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ABSTRACT:

This document is the third report on the HPC-Europa3 Transnational Access activity. It covers the third reporting period (Months 37-60, i.e. 1 May 2020 – 30 April 2022). 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.

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Executive summary

HPC-Europa3's Transnational Access programme offered researchers in Europe, working in any field of computational science, the opportunity to visit another researcher in a similar field in one of 9 European countries where there was a project consortium partner, while gaining access to some of the most powerful High Performance Computing (HPC) facilities in Europe. A limited number of places were also available for researchers working in other countries.

Over the 5-year project lifetime, HPC-Europa3 aimed to support 1098 research visits, and to provide more than 90 million core-hours of computing access.

This document is the third report on the HPC-Europa3 Transnational Access activity. It covers the final reporting period (Months 37-60, i.e. 1 May 2020 – 30 April 2022). 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, as well as the scientific impact of the project.

1 Introduction

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

The central activity of HPC-Europa3 was the Transnational Access research visit programme, which was supported by the associated Networking Activities and Joint Research Activities. The programme funded collaborative research visits of up to 3 months' duration for computational scientists working in any discipline which can benefit from access to extremely powerful computing facilities. Nine of the ten consortium partners participated in the Transnational Access activity:

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

Visits could be made to any research group, academic or commercial, in any of the countries in which the Transnational Access partners were based, but not to a group within the same country where the visitor was working.

The programme was open to researchers of any level, from postgraduate to full professor, from research groups in the EU countries and Associated States¹. A limited number of places were also available for researchers from outside Europe.

Applicants were expected to demonstrate that they were motivated by two factors:

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

During their visits, researchers and hosts were encouraged to work closely together, with the visitor integrated as closely as possible into the host research group. Meanwhile, the relevant HPC centre provided 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 it provides statistics on the applications received and visits carried out during the final reporting period of the programme.

This has been an unusual and particularly challenging period to run a Transnational Access programme, given the lengthy disruption to everyday life caused by the Covid-19 pandemic, which had a major impact on the programme for more than 18 months. The last 2 years of the programme were characterised by a long period during which there were very, very few visits due to the restrictions on international travel, followed by an extremely busy period in the final 6-8 months when

¹ Associated States: Albania, Armenia, Bosnia and Herzegovina, Faroe Islands, Georgia, Iceland, Israel, Moldova, Montenegro, North Macedonia, Norway, Serbia, Switzerland, Tunisia, Turkey, Ukraine

travel restrictions were eased. This report also provides details of the adaptations which were made to the way the programme was run in the face of this challenge, such as the introduction of virtual visits for those who were unable to carry out their planned visits in person within the available timeframe.

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 were launched 4 times per year throughout the programme, with closing dates each February, May, September and November.

Calls were issued on this same schedule throughout the pandemic. As each closing date approached, it was always unclear for how much longer the travel restrictions would continue. As the evaluation process takes 4-6 weeks from the closing date, giving a likely period of 3-4 months between a call being launched and an applicant being informed of the panel's decision, it always seemed at the launch of each call that travel restrictions would probably have eased by the time successful applicants were informed.

Unfortunately, the travel restrictions continued for far longer than anyone could have foreseen, and the assurances to applicants that things would hopefully have improved by their proposed start date began to feel somewhat hollow after a couple of calls during the pandemic. Further, word of mouth has always been an extremely important tool for promoting the programme, but with no face-to-face events taking place and everyone working from home, this was greatly reduced. All of this caused a re-evaluation of the outreach strategy.

During the relatively quiet period of summer 2020, the HPC-Europa3 team was able to undertake the time-consuming task of initiating personal contact with individual researchers. Partners followed up with everyone who had been named as a potential contact in the visitor and host questionnaires, and contacted anyone who was not already within the HPC-Europa3 network who had engaged with the social media accounts (i.e. anyone who had liked, reposted or commented on posts). However, this generated few responses, and the vast majority of replies suggested that the programme was certainly of interest, but the timing was not right to consider a visit to a research group in another country. In all, we are aware of only one application which arose as the result of this direct contact. However, it should be noted that this was a successful application from a less-represented country (Croatia), and therefore a very positive outcome.

As the pandemic continued, the outreach activity began to focus primarily on dissemination of the results, and less on the opportunity to spend time abroad – on the end results, rather than the visits themselves. Fortunately, the programme had then been underway for some time and there were plenty of successes to be publicised.

2.1 *Publicity materials and online content*

No new printed publicity materials were created during this period, as there were no opportunities to display or distribute these at face-to-face events, such as conferences and training events, as would normally happen. Instead, the focus was on online content.

2.1.1 Project website

The website² 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 *Visitors area*³ highlights visitor experiences and successes via success stories, blog articles and short videos. There is also a link to the searchable list of project abstracts. 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

² <http://www.hpc-europa.org>

³ <https://www.hpc-europa.org/visitors>

of disciplines from which they come. This content is promoted via social media and may also be publicised via HPC-Europa3 newsletters, partner newsletters or partner blogs.

2.1.2 HPC-Europa3 newsletters

Four HPC-Europa3 newsletters were published during this period.

- 5th issue: Covid-19 update; Successful visits to Sweden; New HPC systems at EPCC.
- 6th issue: TAM 2020 update, including best talk and best poster awards; Cineca overview.
- 7th issue: Personal stories of 3 lockdown visits; BSC overview.
- 8th issue: Announcement of last call; statistics about backgrounds of applicants.

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 1889 subscribers.

2.1.3 Articles in partner centre newsletters

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 EPCC News⁴, also published as EPCC blog articles:
 - *HPC-Europa3 visitor programme* – published in EPCC News (issue 87, p20) and also as an EPCC blog article, June 2020⁵
 - *TAM 2020: HPC-Europa3 Transnational Access meeting*, plus small side feature *First post-lockdown HPC-Europa3 visitor arrives in Edinburgh* – published in EPCC News (issue 88, p29), and also as an EPCC blog article, November 2020⁶
 - *HPC-Europa3: Transnational Access in the time of Covid-19* – published in EPCC News (issue 89, pp20-21), and part-published as an EPCC blog article, September 2021⁷
 - *End of an era* – published in EPCC News (issue 91, p23), and also as an EPCC blog article, May 2022⁸.

⁴ <https://www.epcc.ed.ac.uk/whats-happening/newsletters-brochures>

⁵ <https://www.epcc.ed.ac.uk/whats-happening/articles/hpc-europa3-visitor-programme>

⁶ <https://www.epcc.ed.ac.uk/whats-happening/articles/hpc-europa3-transnational-access-meeting-tam2020>

⁷ <https://www.epcc.ed.ac.uk/whats-happening/articles/hpc-europa3-huawei-programming-languages-research-laboratory>

⁸ <https://www.epcc.ed.ac.uk/whats-happening/articles/end-era>

2.1.4 Blog articles

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 webpage⁹, and can also be found on some partners' websites. Examples include:

- HPC-Europa3 exchange visit: 'Every discussion enriches the individual'¹⁰
- HPC-Europa3 report: studying the strong force between quarks and gluons¹¹
- Modelling triple stellar interactions during a pandemic¹²
- HPC-Europa3 visit: Investigating the opto-electronic properties of small nanoalloys during a pandemic¹³
- HPC-Europa visit report¹⁴

2.1.5 YouTube

The HPC-Europa3 YouTube channel has a series of short video interviews with visitors, recordings of visitor talks, and a playlist including webinars providing an overview of HPC-Europa. This can be found at: https://www.youtube.com/channel/UC9uOpFQGP9V0TQPXFUOgs_A/playlists

2.2 Methods used to publicise the programme

The various publicity and dissemination materials described in section 2.1 are distributed in a number of different ways.

2.2.1 Network of contacts

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. Networks such as Psi-k have been cited by several applicants as how they first heard of the programme.

All of the electronic publicity material described in section 2.1 is publicised via the HPC-Europa3 mailing lists and social media accounts (see section 2.2.2 below), and those of the project partners.

Reciprocal publicity activities have also continued with the projects and organisations with which HPC-Europa3 signed MoUs in the context of *Work Package 3 – External co-operation for enhancing the best use of HPC*. A list of these entities can be found at <https://www.hpc-europa.org/external>. Applicants have mentioned hearing about the programme for the first time during events such as the PRACE / BioExcel Seasonal School and the PRACE Summer of HPC training week.

⁹ <https://www.hpc-europa.org/visitors>

¹⁰ <https://communities.surf.nl/rekendiensten/artikel/hpc-europa3-exchange-visit-every-discussion-enriches-the-individual>

¹¹ <https://www.epcc.ed.ac.uk/whats-happening/articles/hpc-europa3-report-studying-strong-force-between-quarks-and-gluons>

¹² <https://www.epcc.ed.ac.uk/whats-happening/articles/modelling-triple-stellar-interactions-during-pandemic>

¹³ <https://www.epcc.ed.ac.uk/whats-happening/articles/hpc-europa3-visit-investigating-opto-electronic-properties-small>

¹⁴ <https://www.epcc.ed.ac.uk/whats-happening/articles/hpc-europa-tamara-gerber>

2.2.2 Social media

The project social media accounts have been used to publicise closing dates, announce new visits starting, and disseminate visitor success stories, blog articles, newsletters, video testimonials, and any other project news.

Social media accounts can quickly reach new audiences when content is reposted. We make use of the “mention” feature to increase our reach, e.g. when new visitors start we “mention” any accounts belonging to the visitor and host, and their respective research groups and/or institutes. As previously mentioned, this pointed us to a number of new contacts who were interested in HPC or computational science, but who were not within our existing networks.

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 1096 followers, an increase of 425 (63%) over Months 37-60, equating to approximately 17 new followers per month.
 - To date the project has issued 1182 tweets, of which 562 were in Months 37-60.
 - The project’s tweets were liked 1354 times in Months 37-60, and were retweeted 518 times in the same period.
 - 123 tweets in this period have had an engagement rate of 2% or higher, 9 tweets were retweeted 10 or more times, and 21 were liked 10 or more times.
- **Facebook:** <https://www.facebook.com/hpceuropa/>
 - The Facebook account is also used to promote project news; closing dates and other events, such as seminars and workshops, are created as “Events” so that people can register interest and receive reminders.
 - The Facebook account currently has 251 followers, an increase of 46 (22%) in the last 24 months.
- **LinkedIn:** <https://www.linkedin.com/company/29022707/>
 - The LinkedIn account is also used to promote project news; closing dates and other events, such as seminars and workshops, are created as “Events” so that people can register interest and receive reminders.
 - The LinkedIn account currently has 248 followers, an increase of 132 (53%) over the last 24 months.

2.3 Dissemination of project achievements

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, and so the true impact can only be seen some considerable time after the end of the programme.

In addition to the publicity methods mentioned above, such as newsletters, blog articles, and social media posts, 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 is available to download from

the HPC-Europa3 website. Three project directories have been produced¹⁵, and it is hoped that time will be available after the end of the programme to create a fourth one, featuring the visits from the final reporting period. Due to the pandemic travel restrictions and the resulting postponements of many visits, the majority of these visits took place in the last months of HPC-Europa3, meaning that it was not possible to produce the final project directory during the lifetime of the programme.

- The **user group meetings, TAM** (the Transnational Access Meeting) give visitors the opportunity to present the work resulting from their visit, via either a talk or a poster. In 2020 and 2021 these were held as virtual events instead of the planned face-to-face events, due to the pandemic.
- A series of **Transnational Access Success Stories** was produced¹⁶.
- **Visitor talks**, previously given within the partner centres and/or host departments, have been more commonly held online as webinars since the pandemic began¹⁷.
- Visitors are asked to include an **official acknowledgement** of HPC-Europa3 in journal publications and conference presentations.

2.4 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.

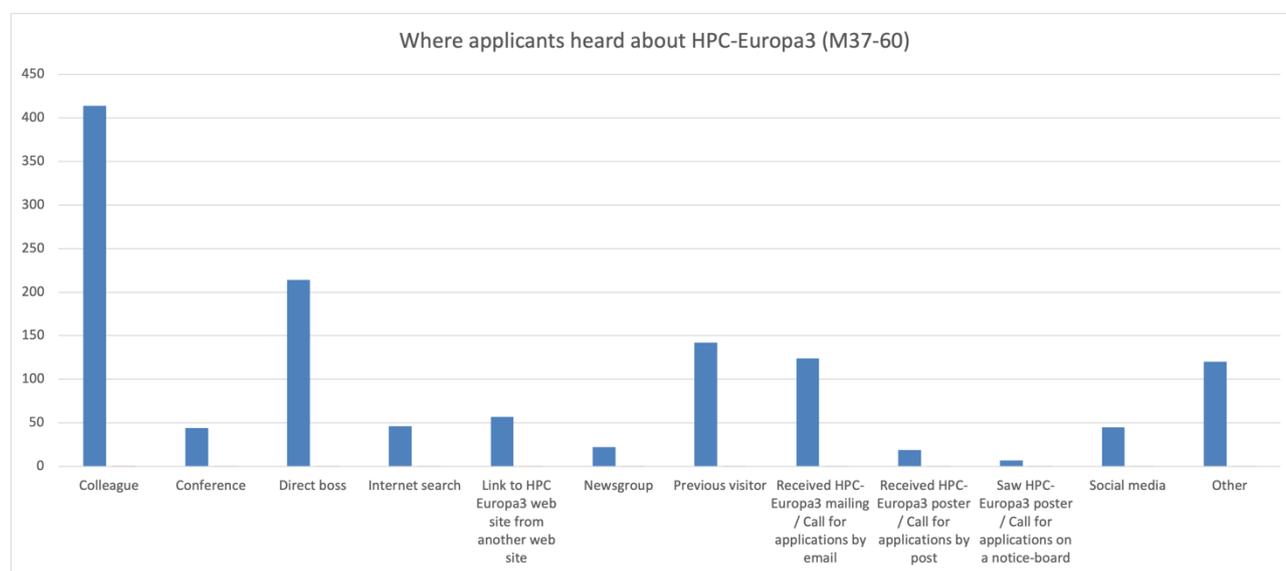


Figure 1: Where applicants heard about HPC-Europa3 (M37-60)

Overall, the relative distribution of sources of information about the programme remains very similar to previous years, with a few changes which are likely to be related to the pandemic.

More than half of applicants (55%) said that they had heard about the programme from a colleague, and more than a quarter of applicants (28%) heard about it from their direct boss, while 19% said that they had heard about the programme from a previous visitor. As in previous periods, this demonstrates

¹⁵ Available to download at https://www.hpc-europa.org/public_documents

¹⁶ Available at https://www.hpc-europa.org/public_documents

¹⁷ Some of these were recorded and are available online, e.g. some can be found among the courses and webinars listed at <https://www.archer2.ac.uk/training/materials/>

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, i.e. did they receive a mailing, hear about it at a conference, were already a visitor themselves, or found out about it some other way?

In total 17% of applicants had received the call for applications by email, showing that this remains an effective way of reaching people.

Some 8% of applicants heard about the programme via links on other websites, most likely due to the co-operations established under WP3. A further 6% found the programme via an internet search – however, we cannot be sure what prompted this search without further details. Meanwhile, 6% of applicants heard about it via social media. Although the proportion of applicants citing social media has not grown significantly (up from 5% in the previous reporting period), this of course equates to a larger number of applicants in total.

