Luxembourg and Malta, and 10 of the 16 Associated States. A further 18 applications were received from a total of 12 other countries.
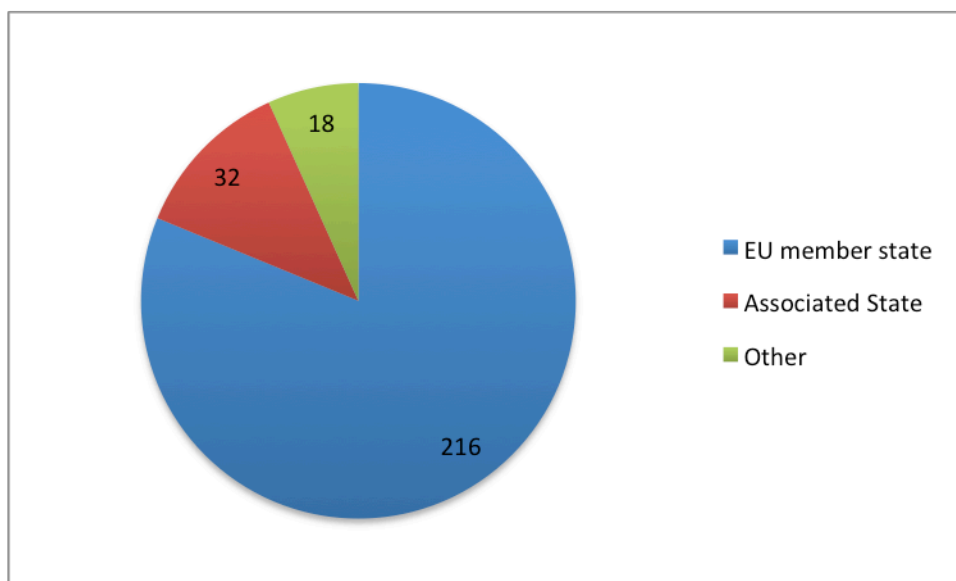

Figure 2: Country of home institute (applicants)

Table 5 gives a full breakdown of how many applications have originated from each country.

It is perhaps not surprising to see that the countries from which the most applications have been received are countries with large populations, where there is with a long tradition of using HPC within the research community at large, and a project partner with long experience of working in previous HPC-Europa programmes: the most applications have come from Spain (41), Italy (36), and the UK (28). Germany (17), France (12) and Greece (10) are all well represented, as too is Poland, the country with most applications which does not have an HPC-Europa partner.

Country (EU)	No. of applicants	Country (Associated State)	No. of applicants	Country (other)	No. of applicants
Austria	2	Albania	0	Argentina	1
Belgium	1	Armenia	3	Belarus	1
Bulgaria	2	Bosnia and Herzegovina	1	Cameroon	1
Croatia	3	Faroe Islands	0	India	1
Cyprus	1	Georgia	0	Iran	2
Czech Republic	6	Iceland	0	Kenya	1
Denmark	5	Israel	2	Korea	1
Estonia	1	Moldova	1	Morocco	2
Finland	6	Montenegro	0	New Zealand	1
France	12	Norway	2	Nigeria	2
Germany	17	Serbia	4	Russia	3
Greece	10	Switzerland	4	U.S.A.	2
Hungary	5	Macedonia (FYROM)	0		
Ireland	1	Tunisia	1		
Italy	36	Turkey	4		
Latvia	4	Ukraine	10		
Lithuania	3				
Luxembourg	0				
Malta	0				
Netherlands	9				
Poland	11				
Portugal	6				
Romania	2				
Slovakia	1				
Slovenia	1				
Spain	41				
Sweden	2				
United Kingdom	28				
TOTAL	**216**		**32**		**18**

Table 5: Country of home institute (applicants)

We can see that applications have been received from a total of 48 countries, which is encouraging, as it shows that the programme is known far beyond the borders of the countries of the HPC-Europa partner centres.

However, when it comes to the success rate of the applicants, there is a clear distinction between EU countries and non-EU countries, with the lowest rates of acceptance from Associated States.

