PRACE

PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

PRACE days 18

Executive Summary

PRACEdays 18

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PRACE days 18

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PRACEdays18

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Foreword

Serge Bogaerts, PRACE Managing Director and Chair of the Organisation & Programme Committee of the European HPC Summit Week 2018

PRACEdays18, this year hosted by the University of Ljubljana, was the fifth edition of our annual flagship conference, which brings together people from all walks of life involved in the world of high performance computing. It took place as part of the wider European HPC Summit Week, which was being held for the third time. From all of us at PRACE, I would first like to extend a heartfelt thankyou to all who attended and made the conference, the lively and exciting event that it has become, as well as to all those from our host nation of Slovenia who made us feel very welcome.

The theme of this year's PRACEdays was "HPC for innovation: When science meets industry". As HPC continues to make inroads into new domains and proves itself useful for an ever-expanding number of tasks, we want to ensure that both academics and industrial users feel supported by PRACE. After all, basic research is of great importance, but so are the technologies that we derive from it that help people in their daily lives.

As ever, the event this year saw a number of presentations from both the scientific and industrial users of the machines we oversee. It was truly astounding to see some of the computational work which is being carried out by the many great minds that we work with. The scale of some of the simulations that Europe's most powerful Tier-0 supercomputers can support never ceases to amaze me, from the thermophoretically-powered micromachines of Marisol Ripoll (page 19) to the binary neutron stars of Luciano Rezzolla (page 20).

A lot of what we do at PRACE is focused on the European HPC ecosystem, but that does not mean that we exist apart from the rest of the world! This year's talk from Allan Williams, associate director of the Australian National Computing Infrastructure, provided a fascinating insight into the history of HPC in Australia as well as a look at the ways in which we can collaborate more closely in the future.

Two of our main sessions this year were the PRACE User Forum and the panel session entitled "Centres of Excellence and High-Level Support Teams: What problems can they solve for me?". We wanted this year's event to provide all those attending both the opportunity to speak out to the community about their HPC experiences, as well as the chance to hear from some of our experts about what we are doing to support them. Both of these sessions were designed with the users of PRACE computers in mind, and we hope you found them useful and informative.

I would like to personally congratulate Professor Xiaoxiang Zhu, the winner of the 2018 PRACE Ada Lovelace Award for HPC. She expressed the desire to act as a role model for women looking to work in both HPC and other STEM disciplines, as well as to increase the number of principal investigators leading PRACE projects, and I colud not agree more with her sentiments.

The number of participants at PRACEdays in 2018 was an all-time high, which demonstrates the growth of HPC as a discipline in itself. We hope to see even more of you at PRACEdays19 in Poznań, Poland, 13-17 May 2019, which will be hosted by the Poznań Supercomputing and Networking Center.

PRACEdays18: Summary

The fifth edition of PRACEdays took place 29-31 May 2018 in Ljulbljana, Slovenia, with people from all walks of life in science and industry brought together by their shared interest in the world of high performance computing. The theme this year was about combining scientific and industrial knowledge to produce innovation, bringing the fruits of HPC to the masses.

This year's event was held in the University of Ljubljana's Faculty of Law, which sits just a stone's throw from the edge of the winding Ljubljanica river. Attendees gathered in the morning to hear from some of PRACE's central figures as well as local dignitaries and politicians.

The first session saw Chair of the PRACE Council Anwar Osseryan provide an overview of the organisation's achievements, giving an idea of the breadth and scale of the research that it supports, as well as the diversity of activities it oversees to help both science and industry.

Representing the Slovenian government was Maja Makovec Brenčič from the Ministry of Education, Science and Sport. She explained how politicians and other policymakers are increasingly looking to HPC-based research to help them make more informed decisions about subjects ranging from climate change to transport. By harnessing the power of the immense amount of data that is collected nowadays, it is possible to create real impact in the daily lives of people around the world.

PRACEdays18 was all about innovation this year, and this feeling was represented through speeches throughout the course of the conference. The PRACE SHAPE (SME HPC Adoption Programme in Europe) Programme, which was created to support SMEs throughout Europe by providing them with HPC resources, threw a number of interesting talks out this year. We heard from InventMedical, who have created custom-made helmets for babies with cranial deformities, as well as companies who have been using HPC to optimise performance of state-of-the-art vehicles in Europe.

