D2.4 - Second Transnational Access summary report

Deliverable No.:	D2.4
Deliverable Name:	Second Transnational Access summary report
Contractual Submission Date:	30/04/2020
Actual Submission Date:	30/04/2020
Version:	V1.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 730897.

COVER AND CONTROL PAGE OF DOCUMENT	
Project Acronym:	**HPC-Europa3**
Project Full Name:	Transnational Access Programme for a Pan-European Network of HPC Research Infrastructures and Laboratories for scientific computing
Deliverable No.:	D2.4
Document name:	Second Transnational Access summary report
Nature (R, P, D, O):	R
Dissemination Level (PU, PP, RE, CO):	PU
Version:	V1.0
Actual Submission Date:	30/04/2020
Author, Institution: E-Mail:	Catherine Inglis, UEDIN-EPCC c.inglis@epcc.ed.ac.uk
Other contributors	Debora Testi, Cineca

ABSTRACT:
This document is the second report on the HPC-Europa3 Transnational Access activity. It covers the second reporting period (Months 19-36, i.e. 1 November 2018 – 30 April 2020). 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 dissemination activities and selection procedure.

KEYWORD LIST:
Transnational Access, research visits, HPC

MODIFICATION CONTROL			
Version	**Date**	**Status**	**Author**
0.1	24/04/2020	Draft	Catherine Inglis, UEDIN-EPCC
0.2	28/04/2020	Revised draft after internal review	Catherine Inglis, UEDIN-EPCC Debora Testi, Cineca
1.0	30/04/2020	Final version	Catherine Inglis, UEDIN-EPCC

TABLE OF CONTENTS

Executive summary

HPC-Europa3's Transnational Access programme offers researchers in Europe, working in any field of computational science, the opportunity to visit a researcher in a similar field in one of 9 European countries where there is a project consortium partner, while gaining access to some of the most powerful High Performance Computing (HPC) facilities in Europe.

Over the project lifetime, HPC-Europa3 aims to support 1098 research visits[1], and provide more than 900 million core-hours of computing access.

This document is the second report on the HPC-Europa3 Transnational Access activity. It covers the second reporting period (Months 19-36, i.e. 1 November 2018 – 30 April 2020). 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 and selection procedure.

[1] This is 10% less than the target stated in the previous 18-month report, due to a Contract Amendment which has come into effect in the meantime.

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, academic or commercial, in any of the countries in which the Transnational Access partners are based, but may not be made to a group 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 few places are also available for researchers from outside Europe.

Visits 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 through 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 visitor 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 second 18-month period 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 and host feedback, and an overview of some project successes.

2 Outreach and publicity

HPC-Europa3 Calls for Applications are issued 4 times per year, with closing dates in February, May, September and November.

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 in France, which is the only partner which does not offer Transnational Access visits.

The team aims to publicise the programme widely in all of the 44 eligible countries[2]. Online meetings are held between calls to review activities for the previous call and plan actions for the next closing date. However, publicity is an ongoing effort which continues throughout the whole call cycle.

The marketing and publicity strategy is set out in Deliverable 2.1, Marketing Plan[3].

2.1 Project webpage, newsletters and other marketing materials

The project webpage (http://www.hpc-europa.eu) is the main source of information for applicants, accepted visitors, and hosts. It includes the link to the secure online portal for applicants, hosts, reviewers and HPC-Europa3 consortium members, with each category of user having a different view.

The initial website was put together quickly at the start of the programme, for the launch of the first Call for Applications. After the first few calls, a full review of both the content and structure was carried out, and a revised version of the website was launched in August 2019.

The webpage revision was driven by feedback from the various categories of users. It was also informed by the most common questions addressed to the email address for general enquiries (staff@hpc-europa.org), which helped to identify which information was missing or difficult to find.

The main objectives were to introduce a cleaner design, with a more logical structure which was simpler to navigate, and to increase the amount of information on the webpage, including results from the visits and some more engaging content, such as visitor testimonials in blog or video format.

In particular, the new ***Visitors area***[4] was added in order to highlight visitor experiences and successes. It includes a link to the searchable list of project abstracts, so potential applicants and hosts can see what sort of work has been carried out under the programme. It also includes links to success stories, blog articles and short videos (discussed further in section 2.2). This section of the website aims not only to showcase the positive outcomes of the visits, but also to highlight the varied profiles of the visitors and the range of disciplines from which they come. Personal anecdotes from visitors are believed to be an effective way to convince people to apply.

There is also a ***Public documents***[5] section of the website, which contains links to webinars about the programme, public deliverables, downloadable copies of the logo, flyer, poster and roll-up (for any stakeholders who wish to publicise the programme), and the project newsletters.

[2] All 27 EU member countries plus the UK, and the Associated States (Albania, Armenia, Bosnia-Herzegovina, Faroe Islands, Georgia, Iceland, Israel, FYR Macedonia, Moldova, Montenegro, Norway, Serbia, Switzerland, Tunisia, Turkey and Ukraine).
[3] https://b2share.eudat.eu/records/4a19b5b3428f41eeb581d5a6fac6ce2f
[4] https://www.hpc-europa.org/visitors
[5] http://www.hpc-europa.eu/public_documents

Two new HPC-Europa3 newsletters were published during this period. The first included an overview of the programme, testimonials from a visitor and a host, and a feature about SURFsara, the partner centre in the Netherlands. The second newsletter featured some statistics about the visitors over the first 3 years of the programme, a visitor success story, and a feature about CSC, the partner centre in Finland.

As well as being available from the Public Documents section of the website, the project newsletters are publicised via social media accounts and distributed to the subscription email list, which currently has 1819 subscribers.

The consortium also monitors the website monthly via Google analytics. From this it can be seen that the number of visits to the website has progressively increased from November 2018, and in particular from August 2019 after the website was redesigned. From the demographic information we can see that the majority of visitors to the website are between 25 and 34 years old, and two thirds of them are male. For other indicators such as time spent on the site, or returning visitors versus new visitors, the values fluctuate, increasing as each call deadline approaches, as would be expected.

Centres are encouraged to publicise the programme via their own websites, newsletters and social media accounts. Some examples of articles produced by project partners include:

- Articles in PDC newsletter:
  - *Visit from Vilnius via HPCE3* – published in PDC newsletter no.2, 2018[6]
  - *HPCE3: 18 months of achievements* – published in PDC newsletter no.1, 2019[7]
- Articles in EPCC News, also published as EPCC blog articles:
  - *Building research collaborations across Europe* – published in EPCC News (issue 85, p17) and also as an EPCC blog article, EPCC, May 2019[8]
  - *HPC-Europa3: "An excellent way to have international collaborations with excellent scientists"* – published in EPCC News (issue 86, p19) and also as an EPCC blog article, December 2019[9]
- LinkedIn article:
  - *Computer too small?* – LinkedIn article by Lykle Voort, SURFsara, February 2020[10]

An HPC-Europa3 article appeared in the 2018 Cineca annual report[11].

The Call for Applications is included in the PDC industry newsflashes[12].

Visitors are encouraged to write blog articles about their visits, which are publicised via the various social media channels. These can be found on the ***Visitors area*** of the webpage, and can also be found on some partners' websites, e.g. at https://www.epcc.ed.ac.uk/blog/tags/hpc-europa.

[6] https://www.kth.se/polopoly_fs/1.865417.1550156936!/Newsletter2018-2-final-lres.pdf#Newsletter18-2-final.indd%3A.66396%3A726
[7] https://www.kth.se/polopoly_fs/1.912243.1560904472!/Newsletter2019-1-final-lres-spreads.pdf#Newsletter19-1-20190610.indd%3A.71337%3A789
[8] http://www.epcc.ed.ac.uk/sites/default/files/EPCC%20News%2085.pdf; http://www.epcc.ed.ac.uk/blog/2019/building-research-collaborations-across-europe
[9] http://www.epcc.ed.ac.uk/sites/default/files/EPCC%20News%20PRINT%2086.pdf; http://www.epcc.ed.ac.uk/blog/2019/12/hpc-europa3-excellent-international-collaborations-excellent-scientists
[10] https://www.linkedin.com/pulse/computer-too-small-lykle-voort/
[11] http://www.hpc.cineca.it/sites/default/files/u153/REPORT_2018.pdf
[12] https://www.pdc.kth.se/research/business-research/newsflashes-1.737499

Some partners produce their own publicity material for the programme. A recent example of a flyer from CSC, highlighting all the visits to Finland, can be found at: https://a3s.fi/hpce3/CSC-HPCE3-flyer.pdf. There is also a general version which does not highlight the visits to Finland, which can be used by any partner, at https://a3s.fi/hpce3/HPCE3_flyer_2020.pdf.

CSC also used this same visit data to produce an animated map showing the origin and destination country over time of all visits so far. The map can be found at http://hpce3visits.rahtiapp.fi/, and has been used to promote the programme via social media. The map was made before the Covid-19 lockdown period and it included the planned dates for upcoming visits, which explains why it appears to show a high number of visits continuing to happen during the lockdown period.

For the first Transnational Access Meeting in October 2018, all attendees received an HPC-Europa3 branded reusable water bottle. For the second meeting, a branded mug has been produced. We hope that the visitors and SUSP members continue to use these items for a long time to come, and raise awareness of the programme while doing so.

2.2 Social media

The project social media accounts are used to publicise closing dates, announce new visits starting, and disseminate visitor success stories, blog articles, video testimonials, and other project news. The accounts have also been used to announce and report on project events such as the three SME workshops organised in *Work Package 3 – External co-operation for enhancing the best use of HPC.*

Social media accounts have great potential to raise the profile of the project beyond our existing network, as we reach new people whenever our followers repost our announcements. When announcing new visits on Twitter, we "mention", where possible, the visitor, the host, and their respective research groups and/or institutes. This often results in reposts from those accounts, which are generally outside our network and often have a very large reach.

The project has the following social media accounts:

- **Twitter:** https://twitter.com/HPCEuropa3
  - This is the principal social media channel used by the project.
  - The account has 671 followers, an increase of 427 in the last 18 months.
  - To date we have issued 620 tweets, 440 of these in the last 18 months.
  - The project tweets have had 827 likes over these 18 months, compared to 185 in the previous 18 months, and they have been retweeted 474 times, compared to 135 times in the previous 18 months.
  - 25 tweets in this period have had an engagement rate of 2% or higher, 10 tweets were retweeted 10 or more times, and 16 were liked 10 or more times.
- **Facebook:** https://www.facebook.com/hpceuropa/
  - The Facebook account currently has 205 followers, an increase of 96 in the last 18 months.
  - Posts have received 144 likes to date.
- **LinkedIn:** https://www.linkedin.com/company/29022707/
  - The LinkedIn account currently has 116 followers. This account had only recently been set up at the end of the last reporting period.
  - Over the last 12-month period, there have been 28 posts which have generated 46 reactions and 115 clicks.
  - The highest "clicks per impression" rate was 5.83% for a post targeted specifically at potential hosts.

The project also has a **YouTube channel**, which has a series of short video interviews with visitors and a playlist including webinars providing an overview of HPC-Europa. The channel can be found at: https://www.youtube.com/channel/UC9uOpFQGP9V0TQPXFUOgs_A/playlists.

2.3 Methods of publicising the programming

Each Call for Applications is sent to all relevant contacts by email and included in the partners' regular mailings to their user communities. Contacts include research councils, scientific networks, and individual researchers, including former visitors and host researchers.

As described in sections 2.1 and 2.2, the programme is publicised online via the HPC-Europa3 website, social media accounts and newsletters, as well as via those of the project partners. Under *Work Package 3 – External co-operation for enhancing the best use of HPC*, a number of MoUs were agreed with other relevant initiatives in order to engage in reciprocal publicity activities. The list of initiatives with which HPC-Europa3 currently has MoUs can be found at https://www.hpc-europa.org/external.

Organisations such as PRACE[13] and BioExcel[14] have a strong focus on training activities, with a similar target demographic to HPC-Europa3, so reciprocal publicity is very appropriate. We stay in regular contact with PRACE Training Centres to ask them to publicise the programme at their many courses and workshops, with a particular focus on the training centres in countries where there is no HPC-Europa3 partner, such as IT4I in the Czech Republic. We encourage them to incorporate the two-slide PowerPoint overview into one of the course presentations, and for larger events we suggest that they download and print publicity material from the webpage. If necessary, and with enough notice, we can send printed copies of publicity materials.

[13] www.prace-ri.eu
[14] http://bioexcel.eu/

Project partners also look for any relevant events which their colleagues will be attending, and ask them to publicise the programme in whichever way they can (displaying a poster or pull-up, handing out flyers, including the PowerPoint overview slides in their presentations, or simply mentioning the programme to potential applicants). When sending the Call for Applications by email, we also remind visitors and hosts that they can help us in the same way.

Direct contact has always played a very important role in publicising the programme, and section 2.6 shows that most applicants hear about the programme from a colleague, their direct boss, or a former visitor. With almost 400 HPC-Europa3 visits now having taken place, the word-of-mouth effect should continue to have a growing impact.

2.4 Dissemination of project achievements

More than 2 years after the first visits finished, there are increasing numbers of project achievements and successes to publicise. By highlighting any novel and/or world-class research that is carried out with the support of the programme, the profile of HPC-Europa3 can be greatly raised.

Examples of project successes include publications arising from research carried out during the visit, collaborative links lasting long after the visit, and visitors gaining new research posts as a result of links made or skills gained during their visits. These are discussed further in section 6.