Unsurprisingly, the proportion of people who had heard about the programme at a conference had decreased compared to the previous period (down from 9% to 6%), which is not surprising as few face-to-face events took place during the 2-year reporting period, due to the pandemic. Very few had received the call by post (3%), and as paper publicity materials were not distributed during this period, these applicants must have already received the information prior to this reporting period. Only 1% reported having seen information on a notice-board, which is also not surprising given that most people were working from home for most of the period, and any notice-board information must have been on display for some time.

Applicants citing “newsgroup” as the source are likely to be referring to a subscription mailing list (such as Psi-k), as newsgroups are not generally used for HPC-Europa3 publicity currently.

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 existing categories, e.g. a previous visitor, their direct boss, or receiving the call for applicants by email (forwarded by the original recipient rather than received directly from HPC-Europa3).

Under “other”, applicants also cited articles in partner centre newsletters or user communications, while in a good number of cases they had heard about it from their host, who had encouraged them to apply.

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. The process described below remains unchanged from the previous reporting periods.

3.1 Selection process for HPC-Europa3 applications

The evaluation and selection process is a two-stage procedure, with each stage taking 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), $\beta+$ (probably accept), $\beta-$ (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**, or 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), $\beta+$ (probably accept), $\beta-$ (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 $\beta+$, Host Support Form is **very enthusiastic** or **enthusiastic**);
- **Fast-track reject** – all reviews are negative (Technical Evaluations and SUSP reviews are all $\beta-$ 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, reduced allocation of HPC resources compared to the request, 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 for 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.

At the final selection meeting in December 2021, more conditional acceptances were given than would ordinarily have been the case, as there was not the usual possibility to provide feedback and encourage the applicant to resubmit for the next call. Instead, the feedback was provided in the context of a conditional acceptance, with the visit being fully approved upon satisfactory resolution of the issues. This provided all candidates with a fair opportunity to address the reviewers' comments.

3.2 Closing dates and selection meetings in third reporting period

Seven Calls for Applications were launched during this reporting period, with all of the corresponding selection meetings being held by online videoconference. In normal times, a face-to-face selection meeting would have been held in conjunction with each Transnational Access Meeting (TAM), but during this period these were of course also held online due to Covid-19.

Call number	Closing date	Selection meeting
12	14 th May 2020	22 nd June 2020
13	17 th September 2020	15 th October 2020
14	12 th November 2020	14 th December 2020
15	18 th February 2021	24 th March 2021
16	13 th May 2021	14 th June 2021
17	9 th September 2021	11 th October 2021
18	11 th November 2021	13 th December 2021

Table 1: HPC-Europa3 closing dates and selection meetings, M37-60

3.3 Members of the Scientific Users Selection Panel

The HPC-Europa3 Scientific Users Selection Panel (SUSP) initially consisted of 22 members, with a distribution of scientific backgrounds closely matched to the proportion of applicants from the various disciplines under the previous HPC-Europa3 programme.

However, the panel was expanded to 36 members as the programme progressed. This addressed the evolving distribution of scientific backgrounds of the proposals. More reviewers were needed for certain fields, and with more reviewers on the panel overall, it is also easier to find a close match between the reviewers' expertise and the applications assigned to them. Increasing the panel size also aimed to spread the load of reviews more evenly among the panel members, and to make the process more manageable when some panel members were unavailable for certain calls.

The current membership of the panel is given in Annex I.

4 Application and Visit Statistics

4.1 Overview of applications received and approved in Months 37-60

During the third reporting period, there were 7 Calls for Applications, for which 467 applications were received in total. Application numbers were unsurprisingly quite low during the times of the greatest restrictions on travel, and indeed on every aspect of daily life. This was disappointing after numbers had been boosted to a record 193 applications for the February 2020 call, following a major outreach push. In May 2020, just a few weeks after full lockdown was imposed in most countries, only 59 applications were received. At that point, however, people still hoped that the restrictions would be short-lived. By September 2020, with restrictions only partly relaxed and international travel still difficult, only 30 applications were received. Application numbers remained below 50 for each of the following 3 calls, and only recovered for the final two calls, in late 2021, as travel was beginning to become easier again (91 applications in September 2021, 156 in November 2021).

Of the 467 applications received during this period, 391 were approved, giving an overall acceptance rate of 84% for this period. This is a bit higher than the previous reporting period (79%), which is at least in part due to the higher number of conditional acceptances given at the final selection meeting. Conditional acceptances were given to those applicants who would ordinarily have been rejected with feedback to help them reapply for the next closing date.

HPC-Europa3 centre	Applications received M37-60	Applications accepted M37-60	Acceptance rate M37-60	Total applications received M1-60	Total applications accepted M1-60	Acceptance rate M1-60
BSC	87	74	85%	235	188	80%
CINECA	104	83	80%	200	162	81%
CSC	45	42	93%	129	116	90%
EPCC	89	72	81%	281	205	73%
GRNET	9	8	89%	43	34	79%
HLRS	66	54	82%	158	126	80%
ICHEC	8	6	75%	22	15	68%
KTH-PDC	3	3	100%	60	51	85%
SURFsara	56	49	88%	119	107	90%
Total	467	391	84%	1247¹⁸	1004	81%

Table 2: Applications per centre M37-60

¹⁸ NB In total, 1249 applications were received over the project lifetime, but two applications were to hosts in countries which did not have an HPC-Europa3 partner in them (Denmark and Portugal). We offered the applicants the chance to identify an alternative host in an eligible country, but as both of these particular applications had been motivated by a desire to collaborate with the specific named hosts, the applicants chose to withdraw their applications instead.

4.2 Overview of visits in Months 37-60

A total of 456 visits began across the 9 partner centres during this period, bringing the total number of visits to 847 (see Table 3 for further details). A further 157 visits were cancelled, the vast majority of them due to the Covid-19 pandemic.

Prior to the pandemic, visits lasted between 3 and 13 weeks, with a small number of visits approved for 2 weeks where there was clear evidence that the applicant had solid HPC skills and a strong existing collaboration with their host.

However, in response to the travel restrictions, “virtual visits” were introduced (see further information in section 4.2.1). These were operated in different ways at different centres, and while some centres provided more intense mentoring and support for the approved number of weeks, others provided less comprehensive support, but for a longer period of time. Hybrid visits were also introduced, in response to demand from some visitors. These “hybrid visits” were carried out partly remotely and partly in the research lab, with the visit to the host lab being for a shorter period of time than requested, and often for only 1-2 weeks, as circumstances allowed. Some visits were longer than the usual maximum visit length, due to Covid complications. As the definition of a visit has been rather flexible during this most recent period, statistics relating to visit lengths are not given in this report.

HPC-Europa3 centre	Visits started M37-60	Total visits M1-60	Target number of visits (M1-60)	Deviation from target	Cancelled visits M1-60 ¹⁹
BSC	90	170	189	-19	18
CINECA	100	147	162	-15	16
CSC	48	91	171	-80	25
EPCC	84	171	180	-9	27
GRNET	12	26	36	-10	8
HLRS	51	100	135	-35	26
ICHEC	11	17	18	-1	4
KTH-PDC	12	44	36	+8	7
SURF	48	81	171	-90	26
Total	456	847	1098	-251	157

Table 3: Number of visits and deviation from target

The total number of visits supported by the programme over the 5 years was 847, below the target number of 1098. However, HPC-Europa3 was clearly very strongly impacted by the Covid-19 pandemic, which effectively paused the programme for around 18 months, from mid-March 2020 until mid-September 2021. This was an unprecedented global situation which could not have been foreseen.

¹⁹ Note that for some centres the sum of “Total visits M1-60” plus “Cancelled visits M1-60” (Table 3) is different from “Total applications accepted M1-60” (Table 2) as some applications were transferred to other centres. In total, 6 were transferred from EPCC to ICHEC and 1 from EPCC to Cineca.

A 6-month project extension was granted due to the pandemic, and the timing of this extension (November 2021-April 2022) was extremely useful, as international travel only began to be relatively easy again in autumn 2021. It was particularly helpful as many of the long-postponed visits were able to take place in these final 6 months. In fact, almost all of the visits in M37-60 took place within the 6 months of the extension. The extension also allowed the programme to launch two additional calls for applications, for which good numbers of applications were received, as people were beginning to have more confidence to plan international travel.

It can be seen from Table 3 above that at most centres, around half the total number of visits for the programme took place in this final reporting period – and considerably more than half in the case of Cineca. Given that most visits in the period took place in the final 6 months, it can be seen that this was a truly exceptionally busy period for all partner centres. The one major exception was KTH, who had already nearly reached their target number when the pandemic began.

The table also shows that a very large number of approved visits were cancelled – around 15% of the total number of accepted applications. The vast majority of these were due to the pandemic, with people unwilling to travel and/or unable to do so within the available timeframe, typically due to completing their Ph.D., changing job or leaving research altogether. Without those cancellations, most centres would have come close to, or even exceeded, their target.

At the final call, more applications were approved for EPCC than there were available places. However, with many pending visits considered to be at high risk of cancellation, all good applications were approved, and the Transnational Access team at EPCC worked with the team at ICHEC to identify applications which would be suitable to transfer to ICHEC. As these two centres work together in a loose “British Isles” partnership in WP5, and visitors to either centre can be hosted by researchers in either the UK or Ireland, this was relatively straight-forward, as no change of host was required – it was simply a matter of identifying which projects were well suited to the HPC facilities at ICHEC. It is not always possible to transfer visitors to another centre due to specific hardware or software issues which may mean that the work is not feasible on the available systems.

As a result of this, 4 visits were transferred to ICHEC, which filled all the places available there at that time. Unfortunately, due to a further cancellation, ICHEC eventually fell one visit short of their target. Meanwhile, 5 remaining applicants to EPCC were put on a waiting list, in case of cancellations, and all were in fact eventually offered a place. Four of them were able to take up the offer, although in some cases for a shorter visit than proposed, with 3 of them carrying out their visit remotely.

4.2.1 Virtual visits

Due to the pandemic, virtual visits were introduced to allow anyone who was unable or unwilling to carry out their visit in person to do so remotely instead. Visitors were given remote access to the HPC facilities and support from the relevant HPC centre, while collaborating remotely with their host supervisor. While this was never going to match the experience of visiting the host research group in person and being immersed into that environment, it did still allow projects to proceed which might otherwise have been cancelled. Additionally, some hybrid visits took place, where the visit was partly or mainly carried out remotely, with a shorter visit period to the host group, as circumstances allowed. During such unpredictable times, flexibility was key to enabling as many visitors get the most benefit from the programme in the way that best suited them.

Virtual visits were not an option under HPC-Europa3 prior to the pandemic, although they had been an option in HPC-Europa2 (2009-2012). Under HPC-Europa2 there was not a high uptake of such visits, which did not really seem to sit well within the scope of the programme, and they were mostly

used by researchers who had already had a face-to-face visit, to obtain some additional HPC resources to carry out some follow-up work on their project. The hosts were not always very active in these visits, and these were not something that the HPC-Europa3 co-ordinators were particularly keen to continue.

However, a decade later, the tools for collaborating remotely had become much more widespread and reliable, and the pandemic forced a change in everyone's working practices. Compared to previous programmes, many more visits under HPC-Europa3 have taken place in cities other than where the partner centres are, so the technical support staff were already more used to supporting their visitors remotely when the pandemic began.

For all these reasons, the move to virtual visits, where necessary, was easier than it might have been some years earlier, and the vast majority of the visits were highly successful, with publications expected to follow. It has been pleasing to see that the feedback from these virtual visits has been overwhelmingly positive, even in the many cases where visitor and host had not met in person or had not had any previous collaboration. As working practices have changed, virtual visits may be a more viable option for future Transnational Access programmes.

4.3 Access planned and delivered

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

TA centre	Access planned (AU) – minimum quantity of access to be provided (M1-60)	Access delivered M37-60	Visits started M37-60	Average access allocated per user-project M37-60	Total access delivered M1-60	Visits M1-60	Average access allocated per user-project, M1-60	Average quantity of access to be delivered per user (planned)
BSC	8.203.125	7.729.182	90	85.880	11.953.575	170	70.315	43.403
CINECA	31.034.483	30.138.192	100	301.382	45.590.812	147	310.142	191.571
CSC	10.674.157	13.397.532	48	279.115	19.648.230	91	215.915	64.422
EPCC	23.529.412	39.192.705	84	466.580	45.984.909	171	268.918	130.719
GRNET	n/a	501.970	12	41.831	2.960.018	26	113.847	n/a
HLRS	11.752.454	19.200.000	51	376.471	25.206.192	100	252.062	87.055
ICHEC	1.503.759	1.361.033	11	123.730	1.523.396	17	89.612	83.542
KTH-PDC	5.882.353	1.589.900	12	132.492	6.054.660	44	137.606	163.399
SURF	12.500.000	2.566.090	48	53.460	3.830.344	81	47.288	73.099
Total	105.079.743	115.676.604	456	253.677	162.752.136	847	192.151	95.701

Table 4: Summary of access planned and access delivered, M37-60

Table 4 shows that the amount of access delivered over the project lifetime was more than 50% above the minimum to be provided. Almost all of the partner centres met their target, and many exceeded this – some by a considerable amount.

The total access delivered in this final reporting period was significantly more than in the previous two reporting periods combined. This is partly due to the fact that more than half the visits took place in this final reporting period. Additionally, many users continue to use the resources after their visits are complete, and so the figures for Months 37-60 will include some users whose visits ended in the previous period. A number of those visitors cut short their visits in spring 2020 due to the Covid-19 pandemic, but continued to use the resources to carry on with their project remotely.

Further, in the early phase of the programme, partner centres are typically rather cautious about allocating very large amounts of compute time to individual users. This is to ensure that sufficient resources remain to guarantee that the average allocation, at least, can be provided to all users over the project lifetime. If the resources are available, and their work justifies this, visitors coming towards the end of the programme may benefit from larger allocations.

As always, the requirements of the users in this period varied enormously, depending on the focus of the work done during their visit. Some focus more on code development during their visit, and so use

less time, while others carry out significant numbers of large production runs, and can easily use several times the average allocation.

4.4 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)

4.4.1 Country of Research Group

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 37-60, applications were received from a total of 52 different countries, of which 21 were EU member states, 7 were Associated States, and 24 were other countries. The proportion of applications from third countries in this period was twice that of the previous reporting period (22% compared to 11%). Awareness of the programme naturally grew as more researchers from these countries took part, and as their participation was publicised via social media activities. Up to 20% of the access could be granted to 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, as it was still a member of the EU at the start of the programme.