The conference this year had a strong focus on networking and collaboration between the many organisations that have a finger in the HPC pie, and the addition of associate director of the National Computational Infrastructure of Australia Allan Williams, who gave to delegates a run-down of the history of HPC in Australia, as well as a feel for how collaboration between Europe and Australia might exist in the future, was welcome.

It is easy to play down the ability of the largest supercomputers in the world when you work in the field, but there were a number of times during the conference when we were reminded of the power that reside in them. From the session about saving energy when running supercomputers, to the visualisations which really demonstrated to us the level of detail which these computers give to use, it was a humbling experience to hear how these machines have helped us.

As always, some of the main sessions of this year were aimed at you, the users of HPC. The User Forum and the panel discussion both brought about some lively debate, with the newly formed High-Level Support Teams and the Centres of Excellence

taking up much of the discussion. The level of feedback this year was beyond our expectation, and it was a truly valuable lesson to hear straight from the users' mouths about how the infrastructure of PRACE can support the users of HPC to a greater level.

The theme of this year's conference, as in the past, was about bringing together science and industry to create innovation. It was inspiring to see success stories from both sides of the HPC ecosystem talking this year, and it was hard to deny the power of hearing from the industrial partners who have been granted HPC resources about how the use of supercomputers has propelled their businesses into the future.

At last year's conference we saw Minna Palmroth of the University of Helsinki, present her spectacular visuals of near-Earth space weather, and continuing in the same astrophysics vein this year was Luciano Rezzolla of the Goethe University Frankfurt, who gave a keynote speech about his work on binary neutron stars. He explained how these systems are not only a strong source of gravitational waves, but can also be used to explain the mechanics behind short gamma-ray bursts, as well as the abundance of certain heavy elements such as gold and platinum in the universe.

Following the introductory sessions, parallel workshops were held throughout the week by both PRACEdays18 and other HPC initiatives such as ETP4HPC, EuroLab4HPC, EXDCI and FETHPC projects. The topics of those workshops covered all HPC-related topics, from architecture to applications, and gave an overview of the latest development in the path to the use of exascale computers.

The end of the conference also saw the award of the PRACE Ada Lovelace Award for Women in HPC 2018, which was won this year by Professor Xiaoxiang Zhu of the Technical University of Munich (TUM), Germany, for her outstanding contributions to and impact on HPC in Europe. Her research has led to the development of explorative algorithms that improve information retrieval from remote sensing data, in particular those from the current and next generation of Earth observation missions. Her sentiments of becoming a figurehead for women in both HPC and the wider world of STEM subjects were welcomed by all.

The PRACE Award for Best Scientific Presentation was given to Vincent Moureau, CORIA CNRS-UMR6614, Normandie Université, INSA et Université de Rouen, France for his presentation "HPC for the simulation of turbulent combustion in aeronautical engines".

The action at this year's conference has shown us all that the world of HPC is developing fast and, as was highlighted by a number of speakers, it is a discipline that many scientists and businesses now rely upon in order to stay competitive. Luciano Rezzolla said it best when he answered a question about how he works: "I like to think I'm always working with three codes: the one I'm using, the one I'm developing, and the one I'm dreaming of!"

PRACE User Forum 2018

The PRACE User Forum is an independent entity where PRACE users can discuss their experiences and express their future needs as well as feedback on the current services and resources that PRACE provides. The aim at this year's event was to provide an effective mechanism through which users of Tier-0 supercomputers can give feedback to PRACE.

At a session run by the PRACE User Forum at PRACEdays18, delegates gathered to come and hear exactly how each proposal is evaluated after it has been submitted. Hosted by Troels Haugbølle, Chair of the PRACE User Forum, it encompassed a number of talks as well as an open-ended Q&A session which allowed people to ask questions of any level about the inner workings of PRACE.

For many of the people watching (including those at home viewing the livestream on YouTube), it was particularly interesting to hear just how rigorous the process of peer review is. Anyone can apply to use a supercomputer, but that does not mean that everyone will be successful. Maria-Grazia Giuffreda, member of the PRACE Board of Directors, began the session by explaining exactly why each proposal is so closely scrutinised: "Anyone looking to use a Tier-0 computer needs to understand that these are not toys for them to play around with; these are some of the most powerful and expensive-to-use pieces of scientific equipment around, and as such we need to know that they are being used to their full capacity and for outstanding science."