For EU countries, the acceptance rate was 83% (146 approved out of 176 reviewed at the first 4 selection panel meetings), while for Associated States the acceptance rate was 48% (12 of 25 accepted) and for other countries it was 53% (8 of 15). This discrepancy may be due to a number of factors – it is likely that applicants within the EU are better informed about the purpose and pre-requisites of the programme, for example, and may be more experienced at putting together a research proposal, especially when this needs to be written in English. It may be that publicity towards researchers in Associated States needs to be better targeted, in order to identify the correct people, and they may need additional help to submit a successful application. This has been the rationale behind setting up the Regional Access Programme within HPC-Europa3, but many of the target

countries for that programme are newer members of the European Union. It is worth noting that the Associated States applicants who have been successful are, in the main, from wealthy countries with well-developed research facilities (Israel, Norway, Switzerland), as well as from Serbia and Ukraine.

4.3.2 Scientific discipline

While by far the largest number of applicants come from chemistry (71) or physics (58) – disciplines in which the use of HPC and of computational methods in general are well-established – there is a good spread across a wide range of disciplines, even including one application from the social sciences, as shown in Table 6.
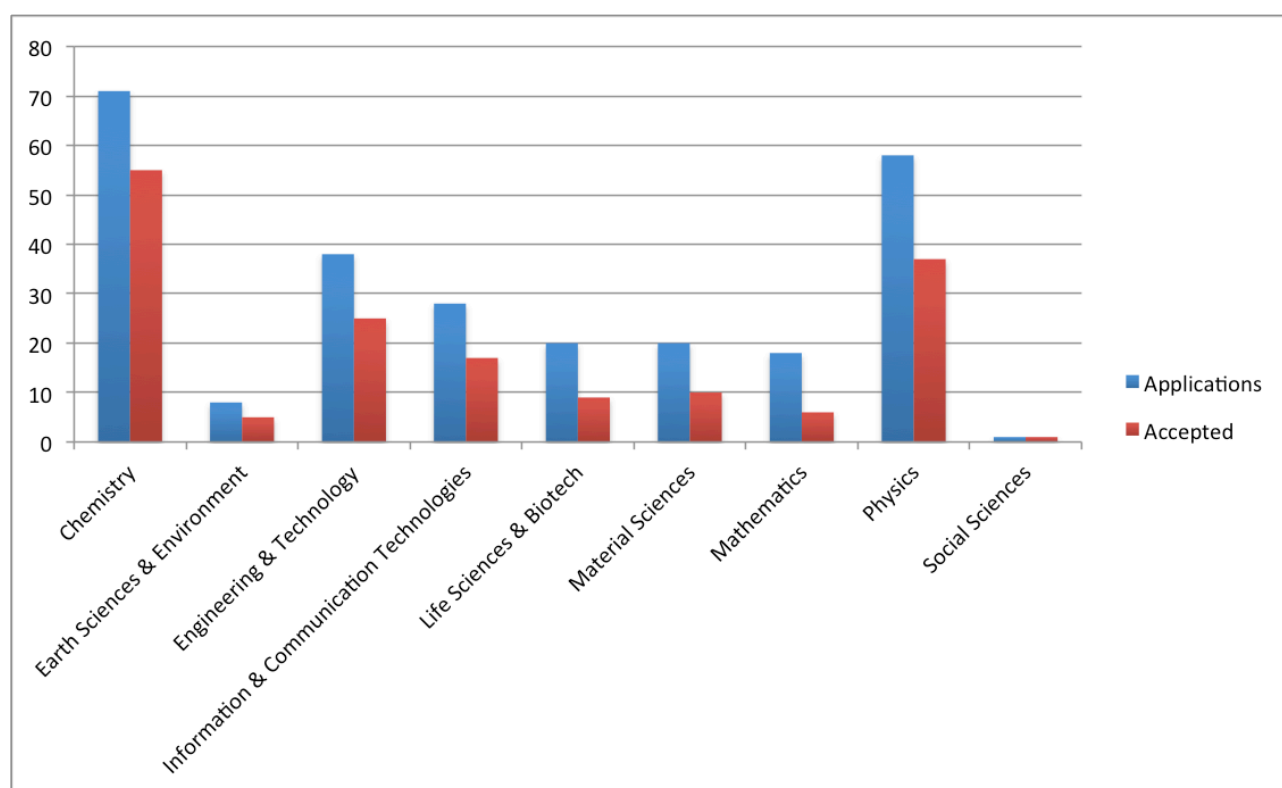