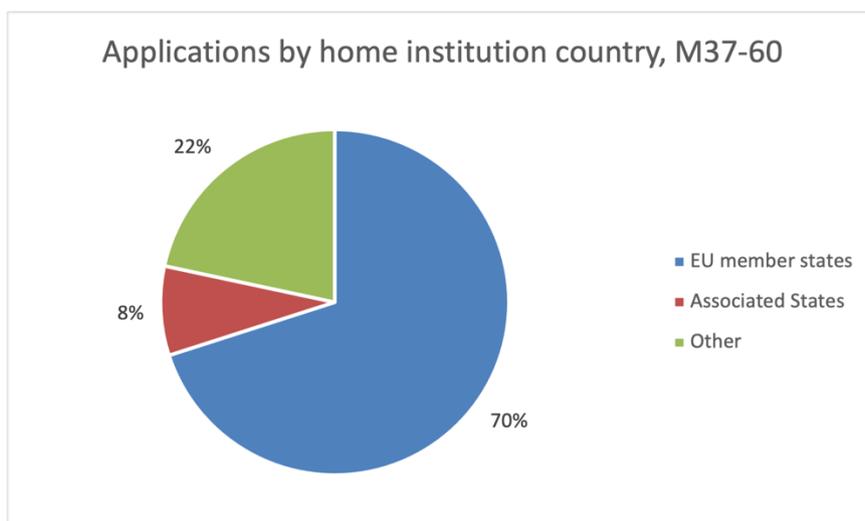


Figure 2: Location of home research institute (applicants)

Table 5 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	Iceland	4	3	Algeria	2	1
Belgium	12	12	Israel	1	1	Argentina	3	3
Croatia	7	6	Serbia	4	4	Australia	1	1
Czech Republic	7	7	Switzerland	4	4	Brazil	6	6
Denmark	4	4	Tunisia	5	4	Cameroon	2	1
Finland	19	15	Turkey	16	10	Canada	1	1
France	20	17	Ukraine	5	4	Chile	3	2
Germany	28	26	TOTAL	39	30	China	10	5
Greece	10	9				Colombia	3	3
Hungary	3	2				Congo	2	2
Ireland	8	6				India	15	10
Italy	55	50				Iran	12	6
Lithuania	1	1				Jordan	1	1
Netherlands	7	7				Kazakhstan	1	1
Poland	17	13				Korea	1	1
Portugal	10	8				Mexico	1	1
Romania	5	3				Morocco	3	2
Slovakia	2	2				Nigeria	16	7
Spain	52	48				Pakistan	2	2
Sweden	5	5				Russia	5	5
United Kingdom	51	44				Singapore	2	2
TOTAL	327	289				Taiwan	1	1
						United States of America	7	7
						Vietnam	1	1
						TOTAL	101	72

Table 5: Applications received by country of research group (M37-60)

As has been seen in the past, the highest numbers of applications have come from the countries with large populations where well-established HPC infrastructures have led to HPC skills being embedded in the research communities.

The three countries with the longest history of running Transnational Access programmes again top the list: Italy (55), Spain (52) and the UK (51). These are also countries with a very active HPC-Europa3 host community, who also encourage their group members to participate.

The next highest number of applications came from 3 more countries with HPC-Europa3 partners in them: Germany (28), France (20) and Finland (19). Next was Poland (17), showing a slight increase over previous years. This may be due to increased awareness of HPC in general due to the very active Polish National Competence Centre established under the EuroCC initiative.

However, after this some new patterns emerge, with the next countries all being non-EU countries: Nigeria (16), Turkey (16) and India (15). Nigeria and India show a striking increase, up from 7 and 9 applications respectively for the whole of the previous 36-month period. This demonstrates both the power of the “word of mouth” effect, as some visitors came from the same institutes as previous visitors, and the importance of publicising the diversity of researchers taking part in the programme, which allows researchers to see that, for example, others from their country have participated.

There continues to be a clear difference in the acceptance rates of applicants from EU countries (88%) and non-EU countries (73%), although this has closed a little since the previous 18-month period. 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 prerequisites of the programme, and may be more used to writing research proposals in English.

4.4.2 Scientific discipline

As in previous reporting periods, we can see that the highest number of applications come from the fields of physics (147) and chemistry (133) – 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, including a small number of applications from the humanities.

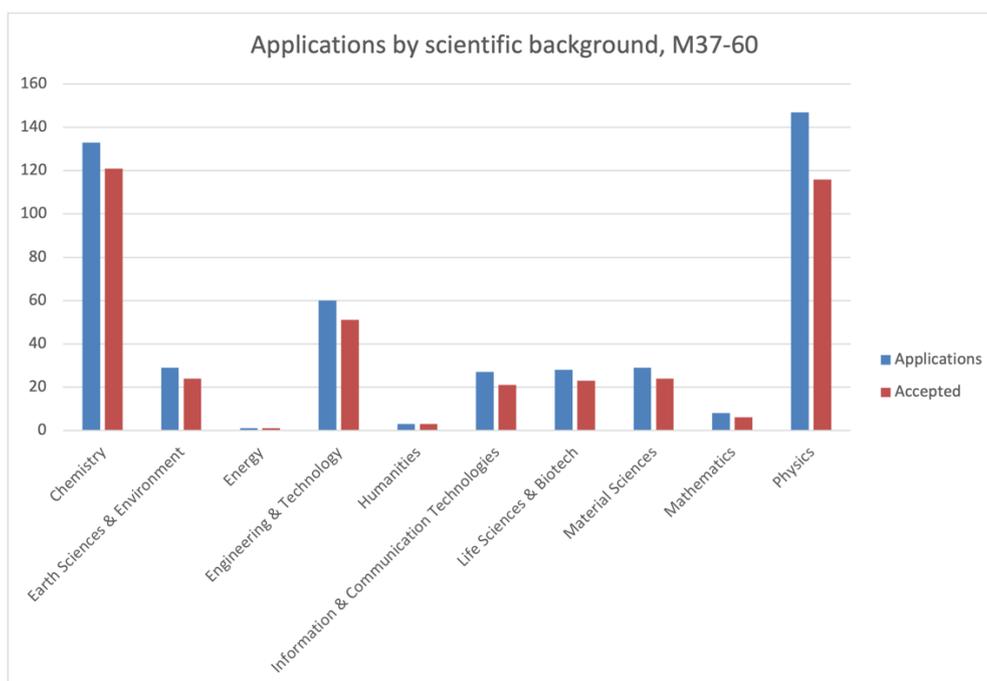


Figure 3: Applicants by scientific discipline

4.4.3 Demographic information

4.4.3.1 Gender

It has previously been noted that the number of female researchers applying for, and being accepted for, HPC-Europa3 has seen a significant increase compared to the previous programmes, where female participation was around 16-20%. It is pleasing to see that the trend has continued during this reporting period, with female applicants representing a record 28% of the total. There was no difference between the percentage of applicants and the percentage of those accepted, which also stood at 28% female.

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 Figure 3) – the disciplines which make most use of HPC.

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

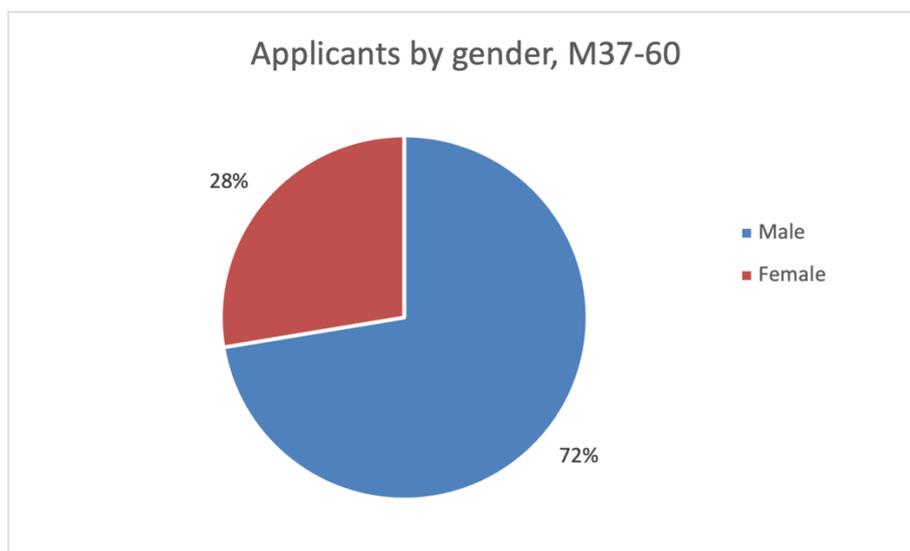


Figure 4: Applicants by gender

4.4.3.2 Age

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

Applicants ranged in age from 21 to 80, covering the full spectrum of academic career stages. The mean age was 32, the median age 30, and the mode 26, 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 4.4.3.3 below.

4.4.3.3 Career stage

During this reporting period, we have seen a shift to a higher proportion of undergraduate applicants. Previously there had been a roughly equal split of postgraduate students, postdoctoral researchers and experienced researchers, although in the second reporting period the proportion of postgraduates had

shown a slight increase compared to the previous period. However, during this period, the percentage of postgraduates has jumped from 41% to 47%, now nearly making up half of all applications, with a corresponding decrease in applications from post-docs and experienced researchers. The percentage of undergraduates has also increased from 3% to 8%, meaning that undergraduate and postgraduate research students combined now account for 55% of applications, compared to 44% previously.

The Covid-19 pandemic may be behind this increased proportion of younger participants. Younger people are likely to have been more prepared to travel again when restrictions began to be lifted, especially as they typically have greater flexibility with their schedules if circumstances were to change suddenly. Further, such students have a shorter window of opportunity to apply before moving on to their next career, and may have wanted to take the chance while they could.

There was very little 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.

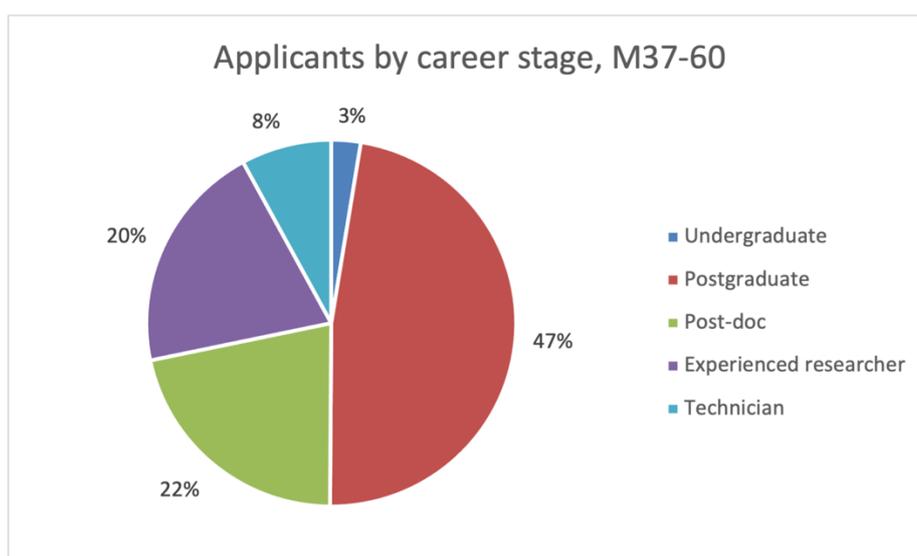


Figure 5: Applicants by career stage

5 Visit Feedback

Both visitors and hosts are asked to complete a questionnaire at the end of each visit. During this reporting period, 350 visitor questionnaires and 201 host questionnaires have been returned.

5.1 Visitor questionnaires

Once again, visitors reported a very high level of satisfaction with the programme, with only 3 of the 350 respondents saying they were *dissatisfied* or *very dissatisfied*, while the remainder were *satisfied* (18%) or *very satisfied* (81%) with the experience overall, giving an overall satisfaction rate of 99%.

Only one respondent gave an overall rating of “very dissatisfied”. This was due to a combination of factors, including technical problems with the HPC work, a feeling of isolation due to being in a new place at a time when most of the host department were still working remotely due to Covid, and the high cost of accommodation in the host city combined with the fact that the expenses were not paid up-front at the start of the visit. However, the work will be presented at a conference in June and the visitor believes ongoing collaboration is likely – and, despite all of the negative factors, the visitor nevertheless concluded, “I still think providing people with HPC resources and research collaboration opportunities is great. If there was no covid and the city was [a different one], I would recommend.”

Five respondents said that they would not recommend the programme. However, this included the “very dissatisfied” respondent, who, as noted above, said they would in fact recommend it in different circumstances. A further two respondents said that this was because the programme was ending, so there was no point in recommending it – these were not a judgement on the inherent value of the programme. Indeed one of these provided an additional comment, “The program as such is wonderful and it would be great if there could be a similar program in the new Horizon Europe framework.”

Other reasons given for not recommending the programme related to the reimbursement of expenses: the processes involved, the amount which could be reimbursed, the lack of flexibility in terms of what could be reimbursed, and the timescale for reimbursement.

While some visitors reported dissatisfaction with individual issues in their questionnaires, very few reported that they were *dissatisfied* with more than 2 issues. Issues which led to dissatisfaction were often one-off issues outside the immediate control of the programme, such as very specific hardware or software issues, or constraints on visitor access due to the Wassenaar Arrangement.

The most cited reasons for dissatisfaction were:

- Accommodation. Many felt that the budget was too low, and commented on the difficulty in finding short-term accommodation in an unfamiliar town when not physically there. Some felt that the HPC-Europa3 team should do more to help with this.
- Reduced allocation of compute time compared to what was requested in the application. Here it should be noted that where the panel approves a reduced amount of time, this is stated in the acceptance letter and the offer is conditional on the applicant confirming that useful work can still be done with the reduced allocation.
- Visit length shortened. In some cases this was on the selection panel’s recommendation, in others it was due to a lack of time to arrange the visit before the end of the programme, either because the visitor had applied for the last call and/or due to Covid delays. For some visitors this was compounded by delays in obtaining a visa, an issue which has become a more common problem now that more participants come from outside Europe. Here it should be

noted that the timing of the last call was expected to allow all decisions to be sent before the Christmas holidays, so that all applicants, even those who had requested 13-week visits, could have time to arrange their visits. The fact that the programme was ending on 30th April was widely publicised.

- Late communication of the evaluation. Most people citing this as a reason for dissatisfaction had applied at the final call. As stated above, the intention had been that all applicants would receive the decisions before the Christmas holidays. Unfortunately, due to a small number of reviewers not submitting their evaluations before the meeting, this was not possible. Some reviews came in late, and others had to be reassigned to other members of the panel. Further, many more conditional acceptances were given for this call than would normally be the case, as weaker applicants would not have the usual opportunity to address feedback and reapply. This resulted in an exceptionally heavy communication workload between applicants and panel members, via the HPC-Europa3 Transnational Access co-ordinator. Lastly, EPCC had received more applications than it could accept, but until all of the reviews were received, a priority list for acceptance could not be finalised, which also created delays. As discussed in section 4.2, some applicants were then transferred from EPCC to ICHEC, and five applicants were placed on a waiting list. These five were all eventually offered a place due to cancellations, but one was not able to take up the offer, and 3 of the others had to carry out a virtual visit instead due to lack of time to arrange the logistics. While it is understandable that several individual applicants felt disappointed and disadvantaged by the late response, an enormous amount of work was going on in the background to try to ensure that everyone was treated fairly and had an opportunity to participate if at all possible.

With a 99% overall satisfaction rate, it is clear that while there were some specific sources of dissatisfaction, on the whole these did not detract majorly from the experience. All visitors who responded said that they expected to publish the results of the work carried out during the visit. 98% of respondents rated their collaboration with their host as *satisfactory* or *very satisfactory*. When asked whether lasting links would have been formed with the host group, 75% replied *certainly*, 19% said *probably*, and 5% said *maybe*.

Below is a selection of the many positive comments to be found in the questionnaires. Quotes such as these have been used for publicity material and publicised via social media accounts.