Each proposal is assessed by both technical staff and three scientific peers. The cost of running a supercomputer is so high that it is not feasible to waste time on them, so technical staff look to see that the team making the proposal are ready to hit the ground running on day one. This is why all applicants are recommended to apply for PRACE Preparatory Access, which allows them to test and benchmark their code first. Technical reviewers also assess whether or not the proposed methods will actually help the applicants achieve their results, and may ask for more information to clarify this.

Scientific reviewers are obviously there to examine the excellence of the science, looking at methodology, the feasibility of the research plan, and the qualifications and academic track record of those applying. In the next step, two rapporteurs look at the scientific reviews independently and then come together to agree on a grade for each proposal. "When these discussions happen, the decisive criterion will ultimately be scientific excellence," explained Giuffreda.

All proposals are then discussed in the presence of the PRACE Access Committee, where the rapporteurs and technical staff provide their input and thoughts about each of them. Proposals for similar problems will be examined more thoroughly to decide which is superior, in order to provide a final ranked list of all the proposals received, including a scientific quality threshold under which proposals would not be funded even if resources were available.

But the process does not end there. At the Resource Allocation Session it is then decided exactly how many hours each proposal is allocated, based on the recommendations of the Access Committee and other constraints on PRACE resources.

How to write a successful proposal

The second talk of the session came from Luca Marsella, ETH Zurich/CSCS. As a member of the PRACE Access Committee, he was there to provide recommendations about how to write a successful proposal. He began by providing an overview of the key elements that are needed. These include demonstrating scientific excellence and impact, showing the transformative qualities of the research, and making the proposal relevant to the scope of the call. The mathematical numerical methodology should be described in detail, and there should be a solid plan in place for both dissemination of the research through relevant channels and for the ooverall management of the project.

Marsella then guided everyone through a proposal template **http://www.prace-ri.eu/prace-project-access/** to demonstrate exactly what is needed to satisfy the scientific and technical reviewers.

From left to right: Troels Haugebølle, Maria-Teresa Para, William Sellers, Luciano Rezolla, Maria-Grazia Giuffredda, Luca Marsella, Derek Groen, Turlough Downes, Koen Hillewaert

Open discussion for PRACE users

The intricate breakdown of how to write a successful proposal for a PRACE project was followed by an open session in which the entire audience was able to ask questions.

Lee Margetts, Chair of the PRACE Industrial Advisory Committee, raised some important issues about the differences between scientific and industrial use of PRACE computers. "If we took a hypothetical scientist from industry, and one from public body, then put them through the process of seeing whether they were worthy of using HPC resources, I think both would do an equally good job in 99 per cent of the criteria which are asked. However, when it comes to prioritisation of projects, I believe a company would have difficulty ranking up with the scientific excellence of universities. This is why I think we need to measure innovation excellence as well as scientific excellence, which could perhaps come in the form of a separate access programme."

"We need to measure innovation excellence as well as scientific excellence in order to support industry"

Koen Hillewaert, Centre de Recherche en Aeronautique (Cenaero), Belgium agreed, but amongst the panel there was some disagreement about the level of industrial involvement which is appropriate, with some believing that public money should be sparingly given out to private enterprises, citing issues of transparency and fair financial play.

Another question from the audience brought up the subject of resources such as the John Hopkins Database for Turbulence, which provides free access to multi-terabyte turbulence databases, residing on several nodes and disks on cluster computers stored in small 3D sub-cubes. These can be used straight from the website, so can PRACE do something similar? The general consensus from the panel was that this would be down to domain specific organisations, with Centres of Excellence possibly playing a role.

A number of people in the audience had more questions about applications for core hours, including whether or not it can harm an application if too many or too few hours are asked for. PRACE does provide guidelines for such questions, and of course the Access Committee has the power to decrease or increase access requests based on various factors. The overall sentiment was that a good proposal is needed for everyone, as every single bit of it will be strongly scrutinised!

Finally, a PRACE user asked about the best way to prepare for exascale computing. At present, the best way to go about this is through PRACE Preparatory Access, which gives users the chance to test code and benchmark it on their chosen system. We invite every one of our users reading this to visit: **www.prace-ri.eu** for more information about how we can support your work.