Table 6: Applicants and accepted applicants by discipline

4.3.3 Demographic information (gender, age)

In the first 18 months of the programme, female researchers have accounted for 23% of applications and 25% of those accepted. In previous programmes, the proportion of female participants was generally around 16-20%, so this is an encouraging sign that might indicate that females are engaging more with computational science. It is also good to see that there is not a major difference between the percentage of applications submitted and the percentage of applications accepted when it comes to gender. However, the overall numbers are small so the statistics may not be too significant at the moment. This is something which the consortium will monitor over the coming period.
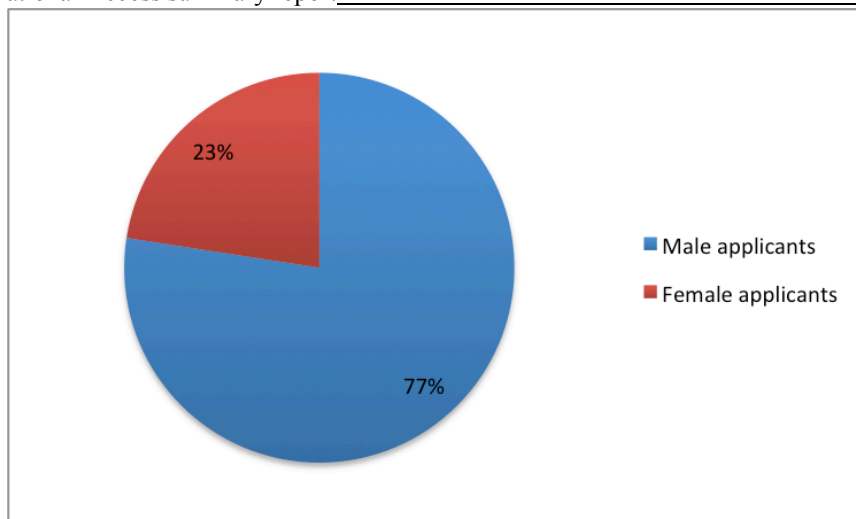
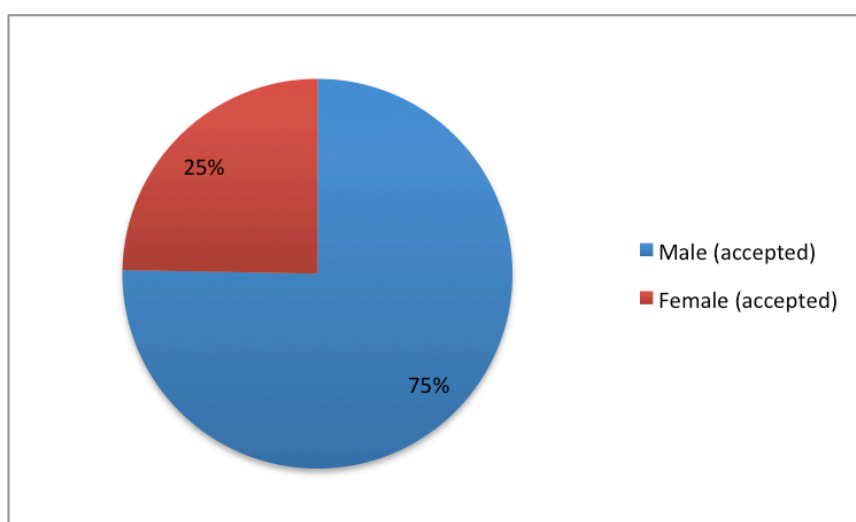**Figure 3: Applicants by gender**

Figure 4: Accepted applicants by gender

The programme attracts applicants of all ages, at all stages of their research career.

Applicants ranged in age from 23 to 68. The mean age was 35, the median age 33, and the mode 27. There was no statistical difference between applicants and those accepted in terms of age. The mean, median and mode ages all suggest that, as in the past, the "average" visitor is likely to be a senior post-graduate or post-doctorate researcher (see also 4.3.4 below). This is perhaps not surprising as these people are the most likely to have the flexibility to be able to spend some time abroad, without the complex work or family commitments of more senior researchers.