“This programme is simply fantastic, at every possible level. I cannot fault a single aspect of it, and could only suggest very minor improvements.”

“This was a great experience and I had the opportunity to learn a lot and significantly improved my work thanks to the resources provided.”

“The programme is very well managed and the support I received throughout it was beyond my expectations!”

“I am glad about the experience of the HPC-Europa3 Program. The group was great, and the working conditions were excellent. I had the opportunity to perform my calculations using extra computational means and increase my confidence in my work and develop my Ph.D. project. I learned a lot and was very productive, even in the context of a pandemic. It exceeded my expectations.”

“I have thoroughly enjoyed my research visit to EPCC. The research experience I gathered there is rewarding and will encourage me to build a successful academic career.”

“Even now that the access to HPC resources is more widespread, such program is great added value.”

“I would like to express my sincere gratitude to the HPC-Europa3 team and the European Commission for making this experience possible. As a young and aspiring researcher, this visit motivated me to continue my academic career and reinforced my interest in HPC. It also motivated me to reach out to forge international collaborations and networks. Thank you so much!”

“Well done! Long live HPC-EUROPA!”

5.2 Host questionnaires

Hosts also report a high level of satisfaction, with 97% saying that they were *satisfied* or *very satisfied* overall with the visits which they have hosted (with 80% saying that they were *very satisfied*).

No hosts reported being *very dissatisfied* overall, although five were *dissatisfied*. This included one whose visitor had barely begun his visit when the pandemic restrictions started, and who then declined to work on the project remotely after returning home, so no progress was made on the project. One host cited a number of issues which made full engagement difficult, “e.g. delay, illness, injury etc”. Two of the hosts cited the need for better definition of the goals of the project before the visit, and one had a poor relationship with the visitor. It should be noted that this host had other visitors at around the same period and was *very satisfied* with the other visits – the dissatisfaction in this particular case was due to the interaction with the specific visitor.

97.5% of respondents rated the scientific value of the work performed during the visit as *good* or *excellent*, with 2 respondents stating that it was *poor* and 1 that it was *very poor*. One also replied *not sure*, stating that in their view scientific value can only be measured in publications and they were unsure at the time of completing the questionnaire whether any publications would arise from the work done. Of those who stated the value of the work was *poor*, one was the host of the visitor mentioned above who had to return home abruptly due to the pandemic and declined the offer to collaborate remotely; another felt the visitor should have done much more preparation for the visit. The host who rated the value of the work as *very poor* commented that the visitor came with his idea of what he would do and did not need, or appear interested in, any help from the host department.

95% 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. Of the respondents who rated the visit *not very useful* or *not useful at all* to their host department, most cited either the lack of interaction via departmental seminars and group meetings, due to the pandemic, or the difficulty in extending the collaboration to the wider department in the case of virtual visits. However, two of the respondents noted that the visit was nevertheless useful at the group level, if not to the wider department.

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

100% of respondents also said that they would be happy to host another visitor in the future, and many noted their support for a future programme in their questionnaires. A number of hosts have contacted the HPC-Europa3 team directly to ask whether there will be a future HPC-Europa programme, as they have found it to be both useful and interesting. Here is a selection of comments from some of the hosts:

- “I was very satisfied with this visit and actually also all other visits in the past 5 years. I strongly support the creation of a follow-up program: HPC Europa 4!”
- “I hope this programme can continue in the future as it has benefitted a wide range of scientific areas.”

- “Please set up a new HPC-Europa 4 program. I would most strongly support this.”
- “Please continue this network action in terms of HPC-Europa 4. It would have our strongest possible support”.

As with the visitor questionnaires, we use selected quotes from the host questionnaires to publicise the programme, especially when promoting it to potential hosts.

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

We are now aware of 233 publications and conference presentations which have acknowledged HPC-Europa3. A full list of these can be found in Annex II.

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.

This is a particularly relevant point in the case of HPC-Europa3, where the Covid-19 pandemic meant that many visits were postponed and a much higher proportion of the visits than would be expected took place in the final six months of the programme. We expect to see much scientific output over the coming 12-24 months from these visits.

6.2 Long-term collaborations

In this 24-month period, 29 applicants successfully submitted applications for follow-up visits to a host researcher with whom they had already had an HPC-Europa3 visit.

We continue to see visitors securing research positions in their former host departments. Some examples follow below.

- Fabio del Sordo, formerly of the FORTH Institute of Astrophysics (Greece), has secured a post at the INAF Astrophysical Observatory of Catania (Italy), where he had 2 successful HPC-Europa3 visits host by Dr Alfio Bonanno.
- Mats Simmermacher had successfully reapplied for a second HPC-Europa3 visit to his host Dr Adam Kirrander, School of Chemistry at the University of Edinburgh (UK). However, this second visit was cancelled due to Mats securing a full-time research position in this department.
- Giuseppe Negro, formerly of the University of Bari (Italy), had previously secured a 4-month post-doctorate research post in his former host group at the School of Physics and Astronomy at the University of Edinburgh (UK) after his second HPC-Europa3 visit. Following a third successful HPC-Europa3 visit to the same group, he has now secured a further post-doctoral research position there.

We have also seen visitors return to their host groups for follow-on research visits with alternative funding. One example is Argyrios Anagnostopoulos, who is continuing to make visits to his host, Prof. Simone Meloni at the University of Ferrara. We are also aware of visits that are planned beyond the lifetime of the project. For example, Apinya Ngoipala of the University of Limerick (Ireland) was accepted at the final call, but was not able to arrange a visa in time to carry out an in-person visit to her host Prof. Volker Deringer at the University of Oxford. The visit was carried out as a virtual visit instead, but Volker now plans to visit Apinya and her group leader in Ireland in June.

More examples of research highlights, long-term collaborations, and visitors obtaining research positions as a result of their visit can be found in the success stories from the individual HPC-Europa3 partner centres, which can be found at https://www.hpc-europa.org/public_documents under “Deliverables”.

7 Transnational Access Meeting (TAM)

HPC-Europa3 planned to hold 3 user group meetings over the project lifetime. These events, known as TAM – the **T**ransnational **A**ccess **M**eeting – give visitors the chance to present the work done in their HPC-Europa3 project as either a talk or a poster. All attendees are expected to present their work. For junior researchers, the event provides a relaxed and welcoming environment to give what may be their first ever conference talk. Participants have always given very positive feedback about these events, in HPC-Europa3 and previous programmes.

7.1 Second Transnational Access Meeting – TAM 2020

The first HPC-Europa3 TAM took place in Edinburgh in October 2018, and was a great success. The second TAM was organised by BSC and had been due to take place in Barcelona on 31st March 2020. However, this meeting had to be postponed due to the Covid-19 pandemic. It was initially rescheduled to take place in October 2020, in Barcelona as planned. However, as the pandemic continued, it became clear that it was still not going to be possible to hold the event in person by October, so the TAM was converted to an online format, held on 22nd and 23rd of October 2020.

There were clearly some new issues to consider when running the event online instead of in person – such as how to carry out the vote for best poster and best talk – but the event went very smoothly and feedback was very positive. All respondents agreed or strongly agreed that the content of both the keynote talk and the visitor presentations was interesting and useful, that the conference met their expectations, and that they would recommend attending TAM to others. All respondents were satisfied or very satisfied with the organisation of the event and the pre-event communication, and just 1 of the 16 respondents was dissatisfied with the online platform.

While the networking opportunities of a face-to-face meeting were obviously lacking, the online format allowed the event to be opened up to a much wider audience, including visitor hosts and interested people with no direct connection to the programme. In total over 100 people registered for the event, whereas normally attendance would be limited to around 40.

The event opened with a welcome talk by Dr. Sergio Girona, Operations Director at BSC, and was followed by a very interesting keynote lecture by John Davis, of the Laboratory for Open Computer Architecture (LOCA) at BSC: “*LOCA: Embracing Open Source Hardware to create an Open Source Ecosystem*”.²⁰

Over the 2 days, 21 visitors gave talks and a further 9 presented posters. The interdisciplinary nature of HPC-Europa3 is really highlighted at TAM, and at this event the presentation topics varied from

²⁰ Slides available at https://drive.google.com/file/d/1TZ_2g67-U6hgwx8Ad9m7sebsNsRRZKw0/view?usp=sharing.

“Unveiling tropical forests: new approaches using 3D terrestrial LiDAR” to “Stellar magnetic fields: stability and dynamos” and “The $\alpha 1$ subunit of the Na,K-ATPase facilitates unconventional secretion of fibroblast growth factor 2 from tumor cells”.

At the end of the first day of the event, Jordi Mas of BSC treated the attendees to a “virtual tour” of one of Barcelona’s most famous landmarks, the Sagrada Familia, since they had been unable to travel to the city and see it for themselves.

The best talk award was given to Martí López of the University of Barcelona (Spain), for *“Insights of the CO₂ adsorption on doped TiC”*, and the best poster award was given to Meilani Wibowo of the University of Nottingham (UK) for *“Combined RAS-srDFT for the study of electron transfer processes”*.

The programme, book of abstracts, the e-Posters, and slides from some of the talks can all be found at: <http://www.hpc-europa.eu/2ndTAM>.

7.2 Third Transnational Access Meeting – TAM 2021

The third HPC-Europa3 TAM, organised by SURF, was held on the 3rd and 4th of November 2021. Once again the event had to take place online, as Covid-19 travel restrictions continued to prevent the planning of in-person events. Registration numbers were somewhat lower for this TAM – perhaps because the novelty of online meetings had worn off and people were tired of presenting online. Nevertheless, 14 talks and 8 posters were presented, again covering a wide range of topics, including “Delineating the role of MALT1 in adaptive immunity and disease comorbidities”, “Modelling radar waves in clayey till using gprMax” and “Chemical properties of simulated galaxy clusters”.

The lower number of visitor talks presented the opportunity to invite more guest speakers, which brought some interesting perspectives to the event. The meeting began with a welcome from Walter Lioen (Head of Research Services at SURF) and a fascinating talk by Prof. Wim Nieuwpoort (Rijksuniversiteit Groningen), a pioneer of the Dutch national infrastructure for scientific calculations. This was followed by a guest lecture by Prof. Céilia Fonseca Guerra (Vrije Universiteit Amsterdam), who is not only a distinguished researcher but also has long involvement with the HPC-Europa3 programme as a host researcher. After lunch on the first day, another HPC-Europa3 host, Assoc. Prof. Hieab Adams (Erasmus University Medical Center, Rotterdam), gave a guest lecture. On the second day there were two further guest lectures, from Assoc. Prof. Ana Lucia Varbanescu (Universiteit van Amsterdam) and Assoc. Prof. Thomas la Cour Jansen (Rijksuniversiteit Groningen). The multidisciplinary character of HPC-Europa3 was again highlighted by the fact that these guest speakers came from the fields of applied theoretical chemistry and supramolecular quantum biochemistry, epidemiology, parallel computing, and theory of condensed matter.

Posters were presented in a virtual room using Gather Town, which worked well, allowing attendees to view the posters and ask the presenters questions directly.

The best talk award was given to Giovanni La Penna of the Italian National Research Council (CNR), for *“Measuring Shared Electrons in Extended Molecular Systems: Covalent Bonds from Plane-Wave Representation of Wave Function”*, and the best poster award was given to Mirko Vanzan of the University of Padova (Italy) for *“A computational study on the opto-electronic properties of various AuRh nanoclusters obtained through different synthetic processes”*.

8 Conclusion

This reporting period covers a time of unprecedented challenge for the HPC-Europa3 programme, with a period of around 18 months during which very few visits were able to take place, due to the global Covid-19 pandemic, followed by a 6-month period of frenetic activity as visitors rushed to carry out their visits before the programme ended.

The programme fell short of its target number of visits by quite a long way, which is disappointing given that the call before the first lockdown had seen the biggest number of applications ever received for any HPC-Europa programme (or any of its predecessors). However, with international travel restrictions in place for much of this period, it is unsurprising that application numbers were low for 5 of the 7 calls in the period, and that many visits were cancelled.

However, there are many positives to highlight.

- The programme adapted successfully to the challenges of the Covid-19 pandemic, introducing flexibility via virtual visits and hybrid visits, which have been much more successful than had been anticipated based on previous experience of virtual visits.
- Satisfaction levels were extremely high, both among visitors and hosts.
- High-quality scientific outputs continue to arise from visits, and all visitor questionnaire respondents said that they expected to publish the results of the work done during their visit.
- Participants continue to report that the experience gained or connections made during their visit have helped them secure their next research post.
- Two successful user group meetings were held, with very positive feedback received.
- Applications continued to come from a wide range of countries, with an increasing number coming from developing countries, and a wide range of scientific disciplines, including applications from the humanities in this reporting period.
- Visitors were from a very wide age range and a mix of different career stages.
- A record high of 28% of applications were from female researchers, which is a good representation given the proportion of females working in STEM research.
- While application numbers fell during the pandemic, they bounced back as the travel restrictions were relaxed in the final months of the programme.
- Although the programme was effectively almost completely paused for 18 months, an unprecedented number of visits took place in the final 6 months of the programme. More than half of all visits took place in this reporting period, and of those, most took place in those final 6 months.

In conclusion, the programme was highly impacted by the Covid-19 pandemic, and this greatly contributed to the shortfall in visitor numbers. However, the programme was extremely successful overall, demonstrably bringing great benefits to almost everyone who participated, either as visitors or host researchers. These include short-term benefits, such as the experience gained both professionally and personally when living and working in another country, medium-term benefits, such as scientific publications and conference presentations arising from the visits, and long-term benefits, such as continuing collaborations and career moves resulting from the visit. The programme was successful in adapting to the challenges of the pandemic, with feedback from virtual visits mostly being as positive as that for visits carried out in person. There is great demand for a continuation of the programme, both from visitors and hosts.