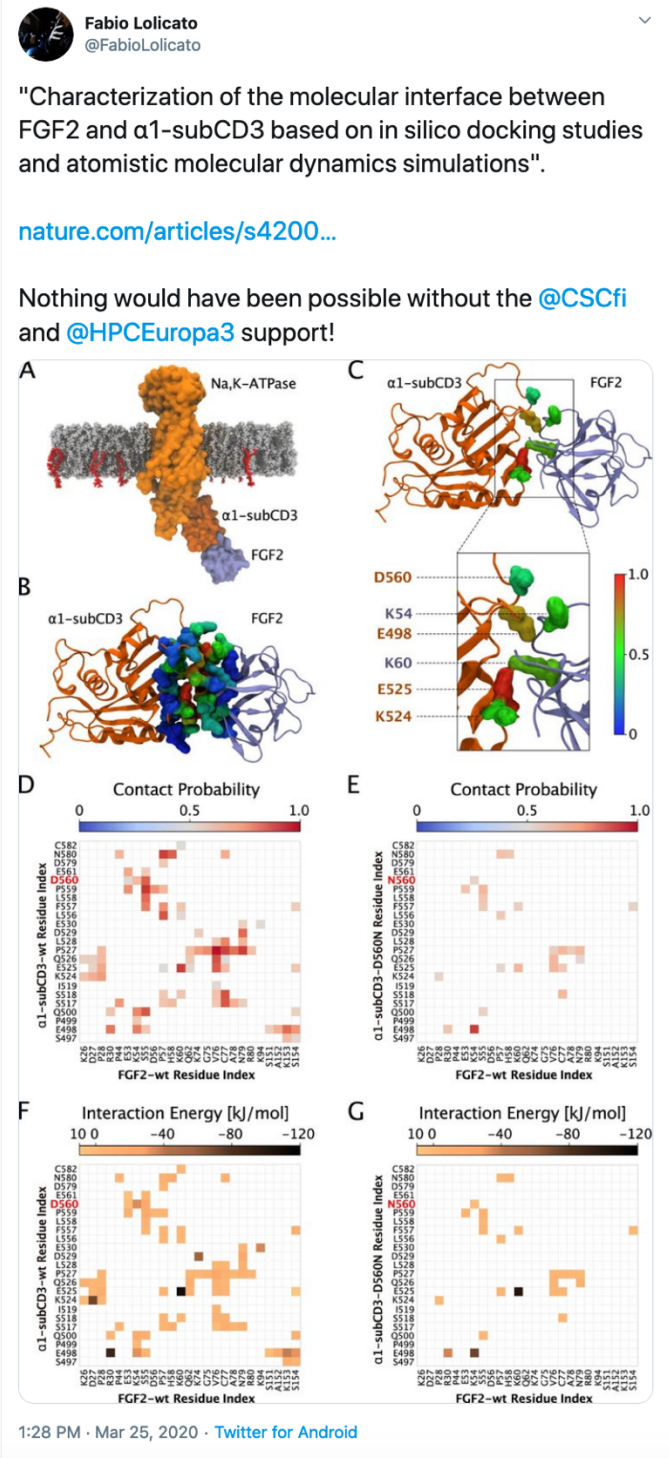
Many of these results will not be seen until some time after the visits are complete. In particular, due to the length of time it can take for journal articles to be reviewed and published, we expect that publications arising from HPC-Europa3 visits will appear between 6 months and 3 years later. Therefore, the results which are emerging now are often from some of the earliest visits under this programme.

Project achievements are disseminated in the following ways:

- The project directory, a compilation of the visitors' project reports, is distributed in electronic format to contributing authors and their hosts and other interested parties, and is available to download from the HPC-Europa3 website[15]. The second project directory is currently in production.
- All visitors are invited to attend the user group meeting, TAM (the Transnational Access Meeting), to present the work resulting from their visit, via either a talk or a poster.
- Visitors are asked to include an official acknowledgement of HPC-Europa3 in journal publications and conference presentations.
- Each centre will produce a "Transnational Access success story" as a deliverable – CSC has already produced one[16].
- Project successes are publicised via social media, and particularly successful projects are featured in the HPC-Europa3 newsletters.
- Partner centres may also publicise visitor successes – for example, a visitor's publication in the prestigious Physical Review Letters was the subject of an EPCC blog article: https://www.epcc.ed.ac.uk/blog/2019/hpc-europa3-visitor-published-paper-physical-review-letters

[15] https://b2share.eudat.eu/api/files/a0f8ce32-4d45-4e24-a667-59dc869e9af5/HPCE3_First_ProjDirectory.pdf
[16] https://b2share.eudat.eu/api/files/2d819a8f-f92c-4188-8aa6-e85fc810918b/HPCE3_D9.1_CSC_Success_story_v2.0.pdf

Below are a couple of examples of visitors acknowledging HPC-Europa3 when announcing publications on Twitter. Such tweets can potentially have a powerful impact in terms of publicising the programme.



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 of researchers from groups which are part of well-established HPC user communities. The Regional Access Programme introduced in HPC-Europa3 recognises this issue.

2.5.1 Regional Access Programme

The Regional Access Programme gives priority to researchers from groups in under-represented countries, focusing on two separate regions: the Baltic States[17], and South East European Countries[18]. Researchers from these regions who have little or no previous HPC experience are given priority when applying to GRNET in Greece and KTH-PDC in Sweden. They gain access to smaller amounts of HPC resources on less powerful, although still significant, HPC resources, providing a much-needed first step for inexperienced users to get started with HPC. In the past, such applicants were typically not approved by the selection panel, as they were judged not to have a sufficient need for the large-scale HPC resources offered by the programme.

GRNET and KTH-PDC have made constant efforts to publicise the programme via their extensive network of existing contacts in these regions.

HPC-Europa3, along with Riga Technical University, University of Tartu and KTH, is an organising partner of the 4th Baltic HPC and Cloud Conference[19]. Unfortunately, this event, which was scheduled to take place in April 2020, has now been postponed until April 2021 due to the Covid-19 pandemic. The event was expected to be a major opportunity to promote the HPC-Europa3 programme within

[17] Estonia, Latvia, Lithuania
[18] Albania, Armenia, Bosnia-Herzegovina, Bulgaria, Croatia, Cyprus, Georgia, Hungary, Israel, FYR of Macedonia, Moldova, Montenegro, Romania and Serbia
[19] https://hpc.rtu.lv/4th-baltic-hpc-and-cloud-conference/?lang=en

the Baltic region, and it is unfortunate that it will now take place close to the expected date of the final Call for Applications for HPC-Europa3.

The success rate for applications to the Regional Access Programme is discussed in section 4.3.1.

2.5.2 Identifying new contacts

Continuous efforts must be made to identify emerging communities and new individuals and research groups who could be potential visitors or hosts. We have identified different categories of potential new users, and will target them as follows:

- **Tier-2 users ready to move to Tier-1:** Partner centres ask operators of Tier-2 facilities to publicise the programme to their users as an ideal way of progressing to Tier-1 level, with technical support provided.
- **Emerging communities:** Research areas of applicants are monitored in order to try to identify areas where there is new uptake of HPC; leverage can be gained through some partner centres' existing efforts to address emerging communities. Specific case studies may be prepared where there have been visitors from any identified communities.
- **Research groups in under-represented countries:** The latest applicant numbers will be analysed to see which countries remain under-represented, and partners will work to identify new contacts in the countries assigned to them in the Marketing Plan (D2.1). There has been a considerable increase in applications from Turkey, for example, after employing the following 2 approaches:
    - Gaining the help of national science funding bodies (e.g. Tübitak, the Scientific and Technological Research Council of Turkey) and other organisations such as the British Council, which have large networks of contacts and are seen as trusted sources of information;
    - Providing summary information about successful applicants from the relevant country, which can help to show that researchers from a similar background have been accepted onto the programme.
- **New user groups in established fields:** Our existing contacts can help us to identify new contacts. For example, visitor and host questionnaires both ask for suggestions about where to publicise the programme. We look for major events such as discipline-specific conferences, and if a public list of delegates is available, we check to see if anyone in our network is attending so that we can ask them to publicise the programme.

We have analysed our Twitter followers to identify any who fall into the above categories, and have contacted some of them directly to encourage them to consider applying and / or to publicise the programme within their communities.

Identifying new contacts is a very time-consuming, but necessary, process. In the final reporting period of the programme, now that a large number of visits have taken place and there are some excellent outcomes to report, we will use more targeted marketing when contacting new users. This could be in the form of specific case studies (featuring visitors from a target country or discipline, or a Tier-2 user moving to Tier-1, for example), or simply in the form of relevant agglomerated statistics.

2.6 Where did applicants hear about HPC-Europa3?

The application form asks applicants where they heard about HPC-Europa3. This information is summarised in Figure 1. 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.

More than half of applicants (55%) said that they had heard about the programme from a colleague, and more than a quarter of applicants (26%) heard about it from their direct boss. This demonstrates the importance of the "word of mouth" factor. What we cannot tell from this, however, is where the colleague or direct boss had heard about the programme.

In total 19% of applicants had received the call for applications by email, showing that this is still an effective way of reaching people.

Meanwhile, 44 people (9%) said they had heard about the programme at a conference, demonstrating that it is important to seek ways to gain leverage from visitors or colleagues attending such events.

5% of applicants had heard about the programme through social media, with this being more significant in the most recent 12 months, as our social media activity has increased and our number of followers has grown.

Although 16% of applicants said they had heard about the programme from some "other" source, on closer examination "other" often equates to one of the given categories, e.g. their Ph.D. supervisor (direct boss) or a colleague. However, some had heard about it from their host, who had encouraged them to apply, while others had heard about it through user communications from their local HPC centre.

Only a very small proportion (2%) of applicants had seen a poster or the call for applications on a notice-board. Notice-boards are much less used now for student information, and most of our publicity is done online, which has many advantages: it is quicker, more cost-efficient, easier for the target to disseminate the message further, and in some cases, it allows tracking of subsequent actions, whereas with a paper mailshot it is very difficult to find out whether the letter was read and the poster displayed. The poster was sent with a mailshot announcing the return of the programme at the beginning of the project lifetime, but this has not been repeated since, and posters and flyers are usually distributed in small bundles at events which contacts are attending, which should be a more effective way of ensuring that they reach a relevant audience.

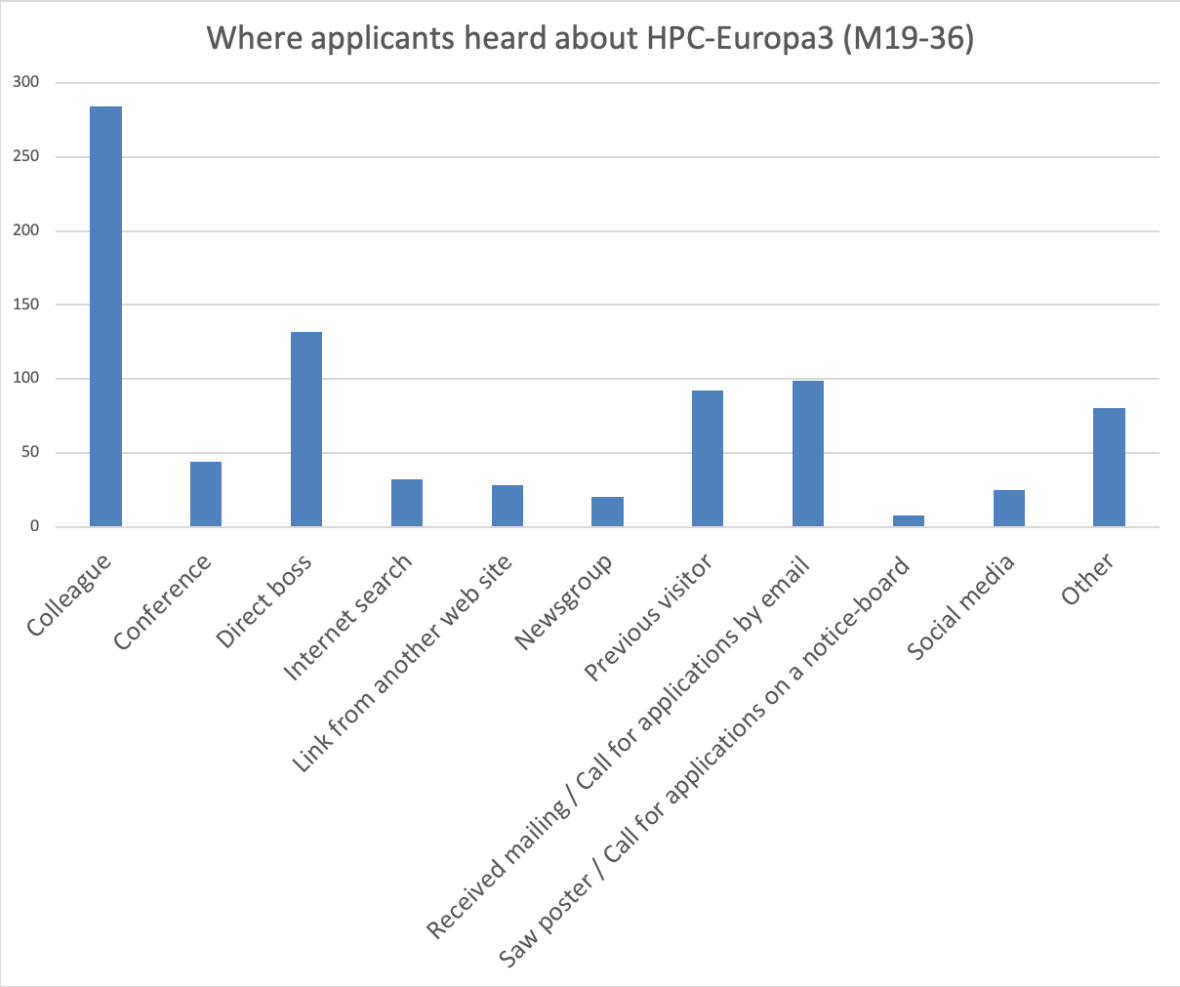


Figure 1: Where applicants heard about HPC-Europa3

During Months 19-36, there were six calls for application, and 514 eligible applications received. However, 37% of these (191 applications) were received for the most recent call (Call 11), which saw a threefold increase in the number of applications compared to the average received over all of the previous 10 calls.