Panel discussion: Centres of Excellence and High-Level Support Teams: What problems can they solve for me?

The panel discussion this year was broadly aimed at discussing the Centres of Excellence and High-Level Support Teams, but ended up covering a wide range of topics, reflected by the diverse panel who brought their own unique experiences and perspectives to the session. Jacki Davis did a fantastic job of moderating the interactive session, which involved not only the panel members but also the entire audience that had congregated.

The panel:

Lee Margetts: *Senior Lecturer of Structural integrity at University of Manchester, Chair of the PRACE Industrial Advisory Committee*
Sinéad Ryan: *Chair of Theoretical High Energy Physics at Trinity College Dublin, Chair of the PRACE Scientific Steering Committee*
Xiaoxiang Zhu: *Professor of Signal Processing in Earth Observation at the German Aerospace Center (DLR) and Technical University of Munich (TUM), Winner of the PRACE Ada Lovelace Award for HPC 2018*
Paul Gibbon: *Head of Computational Science Division at the Juelich Supercomputing Centre, Co-Manager of the Energy Centre of Excellence, coordinator of High-Level Support Teams.*
Erwin Laure: *Professor for HPC and director of PDC Centre of HPC at the Royal Institute of Technology in Stockholm*
Luca Marsella: *Computational Scientist, Swiss National Supercomputing Centre, Eidgenössische Technische Hochschule Zürich*

The session started with a discussion of where the panellists believed most support was currently required for users. For a number of disciplines which have only recently started exploring the possibilities of HPC, making the jump from Tier-1 computing to Tier-0 is where the most support is needed, according to Sinéad Ryan. For the more mature disciplines, the challenge is to help them develop applications at much larger scales that push Tier-0 machines to their limits.

PRACE has created an effective system for collaboration between member states, with plenty of infrastructure and support to help scientists along the route from Tier-2 to Tier-0 computing. However, as Lee Margetts pointed out, this route is not currently open to industry, and this needs to be addressed. As well as this, more thought needs to go into how the scientific results of PRACE projects are leveraged to benefit society. There needs to be a clearly defined "innovation pathway" to the marketplace that takes intellectual property and makes use of it.

The High-Level Support Teams, although only in their nascent stage (Paul Gibbon mentioned that they had only had their first coordination meeting the day before the panel discussion took place), have a real opportunity to provide the kind of cross-disciplinary support that is often needed in HPC projects. They are now reaching out to researchers across Europe to begin working with them and devising the best methods for helping them.

The feeling amongst the HPC community at present is that the Centres of Excellence have so far had mixed levels of success. On the positive side, they provide efficient scaling and are able to create and refine software for use by the academic community on the larger computers in Europe. However, challenges arise when moving up the ladder from Tier-2 to Tier-0. Hardware is becoming more heterogeneous, explained Erwin Laure, and the Centres of Excellence are struggling to keep up with this. For the users, it is now an increasingly complex task to work out what combination of software and hardware is most appropriate for their work. They need holistic support from people with in-depth knowledge of not only the hardware and software but also the science, which is difficult to provide.

Luca Marsella agreed, noting that adapting code for Tier-0 computers requires not just software skill and domain-specific knowledge, but also the ability to work well with the people involved. Xiaoxiang Zhu was keen to point out that more work needs to be done in supporting the creation of scientific visualisations that can convey results more easily to the general public. There are petabytes of data freely available to use, and in the future we will need hybrid systems that use both CPUs and GPUs to help use this.

"For users, it is now an increasingly complex task to work out what combination of software and hardware is most appropriate for their work"

Erwin Laure urged for a much closer interaction between the Centres of Excellence and the High-Level Support Teams in the future, with improved levels of collaboration and tight synchronisation. Without this, there is a great risk of duplication of effort. The High-Level Support Teams are essential for the Centres of Excellence as they have a closer working relationship with the users, and have their fingers on the pulse as to what the users need in terms of the machines and the difficulties that many have in using them, as well as the functionalities that are being requested.

Paul Gibbon agreed, saying that he believes the role of High-Level Support Teams will evolve as time goes on, especially when the second generation of Centres of Excellence appear. This will allow them a greater understanding of what applications are being used. At present they are focusing on helping users deal with the incoming impact of exascale computing, and they will continue to do so for the meantime.