Annex I Membership of Scientific Users Selection Panel (SUSP)

Astrophysics		
Prof. Stefano Borgani	Astronomical Observatory of Trieste, University of Trieste	Italy
Prof. Gustavo Yepes	Department of Theoretical Physics, Autonomous University of Madrid	Spain
Chemistry		
Dr. Mark Abraham	<i>Formerly of</i> Department of Theoretical Physics, KTH Royal Institute of Technology and SciLifeLab	Sweden
Prof. dr. Ria Broer	Department of Theoretical Chemistry, Groningen University	The Netherlands
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. Eliseo Ruiz	Faculty of Chemistry, University of Barcelona	Spain
Prof. Dage Sundholm	Department of Chemistry, University of Helsinki	Finland
Computer Sciences		
Dr. Lilit Axner	PDC Center for High Performance Computing, KTH Royal Institute of Technology <i>NB Lilit joined the panel after KTH had already allocated all of their Transnational Access places and had stopped accepting new applications.</i>	Sweden
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



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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
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
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

Annex II List of publications and conference proceedings

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

1. Acapulco J., Meysami S.S., Babenko V., Evers K., Jones R., Swart M., Grobert N., "In Situ Experimental and Theoretical Studies of the Nucleation and Growth Towards Controlling the Morphology of Boron Nitride Nanotubes Using Chemical Vapour Deposition Techniques" Poster presentation, 2018 MRS Fall Meeting and Exhibit, Boston, Massachusetts, USA.
2. Aarva A., Deringer V.L., Sainio S., Laurila T., Caro M.A., "Understanding X-ray Spectroscopy of Carbonaceous Materials by Combining Experiments, Density Functional Theory, and Machine Learning. Part I: Fingerprint Spectra", *Chem. Mater.*, 31, 22, 9243–9255, 2019. doi:10.1021/acs.chemmater.9b02049
3. Aarva A., Deringer V.L., Sainio S., Laurila T., Caro M.A., "Understanding X-ray Spectroscopy of Carbonaceous Materials by Combining Experiments, Density Functional Theory, and Machine Learning. Part II: Quantitative Fitting of Spectra", *Chem. Mater.*, 31, 22, 9256–9267, 2019. doi:10.1021/acs.chemmater.9b02050
4. Acebrón J.A., Herrero J.R., Monteiro J., "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*, Volume 79, Issue 12, Pages 3495–3515, 2020. doi: 10.1016/j.camwa.2020.02.013
5. Adebambo P.O., Osafire O.E., Laoye J.A., Idowu M.A., Adebayo G.A., "Electronic fitness function, effective mass and thermoelectric properties of Rh-based (-ScTe; -TiSb; -VSn) alloys for thermoelectric generator applications", *Computational Condensed Matter* Volume 26, 2021, e00523. <https://doi.org/10.1016/j.cocom.2020.e00523>
6. Ahmoum H., Boughrara M., Sukor Su'ait M., Kerouad M., "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>
7. Ahmoum H., Boughrara M., Sukor Su'ait M., Li G., Chopra S., Wang Q., Kerouad M., "Understanding the effect of the carbon on the photovoltaic properties of the Cu₂ZnSnS₄", 251, 123065, 2020.
8. Ahmoum H., Chelvanathan P., Sukor Su'ait M., Boughrara M., Li G., Gebauer R., Sopian K., Kerouad M., Amin N., Wang Q., "Sol-gel prepared Cu₂ZnSnS₄ (CZTS) semiconductor thin films: Role of solvent removal processing temperature", *Materials Science in Semiconductor Processing*, 132, 105874, 2021.
9. Ahmoum H., Li G., Piao Y., Liu S., Gebauer R., Boughrara M., Sukor Su'ait M., Kerouad M., Wang Q., "Ab-initio, Monte Carlo and experimental investigation on structural, electronic and magnetic properties of Zn_{1-x}Ni_xO nanoparticles prepared via sol-gel method", <https://doi.org/10.1016/j.jallcom.2020.157142>
10. Aldinucci M., Cesare V., Colonnelli I., Martinelli A.R., Mittone G., Cantalupo B., Cavazzoni C., Drocco M., "Practical parallelization of scientific applications with OpenMP, OpenACC and MPI", *Journal of Parallel and Distributed Computing*, Volume 157, Pages 13-29, ISSN 0743-7315, 2021. <https://doi.org/10.1016/j.jpdc.2021.05.017>.
11. Alekseev A.Y., Migas D.B., Filonov A.B., Borisenko V.E., Skorodumova N.V., "Structural stability and electronic properties of 2D alkaline-earth metal silicides, germanides, and stannides", *Jpn. J. Appl. Phys.* 59, SF0801, 2020.
12. Alessandri R., Barnoud J., Gertsen A.S., Patmanidis I., de Vries A.H., Souza P.C.T., et al. "Martini 3 Coarse-Grained Force Field: Small Molecules", *ChemRxiv*. Cambridge: Cambridge Open Engage; 2021. doi: 10.33774/chemrxiv-2021-1qmq9
13. Amato M., Ossicini S., Canadell E., Rurali R., "Preferential Positioning, Stability, and Segregation of Dopants in Hexagonal Si Nanowires", *Nano Lett.* 19, 866-876, 2019.
14. Aquilante F, et al, "Modern quantum chemistry with [Open]Molcas", *J. Chem. Phys.*, 152, 214117, 2020. <https://doi.org/10.1063/5.0004835>
15. Aseeri S., Muite B.K., Takahashi D., "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, 2019.
16. Ashari Astani N., Najafi F., Maghsoumi A., Huma K., Azimi L., Karimi A., Ejtehadi M.R., Gumbart J.C., Naseri N., "Molecular Machinery Responsible for Graphene Oxide's Distinct Inhibitory Effects toward *Pseudomonas aeruginosa* and *Staphylococcus aureus* Pathogens", *ACS Applied Bio Materials*, 2020.
17. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190203)" [Data set], Zenodo, 2019. <http://doi.org/10.5281/zenodo.2195952>
18. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190204)" [Data set], Zenodo, 2019. <http://doi.org/10.5281/zenodo.2556556>
19. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190207)" [Data set], Zenodo, 2019. <http://doi.org/10.5281/zenodo.2559260>
20. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190228)" [Data set], Zenodo, 2019. <http://doi.org/10.5281/zenodo.2580088>

21. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190307) [Data set]", Zenodo, 2019. <http://doi.org/10.5281/zenodo.2586614>
22. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190326) [Data set]", Zenodo, 2019. <http://doi.org/10.5281/zenodo.2607897>
23. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190513) [Data set]", Zenodo, 2019. <http://doi.org/10.5281/zenodo.2784400>
24. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhao M., "Dynamics of Phase Separation from Holography (Version v20190918) [Data set]", Zenodo, 2019. <http://doi.org/10.5281/zenodo.3445360>
25. Attems M., Bea Y., Casalderrey-Solana J., Mateos D., Zilhão M., "Dynamics of Phase Separation from Holography", JHEP, 01, 106, 2020. doi:10.1007/JHEP01(2020)106, arXiv:1905.12544 [hep-th].
26. Auclair P., Caprini C., Cutting, D., Hindmarsh M., Rummukainen K., Steer D.A., Weir D.J., "Generation of gravitational waves from freely decaying turbulence", eprint = "2205.02588", 2022. <https://inspirehep.net/literature/2077620>
27. Baratto C., Faglia G., Tkachenko N., Holovanova V., Nazarchuk B., Golovanov V., "On the alignment of ZnO nanowires by Langmuir – Blodgett technique for sensing application", Applied Surface Science, 528, 146959, 2020.
28. Baratto C., Golovanova V., Faglia G., Dang T., Hakola H., Niemi T., Tkachenko N., Nazarchuk B., Golovanov V., "Effect of light activation on chemical gas sensor based on aligned nanowires", The Proc. of the IEEE Sensors 2020, WTC, Rotterdam, The Netherlands, October 25-28, 2020.
29. Behbahani A.F., Motlagh G.H., Vaez Allaei S.M., Harmandaris V.A., "Structure and Conformation of Stereoregular Poly (methyl methacrylate) Chains Adsorbed on Graphene Oxide and Reduced Graphene Oxide via Atomistic Simulations", Macromolecules, 52(10), pp 3825-3838, 2019.
30. Behbahani A.F., Vaez Allaei S.M., Motlagh G.H., Eslami H., Harmandaris V.A., "Structure, Dynamics, and Apparent Glass Transition of Stereoregular Poly (methyl methacrylate)/Graphene Interfaces through Atomistic Simulations", Macromolecules, 51 (19), pp 7518–7532, 2018.
31. Bellentani L., Bordone P., Oriols X., Bertoni A., "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.
32. Bellentani L., Bordone P., Oriols X., Bertoni A., "Parallel implementation of the Split-Step Fourier method for exact two-electron dynamics in Hall interferometers", Invited Talk at WHPTCAD seminar at IWCN 2019 (Evanston) (<http://www.iue.tuwien.ac.at/iwcn2019/wp-content/uploads/2019/05/WHPTCAD-2019-Book-of-Abstracts-May-17.pdf>)
33. Bellentani L., Colomes E., Zhan Z., Bordone P., Bertoni A., Oriols X., "On the Incompatibility Between Frensel's Inflow Boundary Conditions and Stationary Wigner Distribution Functions: The Problem and the Solution", Talk at IW2 seminar at IWCN 2019 (Evanston) (<http://www.iue.tuwien.ac.at/iwcn2019/wp-content/uploads/2019/05/IW2-2019-Book-of-Abstracts-May-17.pdf>)
34. Berger R.J.F., Viel A., "The principle underlying antiaromaticity", eprint arXiv:1811.08959, 11, ARXIV, Physics - Chemical Physics, 2018arXiv181108959B, 2018.
35. Bombin R., Cikojević V., Sánchez-Baena J., Boronat J., "Finite-range effects in the two-dimensional repulsive Fermi polaron", Phys. Rev. A, 103, L041302, 2021. doi: 10.1103/physreva.103.l041302
36. Bonanno A., Corsaro E., Del Sordo F., Pallé P.L., Stello D., Hon M., "Acoustic oscillations and dynamo action in the G8 sub-giant EK Eridani", Astronomy & Astrophysics, Volume 628, 2019.
37. Bonilla M.R., García Daza F.A., Ranque P., Aguesse F., Carrasco J., Akhmatskaya E., "Unveiling Interfacial Li-Ion Dynamics in Li7La3Zr2O12/PEO(LiTFSI) Composite Polymer-Ceramic Solid Electrolytes for All-Solid-State Lithium Batteries" ACS Appl. Mater. Interfaces, 13, 26, 30653–30667, 2021. <https://doi.org/10.1021/acsami.1c07029>
38. Bortoli M., Bruschi M., Swart M., Orian L., "Sequential oxidations of phenylchalcogenides by H2O2: insights into the redox behavior of selenium via DFT analysis", New J. Chem., 44, 6724-6731, 2020.
39. Broekgaarden F.S., Justham S., de Mink S.E., Gair J., Mandel I., Stevenson S., ... & Neijssel C.J., "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.
40. Bussov M., Nätilä J., "Segmentation of turbulent computational fluid dynamics simulations with unsupervised ensemble learning", Signal Processing: Image Communication, 2021. <http://arxiv.org/abs/2109.01381>
41. Candelaresi S., Del Sordo F., "Stabilizing Effect of Magnetic Helicity on Magnetic Cavities in the Intergalactic Medium", ApJ, 896, 86, 2020. doi: 10.3847/1538-4357/ab8dc0
42. Cappellini G., Bosin A., Serra G., Furthmueller J., Bechstedt F., Botti S., "Electronic and Optical Properties of Small Metal Fluoride Clusters", ACS Omega, 2020. <https://dx.doi.org/10.1021/acsomega.0c01317>
43. Carena L.N., Gonnella G., Lamura A., Negro G., Tiribocchi A., Eur. Phys. J. E, 42: 81, 2019

44. Carezza L.N., Gonnella G., Marenduzzo D., Negro G. "Chaotic and periodical dynamics of active chiral droplets", *Physica A: Statistical Mechanics and its Applications*, Vol 559, 125025, 2020.
<https://doi.org/10.1016/j.physa.2020.125025>
45. Carezza L.N., Gonnella G., Marenduzzo D., Negro G., "Rotation and propulsion in 3D active chiral droplets", *PNAS* October 29, 2019 116 (44) 22065-22070; first published October 14, 2019
<https://doi.org/10.1073/pnas.1910909116>
46. Carezza L.N., Gonnella G., Marenduzzo D., Negro G., *Proc. Natl. Acad. Sci.*, 116, 22065, 2019.
47. Caro M.A., "Optimizing many-body atomic descriptors for enhanced computational performance of machine learning based interatomic potentials", *Phys. Rev. B* 100, 024112, 2019.
48. Chesnokov A., Gryaznov D., Skorodumova N.V., Kotomin E.A., Zitolo A., Zubkins M., Kuzmin A., Anspoks A., Purans J., "The local atomic structure and thermoelectric properties of Ir-doped ZnO: hybrid DFT calculations and XAS experiments", *J. Mater. Chem. C*, 9, 4948-4960, 2021. DOI:10.1039/D1TC00223F
49. Cikojević V., Poli E., Ancilotto F., Vranješ-Markić L., Boronat J., "Dilute quantum liquid in a K-Rb Bose mixture", *Phys. Rev. A* 104, 033319, 2021. Doi: <https://doi.org/10.1103/physreva.104.033319>
50. Cikojević V., Vranješ Markić L., Boronat J., "Finite-range effects in ultradilute quantum drops." arXiv preprint arXiv:2001.09086, 2020.
51. Cikojević V., Vranješ Markić L., Pi M., Barranco M., Ancilotto F., Boronat J., "Dynamics of equilibration and collisions in ultradilute quantum droplets", *Phys. Rev. Research*, 3, 043139, 2021.
doi:10.1103/physrevresearch.3.043139
52. Cikojević V., Vranješ Markić L., Pi M., Barranco M., Ancilotto F., Boronat J., "TDynamics of equilibration and collisions in ultradilute quantum droplets", 2021. <https://arxiv.org/abs/2104.09102>
53. Cikojević V., Vranješ Markić L., Pi M., Barranco M., Boronat J., "Towards a QMC-based density functional including finite-range effects: excitation modes of a 39K quantum droplet", *Phys. Rev. A* 102, 033335, 2020. DOI: 10.1103/PhysRevA.102.033335
54. Cloutier B., Muite B.K., Parsani M. "Fully Implicit Time Stepping Can Be Efficient on Parallel Computers". *Supercomputing Frontiers and Innovations*, 6 (2), 75–85, 2019. doi:10.14529/jsfi190206
55. Conley K.M., Cocchi C., Ala-Nissila T., "Formation of Near-IR Excitons in Low-Dimensional CuSbS₂", *J. Phys. Chem. C*, 125, 38, 2021. doi: 10.1021/acs.jpcc.1c06530
56. Coronado-Barrientos E., Antonioletti M., Garcia-Loureiro A., "A new AXT format for an efficient SpMV product using AVX-512 instructions and CUDA", *Advances in Engineering Software*, vol. 156, pp. 102997, 2021. <https://doi.org/10.1016/j.advengsoft.2021.102997>
57. Cosco F., Talarico N.W., Tuovinen R., Lo Gullo N., "Spectral properties of correlated quantum wires and carbon nanotubes within the Generalized Kadanoff-Baym Ansatz", 2020. <http://arxiv.org/abs/2007.08901>
58. Damasso M., Del Sordo F. (equally contributing) "Expectations for the confirmation of Proxima c from a long-term radial velocity follow-up", *MNRAS* 2020.
59. Danielis N., Vega L., Fronzoni G., Stener M., Bruix A., Neyman K.M., "AgPd, AuPd, and AuPt Nanoalloys with Ag- or Au-Rich Compositions: Modeling Chemical Ordering and Optical Properties", *The Journal of Physical Chemistry C*, 125 (31), 17372-17384, 2021. DOI: 10.1021/acs.jpcc.1c04222.
60. Daskalakis V., Maity S., Hart C.L., Stergiannakos T., Duffy C.D.P., leinekathöfer U., "Structural Basis for Allosteric Regulation in the Major Antenna Trimer of Photosystem II", *J. Phys. Chem. B*, 123, 45, 9609-9615, 2019.
61. Daskalakis V., Papadatos S., Kleinekathoef, U., "Fine tuning of the photosystem II major antenna mobility within the thylakoid membrane of higher plants", *Biochim. Biophys. Acta – Biomembranes*, 1861, 183059, 2019.
62. Daub C.D., Riccardi E., Hanninen V., Halonen L., "Path sampling for atmospheric reactions: Formic acid catalysed conversion of SO₃ + H₂O to H₂SO₄", *PeerJ Physical Chemistry*, submitted September 2019.
63. Davidovic D., Quintana-Orti E.S., "Structure-Aware Calculation of Many-Electron Wave Function Overlaps on Multicore Processors", in *Parallel Processing and Applied Mathematics*, pp. 13-24, 2020.
<http://fulir.irb.hr/5415/>
64. De Fazio D., Aguado A., Petrongolo C., "Non-adiabatic Quantum Dynamics of the Dissociative Charge Transfer He⁺⁺H₂ → He⁺H+H⁺", *Frontiers in Chemistry*, 7, 2019. DOI=10.3389/fchem.2019.00249
65. de Melo P.M.M.C., Zanolli Z., Verstraete M.J., "Optical Signatures of Defect Centres in Transition Metal Dichalcogenide Monolayers", 2020. <http://arxiv.org/abs/2010.10222>
66. de Melo P.M.M.C., Zanolli Z., Verstraete M.J., "Optical Signatures of Defect Centers in Transition Metal Dichalcogenide Monolayers", *Adv. Quantum Technol.*, 4: 2000118, 2021.
<https://doi.org/10.1002/qute.202000118>