When looking at the *relative* numbers of how many applicants had heard about the programme in each way for Call 11, there was no significant change compared to previous calls.

However, for that call, a particularly strong focus was put on contacting our network of hosts, to ask them not only to publicise the programme among their own contacts, but also to suggest that they encourage suitable researchers to apply to visit them. It is hard to know for certain whether this "host-driven" approach is the reason for the great increase in application numbers, but as this was the main difference from previous calls, we believe it was certainly a factor. We do not intend to repeat this procedure for every call, as many of our hosts are senior researchers who are very busy, and we prefer not to dilute the impact and be seen as "spam". However, we plan to take this approach perhaps twice a year from now on, and it will be interesting to see whether the same results are seen again.

3 Evaluation and Selection Process

The HPC-Europa3 selection process aims to give all candidates a fair review, while at the same time keeping the review process relatively 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** – 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** – 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 provided in terms of the host being **very enthusiastic**, **enthusiastic**, having **some interest** or **no interest**.

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. As with Technical Evaluations, 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 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 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 – for example 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.

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 increased or reduced 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-Europa3 team aims to communicate all decisions to applicants within 2 weeks of the meeting.

3.2 Closing dates and selection meetings in second reporting period

Six Calls for Applications were launched during this reporting period, with all of the corresponding selection meetings being held by online videoconference. The selection meeting corresponding to the 11th call was planned to be a face-to-face meeting, but this had to be postponed due to the COVID-19 pandemic. The meeting has been provisionally rescheduled for October 2020.

Call number	Closing date	Selection meeting
6	15th November 2018	17th December 2018
7	21st February 2019	2nd April 2019
8	14th May 2019	24th June 2019
9	19th September 2020	28th October 2019
10	20th November 2019	10th December 2019
11	20th February 2020	30th March 2020

Table 1: HPC-Europa3 closing dates and selection meetings, M19-36

3.3 Members of the Scientific Users Selection Panel

The HPC-Europa3 Scientific Users Selection Panel (SUSP) initially consisted of 22 members.

However, in order to try to more closely match the reviewers' scientific backgrounds to the applications assigned to them, and also to spread the load of reviews more evenly among the reviewers, we have now increased the number of panel members to 35. This includes 2 new members in the field of mathematics, which was an area previously covered by the computer sciences experts, but in which we had come to need additional experts. We believe that, particularly in the light of the large number of applications received for the most recent call, we could still benefit from expanding this further, and in the next couple of months we will invite some additional experts to join the panel from the specific areas which we have identified as short of reviewers.

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

Name	Institute	Country
Astrophysics		
Prof. Gustavo Yepes	Department of Theoretical Physics, Autonomous University of Madrid	Spain
Chemistry		
Dr. Mark Abraham	*Formerly of* Department of Theoretical Physics, KTH Royal Institute of Technology and SciLifeLab	Sweden
Prof. Andrea Cavalli	Department of Pharmacy and Biotechnology, University of Bologna	Italy
Dr. Valentina Erastova	School of Chemistry, University of Edinburgh	United Kingdom
Prof. Francisco Javier Luque	Faculty of Pharmacy, University of Barcelona	Spain
Prof. Carole Morrison	School of Chemistry, University of Edinburgh	United Kingdom
Dr. Zilvinas Rinkevicius	Theoretical Chemistry and Biology, KTH Royal Institute of Technology	Sweden
Prof. Dage Sundholm	Department of Chemistry, University of Helsinki	Finland
Computer Sciences		
Prof. Eduard Ayguadé	Department of Computer Architecture, UPC – BarcelonaTech	Spain
Dr. Mary Cryan	School of Informatics, University of Edinburgh	United Kingdom
Prof. Dr. Wolfgang Nagel	Center of Information Services and High Performance Computing, TU-Dresden	Germany
Earth Sciences		
Prof. Eleni Katragkou	Department of Meteorology and Climatology, Aristotle University of Thessaloniki	Greece
Engineering		
Dr. Guillaume Houzeaux	CASE – Physical and Numerical Modelling group, BSC (Barcelona Supercomputing Centre)	Spain
Prof. Dr.-Ing. Eckart Laurien	Institute of Nuclear Technology and Energy Systems, University of Stuttgart	Germany
Prof. Phillip Schlatter	Department of Mechanics, KTH Royal Institute of Technology	Sweden
Dr. Prashant Valluri	School of Engineering, University of Edinburgh	United Kingdom
Geophysics		
Prof. Tomaso Esposti Ongaro	National Institute of Geophysics and Volcanology	Italy
Prof. Stefano Salon	Istituto Nazionale di Oceanografia e di Geofisica	Italy

Life Sciences		
Dr. Zoe Cournia	Biomedical Research Foundation, Academy of Athens	Greece
Dr. Berk Hess	SciLifeLab & KTH	Sweden
Material Sciences		
Prof. Mauro Ferrario	Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia	Italy
Prof. Karoliina Honkala	Department of Chemistry, University of Jyväskylä	Finland
Mathematics		
Dr. Colin Cotter	Department of Mathematics, Imperial College London	United Kingdom
Prof. Fiorella Sgallari	Department of Mathematics, University of Bologna	Italy
Meteorology		
Prof. dr. Jordi Vila	Department of Meteorology and Air Quality, Wageningen University	The Netherlands
Physics		
Dr. Anatoly Belonoshko	Department of Physics, KTH Royal Institute of Technology	Sweden
Prof. Marco Bernasconi	Department of Materials Science, University of Milano-Bicocca	Italy
Prof. Stefano Borgani	Astronomical Observatory of Trieste, University of Trieste	Italy
Prof. dr. Ria Broer	Department of Theoretical Chemistry, Groningen University	The Netherlands
Dr. Andreas Hermann	School of Physics and Astronomy, University of Edinburgh	United Kingdom
Dr. Timo Kiviniemi	Department of Applied Physics, Aalto University	Finland
Prof. Kari Rummukainen	Department of Physics, University of Helsinki	Finland
Prof. Silvano Simula	Department of Mathematics and Physics, Roma Tre University	Italy
Prof. Federico Toschi	Departments of Applied Physics and of Mathematics and Computer Science, Eindhoven University of Technology	The Netherlands
Physics / Biogenetics		
Prof. Giovanni Bussi	International School for Advanced Studies (SISSA)	Italy

Table 2: Membership of Scientific Users Selection Panel (SUSP), April 2020

4 Application and Visit Statistics

4.1 Overview of applications received and approved in Months 19-36

During the second reporting period, there were 6 Calls for Applications, for which 516 applications were received in total. Of these, 2 applications were for hosts in Denmark and Portugal, where visits are not possible because there is no associated HPC-Europa partner there. Both applicants chose to withdraw their application rather than identify an alternative host in a participating country, leaving 514 valid applications.

Of these, 4 are still awaiting final decisions from the selection panel at the time of writing, following the most recent selection meeting.

Of the 510 applications for which decisions have been taken during this period, 405 were approved, giving an overall acceptance rate of 79% for this period.

HPC-Europa3 centre	Applications received M19-36	Applications awaiting decision	Applications accepted M19-36	Acceptance rate[20] M19-36	Total applications received M1-36	Total applications accepted M1-36	Acceptance rate M1-36
BSC	91	1	73	81%	148	113	76%
CINECA	67		55	82%	96	80	83%
CSC	65	1	54	84%	84	73	87%
EPCC	121		84	69%	192	131	68%
GRNET	19		14	74%	34	26	76%
HLRS	67	1	50	76%	92	71	77%
ICHEC	9		7	78%	14	11	79%
KTH-PDC	34		30	88%	57	48	84%
SURFsara	41	1	38	95%	63	58	92%
Total	**514**	**4**	**405**	**79%**	**782**	**611**	**78%**

Table 3: Applications per centre M19-36

A total of 252 visits began across the 9 partner centres during this period, bringing the total number of visits started to 398 (see Table 4 for further details). A further 190 approved visits are yet to begin, taking the current confirmed number of expected visits to 588[21]. Most of the visits which have not yet started were approved at the selection panel meeting which took place shortly before the time of writing. Others were scheduled to take place after the end of this reporting period, and a number of

[20] Based on "Applications accepted" divided by ("Applications received" less "Applications awaiting decisions")
[21] 23 visits have been cancelled (see Table 4: Number of visits per centre and average visit lengthTable 4)

visits which were due to start in March or April 2020 have had to be postponed due to the Covid-19 virus.

Visits can last from between 2 and 13 weeks, and visits of all lengths are common, with around 17% lasting 3 weeks or under and around 12% of visits during this period lasting the maximum 13 weeks. The median visit length during this period was 6 weeks, and the mode was 4 weeks. The mean visit length is 7.2 weeks, while the average requested visit length was slightly higher at 7.7 weeks. Although the panel recommends both lengthening as well as shortening proposed visit durations, it is more common that they recommend reducing the duration, as often they judge that some of the proposed work can be done before or after the visit, and does not justify the expense of staying longer.

HPC-Europa3 centre	Visits started M19-36	Visits completed M19-36	Total visits started M1-36	Total visits completed M1-36	Cancelled visits M1-36	Accepted visits still to begin[22]	Average requested visit length (weeks) M19-36	Average visit length (weeks) M1-36[23]
BSC	50	54	80	79	4	29	8.5	8.0
CINECA	38	36	50	45	4	26	8.3	7.3
CSC	28	28	44	43	1	28	6.2	5.2
EPCC	56	59	88	85	2	41	7.8	7.9
GRNET	9	8	14	13	3	9	8.5	8.9
HLRS	32	32	50	47	2	19	7.2	6.9
ICHEC	4	4	6	6	1	4	5.6	6.3
KTH-PDC	16	19	32	32	0	16	6.7	6.2
SURFsara	19	17	34	29	6	18	9.2	7.5
Total	**252**	**257**	**398**	**379**	**23**	**190**	**7.7**	**7.2**

Table 4: Number of visits per centre and average visit length

As mentioned above, the current expected number of visits, including those which have begun and those which are yet to begin, is 588. This is still a very long way short of the reduced target number of 1098 visits.

[22] At the time of writing this report, a large number of accepted visits had still to start; this was mainly due to there having been a selection meeting shortly before the time of writing, with 150 applications approved; additionally, a number of visits that were due to start in March and April were postponed due to the Covid-19 pandemic.

[23] Average visit length is given across the full project lifetime so far, rather than for the reporting period, to minimise the impact of visits starting and finishing in different reporting periods, which would appear shorter than the real duration. Visit length is given for completed visits only.

We currently plan for 4 more regular closing dates (May, September and November 2020, and February 2021). However, it is likely that we will hold a final closing date in May 2021. This would allow a small number of visits to be approved – these visits would have to take place in a fairly short timescale in the final months of the programme, and some centres may already have met their target by this point. Therefore, we will not consider this possible closing date when calculating the target number of applications per remaining call, but it should be noted that this may provide an additional opportunity to reach the target.

The deviation from target varies considerably between the centres, with CSC and SURFsara farthest from the target, while KTH-PDC is ahead of its target and will not be accepting any more applications for the next closing dates.

By adjusting the figures to take account of the visits still to begin, we can see how many applications each centre still needs to approve in order to reach its target. CSC and SURFsara need 99 and 120 further approved applications respectively, equating to 25 and 30 approved applications per call, assuming 4 more calls (see second-last column of Table 5).

BSC and Cineca also need a total of 80 and 86 further visits to be approved respectively, or 20 and 22 per call. The total average number of applications to be approved per call to reach the target is 128. While these targets seem very challenging given the deviation from target so far, it should be noted that at the most recent closing date, 191 applications were received, of which 150 were approved. Therefore, if application numbers can be sustained at even 80% of this last call – with a similar acceptance rate – the target would in fact be achievable.

However, when taken on a per-centre basis, some centres would be above their target and others would still be below, which might require some reallocation of applications between centres. While this may be possible in many cases, it will not be for all, as in some cases there are hardware or software issues which prevent a specific project being feasible at a given centre, and of course it may also be difficult to identify an appropriate host supervisor in an alternative country.

HPC-Europa3 centre	Target number of visits M1-48	Planned visits M1-36 (linear allocation)[24]	Visits started M1-36	Deviation from plan[25]	Remaining visits to reach target[26]	Accepted visits not yet begun	Remaining applications to approve to reach target	Target number visits to accept at each call (assuming 4 more calls)
BSC	189	117	80	-37	109	29	80	20
CINECA	162	100	50	-50	112	26	86	22
CSC	171	106	44	-62	127	28	99	25
EPCC	180	111	88	-23	92	41	51	13
GRNET	36	22	14	-8	22	9	13	4
HLRS	135	83	50	-33	85	19	66	17
ICHEC	18	11	6	-5	12	4	8	2
KTH-PDC	36	22	32	+10	4	16		
SURFsara	171	106	34	-72	137	18	119	30
Total	**1098**	**678**	**398**	**-280**	**700**	**190**	**510**[27]	**128**[28]

Table 5: Planned visits and deviation from target

The consortium is committed to sustaining efforts to publicise the programme widely in order to maintain this increased number of applications. However, the partners need to plan carefully for the remaining period, to ensure the availability of both computing resources and staff support time for a large number of visitors at any given time. Up to 7 new visits per month (in the case of CSC) would need to begin in order for targets to be reached.