4.3.4 Level of seniority

Applications to the programme came from a roughly equal split of postgraduate students, post-doctorate researchers and experienced researchers, although the percentage of postgraduates was slightly higher than the others. This has been seen in previous programmes, and is likely to be due to the flexible working conditions of postgraduates, who have fewer teaching commitments than many senior researchers, and who are also less likely to have personal circumstances which make spending an extended period of time away from home difficult. A small percentage of applicants categorised

themselves as technician/researchers. There was also one application from an undergraduate – however this application was not approved by the selection panel. Undergraduates are not excluded from applying to the programme, but it is rare for them to be accepted, as they have little experience of independent research work, and their research is rarely at a level appropriate for publications in refereed scientific journals. However, some applicants class themselves as undergraduates when they hold a first degree and are working towards a research Master's qualification.

There was very little difference in terms of the percentage of applicants and percentage of those accepted when considering the level of seniority, as shown in the charts below. The undergraduate applicant has not been included here as 1/266 would be shown as 0%, and removing the undergraduate did not change the overall percentages for the other applicants.
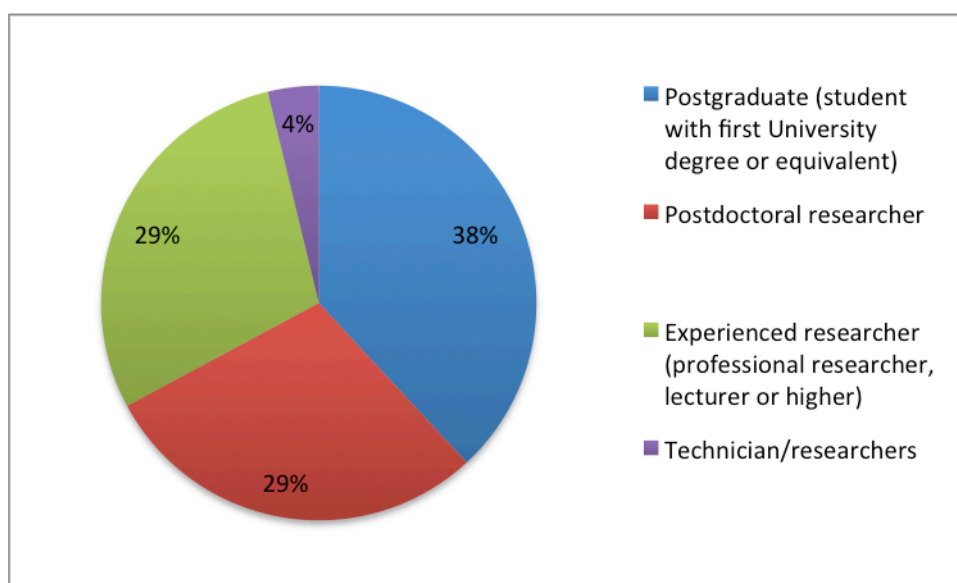

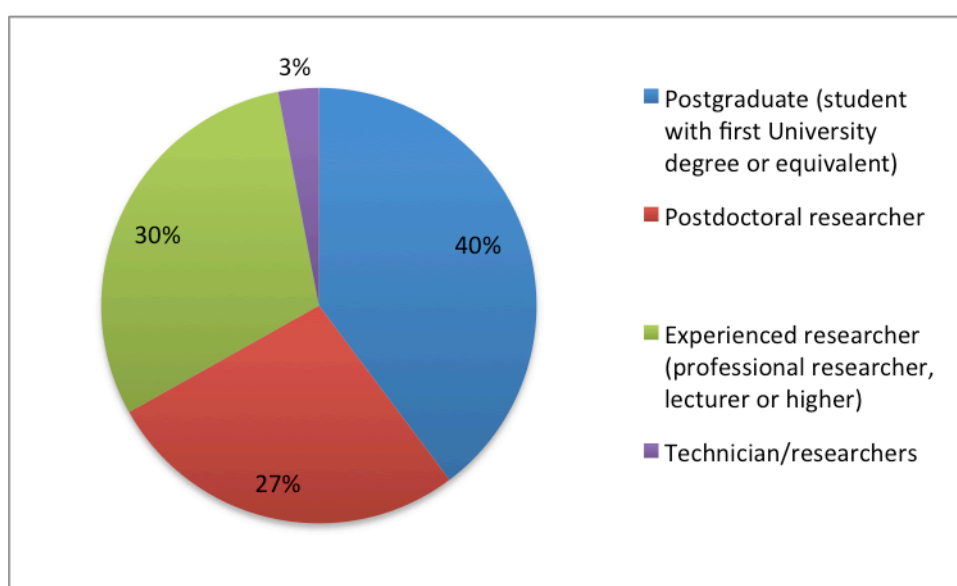**Figure 5: Applicants by level of seniority**

Figure 6: Accepted applicants by level of seniority

5 Visit Feedback

Both visitors and hosts are asked to complete a questionnaire at the end of each visit.