Jacki Davis then addressed another question to the panellists: what do they believe is the best way to identify the needs of researchers? Luca Marsella pointed out that Tier-0 applicants have already been through a rigorous process by the time they get granted time on the computers, and that the PRACE Preparatory Access should be enough to provide users with everything they need. Of course, the High-Level Support Teams should now be there to provide extra advice, and will strive to be in contact with researchers as much as possible.

Erwin Laure illustrated the difficulties that the Centres of Excellence have been facing. He explained the tension that exists between the tasks of having to maintain software quality, implementing new features that are requested by the scientific community, and also looking forward and working on the hardware of the future. Getting all of these things done together in the right balance with finite resources is the great challenge they need to overcome.

Paul Gibbon took a different angle, saying that he believes the best approach is to encourage people to help themselves. This can be done, for instance, by making audits a standard part of algorithm development. He believes this needs to become part of the culture for developing large scale applications for Tier-0 and Tier-1 computers.

Maintaining software on leading edge hardware is undoubtedly a highly complex task, and it may require an increase in funding for the Centres of Excellence if it is to reach the level that many would like to see. Exascale is important, of course, but it is also important to support users working at other levels of the supercomputing ecosystem. Erwin Laure made it clear that this will be a main objective of the Centres of Excellence when the inevitable increase in funding does occur.

The Centres of Excellence have the experience to show people the pathway from the smallest computers to the most powerful ones, and try to make these recommendations as clear as possible. This does however, require numerous people with a variety of skillsets, including domain scientists,

mathematicians, and those with HPC expertise. These people do exist, but more funding will be needed to hire them.

Lee Margetts mentioned the recent developments in some areas of HPC code which he believes are being ignored by the Centres of Excellence and High-Level Support Teams at present. Erwin Laure agreed that this needs to be addressed, but a much longer term perspective will be needed to make this happen. Paul Gibbon countered, arguing that the Centres of Excellence are not the right instrument for supporting codes at this very early stage. There needs to be a tipping point reached within a community when a code becomes a "community code" before they can step in, otherwise there are just too many possible codes to provide support to.

"Obsessing over the top 500 most powerful computers is not useful, but addressing the needs of users is. That is how great science happens"

Jacki Davis rounded up the discussion by asking each of the panellists to provide a vision of the world of HPC they hope to see in the future. Xiaoxiang Zhu described how we are currently experiencing a paradigm shift from computational work to data intensive scientific discovery, which we need to react to quickly. We need a full pipeline starting from data, through analytics, and then to visualisations that can convey the results in a meaningful way. In terms of her field of speciality, Earth visualisation, one look at the Google Earth engine is enough to demonstrate that Europe is falling behind on this. However, there are many other fields such as medical imaging and astrophysics where the same can be said.

We need a landscape for HPC that has scientific excellence as the driver of hardware and software development, said Sinéad Ryan. There is no point in having immensely powerful machines if the people who need them are not able to use them properly. Scientists should therefore play a role in the leadership, helping with algorithmic development, and this should be supported by clearly defined career paths in the field of algorithmic development.

Paul Gibbon described a similar desire, saying that there needs to be more people involved in the co-design of exascale machines. The obsession with the top 500 most powerful computers is not useful, but addressing the needs of users is. That is how great science ends up happening.

Luca Marsella mentioned the importance of scaling up codes to the point where they will be usable by exascale machines, and support will be needed to help restructure codes so that they can be optimised better. This will take a lot of work from the Centres of Excellence and the High-Level Support Teams if it is to be achieved.

Erwin Laure would like to see a vibrant HPC community that looks after long term development, while also providing short term support and encouraging collaboration between different domains. At present there is still fragmentation in the community, and all of the users of supercomputing resources need to be looked after better to help them make the most of them.

Lee Margetts finished by first describing exactly what he did not want to see in the future: a failure to use the innovations made by science to improve society. Working with industry will be essential to ensure this does not happen. We need to be competitive with China and the US, and we can do this by supporting PRACE and using HPC to improve the economy, healthcare and the environment.