Additionally, it is not clear at the time of writing how the Covid-19 pandemic will affect the programme. Currently all new visits are postponed until international travel begins again, which will also result in a bunching of new visits when travel becomes possible again. Further, in the current circumstances, people will be less likely to be planning research visits, which is expected to result in fewer applications for the May 2020 closing date. However, when publicising the closing date, we

[24] Based on linear allocation over 47 months (project lifetime of 54 months, less 7 months at start for project set-up and first call / evaluation)
[25] Visits started minus planned visits M1-36
[26] Target number of visits, less visits started
[27] The discrepancy between this figure (total number of remaining visits minus number of accepted visits) and the sum of the remaining applications per centre (523) is due to the fact that KTH has now approved more than its target number of visitors.
[28] As the numbers per centre have all been rounded up, this is based on the total number of applications to be approved (511) divided by 4.

are taking care to point out that applications for the May closing date normally correspond to visits in the second half of the year anyway, and that there is flexibility with visit dates due to the pandemic.

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)	Access delivered M19-36	Total access delivered M1-36	Average quantity of access to be delivered per user (planned)	Visits started M19-36	Average access allocated per user-project M19-36[29]	Visits started M1-36	Average access allocated per user-project, M1-36
BSC	8.400.000	3.044.879	4.224.393	44.444	50	60.898	80	52.805
CINECA	31.034.483	12.982.620	15.452.620	191.571	38	341.648	50	309.052
CSC	7.392.996	4.033.184	6.264.962	43.234	28	144.042	44	142.386
EPCC	23.529.412	5.078.195	6.792.204	130.719	56	90.682	88	77.184
GRNET	n/a	2.192.679	2.458.048	n/a	9	243.631	14	175.575
HLRS	9.202.454	5.927.428	6.006.192	68.166	32	185.232	50	120.124
ICHEC	1.503.759	151.553	162.363	83.542	4	37.888	6	27.061
KTH-PDC	5.882.353	3.227.920	4.464.760	163.399	16	201.745	32	139.524
SURFsara	9.500.000	847.717	1.264.254	55.556	19	44.617	34	37.184
Total	**96.445.457**	**37.486.175**	**47.089.796**	**87.837**	**252**	**148.755**	**398**	**118.316**

Table 6: Summary of access planned and access delivered, M19-36

Each centre has a minimum quantity of access which is to be delivered over the duration of the contract. Compared to the previous reporting period, the average allocation per visitor has increased – quite significantly, at some centres. At most centres the actual average allocation per visitor is above the planned average.

Additional time granted beyond the minimum quantity to be provided will be contributed in kind by the respective partner centres.

Users' requirements vary enormously, as some visitors focus more on code development during their visit, and therefore use less time, while others carry out significant numbers of large production runs, and can easily use several times the average allocation. Some partners have so far been cautious about allocating very large amounts to any individual users, in order to guarantee that sufficient resources remain to allow all users over the project lifetime to receive at least the average allocation, should their work justify it.

[29] Note that this is approximate as figures include usage by users whose visits were reported as completed in the first reporting period, but who continued to have access to the HPC resources for a period of time after the visit, and also users whose visits were still in progress at the time of reporting.

The final allocation per visitor will of course 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)
- Career stage

4.3.1 Country of Origin

Over the project lifetime, applications have been received from a wide range of countries, including all of the EU member states except Malta, and 13 of the 16 Associated States (all except the Faroe Islands, Georgia and Montenegro). Applications have also been received from countries in each of the other continents (with the exception of Antarctica).

During Months 19-36, applications were received from a total of 57 different countries, of which 27 were EU member states, 10 were Associated States, and 20 were other countries. A maximum of 20% of the access can be provided for researchers from outside the EU and Associated States.

Note that for the purposes of this report, the United Kingdom has been included within the EU member states.

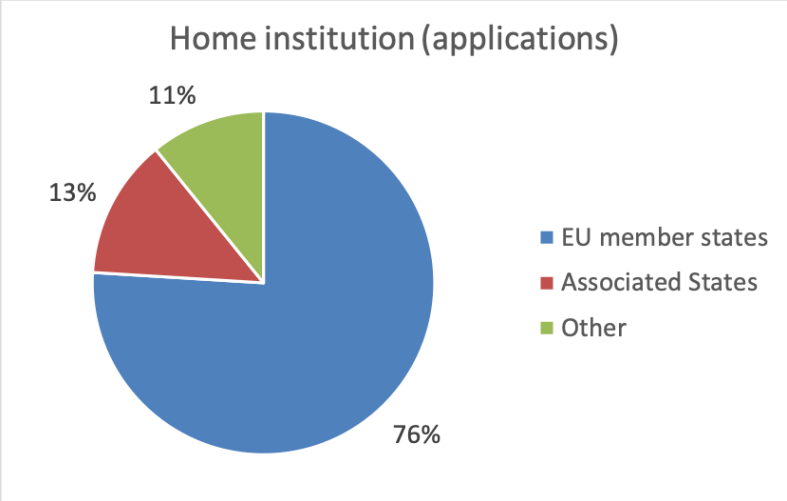


Figure 2: Location of home research institute (applicants)

Table 7 gives a full breakdown of how many applications have been received from each country.

Country (EU)	Applicants	Accepted	Country (Associated State)	Applicants	Accepted	Country (other)	Applicants	Accepted
Austria	4	4	Albania	1	0	Algeria	1	1
Belgium	7	7	Armenia	1	0	Australia	1	1
Bulgaria	5	2	Iceland	2	0	Brazil	4	4
Croatia	5	5	North Macedonia	1	0	Chile	1	1
Cyprus	1	1	Norway	10	10	China	6	3
Czech Republic	18	11	Serbia	10	7	Ecuador	1	1
Denmark	4	3	Switzerland	10	8	Egypt	1	0
Estonia	1	1	Tunisia	3	1	India	8	3
Finland	33	25	Turkey	22	12	Iran	8	4
France	18	15	Ukraine	8	6	Jordan	2	1
Germany	37	29	**TOTAL**	**68**	**44**	Kazakhstan	1	1
Greece	18	16				Kenya	1	0
Hungary	3	3				Korea, Republic of	1	1
Ireland	7	6				Malaysia	2	2
Italy	60	50				New Zealand	1	1
Latvia	2	2				Nigeria	5	2
Lithuania	5	4				Russia	2	2
Luxembourg	1	1				South Africa	1	1
Netherlands	13	11				Sudan	1	0
Poland	17	14				United States of America	8	7
Portugal	10	10				**TOTAL**	**56**	**36**
Romania	4	4						
Slovakia	1	1						
Slovenia	1	1						
Spain	64	48						
Sweden	3	3						
United Kingdom	50	48						
TOTAL	**392**	**325**						

Table 7: Applications received by country of research group (M19-36)

As might be expected, the highest numbers of applications have been received from countries with large populations, where there is a project partner, and where HPC use is well-established in the wider research community. The most applications came from the three countries with the longest history of

running Transnational Access programmes: Spain (64), Italy (60), and the UK (50). These were followed by other countries with project partners: Germany (37) and Finland (33). The latter stands out due to the large increase in application numbers (from just 6 in the previous 18-month period), and also because of the small population of Finland. This is probably due to the very strong links which CSC has with the scientific research community in Finland and their active promotion of the programme within their network.

The next highest number of applications came from Turkey (22), which was also a considerable increase compared to the previous 18-month period, when just 4 were received. This follows specific outreach activities targeted at the Turkish research community.

Next again came France and Greece (18 each), both of which have HPC-Europa3 partners, and the Czech Republic (also 18), which does not have an HPC-Europa3 partner. The increase in applications from the Czech Republic may be due to the growing HPC awareness in that country through the activities of the Czech national supercomputing centre, IT4Innovations (www.it4i.cz). IT4I is a PRACE Training Centre and HPC-Europa3 is in touch with them regularly to ask them to publicise the programme at their training courses.

Among the Associated States, 10 applications were received from each of Norway, Serbia and Switzerland. These are all countries with relatively small populations, but strong technological sectors.

Among the countries outside the EU and Associated States, the most represented countries are the United States of America (8 applications), perhaps not surprisingly, and developing countries which again have a strong technological focus: India (8), Iran (8) and China (6).

There continues to be a clear difference in the acceptance rates of applicants from EU countries (83%) and non-EU countries (65%), although the acceptance rate has increased for both Associated States and third countries since the previous 18-month period, when it was 48% and 53% respectively. We believe that the higher acceptance rate of EU applicants is due to a number of factors, e.g. researchers within the EU are more likely to be aware of the work of other research groups within the EU, and may already have research links between groups, which would make the identification of a suitable host easier. Applicants within the EU are likely to be better informed about the purpose and pre-requisites of the programme, and may be more used to writing research proposals in English.

The Regional Access Programme (see section 2.5.1) was established in HPC-Europa3 to lower the threshold for researchers with little or no HPC experience coming from the target countries. During this last 18-month period, the Regional Access centres, GRNET and KTH-PDC, have received 17 applications from these target countries. Of those applicants, 6 had some previous experience of HPC, although mostly this was modest, e.g. running on a local cluster with 700 cores, or having attended the PRACE/BioExcel seasonal school in 2019. These 6 applicants with some prior experience were all approved; 6 of the 11 who had no previous experience were also approved. This gives an acceptance rate of 55% for applicants from these target countries who had no previous experience of HPC or any similar programme. While significantly lower than the overall acceptance rate for the programme, this is still a much higher success rate than was seen for similar applicants in previous programmes where no such initiative existed. The acceptance rate for all applicants from these countries applying to all HPC-Europa3 centres was 77%, very close to the overall acceptance level.

4.3.2 Scientific discipline

As before, we can see that the highest number of applications come from the fields of physics (162) and chemistry (127) – disciplines in which the use of HPC and computational methods in general have long been used. However, there is a wide range of disciplines represented, and the proportion of applications coming from the life sciences and biotech industry has increased compared to the previous period. This is a field which is increasingly adopting HPC, especially in the areas of genomics, drug discovery and personalised medicine.

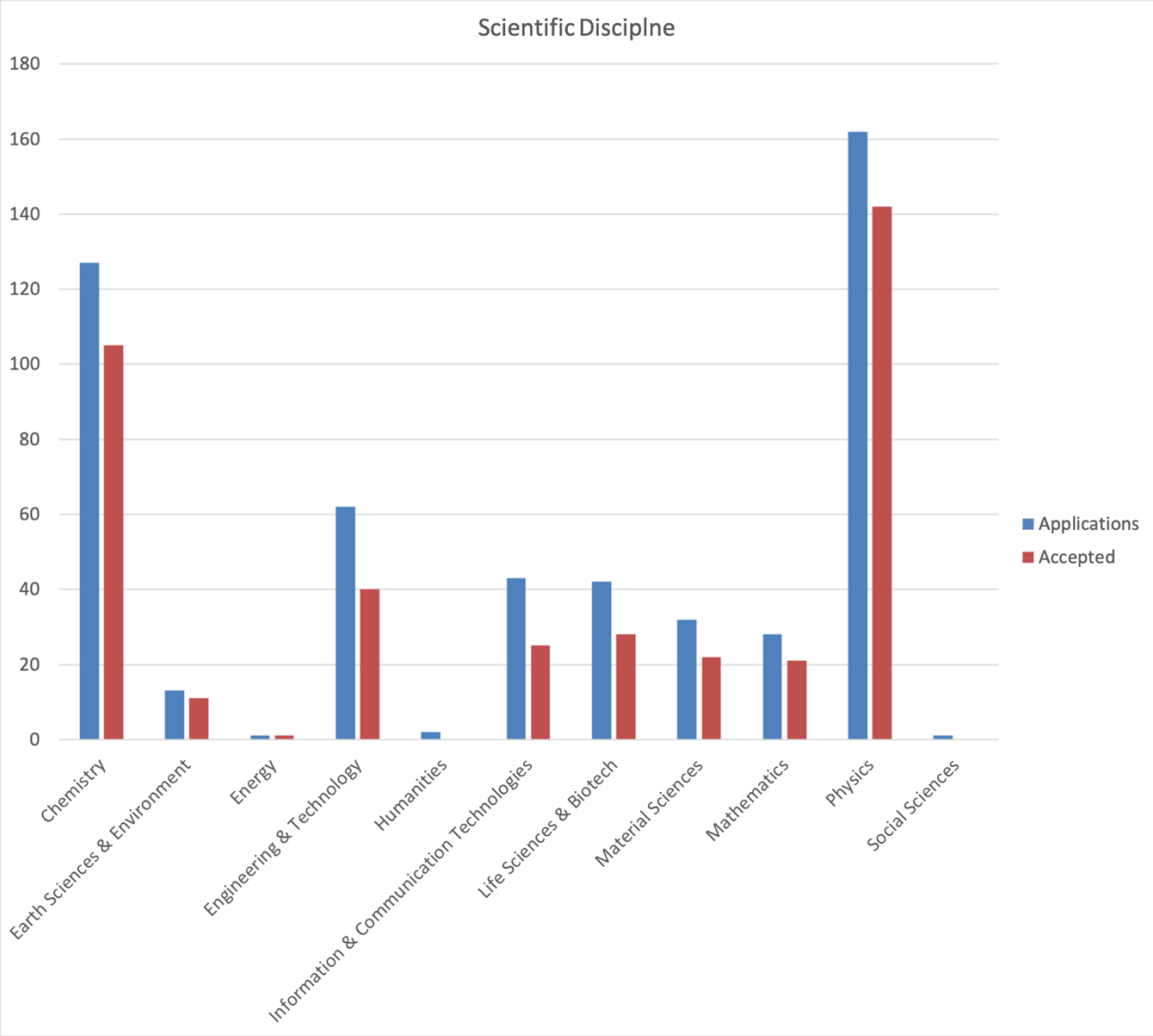


Table 8: Applicants by scientific discipline

4.3.3 Demographic information

4.3.3.1 Gender

In the first 18 months of the programme, we had seen female researchers account for 23% of applications and 25% of those accepted, which was a significant increase compared to previous programmes, where female participation had been around 16-20%.