67. De Santis M., Storchi L., Belpassi L., Quiney H.M., Tarantelli F., "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>
68. Delgado-Callico L., Ferrari P., Bakker J.M., Baletto F., Janssens E., "Benchmarking density functional theory methods for cationic metal-argon complexes", *Theor. Chem. Acc.* 140, 38, 2021.
69. Deringer V.L., Caro M.A., Csányi G., "Machine Learning Interatomic Potentials as Emerging Tools for Materials Science", *Adv. Mater.*, 1902765, 2019. DOI: 10.1002/adma.201902765
70. Deringer V.L., Caro M.A., Csányi, G., "A general-purpose machine-learning force field for bulk and nanostructured phosphorus", *Nat Commun* 11, 5461, 2020. <https://doi.org/10.1038/s41467-020-19168-z>
71. Deringer V.L., Caro M.A., Jana R., Aarva A., Elliott S.R., Laurila T., Csányi G., Pastewka L. "Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory", *Chem. Mater.*, 2018. DOI: 10.1021/acs.chemmater.8b02410
72. Deubner H.L., Graubner T., Buchner M.R., Weigend F., Ivlev S.I., Karttunen A.J., Kraus F., *ACS Omega*, 7, 11995–12003, 2022.
73. Di Gaetano S., Pirone L., Galdadas I., Traboni S., Iadonisi A., Pedone E., Saviano M., Gervasio F.G., Capasso D., "Design, Synthesis, and Anticancer Activity of a Selenium-Containing Galectin-3 and Galectin-9N Inhibitor", *Int. J. Mol. Sci.*, 23, 2581, 2022. <https://doi.org/10.3390/ijms23052581>
74. Di Liberto G., Tosoni S., Illas F., Pacchioni G., "Nature of SrTiO₃/TiO₂ (anatase) Heterostructure from Hybrid Density Functional Theory Calculations", *J. Chem. Phys.* 152, 184704, 2020.
75. Diaz J., Pinna M., Zvelindovsky A.V., Pagonabarraga I., "Large scale three dimensional simulations of hybrid block copolymer/nanoparticle systems", *Soft Matter*, 15, 9325-9335, 2019. doi:10.1039/C9SM01760G
76. Diaz J., Pinna M., Zvelindovsky A.V., Pagonabarraga I., "Nonspherical Nanoparticles in Block Copolymer Composites: Nanosquares, Nanorods, and Diamonds", *Macromolecules*, 52(21), 8285–8294, 2019. doi: 10.1021/acs.macromol.9b01754
77. Diez-Cabanes V., Morales-Garcia A., Illas F., Pastore M., "Understanding the Structural and Electronic Properties of Photoactive Tungsten Oxide Nanoparticles from Density Functional Theory and GW Approaches", *J. Chem. Theory Comput.*, 17, 3462–3470, 2021.
78. Dobrota A.S., Pašti I.A., Mentus S.V., Johansson B., Skorodumova N.V., "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, 2020. <https://doi.org/10.1016/j.apsusc.2020.145937>
79. Dominikowska J., Rybarczyk-Pirek A.J., Fonseca Guerra C., "Lack of Cooperativity in the Triangular X₃ Halogen-Bonded Synthons?", *Cryst. Growth Des.*, 21, 1, 597–607, 2021. <https://doi.org/10.1021/acs.cgd.0c01410>
80. Dotolo S., Facchiano A., "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.
81. Dotolo S., Facchiano A., "Natural-bioactive compounds study by means of bioinformatics approaches", On Abstract book. BITS 5-8 July 2017.
82. Dotolo S., Facchiano A., Pandini A., "Comparative analysis of molecular motions in SIRTUIN2 proteins". On Abstract book. BBCC 18-20, 2017.
83. Dotolo S., Facchiano A., Pandini A., "Detection of the impairment of allosteric communication in Sirtuin2 proteins through molecular dynamics and residue coevolution", BITS 27-29 June 2018.
84. Drach V., Fritzsche P., Rago A., Romero-Lopez F., "Singlet channel scattering in a composite Higgs model on the lattice", *Eur. Phys. J. C*, 82(1):47, 2022. doi: 10.1140/epjc/s10052-021-09914-y
85. Dragoni D., Behler J., Bernasconi M., "Mechanism of amorphous phase stabilization in ultrathin films of monoatomic phase change material", *Nanoscale*, 13, 38, 16146-16155, 2021. doi: 10.1039/d1nr03432d
86. Economo S., Royuela S., Ayguadé E., Beltran V., "A Toolchain to Verify the Parallelization of OmpSs-2 Applications", In: Malawski, M., Rządca, K. (eds) *Euro-Par 2020: Parallel Processing*. Euro-Par 2020. Lecture Notes in Computer Science(), vol 12247. Springer, Cham. https://doi.org/10.1007/978-3-030-57675-2_2
87. Faroughi S.A., Roriz A.I., Fernandes C., "A Meta-Model to Predict the Drag Coefficient of a Particle Translating in Viscoelastic Fluids: A Machine Learning Approach", *Polymers*, Vol 14, Iss 430, p 430, 2022. <https://www.mdpi.com/2073-4360/14/3/430>
88. Ferrari P., Delgado-Callico L., Lievens P., Baletto F., Janssens E., "Stability of cationic silver doped gold clusters and the subshell-closed electronic configuration of AgAu₁₄⁺", *J. Chem. Phys.* 153, 244304, 2020.
89. Ferrari P., Pham H.T., Vanbuel J., Nguyen M.T., Fiellike A., Janssens E., "An octacoordinated Nb atom in the NbAl₈H₈⁺ cluster", *Chem. Commun.*, 57, 9518-9521, 2021.

90. Finelli F., Cerri S.S., Califano F., Pucci F., Laveder D., Lapenta G., Passot T., "Bridging hybrid-and full-kinetic models with landau-fluid electrons: I. 2d magnetic reconnection", *Astronomy & Astrophysics*, 653:A156, 2021. doi:<https://doi.org/10.1051/0004-6361/202140279>
91. Futatani S., "Application of OpenFOAM for non-linear MHD simulations of magnetically confined plasma", Oral talk, 3rd TA visitors meeting (TAM), online meeting, November 3-4, 2021.
92. Gallego A.-J., Gil P., Pertusa A., Fisher R.B., "Segmentation of Oil Spills on Side-Looking Airborne Radar Imagery with Autoencoders", *Sensors*, 18(3): 797, 2018.
93. Gallego A.-J., Pertusa A., Gil P., Fisher R.B., "Detection of bodies in maritime rescue operations using Unmanned Aerial Vehicles with multispectral cameras", *Journal of Field Robotics*, 2018.
94. Garip A.K., Arslan H., Rapetti D., Ferrando R., "A DFT study of chemical ordering and oxygen adsorption in AuPtPd ternary nanoalloys", *Mater. Today Commun.* 25, 101545, 2020. doi:10.1016/j.mtcomm.2020.101545.
95. Gebraad L., Zhang X., Zunino A., Fichtner A., Curtis, A., "Comparing algorithms for Bayesian tomography: SVGD versus HMC", In AGU Fall Meeting 2021.
96. Gent F.A., Snow B., Fedun V., Erdelyi R., "Modelling 3D magnetic networks in a realistic solar atmosphere", arXiv:1904.11421, 2019. <https://ui.adsabs.harvard.edu/abs/2019arXiv190411421G>
97. George J., Hautier G., Bartók A.P., Csányi G., Deringer V.L., "Combining phonon accuracy with high transferability in Gaussian approximation potential models", *J. Chem. Phys.*, 153, 044104, 2020. URL: <https://aip.scitation.org/doi/10.1063/5.0013826>
98. Gianguzzi L., Bazan G., "The Olea europaea L. var. sylvestris (Mill.) Lehr. forests in the Mediterranean area", *Plant Sociology* 56(2): 3-34, 2019. DOI:10.7338/pls2019562/01
99. Gimferrer M., Danes S., Andrada D.M., Salvador P., "Unveiling the Electronic Structure of the Bi(+1)/Bi(+3) Redox Couple on NCN and NNN Pincer Complexes", *Inorg. Chem.*, 60, 23, 17657-17668, 2021. DOI:10.1021/acs.inorgchem.1c02252
100. Gonçalves J.N., Phillips A.E., Li W., Stroppa A., "First-Principles Study of Structure and Magnetism in Copper(II)-Containing Hybrid Perovskites", *Crystals* 10, 12, 2020.
101. Gouveia J.D., Morales-García A., Viñes F., Gomes J.R.B., Illas F., "Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes", *ACS Catal.*, 10, 9, 5049–5056, 2020. <https://doi.org/10.1021/acscatal.0c00935>
102. Gouveia J.D., Morales-García A., Viñes F., Illas F., Gomes J.R.B., "MXenes as promising catalysts for water dissociation", *Applied Catalysis B: Environmental* 260, 118191, 2020.
103. Granda-Marulanda L.P., Builes S., Koper M.T.M., Calle-Vallejo F., "Influence of Van der Waals Interactions on the Solvation Energies of Adsorbates at Pt-Based Electrocatalysts", *ChemPhysChem*, 20, 2968, 2019. <https://doi.org/10.1002/cphc.201900512>
104. Guccione G., Benzi R., Plummer A., Toschi F., "Discrete Eulerian model for population genetics and dynamics under flow", *Phys. Rev. E*, 100, 062105, 2019. doi: <https://doi.org/10.1103/physreve.100.062105>
105. Guerrero G., Del Sordo F., Bonanno A., Smolarkiewicz P.K., "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.
106. Guerrini M., Cocchi C., Calzolari A., Varsano D., Corni S., "Interplay between Intra- and Intermolecular Charge Transfer in the Optical Excitations of J-Aggregates", *J. Phys. Chem. C*, 123, 11, 6831–6838, 2019. doi: 10.1021/acs.jpcc.8b11709
107. Gurova S.-M., Gurov T., Karaivanova A., "Scalability study of MPI algorithm for a predator-prey model with SEIRS epidemic disease", *AIP Conference Proceedings*, vol.2302, pp. 030001-1- 030001-7, 2020. DOI:10.1063/5.0033697, (SJR=0.190).
108. Heshmat M., "Alternative Pathway of CO₂ Hydrogenation by Lewis-Pair-Functionalized UiO-66 MOF Revealed by Metadynamics Simulations", *J. Phys. Chem. C*, 124, 20, 10951–10960, 2020.
109. Heshmat M., "Lewis acidity of carbon in activated carbonyl group vs. B(C₆F₅)₃ for metal-free catalysis of hydrogenation of carbonyl compounds", *ChemPhysChem*, Volume22, Issue14, Pages 1535-1542, 2021. <https://doi.org/10.1002/cphc.202100003>
110. Heshmat M., Ensing B., "Optimizing the Energetics of FLP-Type H₂ Activation by Modulating the Electronic and Structural Properties of the Lewis Acids: A DFT Study", *J. Phys. Chem. A*, 124, 32, 6399–6410, 2020.
111. Hindmarsh M., Lizarraga J., Urio A., Urrestilla J., "Loop decay in Abelian-Higgs string networks", *Phys. Rev. D*, 104, 4, 043519, 2021. doi = 10.1103/PhysRevD.104.043519
112. Iakymchuk R., Barreda M., Graillat S., Aliaga J.I., Quintana-Ortí E.S., "Reproducibility of Parallel Preconditioned Conjugate Gradient in Hybrid Programming Environments", Accepted to IJHPCA, 2020. <https://hal.archives-ouvertes.fr/hal-02427795/document>
113. Iakymchuk R., Barreda M., Wiesenberger M., Aliaga J.I., Quintana-Ortí E.S., "Reproducibility Strategies for Parallel Preconditioned Conjugate Gradient", *JCAM*, vol 371, pages 112697, 2020. DOI: <https://doi.org/10.1016/j.cam.2019.112697>