The PRACE Ada Lovelace Award for HPC 2018

Xiaoxiang Zhu is professor of signal processing in Earth observation at the German Aerospace Center (DLR) and Technical University of Munich (TUM), Germany. In recognition of her work, Professor Zhu was this year awarded the 2018 PRACE Ada Lovelace Award for HPC for her outstanding contributions in the field of HPC in Europe. We spoke to her after the conference to get her thoughts on the award and the wider world of HPC.


Xiaoxiang Zhu

Xiaoxiang Zhu and her team develop explorative algorithms to improve information retrieval from remote sensing data, in particular those from the current and next generation of Earth observation missions. The outstanding achievement of her research work has been to use satellite imagery and supercomputing to predict the risks of structural degradation and damage to city buildings. Furthermore, she and her team are contributing to the first ever global urban models in 3D and 4D. This work has a real social impact as the improved retrieval of geo-information from Earth observation data can be used to better support cartographic applications, resource management, civil security, disaster management, planning and decision making.

3D models can provide precise, static representations of a city, but Zhu and her team have gone one step further. Using HPC, they are now measuring temporal changes down to the centimetre or even millimetre scale to observe whether buildings have been disturbed by uplift or subsidence. To create the 4D models, the next generation of HPC systems and data storage were used to fuse petabytes of Earth observation satellite data and social media data, including images and texts. Such global data sets are a giant leap forwards for urban geography research and can significantly contribute to the United Nations' Sustainability Goal "Sustainable Cities and Communities".

First of all, congratulations on becoming the third winner of the PRACE Ada Lovelace Award for HPC.

Xiaoxiang Zhu: Thank you. Of course, there are many people I would like to thank as well, including Professor Kranzlmüller of the Leibniz Supercomputing Centre, who nominated me because I have done a lot of my computation on the SuperMUC computer.

On the other hand, I would also like to say that this award does not belong to me alone – it belongs to my team, and all of the other people who work in this field with me. And in winning this award, I am delighted to take the responsibility of speaking out for women working in the field of HPC and other STEM fields.

Could you tell us a bit more about your research?

Zhu: We are working in the field of Earth observation, using satellites orbiting the Earth as our sensors to take measurements of the Earth's surface on a global scale. We are then trying to retrieve useful geo-information from this data. I have a team of about 20 people working under an ERC starting grant, who are trying to fuse the many petabytes of satellite data available together to produce the first ever global open models.

The relevance of this work is not that high in Europe because we already have very good models, but if you think about developing countries with huge slum areas, the authorities do not have any reliable information about infrastructure like healthcare, clean water and education at this scale. We are trying to close this gap using Earth observation satellite data along with HPC resources.

In the panel discussion today you mentioned the paradigm shift towards the use of massive amounts of data. Could you elaborate on this?

Zhu : We are currently standing on the brink of a big shift towards data intensive scientific discovery. For example, this is reflected in my field by the European Commission's Copernicus Programme which provides around 30 petabytes of freely accessible data to anyone working in the field of Earth observation. There is also a recent trend towards deep-learning research, which has enabled people to take huge datasets and learn a lot from the data itself. This is happening in many fields now.

How can we support his shift?

Zhu: If we talk about artificial intelligence then there are already quite a few activities going on in Europe. However, if we are talking about data then we are still lagging a bit behind. In the field of Earth observation, there are 30 petabytes of data freely accessible, but only a few scientists in Europe are able to really explore the potential of harvesting this data.

Take a look at the Google Earth engine. They download all the centre data which is made available from European money, and then they are offering services to researchers. You can select areas, and choose simple codes to get global parameter estimations for example. This is great, but you do not yet have the freedom to put everything that you want to calculate there, they have limited run time, and you never know when it might suddenly not be free anymore. But in the end, they are ahead of us and we need to catch up.

"For many researchers, HPC helps them compute faster. For my research, it is the difference between having results and not having them!"

As a woman working in the field of HPC, how do you think more women can be encouraged to get involved?

Zhu: We have too few women, especially in leading positions, in HPC and other STEM fields. There are many initiatives in different countries and even at the European level designed to close this gap and bring greater diversity and a more balanced situation. To have this kind of award is a very good idea. Specifically, in the field of HPC I think a good next step would be to encourage more women to become principle investigators or even to lead some of the Centres of Excellence. We need more female faces everywhere, including the High-Level Support Teams, so that they can really be seen as role models. This would definitely be very helpful for encouraging more women into the field.