It is encouraging to see that this trend has continued during Months 19-36, with female applicants accounting for 24% of the applications received, and 26% of those accepted, showing that females even have a slightly higher acceptance rate overall.

The higher proportion of female applicants in HPC-Europa3 is likely to indicate that there is now a greater number of female researchers working in computational science, as much has been done in recent years to promote careers in computational science, and STEM subjects in general, to young females. Further, in recent years there has been much greater uptake of HPC in the life sciences area, which has always been a discipline with higher numbers of female researchers than areas such as physics and chemistry, which have traditionally been – and still remain (as can be seen in Table 8) – the disciplines which make most use of HPC.

HPC-Europa3 always tries to ensure a balance of genders where possible in its outreach material.

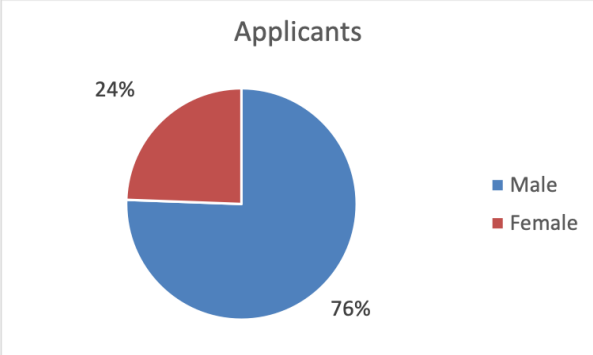


Table 9: Applicants by gender

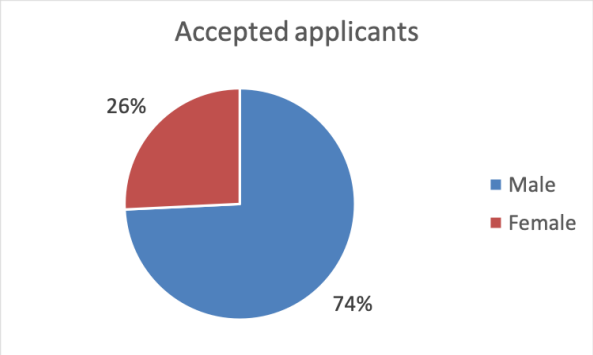


Table 10: Accepted applicants by gender

4.3.3.2 Age

The programme continues to attract applicants of all ages, at all stages of their research career.

Applicants ranged in age from 20 to 69. The mean age was 33, the median age 31, and the mode 27, both for applicants and for those accepted.

As before, the mean, median and mode ages continue to show that the "average" visitor is typically a senior post-graduate or post-doctorate researcher. This is discussed further in section 4.3.3.3 below.

4.3.3.3 Career stage

Applications continue to come from a roughly equal split of postgraduate students, postdoctoral researchers and experienced researchers, although compared to the previous 18-month period there has been a slight increase in the proportion of postgraduates, who now represent 41% of applicants, and a slight decrease in the proportion of experienced researchers. There has also been an apparent

increase in the number of undergraduates applying (and being approved, with 10 out of 12 being accepted). Few undergraduates apply as they usually lack experience of carrying out independent research and it is rare for them to be working at a level which would lead to publications in refereed journals. Further, the teaching-focused structure of the academic year does not lend itself towards undergraduate visits. Most of those who classed themselves as undergraduates were senior students working towards a research Master's qualification.

There was almost no difference in terms of the percentage of applicants and of those accepted in terms of career stage, so only the chart showing applicants has been included.

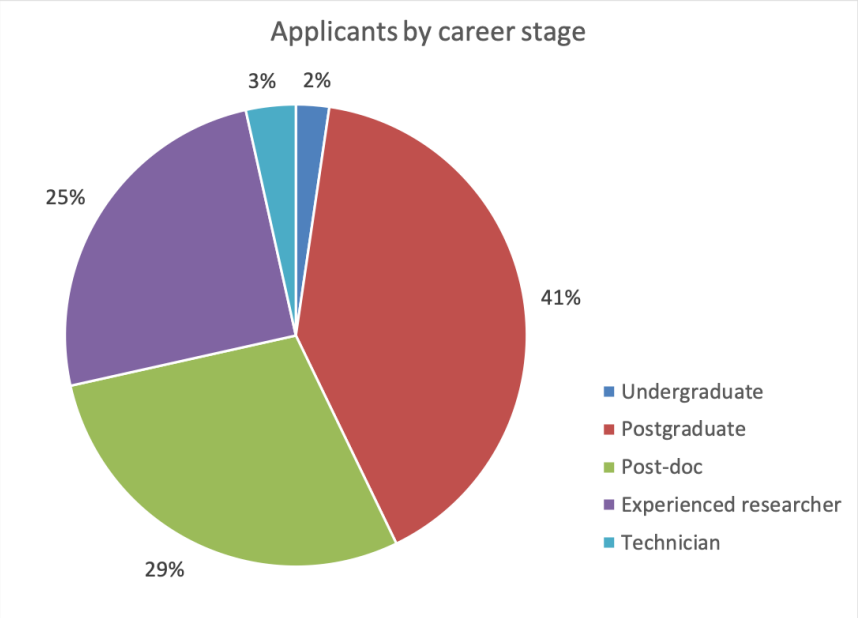


Figure 3: Applicants by career stage

As mentioned in section 4.3.3.2 above, the mean, median and mode ages continue to show that the "average" visitor is typically a senior post-graduate or post-doctorate researcher. Within this age group and at this career stage, applicants have typically acquired suitable research and computing skills and are able to work independently, while still having the flexibility to be able to spend a period of time abroad – unlike more senior researchers who might have to make complex arrangements around work or family commitments.

5 Visit Feedback

Both visitors and hosts are asked to complete a questionnaire at the end of each visit. During this reporting period, 203 visitor questionnaires and 115 host questionnaires have been returned.

5.1 Visitor questionnaires

Visitors continue to report a very high level of satisfaction with the programme, with only 1 of the 203 respondents saying they were *dissatisfied* and that they would not recommend the programme. The remainder were *satisfied* (16%) or *very satisfied* (83%) with the experience overall.

While some visitors reported dissatisfaction with individual issues in their questionnaires, very few reported that they were *dissatisfied* with more than 2 issues, and often these were related (e.g. different aspects of availability of software on the HPC systems).

The most often cited reasons for dissatisfaction related to accommodation: the general difficulties in finding accommodation before arriving in the host city, and the lack of availability of reasonable accommodation within the budget. Following a recent contract amendment which saw a reduction in the target number of visitors, the living and accommodation allowance per visitor has now increased, so this will help to alleviate this issue. Even though this was the single greatest cause of dissatisfaction, only 6% of visitors said they were *dissatisfied* or *very dissatisfied* about the accommodation situation.

In all other respects, satisfaction levels were at 96% or higher. The few cases of dissatisfaction mainly arose from isolated incidents, some of which were outside the control of HPC-Europa3.

It is important to note that 99.5% of respondents were *satisfied* or *very satisfied* with their experience, even in cases where they had reported dissatisfaction with specific issues, such as the level of funding provided, or the panel having granted a reduced amount of compute time or reduced visit length.

There are many extremely positive comments to be found in the questionnaires, and we will continue to select some of these as visitor testimonials to be used to promote the programme.

5.2 Host questionnaires

Hosts also report a high level of satisfaction, with 98% saying that they were *satisfied* or *very satisfied* overall with the visits which they have hosted (with 84% saying that they were *very satisfied*).

Only one host reported being *very dissatisfied* overall, and this was due to a specific issue with the visitor misappropriating data from the host laboratory. One other was *dissatisfied* overall, and this was due to the lack of collaborative research that was carried out. It is important to note that both of these hosts have said that these visits were atypical of their experience of HPC-Europa3 and that they would be happy to host further visitors in the future. (“Most other visits are successful. This one did not work as planned.”)

97% of respondents rated the scientific value of the work performed during the visit as *good* or *excellent*, with 3 stating that it was *poor*. Of these, 2 were the hosts who had said they were *(very) dissatisfied* overall, as detailed above, while in another case it was due to cultural differences between

the research groups ("The visitor comes from a group where the fast production of results for publications is apparently more important than a deeper understanding of the science. It took quite some time to convince him of slowing down and carefully checking methodologies and results.")

96% of respondents rated the visits as *useful* or *very useful* to their department, with 94% saying that there was *definitely* or *maybe* potential for future collaboration with the visitor's group.

100% of respondents said that their relationship with the HPC-Europa3 team was *satisfactory* or *very satisfactory*.

Only one respondent did not wish to host another visitor in the future, and this was due to lack of time (student supervision and upcoming period to be spent abroad).

We have already used some quotes from host questionnaires to publicise the programme, especially when promoting it to potential hosts. We will continue to select comments from questionnaires for this purpose.

6 Research Highlights

HPC-Europa3 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 the host researcher, or someone from their group, goes to the visitor's group), with or without HPC-Europa3 funding.

6.1 Journal publications and conference proceedings

With 379 visits now completed, we are already aware of 101 publications and conference presentations which have acknowledged HPC-Europa3. 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, or even later. Previous experience suggests that the research enabled by the programme continues to lead to publications for 2-3 years after the visits, and so this often means after the programme has ended. Therefore, these lists are never totally representative of the full scientific output of the programme.

We are also currently aware of some visitors who had had papers accepted for conferences which have been postponed due to the Covid-19 pandemic, and so they have not yet included the details of these papers in the HPC-Europa3 database.

Visitors have highlighted the following publications which they believe to be particularly important:

Revisiting Kekulene: Synthesis and Single-Molecule Imaging, *Iago Pozo, Zsolt Majzik, Niko Pavliček, Manuel Melle-Franco, Enrique Guitián, Diego Peña, Leo Gross, Dolores Pérez*, J. Am. Chem. Soc. 2019, 141, 39, 15488-15493, https://doi.org/10.1021/jacs.9b07926

> Prof. Manuel Melle-Franco (University of Aveiro, Portugal) was the visitor; Dr. Diego Peña (CiQUS, Spain) was the host.
>
> Manuel says, "The article we made from my visit to CiQUS in Spain was published in one of the top chemistry broad Journals (JACS) and had quite a lot of impact, with a few newspaper articles, appeared in several blogs and so-on".

Preferential Positioning, Stability, and Segregation of Dopants in Hexagonal Si Nanowires, *Michele Amato, Stefano Ossicini, Enric Canadell, and Riccardo Rurali*, Nano Lett. 19, 866 (2019), https://pubs.acs.org/doi/10.1021/acs.nanolett.8b04083

Prof. Michele Amato (Université Paris-Sud, France) was the visitor; Dr. Riccardo Rurali (ICMAB-CSIC, the Institute of Materials Science of Barcelona) was the host.

Riccardo says that Nano Letters is a prestigious journal, "almost as high as one can go without experiments".

6.2 Long-term collaborations

In this 18-month period, 31 applicants successfully submitted applications for follow-up visits to a host researcher with whom they had already had an HPC-Europa3 visit.

Some reciprocal visits have also been funded, e.g. between Miguel Caro (Aalto University) and Volker Deringer (formerly University of Cambridge, now University of Oxford). This extremely productive collaboration is the focus of D9.1, the CSC Transnational Access success story[30].

We continue to see visitors securing research positions in their former host departments. Examples include:

- Ana Dobrota, formerly of the University of Belgrade (Serbia), who started a post-doctorate position in the group of her former host, Prof Natalia Skorodumova of Materials Science and Engineering at KTH (Sweden);
- Giuseppe Negro, formerly of the University of Bari (Italy), who secured a post-doctorate research post in the School of Physics and Astronomy at the University of Edinburgh (UK), where his two HPC-Europa3 visits were hosted;
- Pavel Janoš, formerly of Masaryk University (Czech Republic), who secured a position in Trieste (Italy), where he was hosted during his visit.

We have also seen visitors return to their host groups for follow-on research visits with alternative funding. One example is Javier Gallego Sánchez (University of Alicante), who returned to his former host group in the School of Informatics at the University of Edinburgh for a further 6-month visit, with funding from the Spanish government's Centre for Industrial and Technological Development[31].

Some visitors and host researchers have contacted us to inform us of research highlights arising from their visits. In some cases the visits took place in the previous reporting period, but these highlights relate to subsequent development of the collaboration after the visits.

Project title: Interaction of intense field with matter and gamma ray source

Visitor: Jian Fuh Ong (Extreme Light Infrastructure - Nuclear Physics (ELI-NP) International Research Center, Romania)

Host: Dr. Vasilis Dimitriou (Hellenic Mediterranean University, Greece)

"Jian Fuh ONG was introduced to the Institute of Plasma Physics and Laser (IPPL) of the Hellenic Mediterranean University in Greece by HPC-Europa3, by the help of GRNET High Performance

[30] https://b2share.eudat.eu/api/files/2d819a8f-f92c-4188-8aa6-e85fc810918b/HPCE3_D9.1_CSC_Success_story_v2.0.pdf
[31] See p.17 of EPCC News issue 85: https://www.epcc.ed.ac.uk/sites/default/files/EPCC%20News%2085.pdf

Computing Services, before the application. He was hosted in IPPL in June and September 2019 when a strong collaboration was established and led to the signing of an MoU between IPPL-HMU and ELI-NP. This collaboration continues by the support of the Action TUMMIE CA17126 - STSM ECOST-STSM-Request-CA17126-46042 grant. It brought us back together to continue our work on accelerators simulations with PIC codes for IPPL-HMU and ELI-NP. The research work we perform will be submitted for publication in the *"Special issue on high field laser-plasma interactions 2020"* of the Journal Plasma Physics and Controlled Fusion."