5.1 Visitor questionnaires

Visitors have reported a very high level of satisfaction with the programme in their questionnaires. Although some visitors did report dissatisfaction with a particular aspect of their visit, of the 108 respondents so far, 100% have declared themselves to be satisfied or very satisfied overall, with 85% in the "very satisfied" category.

The issues with which visitors reported dissatisfaction were:

- The level of the daily allowance, which some feel is insufficient, particularly for those visiting the more expensive cities, and for researchers from countries with a lower average income (some hosts also noted this in their questionnaires);
- The lack of help to find accommodation in certain countries;
- A few specific cases of communication problems with the local administration team – this should hopefully be much less frequent now that the centres all have more experience of running the programme (and indeed we can see an increase in the proportion of "very satisfied" visitors among the more recent visitors compared to those who came at the start of the programme).
- In one case, the amount of CPU time allocated, which was considerably lower than the visitor had requested – this should have been mentioned in the acceptance letter, as in such cases we usually make an offer conditional on the applicant agreeing to a reduced allocation of computing time.

However, all visitors had found the programme to be a positive experience, and we have requested permission from some of the visitors to quote some of their positive comments as visitor testimonials for the webpage and marketing material for the programme.

5.2 Host questionnaires

Hosts also report a high level of satisfaction, with 97% of the 59 respondents to date saying that they have been satisfied or very satisfied overall with the visits which they have hosted (with 83% saying that they were very satisfied).

For those who were dissatisfied overall with the visit (just 2 respondents), this was due specifically to a lack of useful collaborative interaction with the visitor.

The host questionnaires also contain a number of valuable comments which will be used in the near future to promote the programme within the community of (current and potential) host researchers.

6 Research Highlights

Despite the small number of visits completed to date, and the relatively short period of time since the first visits were completed, the programme has already had considerable impact for some of the participants.

Work carried out in the context of the programme has already led to 19 publications and conference presentations being produced. A full list of these can be found in Annex 1.

Due to the inevitable delay between the preparation of a scientific publication and the time when it actually appears in print (typically six months to a year), we expect most of the published scientific output from HPC-Europa3 visits funded in any given year to appear the following year. Further, the research carried out during HPC-Europa visits is typically not carried out in isolation, but is usually part of a wider research focus, and therefore we expect to see publications acknowledging the programme appearing for at least 2 years after some visits.

One of the successes we have seen from HPC-Europa visits in the past is when visitors have secured subsequent research positions in their host departments, and although it is still less than 12 months since the first visitor arrived, we already know of one such case: EPCC visitor Mats Simmermacher has obtained a one-year position, covering a period of sabbatical leave, in his host department, the School of Chemistry at the University of Edinburgh. Had he not carried out his HPC-Europa3 visit there, he may not have heard of this opportunity, and it is likely that his visit contributed to him being able to secure the post.

HPC-Europa aims to build long-lasting collaborative links, leading to joint publications between visitor and host research group, or follow-up research visits (including reciprocal visits, where someone from the host group goes to the visitor's group), with or without HPC-Europa funding. The HPC-Europa team is aware of several examples of subsequent visits which are planned to follow up the research links formed during visits.

7 First Transnational Access Meeting (TAM 2018)

The HPC-Europa3 user group meeting, TAM – the **T**ransnational **A**ccess **M**eeting – is an opportunity for visitors from each of the HPC centres to come together to present the results of the work they have done during their visit. All visitors attending the meeting are required to give a presentation (either a talk or a poster) about their work. For many researchers this represents an early opportunity to present their results, and for junior researchers with little conference experience it offers a chance to gain some experience of presenting their research in a relatively relaxed and friendly environment. In previous HPC-Europa programmes, TAM has led to new collaborative links being formed, sometimes bridging different areas of research, as the cross-disciplinary nature of the programme is reflected in the attendee list.