On another note, I think the opportunities women have nowadays are better than ever, so we need to make sure they use them.

How has working with PRACE helped your research?

Zhu: When people talk about HPC, most people think that it is going to help you to compute faster. Although that is the case for many, for my

Professor Xiaoxiang Zhu receives the 2018 PRACE Ada Lovelace Award for HPC from Sinéad Ryan, Chair of the PRACE Scientific Steering Committee

"We are trying to help developing countries that lack reliable information on healthcare, clean water and education"

research field it is a game changer. The difference is not faster – it's the difference between having results or not having results! We are using radar satellite images of the Earth, which you can think of as being like a single image from a CAT scan of the brain. To put many of these images together we then have to carry out tomographic reconstruction in 3D. If we want to do this for something the size of a city, which is the kind of scale of problem we are facing, we are then looking at something like 10 000 x 5 000 pixels, where for each pixel itself we have to solve huge problems at the scale of hundreds of millions. Even reconstructing a city in this way would be impossible without HPC, let alone what we are trying to do in creating a global map.

What exactly will people be able to do with these maps?

Zhu: We are aiming for a global map, but it will be most significant for developing areas, where proper maps exist, the semantics or the functions of the buildings are not known, and most likely the populations living in areas such as slums are being underestimated. These are the areas where we hope to make a difference.

Virtual prototyping for 3D printed cranial orthoses

Invent Medical are just one of the many SMEs involved in the SHAPE Programme, which aims to bring the benefits of HPC to small companies. **Tomáš Karásek** of IT4Innovations national supercomputing centre spoke at PRACEdays18 about how the process of creating individually customised cranial orthoses for children with head deformities has been improved through the development of a new virtual prototyping tool.

A lack of expertise and lack of resources have in the past acted as barriers to the use of HPC by small businesses in Europe. SHAPE – the SME HPC Adoption Programme in Europe – is a pan-European, PRACE-based programme supporting HPC adoption by SMEs. The programme aims to raise awareness and equip European SMEs with the expertise necessary to take advantage of the innovation possibilities opened up by high performance computing, thus increasing their competitiveness.

"The helmet is more breathable and can be made up to 40% lighter than previous designs"

One inspiring story to come from the SHAPE programme was presented at this year's conference by IT4Innovation's Tomáš Karásek, who has been working alongside progressive healthcare start-up Invent Medical. He talked about his experience with SHAPE and how the company have directly benefited from the use of HPC. They have now incorporated virtual prototyping into their supply chain and production processes, which often involve the use of advanced technologies such as 3D printing.

Karásek talked specifically about how HPC has been used to help the company develop their cranial orthoses. These devices are used to control the effect of head deformities in young children, helping it to grow into the correct shape. The company has successfully treated over 8 000 infants in six countries, with amazing results, but have also seen the drawbacks of standard cranial remoulding orthoses such as weight, thermal discomfort and size.

Each orthosis is designed for the individual head shape of the child based on non-invasive scanning. It is then manufactured using 3D printing, and consists of plastic shells coupled with a locking mechanism. Previously, the inner stiffness of such devices had to be determined manually, which was a time-consuming process to carry out for each patient.

To solve this issue, the SHAPE programme has supported the company in developing a virtual prototyping tool to determine the stiffness of the supporting structure. This involved first carrying out laboratory tests on one selected structure, which were used to create a computer model that correctly described the real structure during physical testing. This model was then refined and the process of prototyping was fully automated, using numerical simulations on three variants of structures to test the developed workflow.

Invent Medical's new virtual prototyping tool has proven to be a huge benefit to all involved in the supply chain. For the patient, the increased customisability of the design means that the helmet is more breathable and can be made up to 40% lighter than previous designs through the use of static structures. Without the support of SHAPE, the creation of this new semi-automated workflow would have been extremely difficult, and it will be interesting to see how the company now progresses.

To find out more about Invent Medical, visit: **www.inventmedical.com**

EaPConnect: Deep learning and medical data mining

The last few years has seen enormous progress in the fields of deep learning and artificial intelligence, with huge potential for use in medicine and industry. At this year's European HPC Summit Week 2018, the EaPConnect project organised a workshop on deep learning and medical data mining.