114. Ibragimova R., Erhart P., Rinke P., Komsa H.-P., "Surface Functionalization of 2D MXenes: Trends in Distribution, Composition, and Electronic Properties", *J. Phys. Chem. Lett.*, 12, 9, 2377–2384, 2021. doi: 10.1021/acs.jpcclett.0c03710
115. Iravani A., "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.
116. Iravani A., Åström J., Ouchterlony F., "Physical Origin of the Fine-Particle Problem in Blasting Fragmentation", *PhysRevApplied*, 10(3):34001, 2018. DOI: 10.1103/PhysRevApplied.10.034001
117. Iravani A., Kukolj I., Ouchterlony F., Antretter T., Åström, J., "Modelling blast fragmentation of mortar and rock". In proceedings of the 12th international symposium on rock fragmentation by blasting Luleå, Sweden, 2018.
118. Ivanovskaya M., Ovodok E., Kotsikau D., Azarko I., Micusik M., Omastova M., Golovanov V., "Structure of titanium carbide and nature of its defects", *RSC Advances*, 10, 25602-25608, 2020.
119. Kapci M.F., Schön J.C., Bal B., "The role of hydrogen in the edge dislocation mobility and grain boundary-dislocation interaction in -Fe", *International Journal of Hydrogen Energy*, Volume 46, Issue 64, Pages 32695-32709, 2021.
120. Khan S.U. et al., "Natural bioactive compounds as a new source of promising G protein-coupled estrogen receptor (GPER) modulators: comprehensive in silico approach." *Journal of Biomolecular Structure and Dynamics*: 1-12, 2021.
121. Klefogiannis I., Amanatidis I., "Physics in nonfixed spatial dimensions via random networks", *Phys. Rev. E* 105, 024141, 2022. <https://journals.aps.org/pre/abstract/10.1103/PhysRevE.105.024141>
122. Klefogiannis, I., Amanatidis, I., "Fractional-quantum-Hall-effect (FQHE) in 1D Hubbard models", *Eur. Phys. J. B*, 94, 41, 2021. DOI: <https://doi.org/10.1140/epjb/s10051-021-00050-w>
123. Knol MJ, Pawlak MA, Lamballais S, Terzikhan N, Hofer E, Xiong Z, Klaver CCW, Pirpamer L, Vernooij MW, Ikram MA, Schmidt R, Kayser M, Evans TE, Adams HHH. Genetic architecture of orbital telorism. *Hum Mol Genet.* 2022 May 4;31(9):1531-1543. doi: 10.1093/hmg/ddab334. PMID: 34791242; PMCID: PMC9071440. <https://pubmed.ncbi.nlm.nih.gov/34791242/>
124. Köpcke B., Steuer M., Gorlatch S., "Generating Efficient FFT GPU Code with Lift", *FHPNC@ICFP*, 1-13, 2019.
125. Kos L., Brank M., Simič G., Penko D., Johnson T., "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.
126. Kos L., Pitts R.A., Simic G., Brank M., Anand H., Arter W., "SMITER: A field-line tracing environment for ITER", *Fusion Eng. and Design*, 2019. DOI:10.1016/j.fusengdes.2019.03.037, arXiv:1903.11547
127. Kuisma M., Rousseaux B., Czajkowski K.M., Rossi T.P., Shegai T., Erhart P., Antosiewicz T.J., "Ultrastrong Coupling of a Single Molecule to a Plasmonic Nanocavity: A First-Principles Study", *ACS Photonics* 9, 1065-1077, 2022.
128. La Penna G., Tiana D., Giannozzi P., "Measuring Shared Electrons in Extended Molecular Systems: Covalent Bonds from Plane-Wave Representation of Wave Function", *Molecules* (special issue dedicated to Linus Pauling), 2021. <https://www.mdpi.com/1420-3049/26/13/4044>
129. Legrand C., Saleppico R., Sticht J., Lolicato F., Müller H.-M., Wegehingel S., Dimou E., Steringer J.P., Ewers H., Vattulainen I., Freund C., Nickel W., "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
130. Lengvinaitė D., Kvedaraviciute S., Bielskutė S., Klimavicius V., Balevicius V., Mocci F., Laaksonen A., Aidas K., "Structural Features of the [C4mim][Cl] Ionic Liquid and Its Mixtures with Water: Insight from a 1H NMR Experimental and QM/MD Study", *Journal of Physical Chemistry B*, 125, 48, 13255–13266, 2021. <https://pubs.acs.org/doi/10.1021/acs.jpcc.1c08215>
131. Lepsik M., Sommer R., Kuhadomlarp S., Lelimousin M., Paci E., Varrot A., 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.*, 177:212-220, 2019.
132. Li G., Ahmoum H., Liu S., Liu S., Sukor Su'ait M., Boughrara M., Kerouad M., Wang Q., "Theoretical insight into magnetic and thermoelectric properties of Au doped ZnO compounds using density functional theory". 562, 67, 2019.
133. Lin Z., Qian L., Campobasso M.S., Bai W., Zhou Y., Ma Z., "Modelling Aerodynamics of a Floating Offshore Wind Turbine Using the Overset Mesh Solver in OpenFOAM, paper OMAE2022-79230, ASME Conference on Ocean", *Offshore and Arctic Engineering*, 5th-10th June 2022, Hamburg, Germany.
134. López M., Viñes F., Nolan M., Illas F., "Predicting the Effect of Dopants on CO2 Adsorption in Transition Metal Carbides: Case Study on TiC (001)", *J. Phys. Chem. C*, 124, 29, 2020.

135. Maćzka M., Gağor A., Stroppa A., Gonçalves J.N., Zaręba J.K., Stefańska D., Pikul A., Drozd M., Sieradzki A., "Two-Dimensional Metal Dicyanamide Frameworks of BeTriMe[M(Dca)₃(H₂O)] (BeTriMe = Benzyltrimethylammonium; Dca = Dicyanamide; M = Mn²⁺, Co²⁺, Ni²⁺): Coexistence of Polar and Magnetic Orders and Nonlinear Optical Threshold Temperature Sensing", *J. Mater. Chem.*, C 8, 11735, 2020.
136. Maio U., Borgani S., Ciardi B., Petkova M., "The seeds of supermassive black holes and the role of local radiation and metal spreading", eprint arXiv:1811.01964, 2019.
<http://adsabs.harvard.edu/abs/2018arXiv181101964M>
137. Maity S., Gelessus A., Daskalakis V., Kleinekathoefer U., "On a Chlorophyll-Carotenoid Coupling in LHCII", *Chem. Phys.* 526, 110439, 2019.
138. Marchetti F., Moroni E., Pandini A., Colombo G., "Machine Learning Prediction of Allosteric Drug Activity from Molecular Dynamics", *J. Phys. Chem. Lett.*, 12, 15, 3724–3732, 2021.
<https://doi.org/10.1021/acs.jpcclett.1c00045>
139. Maronas M., Teruel X., Bull J., Ayguade E., Beltran V., "Evaluating Worksharing Tasks on Distributed Environments," in 2020 IEEE International Conference on Cluster Computing (CLUSTER), Kobe, Japan, pp. 69-80, 2020. doi: 10.1109/CLUSTER49012.2020.00017, url:
<https://doi.ieeecomputersociety.org/10.1109/CLUSTER49012.2020.00017>
140. Melis C., Fugallo G., Colombo L., "Room temperature second sound in cumulene", *PCCP*, 23, 15275b, 2021. DOI:<https://doi.org/10.1039/D1CP00501D>
141. Micera A., Boella E., Zhukov A.N., Shaaban S.M., et al, "Particle-in-Cell simulations of the parallel proton firehose instability influenced by the electron temperature anisotropy in solar wind conditions", published in *The Astrophysical Journal*, 2020. 10.3847/1538-4357/ab7faa
142. Micera A., Zhukov A.N., López R.A., Innocenti M.E., et al, "Particle-in-Cell Simulation of Whistler Heat-flux Instabilities in the Solar Wind: Heat-flux Regulation and Electron Halo Formation", published in *The Astrophysical Journal Letters*, 2020. 10.3847/2041-8213/abc0e8
143. Michalchuk A.A.L., Hemingway J., Morrison C.A., *J Chem. Phys.*, 154(6), 064105, 2021. DOI: 10.1063/5.0036927
144. Migas D.B., Filonov A.B., Borisenko V.E., Skorodumova N.V., "Effect of polaron formation on electronic, charge and magnetic properties of Nb₁₂O₂₉", *J. Alloys Compd.* 821, 153527, 2020.
145. Millara Á.F. et al., "Profile Measurement of Rails in a Rolling Mill: Implementing and Evaluating Autonomic Computing Capabilities", *IEEE Transactions on Industry Applications*, 55(5), 2019.
146. Miró A., "Flow and Heat Transfer of Impinging Synthetic Jets," *Universitat Politècnica de Catalunya*, 2019.
147. Miró A., Soria M., Moulinec C., Cajas J. C., Fournier Y., "Numerical investigations on rectangular and circular synthetic jet impingement". In *Tenth International Conference on Computational Fluid Dynamics (ICCFD10)* (pp. 1–18), 2018.
148. Morales-Salvador R., Gouveia J.D., Morales-García A., Viñes F., Gomes J.R.B., Illas F., "Carbon Capture and Usage by MXenes", *ACS Catal.*, 11, 17, 11248–11255, 2021.
149. Moreno-Álvarez S., Paoletti M.E., Rico-Gallego J.A. et al., "Heterogeneous gradient computing optimization for scalable deep neural networks", *J Supercomput.*, 2022. <https://doi-org.ezproxy.unex.es/10.1007/s11227-022-04399-2>
150. Moreton-Fernandez A., Sierra Y.T.D.L., Gonzalez-Escribano A., Llanos D.R., "Operators for Data Redistribution: Applications to the STL Library and RayTracing Algorithm," in *IEEE Access*, vol. 9, pp. 38557-38570, 2021. doi: 10.1109/ACCESS.2021.3063628.
151. Muite B.K., Aseeri S., "Benchmarking solvers for the one dimensional cubic nonlinear Klein Gordon equation on a single core". *Bench'19. International Open Benchmarking Council*, 2019.
152. Mulks F.F., "Highlighted on supplementary cover (artwork): Organometallics", 39, 2019.
<https://pubs.acs.org/toc/orgnd7/39/10>.
153. Mulks F.F., Hashmi A.S.K., Faraji S.S., "Sesquicarbene Complexes—Bonding at the Interface Between M–C Single Bonds and M=C Double Bonds", *Organometallics*, 39, 1814–1823, 2020. DOI: 10.1021/acs.organomet.0c00102.
154. Navarro A., Lorenzon A.F., Ayguadé E., Beltran V., "Enhancing Resource Management Through Prediction-Based Policies", Part of the *Lecture Notes in Computer Science* book series, 2020. doi:10.1007/978-3-030-57675-2_31
155. Navarro Muñoz A., Lorenzon A.F., Ayguadé Parra E., Beltran Querol V., "Combining Dynamic Concurrency Throttling with Voltage and Frequency Scaling on Task-based Programming Models", In *50th International Conference on Parallel Processing (ICPP 2021)*. Association for Computing Machinery, New York, NY, USA, Article 10, 1–11, 2021. <https://doi.org/10.1145/3472456.3472471>
156. Nikolaev D.M., Manathunga M., Orozco-Gonzalez Y., Shtyrov A.A., Guerrero Martínez Y.O., Gozem S., Ryazantsev M.N., Coutinho K., Canuto S., Olivucci, M., "Free Energy Computation for an Isomerizing

- Chromophore in a Molecular Cavity via the Average Solvent Electrostatic Configuration Model: Applications in Rhodopsin and Rhodopsin-Mimicking Systems", *Journal of Chemical Theory and Computation*, 2021. <https://doi.org/10.1021/acs.jctc.1c00221> Q1
157. Nikolaev D.M., Manathunga M., Orozco-Gonzalez Y., Shtyrov A.A., Guerrero Martínez Y.O., Gozem S., Ryazantsev M.N., Coutinho K., Canuto S., Olivucci, M., "Free Energy Computation for an Isomerizing Chromophore in a Molecular Cavity via the Average Solvent Electrostatic Configuration Model: Applications in Rhodopsin and Rhodopsin-Mimicking Systems", *Journal of Chemical Theory and Computation*, 2021. <https://doi.org/10.1021/acs.jctc.1c00221> Q1
 158. Nordam T., Kristiansen R., Nepstad R., Röhrs J., "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>.
 159. Ntormousi E., Tassis K., Del Sordo F., Fragkoudi F., Pakmor R., "A dynamo amplifying the magnetic field of a Milky-Way-like galaxy", *A&A*, 641, A165, 2020. doi: <https://doi.org/10.1051/0004-6361/202037835>
 160. Ódor G., Gastner M.T., Kelling J., Deco G., "Modelling on the very large-scale connectome", *Journal of Physics: Complexity*, Volume 2, Number 4, 045002, 2021. doi: 10.1088/2632-072x/ac266c
 161. Ódor G., Kelling J., Deco G., "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
 162. Onchis D.M., Istin C., Real P., "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 Online ISBN 978-3-030-29888-3
 163. Onchis D.M., Istin C., Tudoran C., Tudoran M., Real P., "Timely-Automatic Procedure for Estimating the Endocardial Limits of the Left Ventricle Assessed Echocardiographically" in *Clinical Practice, Diagnostics Journal IF 2.489, Diagnostics*, 10(1), 40, 2020. <https://doi.org/10.3390/diagnostics10010040>
 164. Ortolani A., Papi F., Bianchini A., Persico G., Drofelnik J., Campobasso M.S., "Multi-fidelity Analyses of Rotor Loads of Floating Offshore Wind Turbines with Wind/Wave Misalignment", to appear in *Journal of Physics: Conference Series*, 2022.
 165. Ortolani A., Persico G., Drofelnik J., Jackson A., Campobasso M.S., "Computational Fluid Dynamics Analysis of Floating Offshore Wind Turbines in Severe Pitching Conditions", *ASME Journal of Engineering for Gas Turbine and Power*, Vol. 142(12), 2020. DOI: 10.1115/1.4048776.
 166. Ortolani A., Persico G., Drofelnik J., Jackson A., Campobasso M.S., "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", *Journal of Physics: Conference Series*, Vol. 1618, no.5, ref. 052016, 2020. DOI: 10.1088/1742-6596/1618/5/052016. Also presented at TORQUE Conference, virtual event, online, 28th September - 2nd October 2020.
 167. Ortolani A., Persico G., Drofelnik J., Jackson A., Campobasso M.S., "High-Fidelity Calculation of Floating Offshore Wind Turbines under Pitching Motion", paper GT2020-15552, *ASME Turbo Expo Technical Conference*, virtual event, online, 21st-25th September 2020. DOI: 10.1115/GT2020-15552.
 168. Ortuño M.A., Hollóczki O., Kirchner B., López N., "Selective Electrochemical Nitrogen Reduction Driven by Hydrogen Bond Interactions at Metal-Ionic Liquid Interfaces", *J. Phys. Chem. Lett.*, 10, 513-517, 2019. DOI: 10.1021/acs.jpcclett.8b03409
 169. Ossicini S., Marri I., Amato M., Palumbo M., Canadell E., Rurali R., "Ab initio studies of the optoelectronic structure of undoped and doped silicon nanocrystals and nanowires: the role of size, passivation, symmetry and phase", *Faraday Discuss.*, 222, 0, 217-239, 2020. doi = 10.1039/C9FD00085B
 170. Pandey D., Bellentani L., Villani M., Albareda G., Bordone P., Bertoni A., Oriols X., "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.*, 9(11), 2300, 2019.
 171. Pavlyukh Y., Stefanucci G., van Leeuwen R., "Dynamically screened vertex correction to GW", *Phys. Rev. B*, 102, 045121, 2020. doi = 10.1103/PhysRevB.102.045121, url = <https://link.aps.org/doi/10.1103/PhysRevB.102.045121>
 172. Pawlak MA, Knol MJ, Vernooij MW, Ikram MA, Adams HHH, Evans TE. Neural correlates of orbital telorism. *Cortex*. 2021 Dec;145:315-326. doi: 10.1016/j.cortex.2021.10.003. Epub 2021 Oct 22. PMID: 34781092. <https://pubmed.ncbi.nlm.nih.gov/34781092/>
 173. Pecha M., Horák D., "Analyzing l1-loss and l2-loss Support Vector Machines Implemented in PERMON Toolbox", Will be published in *Lecture Notes in Electrical Engineering series*. 2018.
 174. Peeters K., Janssens E., Hansen K., Lievens P., Ferrari P., "Unravelling the electronic nature of the radiative cooling of cobalt clusters", *Phys. Rev. Research* 3, 033225, 2021.