Project title: Coupling molecular-driven cooling and multi-phase star formation

Visitor: Dr. Umberto Maio (Leibniz Institute for Astrophysics, Germany)

Host: Prof. Stefano Borgani (University of Trieste, Italy)

"We used numerical hydrodynamical simulations coupling non-equilibrium molecular chemistry, multi-phase star formation and feedback effects from different stellar populations and multifrequency radiative transfer to investigate early structures and, in particular, the formation path of early supermassive black holes within primordial galaxies.

We found that massive black-hole seeds, of the order of hundreds of million solar masses, might originate from direct collapse of pristine gas in primordial quiescent mini-haloes exposed to powerful nearby stellar radiation (DCBHs). On the contrary, commonly known standard stellar-origin black holes are unlikely to be reliable seeds of supermassive black holes, because they are too small and hence are not able to accrete significant amounts of material from neighbouring regions. The difference among the possible scenarios can be verified by comparing the predicted gas temperature maps in the first half billion years (redshift z=9) for a model with powerful primordial stars (Figure) and a model with standard stellar sources (Figure). In the former case, powerful radiation from the first stars heats cosmic gas up to 10 thousand Kelvin and dissociates molecules. This allows gas in three pristine haloes to collapse and form a massive black hole. In the latter case, radiation from standard stars are not able to heat significantly the surrounding medium, therefore gas in pristine haloes fragments and forms small cold clumps, without being able to generate any massive black-hole seeds. By a closer inspection, we also found that early DCBH host candidates show little molecular content, Lyman-Werner intensities around 1-50 J_21, turbulent motions and the possible occurrence of substructures. Such information on the complex features of the local environment highlight that a very fine balance between chemistry evolution and radiative transfer must be reached in order to form a massive black-hole seed in early times. Nevertheless, this study opens up the opportunity to better understand the processes leading to the formation of such important objects in the cosmic history and the role of early stellar populations in primeval epochs."

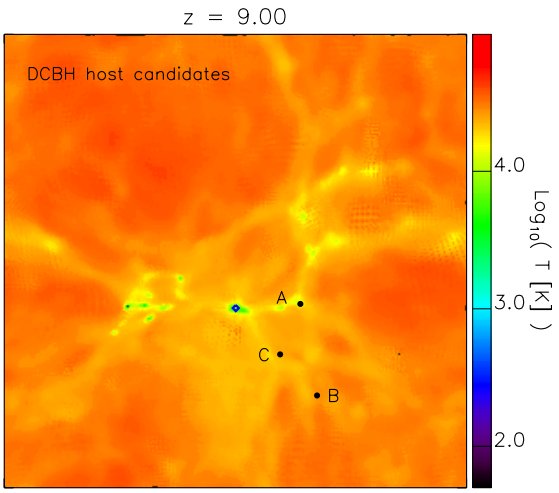


Figure 4

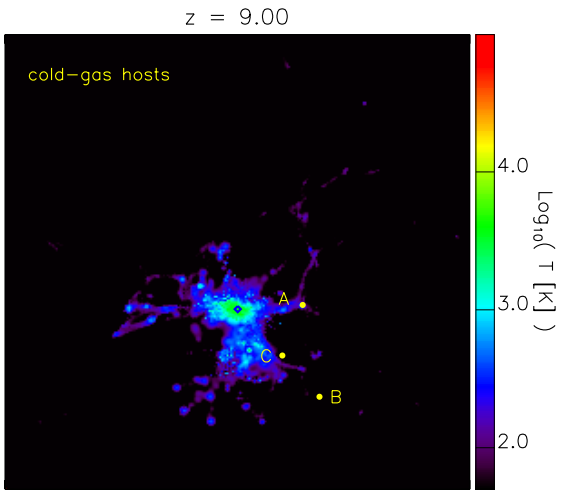


Figure 5

Project title: On the connection between cluster cool-coreness and cosmological shock waves

Visitor: Dr. Susana Planelles (University of València, Spain)

Host: Prof. Stefano Borgani (University of Trieste, Italy)

"Cosmological shock waves, developed as a consequence of the formation and evolution of cosmic structures, play a main role in the energetic balance of the intergalactic medium. In this project we analyse the distribution of shock waves in a sample of 29 galaxy clusters obtained from a set of simulations performed with the code GADGET-3. The simulations include, besides some other physical processes, a prescription for AGN feedback. A grid-based shock-finding algorithm is applied in post-processing to the outputs of the simulations. Besides the dependencies of the shock distribution on cluster mass, redshift (Figure) and baryonic physics, we also analyse in detail its connection with the clusters' core (CC/NCC) and global dynamical state (regular/disturbed). In agreement with previous works, we confirm the fact that internal low-Mach number shocks fill most of the computational volume and process most of the total thermal energy flux. According to cluster core properties, the shock distribution does not show any relevant difference between CC and NCC clusters. However, we find a mild dependence of the radial distribution of the shock Mach number on the clusters' dynamical state, with disturbed systems showing higher shock strengths than regular ones throughout the clusters' volume (Figure)."

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 730897.

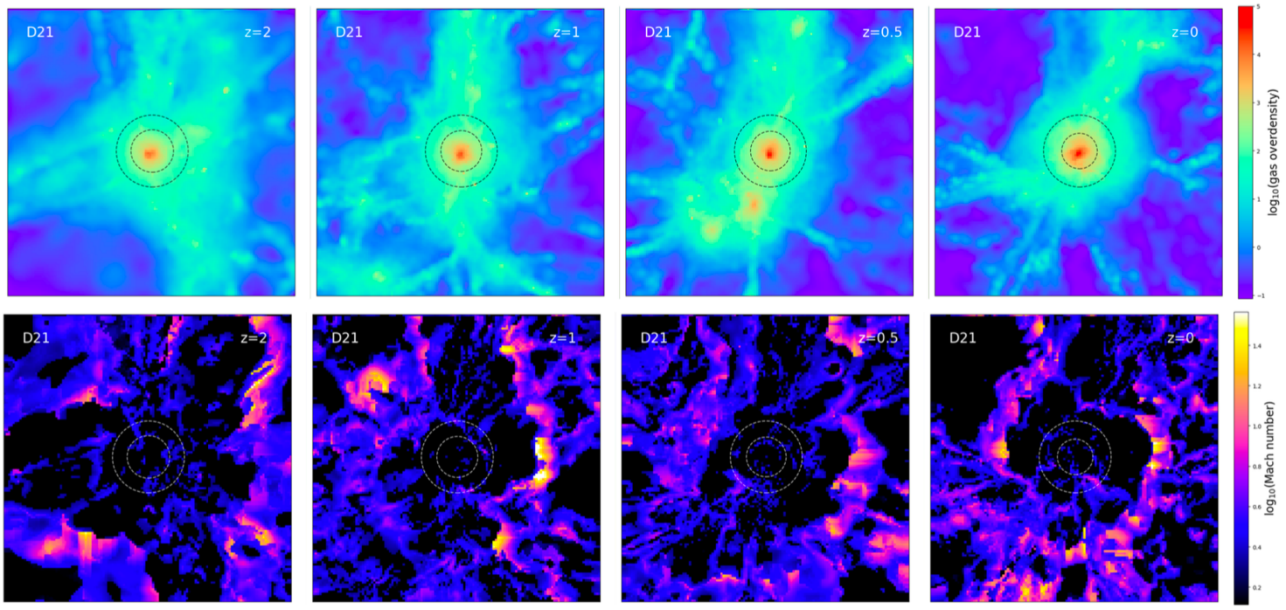


Figure 6: 2-D projections of the gas overdensity (upper panels) and the Mach number distribution (lower panels) around one massive cluster in our sample at different redshifts (from left to right, z =2, 1, 0.5 and 0). Each map, projected along the z-axis and centred on the cluster position, has a length of 8XRvir at each redshift. Circles on the maps represent, respectively, R500 and Rvir of the central cluster.

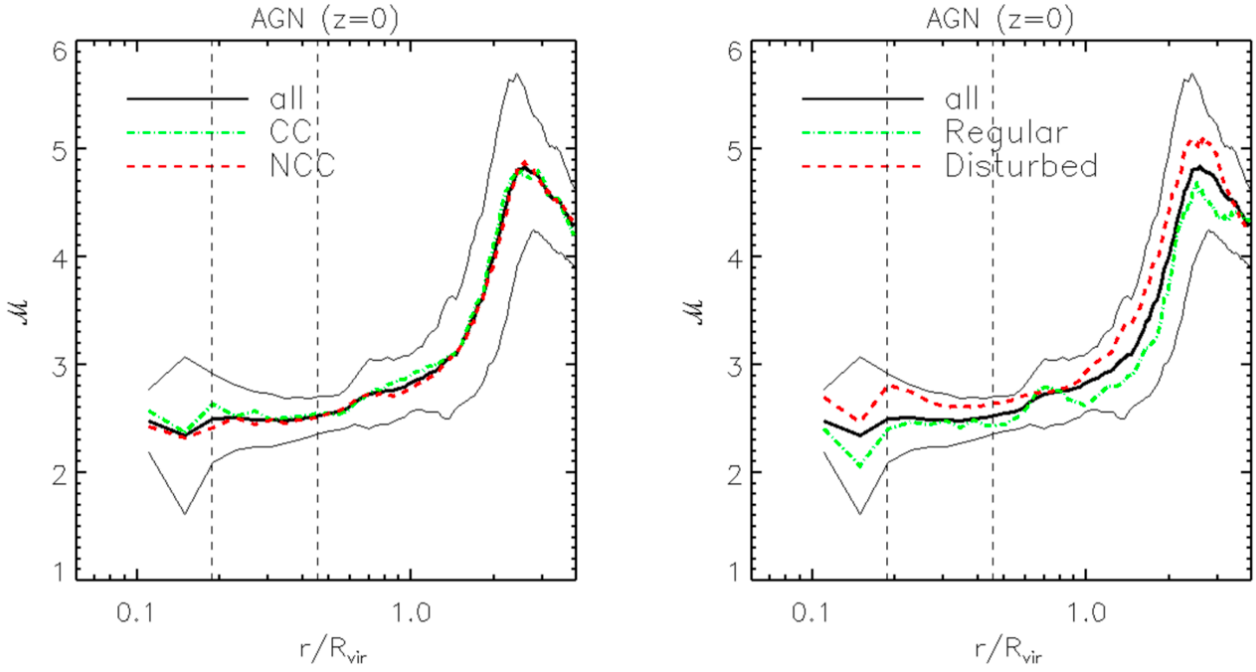


Figure 7: Radial profiles of the mean Mach number for the whole sample of 29 clusters at z = 0 (thick black continuous lines in both panels). Results for the subsamples of CC/NCC and for the regular/disturbed clusters are also shown. Thin black continuous lines in both panels represent 1-σ standard deviation around the mean global profile.

Project title: Role of Sialylation in Epidermal Growth Factor Receptor Deregulation

Visitor: Mr. Mykhailo Girych (University of Helsinki, Finland)

Host: Dr. Ünal Coskun (TU Dresden, Germany)

Mykhailo's visit to Dr. Coskun's lab continued an ongoing collaboration between the University of Helsinki and TU Dresden, investigating human epidermal growth factor receptor (EGFR), which is one of the most significant cancer-related membrane proteins. The host, Dr. Coskun, and the visitor's Ph.D. supervisor, Prof. Ilpo Vattulainen, emphasise the importance of this research, which is expected to have "a massive impact in biomedicine". Background information about this research can be found at:

https://www.gauss-center.de/results/life-sciences/article/unlocking-the-role-of-lipids-in-the-activation-mechanism-of-the-epidermal-growth-factor-receptor-egf/ (article from 2015), and

https://www.gauss-center.de/results/life-sciences/article/revealing-the-mechanism-underlying-the-activation-of-the-insulin-receptor/ (article from 2020).

7 Second Transnational Access Meeting (TAM)

The second HPC-Europa3 user group meeting, TAM – the **T**ransnational **A**ccess **M**eeting – was due to take place in Barcelona on 31st March 2020, with 24 talks scheduled and an additional 14 poster presentations accepted. However, due to the Covid-19 pandemic, this meeting had to be postponed, and is now provisionally scheduled to take place on 23rd October 2020 instead.

8 Conclusion

We can see that the HPC-Europa3 programme is running very smoothly, with very high levels of satisfaction among the participants – both visiting and host researchers – and with many high-level scientific results arising. In particular:

- Applications have been received from a very wide range of countries and scientific disciplines. Visitors come from a wide age range and a mix of different career stages. Female researchers are well represented, bearing in mind that females are less well represented in STEM research careers generally.
- The Regional Access Programme is benefitting the people at whom it is aimed, lowering the threshold for acceptance for new/early HPC users from target countries.
- While visit numbers are still well below target, application numbers increased significantly for the most recent Call for Applications.
- Approximately half of the minimum compute resources to be provided have now been allocated, with many visitors receiving more than the average allocation of time (other visitors' requirements are well below the average amount). The average compute time used per visitor has increased during this reporting period, and we expect that it will increase again in the coming period.
- Visitors and hosts alike report extremely high levels of satisfaction with the programme.
- Visits are giving rise to growing numbers of high-quality scientific outputs, and are helping researchers to build their careers.