The first HPC-Europa3 TAM is being hosted by EPCC in Edinburgh on Tuesday 23rd October 2018, just at the end of this reporting period.

In total, 40 HPC-Europa3 visitors have registered for TAM 2018. Of these, 25 have registered to give a talk, and 12 will present posters. Three further attendees will not present posters at this TAM as they are visitors to EPCC who have just started their visits in October, so are not ready to present their work yet.

Visitors from every centre will be represented, as shown in the table below:

HPC-Europa3 centre	Talk	Poster	New EPCC visitors – no presentation	Total
BSC	5			5
CINECA		1		1
CSC	4			4
EPCC	5	5	3	13
GRNET	2			2
HLRS	4	2		6
ICHEC	1			1
KTH	1	3		4
SURFsara	3	1		4
Total	25	12	3	40

Table 7 TAM 2018 presentations by HPC-Europa3 centre visited

Talks have been scheduled in two parallel sessions, which are broadly themed by discipline. Presentations will cover research in the fields of chemistry, materials science, physics, life sciences and biotechnology, engineering and technology, and information and communication technologies.

The programme for the meeting, including talk and poster titles, can be found on the HPC-Europa3 website at http://www.hpc-europa.org/first-user-group-meeting-edinburgh-uk-23-oct-2018, and will not be reproduced here.

As previously mentioned in this report, the annual face-to-face SUSP meeting has been scheduled in conjunction with TAM, allowing panel members to attend the visitors' presentations to see for themselves some of the users' successful results.

8   Conclusion

In conclusion, we can see that many aspects of the HPC-Europa3 programme have been successful.

- The consortium is now well-established, procedures are all in place, and the day-to-date operation of the programme is going smoothly at all centres.
- Applications have already been received from 36 of the 44 eligible countries, and from a wide range of scientific disciplines. A higher percentage of applicants than in the past are female, and the range of ages of the applicants is very broad, with a good mix of researchers at different stages of their careers.
- Visitors and hosts are generally satisfied or very satisfied with their visits, even where there has been some level of dissatisfaction with a specific aspect of the visit.
- Successful outcomes are beginning to be reported by those whose visits have concluded, and these offer excellent material for promoting the programme.

For those who have already participated in the programme, either as visitors or as hosts, HPC-Europa has, almost without exception, been a very valuable experience, often leading to significant results.

However, the number of applications received and visits carried out so far has been far below what was planned, and the major challenge for the coming months is to focus on publicising the programme and increasing the number of applications significantly.

The consortium partners will make an enormous effort to focus on two priorities in particular:

- improving and expanding the material used to promote the programme, and
- increasing the visibility of the programme.

In terms of improving the material, firstly the webpage will undergo consider redevelopment, to include more information and improved content, and to make it easier to find the information that is there. The visitor reports forming the first project directory will be made available on the webpage and publicised. We will also collate on the website all the disparate items that are scattered across various locations at the moment, such as the visitor blogs which have been posted on the websites of individual centres. More visitor videos will be created and posted on both the YouTube site and the HPC-Europa webpage. We will increase our use of social media, which make it easy for people to share our publicity, and in particular we will investigate the potential of LinkedIn more fully.

However, no matter how good the publicity material is, if the target audience do not see it, it has no value. In order to exploit the material fully, an enormous effort will be made to publicise the programme far and wide. This will include all the activities already undertaken, but these reach mainly those already within our existing networks. To reach beyond these, major efforts will be made by all partners to identify new research groups. This is a time-consuming process which generally has a low yield, so some of this effort will go towards identifying scientific networks and (re-)establishing contacts within research councils, in order to be able to spread the information to a wider audience more quickly, and to have it broadcast by a trusted source.

In conclusion, the programme has begun well and has already led to many successful visits, but an enormous amount of work is now required to publicise the programme extensively in order to significantly increase application numbers. The time and effort to set up the programme from scratch after such a long pause had been somewhat under-estimated, leading to reduced time available to promote the programme, but consortium members should now have more time available to focus on outreach and dissemination, and we expect to see a considerable improvement in application numbers for the upcoming calls.