175. Perini F., Bna S., Pascolo E., Spisso I., Reitz R.D., "Robust preconditioning techniques for iterative solvers in scalable engine simulations using FRESKO", International Multidimensional Engine Modeling Meeting 2019, Detroit, MI, USA
176. Perini F., Busch S., Zha K., Kurtz E., Reitz R.D., "Piston Bowl Geometry Effects on Combustion Development in a high-speed light-duty Diesel Engine" submitted to SAE ICENA2019 conference.
177. Postek E., Schneider Y., Schmauder S., "Impact of WC/Co/diamond sample with peridynamics", SCFE2019, Supercomputing Frontiers Europe 2019, 2019-03-11/03-14, Warsaw (PL), pp.1-4, 2019.
178. Potenti S., Paoloni L., Nandi S., Fusè M., Barone V., Rampino S., "Chemical bonding in cuprous complexes with simple nitriles: octet rule and resonance concepts versus quantitative charge-redistribution analysis", *Physical Chemistry Chemical Physics*, 2020. DOI: 10.1039/D0CP01536A
179. Pozo I., Majzik Z., Pavliček N., Melle-Franco M., Guitián E., Peña D., Gross L., Pérez D., "Revisiting Kekulene: Synthesis and Single-Molecule Imaging", *Journal of the American Chemical Society*, 141 (39), 15488-15493, 2019. DOI: 10.1021/jacs.9b07926
180. Pruszkowska K., Stasyuk O.A., Zep A., Krówczyński A., Sicinski R.R., Solà M., Cyrański M.K., "Chemphyschem: a European Journal of Chemical Physics and Physical Chemistry", *Chemphyschem*, Vol. 23 (2), pp. e202100741, 2022. DOI: 10.1002/cphc.202100741
181. Raievska I., Raievska M., "Local nearrings on finite Abelian groups", International Conference of Young Mathematicians 2021, June 3-5, Kyiv, Ukraine)
(https://www.imath.kiev.ua/~young/youngconf2021/Abstracts_2021.pdf)
182. Raievska I., Raievska M., "The additive groups of local nearrings of order 64", Conference of young scientists "Pidstryhach readings - 2020" (2020, May 26-28, Lviv, Ukraine)
(<http://www.iapmm.lviv.ua/chyt2020/abstracts/Raievska.pdf>)
183. Ranjbar S., Astani N.A., Atabay M., Naseri N., Esfandiari A., Ejtehadi M.R., "Electrochemical and Computational Studies of Bio-mimicked Ti3C2Tx MXene-based Sensor with Multivalent Interface", *Journal of Colloid and Interface Science*, 2022.
184. Reali L., et al, "Mapping the asymptotic inspiral of precessing binary black holes to their merger remnants", *Class. Quantum Grav.*, 37, 225005, 2020.
185. Renault L., Arsouze T., Ballabrera-Poy J., "On the influence of the current feedback to the atmosphere on the Western Mediterranean Sea dynamics", *Journal of Geophysical Research: Oceans*, 126, e2020JC016664, 2021.
<https://doi.org/10.1029/2020JC016664>
186. Renault L., Masson S., Arsouze T., Madec G., McWilliams J.C., "Recipes for how to force oceanic model dynamics", *Journal of Advances in Modeling Earth Systems*, 12, e2019MS001715, 2020.
<https://doi.org/10.1029/2019MS001715> doi: 10.1029/2019ms001715
187. Ribić V., Dapčević A., Skorodumova N., Rečnik A., Luković Golić D., Branković G., "DFT screening of Gd as a dopant in the BiFeO3 superlattice", HPC-Europa Transnational Access Meeting (TAM 2018), 23 October 2018, Edinburgh, UK
188. Ribić V., Dapčević A., Skorodumova N., Rečnik A., Luković Golić D., Branković G., "Structure characterization of Gd doped BiFeO3", 3rd International Meeting on Materials Science for Energy Related Applications, 25-26 September 2018, Belgrade, Serbia
189. Ribić V., Dapčević A., Skorodumova N., Rečnik A., Luković Golić D., Branković G., "First-Principles Calculation of Gd - doped BiFeO3", European HPC Summit Week 2018 - #EHPCSW, May 28th to June 1st 2018, Ljubljana, Slovenia
190. Ribić V., Skorodumova N., Dapčević A., Rečnik A., Luković Golić D., Branković Z., Branković G., "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
191. Ricci E., Vergadou N., Vogiatzis G.G., De Angelis M.G., Theodorou D.N., "Molecular Simulations and Mechanistic Analysis of the Effect of CO 2 Sorption on Thermodynamics, Structure, and Local Dynamics of Molten Atactic Polystyrene", *Macromolecules*, 2020. <https://doi.org/10.1021/acs.macromol.0c00323>.
192. Rodríguez-Espigares I., Torrens-Fontanals M., Tiemann J.K.S., Aranda-García D., Ramírez-Anguita J.M., Stepniowski T.M., Worp N., Varela-Rial A., Morales-Pastor A., Medel Lacruz B., Pándy-Szekeres G., Mayol E., Giorgino E., Carlsson J., Deupi X., Filipek S., Filizola M., Gómez-Tamayo J.C., Gonzalez A., Gutierrez-de-Teran H., Jimenez M., Jespers W., Kapla J., Khelashvili G., Kolb P., Latek D., Marti-Solano M., Matricon P., Matsoukas M.-T., Miszta P., Olivella M., Perez-Benito L., Provasi D., Ríos S., Rodríguez-Torrecillas I., Sallander J., Szttyler A., Vaidehi N., Vasile S., Weinstein H., Zachariae U., Hildebrand P.W., De Fabritiis G., Sanz F., Gloriam D.E., Cordini A., Guixà-González R., Selent J., "GPCRmd uncovers the dynamics of the 3D-GPCRome" bioRxiv 839597; 2019. doi: <https://doi.org/10.1101/839597>

193. Rodriguez-Gutierrez E., Moreton-Fernandez A., Gonzalez-Escribano A., Llanos, D.R. "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>
194. Roet S., Daub C.D., Riccardi E., "Chemistrees: data driven identification of reaction pathways via machine learning", *Journal of Chemical Theory and Computation*, 17 (10), 6193-6202, 2021. DOI: 10.1021/acs.jctc.1c00458
195. Rossi T.P., Shegai T., Erhart P., Antosiewicz T.J., "Strong plasmon-molecule coupling at the nanoscale revealed by first-principles modeling", *Nature Communications* 10, 3336, 2019.
196. Sagresti L., Rampino S., "Charge-Flow Profiles along Curvilinear Paths: A Flexible Scheme for the Analysis of Charge Displacement upon Intermolecular Interactions", *Molecules*, 26, 21, 2021. doi: 10.3390/molecules26216409
197. Sayer T., Sprik M., Zhang C., "Finite electric displacement simulations of polar ionic solid-electrolyte interfaces: Application to NaCl(111)/aqueous NaCl solution", *J. Chem. Phys.* 150, 041716, 2019. <https://doi.org/10.1063/1.5054843>
198. Scarbath-Evers L.K., Todorović M., Golze D., Hammer R., Widdra W., Sebastiani D., Rinke P., "Gold diggers: Altered reconstruction of the gold surface by physisorbed aromatic oligomers", *Phys. Rev. Materials* 3, 011601(R), 2019.
199. Serdaroglu G., Uludag N., Erçag E., "Cyanomethylation of 2,3,4,9-tetrahydro-1H-carbazol-1-one based on using two different reagents: Antioxidant activity and DFT studies", *Journal of Molecular Structure*, 1253, 132262, 2022.
200. Shukla N. et al, "Relativistic collisionless shocks: microphysics and long-term dynamics", under preparation to *Physical Review Letters*.
201. Sieffert N., Thakkar A., Bühl M., "Modelling uranyl chemistry in liquid ammonia from density functional theory", *Chem. Commun.*, 54, 10431, 2018. <http://dx.doi.org/10.1039/C8CC05382K>
202. Simmermacher M., Henriksen N.E., Møller K.B., Moreno Carrascosa A., Kirrander A., *Phys. Rev. Lett.*, 122, 073003, 2019.
203. Simmermacher M., Moreno Carrascosa A., Henriksen N.E., Møller K.B., Kirrander A., *J. Chem. Phys.*, 151, 174302, 2019.
204. Stalevski M., Asmus D., Tristram K., "Towards a new paradigm of dust structure in AGN: Dissecting the mid-IR emission of Circinus galaxy", *Proceedings of the International Astronomical Union*, 15(S356), 50-55, 2019. doi:10.1017/S1743921320002562
205. Stalevski M., Tristram K., Asmus D., "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*, 484, 3334-3355, 2019. DOI: 10.1093/mnras/stz220 <http://adsabs.harvard.edu/abs/2019MNRAS.484.3334S>
206. Stene R.E., Graubner T., Ivlev S.I., Karttunen A.J., Kraus F., "A Symmetric F–H–F Hydrogen Bond in Strontium Bifluoride, Sr[HF₂]₂", *Anorg Z., Allg. Chem.*, e202100374, 2022. doi: 10.1002/zaac.202100374
207. Szatyłowicz H., Marek P.H., Stasyuk O.A., Krygowski T.M., Solà M., "Substituted adenine quartets: interplay between substituent effect, hydrogen bonding, and aromaticity", *RSC Adv.*, 10, 23350-23358, 2020. doi: 10.1039/d0ra04585c
208. Szczepanik D.W., "A simple alternative to the pseudo- π method", *Int. J. Quantum Chem.*, 118, e25696, 2018. doi: 10.1002/qua.25696.
209. Szczepanik D.W., Solà M., "Electron Delocalization in Planar Metallacycles: Hückel or Möbius Aromatic?", *ChemistryOpen*, 8, 2, 219-227, 2019. doi: 10.1002/open.201900014
210. Tanis I., Kostarellou E., Karatasos K., "Molecular Dynamics Simulations of Hyperbranched Poly (ethylene imine) – Graphene Oxide) Nanocomposites as Due Adsorbents for Water Purification", *Phys. Chem. Chem. Phys.*, 2021. DOI: 10.1039/D1CP02461B
211. Tazes I. et al, *Plasma Phys. Control. Fusion*, 62, 094005, 2020.
212. Terranova U., Viñes F., de Leeuw N.H., Illas F., "Mechanisms of carbon dioxide reduction on strontium titanate perovskites", *J. Mater. Chem. A*, 8, 18, 9392-9398, 2020. doi =10.1039/D0TA01502D
213. Tobola F., Lepšík M., Zia S.R., Leffler H., Nilsson U.J., Blixt O., "Imberty, A.; Wiltshi, B. Engineering the ligand specificity of the human galectin-1 by incorporation of tryptophan analogs", *ChemBioChem*, 2022. Accepted, DOI: 10.1002/cbic.202100593
214. Tsipis A.C., Sarantou A.A., "DFT insights into the photocatalytic reduction of CO₂ to CO by Re(i) complexes: the crucial role of the triethanolamine "magic" sacrificial electron donor", *Dalton Trans.*, 50, 14797-14809, 2021. <https://doi.org/10.1039/d1dt02188e>
215. Tsourtou F.D., Peristeras L.D., Apostolov R., Mavrantzas V.G., "Molecular Dynamics Simulation of Amorphous Poly(3-hexylthiophene)", *Macromolecules*, 53, 18, 7810–7824, 2020. DOI :<https://doi.org/10.1021/acs.macromol.0c00454>

216. Tsoutsanis P., "Stencil selection algorithms for WENO schemes on unstructured meshes", *Journal of Computational Physics*: X, Volume 4, 100037, 2019.
<https://www.sciencedirect.com/science/article/pii/S2590055219300538>,
<https://doi.org/10.1016/j.jcp.2019.100037>
217. Tzounis P.-N., Anogiannakis S.D., Theodorou D.N., "Atomistic Simulations of Oligomers used in Directed Self-Assembly Lithography: Estimation of the Interaction Parameter χ ", in preparation.
218. Vanzan M., Jones R.M., Corni S., D'Agosta R., Baletto F., *ChemPhysChem*, e202200035, 2022.
219. Vasilevska I., Tomšič P., Kos I., "Modernization of the PIC codes for exascale plasma simulation", MIPRO 2020, 43rd International Convention, Opatija, Croatia, pp. 209-213, 2020.
<https://ieeexplore.ieee.org/document/9245299>
220. Vega L., Aleksandrov H.A., Farris R., Bruix A., Viñes F., Neyman K.M., "Chemical ordering in Pt–Au, Pt–Ag and Pt–Cu nanoparticles from density functional calculations using a topological approach", *Materials Advances*, 2021.
221. Vencels J., Råback P., Geža V., "EOF-Library: Open-source Elmer FEM and OpenFOAM coupler for electromagnetics and fluid dynamic's", *SoftwareX*, Volume 9, Pages 68-72, ISSN 2352-7110, 2019.
<https://doi.org/10.1016/j.softx.2019.01.007>
222. Viviani M., Käpylä M.J., Warnecke J., Käpylä P. J., Rheinhardt M., "Stellar Dynamos in the Transition Regime: Multiple Dynamo Modes and Antisolar Differential Rotation", *ApJ*, 886, 21, 2019. Doi: 10.3847/1538-4357/ab3e07
223. Westermayr J., Gastegger M., Marquetand P., "Combining SchNet and SHARC: The SchNarc Machine Learning Approach for Excited-State Dynamics", *The Journal of Physical Chemistry Letters*, volume: 11. DOI: 10.1021/acs.jpcl.0c00527
224. Wouters M., Aouane O., Krüger T., Harting J., "Mesoscale simulation of soft particles with tunable contact angle in multicomponent fluids", *Physical Review E*, 100(3) 033309, 2019.
<https://doi.org/10.1103/PhysRevE.100.033309>
225. Wouters M., Aouane O., Sega M., Harting J., "Capillary interactions between soft capsules protruding through thin fluid films", *Soft Matter*, 16, 10910-10920, 2020. doi: 10.1039/d0sm01385d
226. Wouters M., Aouane O., Sega M., Harting J., "Lattice Boltzmann simulations of drying suspensions of soft particles", *Phil. Trans. R. Soc. A.*, 379, 20200399, 2021. <http://doi.org/10.1098/rsta.2020.0399>
227. Zahorska E., Kuhadomlarp S., Minervini S., Yousaf S., Lepsik M., Kinsinger T., Hirsch A.K.H., Imberty A., Titz A., "A rapid synthesis of low nanomolar divalent LecA inhibitors in four linear steps from D-galactose pentaacetate", *Chem. Commun.*, 56: 8822-8825, 2020.
228. Zborowski K.K., Poater J., "Pyrrole and Pyridine in the Water Environment. Effect of Discrete and Continuum Solvation Models", *ACS Omega*, 6, 24693–24699, 2021. <https://doi.org/10.1021/acsomega.1c03437>.
229. Zhou F., Giannakis I., Giannopoulos A., Holliger K., Slob E., "Estimating reservoir permeability with borehole radar", *Geophysics*, 85(4): 1–10, 2020.
230. Ziegler-Borowska M., Mylkie K., Kozłowska M., Nowak P., Chelminiak-Dudkiewicz D., Kozakiewicz A., Ilnicka A., Kaczmarek-Kedziera A., "Effect of Geometrical Structure, Drying, and Synthetic Method on Aminated Chitosan-Coated Magnetic Nanoparticles Utility for HSA Effective Immobilization", *Molecules*, 24, 1925-1942, 2019. DOI: 10.3390/molecules24101925
231. Zinchenko I.A., Vilchez J.M., Pérez-Montero E., Sukhorukov A.V., Sobolenko M., Duarte Puertas S., "The dependence of the gradients of oxygen and nitrogen-to-oxygen on stellar age in MaNGA galaxies" (<https://ui.adsabs.harvard.edu/abs/2021A%26A...655A..58Z/abstract>)
232. Zitz S., Scagliarini A., Harting J., "Lattice Boltzmann simulations of stochastic thin film dewetting", *Phys. Rev. E*, vol. 104 (3), pp. 034801, 2021. doi =10.1103/PhysRevE.104.034801.
233. Zitz S., Scagliarini A., Maddu S., Darhuber A.A., Harting J., "Lattice Boltzmann method for thin-liquid-film hydrodynamics", *Phys. Rev. E*, vol. 100(3), pp. 033313, 2019. doi: 10.1103/PhysRevE.100.033313.