However, there is still a significant shortfall in the number of visits, and only at the most recent closing date was there a marked increase in application numbers. We hope that application numbers will continue to be higher from now on, as a result of the determined efforts of the project partners, combined with a general raised awareness of the programme resulting from the growing number of participants and the increasing numbers of scientific results which can be disseminated. We have seen in this report that it would still be possible to meet the target number of visitors if we can sustain even 80% of the number of applications received for the last call for the remaining calls.

The Covid-19 pandemic also presents a major risk, and has already had an impact on the programme, with the postponement of the TAM, some visits curtailed and others prolonged due to restrictions on travel, and all upcoming visits currently postponed indefinitely. We expect that application numbers may drop in the short-term due to the uncertainty surrounding when international travel might again be possible, although we are working to reassure applicants that visit dates are currently flexible. We are currently discussing various mitigation strategies, while monitoring the developing situation.

Over the coming months, then, we will continue to work hard on publicising the programme, with a particular focus on the following:

- Reaching new researchers who might be aware of the programme:
  - Focusing on under-represented countries and disciplines;
  - Identifying leading research groups in relevant fields who have not participated in the programme yet.
- Strengthening links with the host community:
  - Reminding hosts to encourage possible collaborators to apply to visit them, and to publicise the programme within their departments and to their wider network of contacts.
- Creating more material to publicise the programme:
  - Recording more visitor videos and publicising them on social media, as posts with images, and especially videos, tend to have a higher engagement rate;
  - Creating new targeted marketing material for people in identified groups (e.g. identified countries or disciplines), featuring previous visitors from the same demographic.
- Disseminating the results:
  - All scientific outputs, career moves, and other results will be disseminated widely by the project and the individual partners.

In conclusion, the programme continues to be extremely successful, demonstrably bringing great benefits to almost everyone who participates, either as visitors or host researchers. However, application numbers have continued to be low, and there is a large shortfall of visits to make up during the final 18 months of the programme. Nevertheless, the number of applications received for the last call increased significantly, and sustaining 80% of this number of applications for the remaining calls would allow us to meet our targets. However, a final uncertainty in this period is the effect of the Covid-19 pandemic, which is still an evolving situation, and the consortium is discussing how best to mitigate the risks which this raises.

Annex I: List of publications and conference proceedings

The following publications and conference proceedings acknowledged the support of HPC-Europa3.

1. B. Köpcke, M. Steuwer, S. Gorlatch “Generating Efficient FFT GPU Code with Lift”, FHPNC@ICFP 2019: 1-13.
2. V. L. Deringer, M. A. Caro, R. Jana, A. Aarva, S. R. 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.
3. 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]
4. V. Ribić, A. Dapčević, N. Skorodumova, A. Rečnik, D. Luković Golić, G. Branković, "Structure characterization of Gd doped BiFeO3", 3rd International Meeting on Materials Science for Energy Related Applications, 25-26 September 2018, Belgrade, Serbia.
5. V. Ribić, A. Dapčević, N. Skorodumova, A. Rečnik, D. Luković Golić, Z. Branković and G. Branković, “First-Principles Calculation of Gd - doped BiFeO3”, European HPC Summit Week 2018 - #EHPCSW, May 28th to June 1st 2018, Ljubljana, Slovenia.
6. V. Ribić, N. Skorodumova, A. Dapčević, A. Rečnik, D. Luković Golić, Z. Branković, G. Branković, “Microscopic and Computational Study of Gd-doped BiFeO3”, 5th Conference of The Serbian Society for Ceramics Materials, pp. 112, 11. - 13. Jun 2019, Belgrade, Serbia.
7. V. Ribić, A. Dapčević, N. Skorodumova, A. Rečnik, D. Luković Golić, G. Branković, "DFT screening of Gd as a dopant in the BiFeO3 superlattice", HPC-Europa Transnational Access Meeting (TAM 2018), 23 October 2018, Edinburgh, UK.
8. J.A. Acebrón, J.R. 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", Computers & Mathematics with Applications, Feb 2020.
9. A. Bonanno, E. Corsaro, F. Del Sordo, P.L. Pallé, D. Stello, M. Hon, “Acoustic oscillations and dynamo action in the G8 sub-giant EK Eridani” Astronomy & Astrophysics, Volume 628, 2019.
10. G. Guerrero, F. Del Sordo, A. Bonanno, P.K. Smolarkiewicz, “Global simulations of Tayler instability in stellar interiors: the stabilizing effect of gravity” Monthly Notices of the Royal Astronomical Society, Volume 490, Issue 3, p.4281-4291, 2019.
11. L. Bellentani, P. Bordone, X. Oriols, A. Bertoni, “Coulomb and exchange interaction effects on the exact two-electron dynamics in the Hong-Ou-Mandel interferometer based on Hall edge states”, arXiv:1903.02581v2 [cond-mat.mes-hall] (2019)
12. L. Bellentani, E. Colomes, Z. Zhan, P. Bordone, A. Bertoni, and X. Oriols, Talk at IW2 seminar at IWCN 2019 (Evanston): “On the Incompatibility Between Frensley’s Inflow Boundary Conditions and Stationary Wigner Distribution Functions: The Problem and the Solution” (http://www.iue.tuwien.ac.at/iwcn2019/wp-content/uploads/2019/05/IW2-2019-Book-of-Abstracts-May-17.pdf)
13. D. Pandey, L. Bellentani, M. Villani, G. Albareda, P. Bordone, A. Bertoni and X. Oriols, "A Proposal for Evading the Measurement Uncertainty in Classical and Quantum Computing: Application to a Resonant Tunneling Diode and a Mach-Zehnder Interferometer", Appl. Sci. 2019, 9(11), 2300.
14. L. Bellentani, P.o Bordone, X. Oriols, and A. Bertoni, Invited Talk at WHPTCAD seminar at IWCN 2019 (Evanston): “Parallel implementation of the Split-Step Fourier method for exact two-electron dynamics in Hall interferometers” (http://www.iue.tuwien.ac.at/iwcn2019/wp-content/uploads/2019/05/WHPTCAD-2019-Book-of-Abstracts-May-17.pdf)
15. U. Maio, S. Borgani, B. Ciardi, M. Petkova, “The seeds of supermassive black holes and the role of local radiation and metal spreading”, eprint arXiv:1811.01964, http://adsabs.harvard.edu/abs/2018arXiv181101964M.

16. L.K. Scarbath-Evers, M. Todorović, D. Golze, R. Hammer, W. Widdra, D. Sebastiani, and P. Rinke, “Gold diggers: Altered reconstruction of the gold surface by physisorbed aromatic oligomers”, Phys. Rev. Materials 3, 011601(R), 2019.
17. F. Perini, S. Busch, K. Zha, E. Kurtz, R.D. Reitz, "Piston Bowl Geometry Effects on Combustion Development in a high-speed light-duty Diesel Engine" submitted to SAE ICENA2019 conference.
18. F. Perini, S. Bna, E. Pascolo, I. Spisso, R.D. Reitz, "Robust preconditioning techniques for iterative solvers in scalable engine simulations using FRESCO", International Multidimensional Engine Modeling Meeting 2019, Detroit, MI, USA.
19. E. Rodriguez-Gutiez, A. Moreton-Fernandez, A. Gonzalez-Escribano, and D.R. Llanos, “Toward a BLAS library truly portable across different accelerator types. The Journal of Supercomputing”, 75(11), 7101–7124, 2019. https://doi.org/10.1007/s11227-019-02925-3.
20. A. Miró, M. Soria, C. Moulinec, J.C. Cajas, and Y. Fournier, “Numerical investigations on rectangular and circular synthetic jet impingement”. In Tenth International Conference on Computational Fluid Dynamics (ICCFD10) (pp. 1–18) (2018). Barcelona.
21. A. Miró, “Flow and Heat Transfer of Impinging Synthetic Jets,” Universitat Politècnica de Catalunya, 2019.
22. M. Ziegler-Borowska, K. Mylkie, M. Kozlowska, P. Nowak, D. Chelminiak-Dudkiewicz, A. Kozakiewicz, A. Ilnicka, A. Kaczmarek-Kedziera, “Effect of Geometrical Structure, Drying, and Synthetic Method on Aminated Chitosan-Coated”, Magnetic Nanoparticles Utility for HSA Effective Immobilization Molecules, 2019, 24, 1925-1942, DOI: 10.3390/molecules24101925.
23. M. Ziegler-Borowska, K. Mylkie, M. Kozlowska, P. Nowak, D. Chelminiak-Dudkiewicz, A. Kozakiewicz, A. Ilnicka, and A. Kaczmarek-Kedziera, “Effect of Geometrical Structure, Drying, and Synthetic Method on Aminated Chitosan-Coated Magnetic Nanoparticles Utility for HSA Effective Immobilization”, Molecules, vol 24, 2019, 10, 1925, https://www.mdpi.com/1420-3049/24/10/1925.
24. V.L. Deringer, M.A. Caro, G. Csányi: "Machine Learning Interatomic Potentials as Emerging Tools for Materials Science". Adv. Mater. 2019, 1902765 (DOI: 10.1002/adma.201902765).
25. V. Daskalakis, S. Maity, C.L. Hart, T. Stergiannakos, C.D.P. Duffy, and U. Kleinekathöfer, “Structural Basis for Allosteric Regulation in the Major Antenna Trimer of Photosystem” II (2019) J. Phys. Chem. B, 123, 45, 9609-9615.
26. S. Maity, A. Gelessus, V. Daskalakis, U. Kleinekathoefer, “On a Chlorophyll-Carotenoid Coupling”, in LHCII (2019) Chem. Phys. 526, 110439.
27. V. Daskalakis, S. Papadatos, U. Kleinekathoefer, “Fine tuning of the photosystem II major antenna mobility within the thylakoid membrane of higher plants” (2019) Biochim. Biophys. Acta – Biomembranes, 1861, 183059.
28. D.M. Onchis, C. Istin, P. Real, “Refined Deep Learning for Digital Objects Recognition via Betti Invariants” In: Vento M., Percannella G. (eds) Computer Analysis of Images and Patterns. CAIP 2019. Lecture Notes in Computer Science, vol 11678 (2019). Springer, Cham DOI https://doi.org/10.1007/978-3-030-29888-3_50.
29. M. Darian, O. Codruta Istin, C. Tudoran, M. Tudoran and P. Real, “Timely-Automatic Procedure for Estimating the Endocardial Limits of the Left Ventricle Assessed Echocardiographically” in Clinical Practice, Diagnostics Journal IF 2.489, Diagnostics 2020, 10(1), 40; https://doi.org/10.3390/diagnostics10010040.
30. N. Shukla et al “Relativistic collisionless shocks: microphysics and long-term dynamics”, under preparation to Physical Review Letters.
31. L.N. Carenza, G. Gonnella, A. Lamura, G. Negro and A. Tiribocchi, Eur. Phys. J. E (2019) 42: 81.
32. L.N. Carenza, G. Gonnella, D. Marenduzzo, G. Negro, Proc. Natl. Acad. Sci. 116, 22065 (2019).
33. M.A. Caro, “Optimizing many-body atomic descriptors for enhanced computational performance of machine learning based interatomic potentials”, Phys. Rev. B 100, 024112 (2019).
34. V.L. Deringer, M.A. Caro, G. Csányi. “Machine Learning Interatomic Potentials as Emerging Tools for Materials Science”, Adv. Mater., 1902765 (2019).

35. G. Ódor, J. Kelling and G. Deco, “The effect of noise on the synchronization dynamics of the Kuramoto model on a large human connectome graph” Accepted in Journal of Neurocomputing. preprint : arXiv:1912.06018.
36. A. Ortolani, G. Persico, J. Drofelnik, A. Jackson, M.S. Campobasso, “Cross-comparative analysis of loads and power of pitching floating offshore wind turbine rotors using frequency-domain Navier-Stokes CFD and blade element momentum theory”, TORQUE Conference, The Netherlands, 2020. Under review.
37. A. Ortolani, G. Persico, J. Drofelnik, A. Jackson, M.S. Campobasso, “High-Fidelity Calculation of Floating Offshore Wind Turbines Under Pitching Motion”, paper GT2020-15552, ASME Turbo Expo Technical Congress, 22nd-26th June 2020, London, United Kingdom.
38. V. Cikojević, L. Vranješ Markić, and J. Boronat. "Finite-range effects in ultradilute quantum drops." arXiv preprint arXiv:2001.09086 (2020).
39. M. Wouters, O. Aouane, T. Krüger, and J. Harting, “Mesoscale simulation of soft particles with tunable contact angle in multicomponent fluids”, Physical Review E. 100(3) 033309; https://doi.org/10.1103/PhysRevE.100.033309; 2019.
40. M. Amato, S. Ossicini, E. Canadell, R. Rurali, “Preferential Positioning, Stability, and Segregation of Dopants in Hexagonal Si Nanowires”, Nano Lett. 192, 866-876 (2019).
41. E. Postek, Y. Schneider, S. Schmauder, “Impact of WC/Co/diamond sample with peridynamics”, SCFE2019, Supercomputing Frontiers Europe 2019, 2019-03-11/03-14, Warsaw (PL), pp.1-4, 2019.
42. F.S. Broekgaarden, S. Justham, S.E. de Mink, J. Gair, I. Mandel, S. Stevenson, ... & C.J. Neijssel, “STROOPWAFEL: Simulating rare outcomes from astrophysical populations, with application to gravitational-wave sources”. Monthly Notices of the Royal Astronomical Society, 490(4), 5228-5248, 2019.
43. F.A. Gent, B. Snow, V. Fedun and R. Erdelyi, “Modelling 3D magnetic networks in a realistic solar atmosphere", arXiv e-prints, 2019, 1904.11421, https://ui.adsabs.harvard.edu/abs/2019arXiv190411421G.
44. S. Dotolo, A. Facchiano, A. Pandini, “Comparative analysis of molecular motions in SIRTUIN2 proteins”. On Abstract book. BBCC 18-20, December 2017.
45. 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.
46. S. Dotolo, A. Facchiano, “Natural-bioactive compounds study by means of bioinformatics approaches”. On Abstract book. BITS 5-8 July 2017.
47. 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."
48. L. Gianguzzi, G. Bazan. 2019. The Olea europaea L. var. sylvestris (Mill.) Lehr. forests in the Mediterranean area. Plant Sociology 56(2): 3-34. DOI 10.7338/pls2019562/01
49. V.L. Deringer, M.A. Caro, R. Jana, A. Aarva, S. R. 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.
50. 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.
51. A. Iravani, “Simulation of dynamic fracturing in rock like materials - Fines creation from branching-merging of blast loaded cracks in general and in cylindrical specimens”, Ph.D. thesis, Montanuniversität Leoben, 2020.
52. 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
53. R.J.F. Berger, A. Viel, “The principle underlying antiaromaticity”, eprint arXiv:1811.08959, 11/2018, ARXIV, Physics - Chemical Physics, 2018arXiv181108959B.