Annex 1

Scientific publications produced by HPC-Europa3 visitors:

1. DW Szczepanik, A simple alternative to the pseudo-π method, Int. J. Quantum Chem. 118 (2018) e25696; doi: 10.1002/qua.25696.
2. N Sieffert, A Thakkar, M Bühl, Modelling uranyl chemistry in liquid ammonia from density functional theory. Chem. Commun. 2018, 54, 10431; doi: 10.1039/C8CC05382K.
3. PN Tzounis, SD Anogiannakis, DN Theodorou, Atomistic Simulations of Oligomers used in Directed Self-Assembly Lithography: Estimation of the Interaction Parameter χ, in preparation.
4. P Behbahani, Alireza F, Vaez Allaei, S Mehdi, Motlagh, Ghodratollah H, Eslami, Hossein and Harmandaris, Vagelis A, Structure, Dynamics, and Apparent Glass Transition of Stereoregular Poly (methyl methacrylate)/Graphene Interfaces through Atomistic Simulations. Macromolecules, 2018, 51 (19), pp 7518–7532.
5. AJ Gallego, P Gil, A Pertusa, RB Fisher, Segmentation of Oil Spills on Side-Looking Airborne Radar Imagery with Autoencoders. Sensors, 18(3): 797, 2018.
6. Gallego, Antonio-Javier; Pertusa, Antonio; Gil, Pablo; and Fisher, Robert B. Detection of bodies in maritime rescue operations using Unmanned Aerial Vehicles with multispectral cameras. Journal of Field Robotics, 2018 (under review).
7. M Pecha and D Horák, Analyzing l1-loss and l2-loss Support Vector Machines Implemented in PERMON Toolbox. Will be published in Lecture Notes in Electrical Engineering series. 2018. [in print].
8. VL Deringer, MA Caro, R Jana, A Aarva, SR Elliott, T Laurila, G Csányi, L Pastewka, Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory, Chem. Mater. 2018, in press, DOI: 10.1021/acs.chemmater.8b02410.
9. V Ribić, A Dapčević, N Skorodumova, A Rečnik, D Luković Golić, Z Branković, G Branković, First-Principles Calculation of Gd - doped BiFeO3, European HPC Summit Week 2018 - #EHPCSW, May 28th to June 1st 2018, Ljubljana, Slovenia.
10. J Acebron, JR Herrero, J Monteiro, A highly parallel algorithm for computing the action of a matrix exponential on a vector based on a multilevel Monte Carlo method, submitted on July 25th to Journal Of Computational Physics.
11. A Miró, M Soria, C Moulinec, JC Cajas, Y Fournier, (2018) Numerical investigations on rectangular and circular synthetic jet impingement. In Tenth International Conference on Computational Fluid Dynamics (ICCFD10) (pp. 1–18). Barcelona.
12. S Dotolo, A Facchiano, A Pandini, Comparative analysis of molecular motions in SIRTUIN2 proteins. On Abstract book. BBCC 18-20 December 2017.
13. S Dotolo, A Facchiano, Functional analysis of Aryl Hydrocarbon Receptor main and unknown molecular-genetic pathways involved in human cutaneous malignant melanoma for designing new therapeutic approaches. On Abstract book. ISMB/ECCB 21-25 July 2017.
14. S Dotolo, A Facchiano, Natural-bioactive compounds study by means of bioinformatics approaches. On Abstract book. BITS 5-8 July 2017.
15. S Dotolo, A Facchiano, A Pandini, Detection of the impairment of allosteric communication in Sirtuin2 proteins through molecular dynamics and residue coevolution. BITS 27-29 June 2018.

16. VL Deringer, MA Caro, R Jana, A Aarva, SR Elliott, T Laurila, G Csányi, L Pastewka, Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. Chem. Mater. 2018, in press, DOI: 10.1021/acs.chemmater.8b02410.

17. A Iravani, I Kukolj, F Ouchterlony, T Antretter, J Åström, 2018. Modelling blast fragmentation of mortar and rock. In proceedings of the 12th international symposium on rock fragmentation by blasting Luleå, Sweden.

18. A Iravani, J Åström, F Ouchterlony, Physical Origin of the Fine-Particle Problem in Blasting Fragmentation, PhysRevApplied 10(3):34001. DOI: 10.1103/PhysRevApplied.10.034001.

19. L Kos, M Brank, G Simič, D Penko, T Johnson, Parallel Power Deposition on Plasma Facing Components, poster presentation at the Int. conf. European HPC Summit Week 2018 and PRACEdays 2018, 28 May - 1 June 2018, Ljubljana, Slovenia.