54. 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
55. L. Kos, R.A. Pitts, G. Simic, M. Brank, H. Anand, W. Arter, "SMITER: A field-line tracing environment for ITER", Fusion Eng. and Design (2019), DOI:10.1016/j.fusengdes.2019.03.037, arXiv:1903.11547
56. T.P. Rossi, T. Shegai, P. Erhart, T.J. Antosiewicz, "Strong plasmon-molecule coupling at the nanoscale revealed by first-principles modelling", Nature Communications 10, 3336 (2019).
57. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, "Dynamics of Phase Separation from Holography" Submitted at Journal of High Energy Physics, arXiv:1905.12544 [hep-th].
58. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, (2019). Dynamics of Phase Separation from Holography (Version v20190203) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.2195952.
59. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, (2019). Dynamics of Phase Separation from Holography (Version v20190307) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.2586614.
60. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, (2019). Dynamics of Phase Separation from Holography (Version v20190326) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.2607897.
61. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, (2019). Dynamics of Phase Separation from Holography (Version v20190204) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.2556556.
62. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, (2019). Dynamics of Phase Separation from Holography (Version v20190207) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.2559260.
63. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, (2019). Dynamics of Phase Separation from Holography (Version v20190228) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.2580088.
64. M. Attems, Y. Bea, J. Casalderrey-Solana, D. Mateos, M. Zilhão, (2019). Dynamics of Phase Separation from Holography (Version v20190513) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.2784400.
65. I. Rodríguez-Espigares, M. Torrens-Fontanals, J.K.S. Tiemann, D.Aranda-García, J.M. Ramírez-Anguita, T.M. Stepniewski, N. Worp, A. Varela-Rial, A. Morales-Pastor, B. Medel Lacruz, G. Pándy-Szekeres, E. Mayol, T. Giorgino, J. Carlsson, X. Deupi, S. Filipek, M. Filizola, J.C. Gómez-Tamayo, A. Gonzalez, H. Gutierrez-de-Teran, M. Jimenez, W. Jespers, J. Kapla, G. Khelashvili, P. Kolb, D. Latek, M. Marti-Solano, P. Matricon, M.-T. Matsoukas, P. Miszta, M. Olivella, L. Perez-Benito, D. Provasi, S. Ríos, I. Rodríguez-Torrecillas, J. Sallander, A. Sztyler, N. Vaidehi, S. Vasile, H. Weinstein, U. Zachariae, P.W. Hildebrand, G. De Fabritiis, F. Sanz, D.E. Gloriam, A. Cordomi, R. Guixà-González, J. Selent, "GPCRmd uncovers the dynamics of the 3D-GPCRome", bioRxiv 839597; doi: https://doi.org/10.1101/839597.
66. J. Vencels, P. Råback, V. Geža, "EOF-Library: Open-source Elmer FEM and OpenFOAM coupler for electromagnetics and fluid dynamics", SoftwareX, Volume 9, 2019, Pages 68-72, ISSN 2352-7110, https://doi.org/10.1016/j.softx.2019.01.007
67. M. Lepsik, R. Sommer, S. Kuhaudomlarp, M. Lelimousin, E. Paci, A. Varrot, et al. "Induction of rare conformation of oligosaccharide by binding to calcium-dependent bacterial lectin: X-ray crystallography and modelling study". Eur J Med Chem. 2019;177:212-20.
68. D.B. Migas, A.B. Filonov, V.E. Borisenko, N.V. Skorodumova, "Effect of polaron formation on electronic, charge and magnetic properties of Nb12O29", J. Alloys Compd. 821, 153527 (2020).
69. A.Y. Alekseev, D.B. Migas, A.B. Filonov, V.E. Borisenko, and N.V. Skorodumova, "Structural stability and electronic properties of 2D alkaline-earth metal silicides, germanides, and stannides," Jpn. J. Appl. Phys. 59, SF0801 (2020).

70. M. De Santis, L. Storchi, L. Belpassi, H.M. Quiney, F. Tarantelli "PyBERTHART: A Relativistic Real-Time Four-Component TDDFT Implementation Using Prototyping Techniques Based on Python", J. Chem. Theory Comput. 2020, https://doi.org/10.1021/acs.jctc.0c00053.
71. C.D. Daub, E. Riccardi, V. Hanninen, L. Halonen, "Path sampling for atmospheric reactions: Formic acid catalysed conversion of SO$_3$ + H$_2$O to H$_2$SO$_4$", PeerJ Physical Chemistry, submitted September 2019.
72. I. Pozo, Z. Majzik, N. Pavliček, M. Melle-Franco, E. Guitián, D. Peña, L. Gross, and D. Pérez "Revisiting Kekulene: Synthesis and Single-Molecule Imaging", PNAS October 29, 2019 116 (44) 22065-22070; first published October 14, 2019 https://doi.org/10.1073/pnas.1910909116, Journal of the American Chemical Society 2019 141 (39), 15488-15493, DOI: 10.1021/jacs.9b07926.
73. T. Nordam, R. Kristiansen, R. Nepstad, J. Röhrs, "Numerical analysis of boundary conditions in a Lagrangian particle model for vertical mixing, transport and surfacing of buoyant particles in the water column", Ocean Modelling, vol. 136, pp. 107-119, 2019. DOI: https://doi.org/10.1016/j.ocemod.2019.03.003.
74. M.A. Ortuño, O. Hollóczki, B. Kirchner, N. López. "Selective Electrochemical Nitrogen Reduction Driven by Hydrogen Bond Interactions at Metal–Ionic Liquid Interfaces" J. Phys. Chem. Lett. 2019, 10, 513-517. DOI: 10.1021/acs.jpclett.8b03409.
75. D.W. Szczepanik, "A simple alternative to the pseudo-π method", Int. J. Quantum Chem. 118 (2018) e25696; doi: 10.1002/qua.25696.
76. N .Sieffert, A. Thakkar, M. Bühl, "Modelling uranyl chemistry in liquid ammonia from density functional theory". Chem. Commun. 2018, 54, 10431 (http://dx.doi.org/10.1039/C8CC05382K).
77. M. Simmermacher, A. Moreno Carrascosa, N.E. Henriksen, K.B. Møller, and A. Kirrander, J. Chem. Phys. 151, 174302 (2019).
78. M. Simmermacher, N.E. Henriksen, K.B. Møller, A. Moreno Carrascosa, and A. Kirrander, Phys. Rev. Lett., 122, 073003 (2019).
79. S. Zitz, A. Scagliarini, S. Maddu, A.A. Darhuber, and J. Harting, "Lattice Boltzmann method for thin-liquid-film hydrodynamics", Phys. Rev. E, 100:3, 033313, 2019. doi= {10.1103/PhysRevE.100.033313}.
80. P.-N. Tzounis, S. D. Anogiannakis, D. N. Theodorou: "Atomistic Simulations of Oligomers used in Directed Self-Assembly Lithography: Estimation of the Interaction Parameter χ", in preparation.
81. M. Damasso and F. Del Sordo (equally contributing): Expectations for the confirmation of Proxima c from a long-term radial velocity follow-up, MNRAS 2020
82. F. Zhou, I. Giannakis, A. Giannopoulos, K. Holliger, and Evert Slob, "Estimating reservoir permeability with borehole radar", Geophysics, 2020, 85(4): 1–10. (a proof is to be published in July-Agugust 2020).
83. C. Legrand, R. Saleppico, J. Sticht, F. Lolicato, H.-M. Müller, S. Wegehingel, E. Dimou, J. P. Steringer, H. Ewers, I. Vattulainen, C. Freund and W. Nickel, "The Na,K-ATPase acts upstream of phosphoinositide PI(4,5)P2 facilitating unconventional secretion of Fibroblast Growth Factor 2", Communications Biology volume 3, Article number: 141 (2020), DOI:10.1038/s42003-020-0871-y.
84. M. Stalevski, K. Tristram, D. Asmus, "Dissecting the active galactic nucleus in Circinus – II. A thin dusty disc and a polar outflow on parsec scales", Monthly Notices of the Royal Astronomical Society, 2019, 484, 3334-3355 DOI: 10.1093/mnras/stz220, http://adsabs.harvard.edu/abs/2019MNRAS.484.3334S.
85. B. Cloutier, B.K. Muite, M. Parsani, (2019). "Fully Implicit Time Stepping Can Be Efficient on Parallel Computers. Supercomputing Frontiers and Innovations", 6 (2), 75−85.10.14529/jsfi190206.
86. B.K. Muite, S. Aseeri, (2019). "Benchmarking solvers for the one dimensional cubic nonlinear Klein Gordon equation on a single core." Bench'19. International Open Benchmarking Council.
87. S. Aseeri, B.K. Muite, D. Takahashi, (2019). "Reproducibility in Benchmarking Parallel Fast Fourier Transform based Applications". Companion of the 2019 ACM/SPEC International Conference on Performance Engineering - ICPE '19. Association for Computing Machinery, 5−8.10.1145/3302541.3313105.

88. A.S. Dobrota, I.A. Pašti, S.V. Mentus, B. Johansson, and N.V. Skorodumova, (2020). "Altering the reactivity of pristine, N-and P-doped graphene by strain engineering: a DFT view on energy related aspects". Applied Surface Science, 514, 145937, https://doi.org/10.1016/j.apsusc.2020.145937.
89. Behbahani, Alireza F and Vaez Allaei, S Mehdi and Motlagh, Ghodratollah H and 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.
90. Behbahani, Alireza F and Motlagh, G Hashemi and Vaez Allaei, S Mehdi and Harmandaris, Vagelis A, "Structure and Conformation of Stereoregular Poly (methyl methacrylate) Chains Adsorbed on Graphene Oxide and Reduced Graphene Oxide via Atomistic Simulations", Macromolecules, 2019, 52(10), pp 3825-3838.
91. J. Chem. Phys. 150, 041716 (2019); https://doi.org/10.1063/1.5054843
92. A.J. Gallego, P. Gil, A. Pertusa, and R.B. Fisher, "Segmentation of Oil Spills on Side-Looking Airborne Radar Imagery with Autoencoders". Sensors, 18(3): 797, 2018
93. A.J. Gallego, A. Pertusa, P. Gil, and R.B. Fisher, "Detection of bodies in maritime rescue operations using Unmanned Aerial Vehicles with multispectral cameras". Journal of Field Robotics, 2018
94. M. Bortoli, M. Bruschi, M. Swart, L. Orian "Sequential oxidations of phenylchalcogenides by H2O2: insights in the redox behavior of selenium from a DFT analysis", New J. Chem., 2020, Accepted Manuscript
95. L. Guojian, A. Hassan, L. Shan, L. Shiying, Mohd Sukor Su'ait, B. Mourad, K. Mohamed, W. Qiang. "Theoretical insight into magnetic and thermoelectric properties of Au doped ZnO compounds using density functional theory". 562 (2019) 67.
96. A. Hassan, B. Mourad, Mohd Sukor Su'ait, L. Guojian, C. Siddheshwar, W. Qiang, K. Mohamed. "Understanding the effect of the carbon on the photovoltaic properties of the Cu2ZnSnS4", 251 (2020) 123065.
97. A. Hassan, B. Mourad, Mohd Sukor Su'ait, K. Mohamed. "Electronic and Magnetic Properties of Mn-doped and (Mn,C)-codoped w-AlN with the Presence of N Vacancy". J Supercond Nov Magn (2019). https://doi.org/10.1007/s10948-019-5102-8.
98. P. Tsoutsanis, "Stencil selection algorithms for WENO schemes on unstructured meshes,
99. Journal of Computational Physics: X Volume 4, September 2019, 100037 https://www.sciencedirect.com/science/article/pii/S2590055219300538, https://doi.org/10.1016/j.jcpx.2019.100037.
100. J. Diaz, M. Pinna, A.V. Zvelindovsky, and I. Pagonabarraga, I., 2019. "Large scale three dimensional simulations of hybrid block copolymer/nanoparticle systems". Soft Matter, 2019,15, 9325-9335 . doi:10.1039/C9SM01760G.
101. J. Diaz, M. Pinna, A.V. Zvelindovsky, and I. Pagonabarraga, I., "Nonspherical Nanoparticles in Block Copolymer Composites: Nanosquares, Nanorods, and Diamonds", Macromolecules, 52(21), 8285–8294. doi: 10.1021/acs.macromol.9b01754.