Deep learning and artificial intelligence are both taking bigger and bigger strides with each other as computing becomes more and more powerful. They are implemented in software and trained using large amounts of datasets which are proving are crucial in tackling various challenges in industry, medical diagnosis, quality control, marketing, internet services, gaming, the entertainment industry, and more. However, serious obstacles still prevent their widespread use:

'Teaching' an artificial deep neural network requires a very large amount of data, which is difficult to accumulate and label. This is especially true for sensitive areas such as medical imaging and computerised diagnosis. The task is also hugely computationally expensive. In order to remove these obstacles, EaPConnect used the opportunity of the workshop this year to share their knowledge and medical image data with European partners, to achieve better scientific results, develop deep learning and data mining technologies further, and contribute towards better health services in EU and Eastern Partnership (EaP) countries.

There is a lot of potential for AI development and application in the EaP partners' region, but it will unfold differently in the various countries. Data is critical to the successful application of AI and data concentration may vary, meaning that AI will develop at different rates. Nevertheless, there is an enormous pool of data to work through, so AI adoption may progress slowly.

The EaP region's scarcity of traditional data in many markets could actually set it apart from others. This means that alternative and unstructured data will play a bigger role in AI implementation. The ability to analyse large amounts of alternative data will take things a step further, as AI is expected to unlock the potential of alternative data sets, which originate as a product of a company's operations, opening the door to many new products and services.

"This technology may be able to generate artificial medical images that are indistinguishable from real patient images"

In EaP countries, participants are working on AI and deep learning technology applications in computer-assisted medical diagnosis, new materials development, computational physics, environmental protection and other areas. They are very interested in information on accessing computational resources for long-lasting training of deep CNNs and related information resources. The main hardware characteristic is the availability of recent high-performance computational resources, including using modern accelerators like GPU NVidia graphical cards. Another critical point is creating joint, open-access information resources and crowd sourcing.

The use of patients' image data will continue to be a very sensitive and critical issue in terms of ethics and security, even when data is completely de-personalised. Other obvious topics for consideration are the possible ways of using brand-new technologies such as generative adversarial networks. After training two competitive networks, this technology may be able to generate artificial medical images that are indistinguishable from real patient images. If so, this could open a new era of free use of medical images of 'people who do not really exist' in training algorithms, handbook illustrations, teaching, websites and other resources.

Molecular design of bio-based polyurethanes

Bio-based polyurethanes represent an excellent eco-friendly alternative to the oil-based plastics which are so widely used in our day-to-day lives. **Bela Fiser** of the University of Miskolc has been using computational tools to work out which plant-derived chemicals are most suitable for the synthesis of these new materials.

As the world tries to rid itself of its dependence on oil-based materials, the race is on to try and create more sustainable alternatives. The market for bio-based goods is now rapidly growing, and there is no shortage of creativity in the field, with people using materials ranging from algae to elephant dung to synthesise an ever-expanding range of products.

Bio-based products are wholly or partly derived from materials of biological origin (excluding fossil fuels). As they are derived from renewable raw materials such as plants, they can help reduce CO_2 emissions and offer other advantages such as lower toxicity.

Bio-based products have the potential to make the economy more sustainable and lower its dependence on fossil fuels. For this reason, the EU has in recent years declared the bio-based products sector to be a priority area with high potential for future growth, reindustrialisation, and addressing societal challenges.

Polyurethanes (PUs), are the sixth most widespread group of polymers used in the global market. They are made by reacting di- or oligo-isocyanates with polyols to form various materials with versatile properties, such as heat insulation. Recycling PUs is expensive, however, due to their thermoset character which make them hard to break down. The polyols which are used to make them are also derived from petrochemicals, meaning that they cannot be sustainably produced.

Bela Fiser of the University of Miskolc has been exploring the possibility of designing a new generation of PUs based on natural polyols (carbohydrates) that would be easier to recycle, cheaper, and sustainably produced. The use of these bio-polyols could also improve the biodegradability and mechanical properties of the resultant PUs.

Bela Fiser

"The reactivity of each sugar was compared by simulating all of the possible reaction pathways"

Fiser presented at the Materials and Chemistry session, explaining how he has used computational tools to test the potential of a number of different bio-polyols, including sucrose, maltose, mannitol, glucose and fructose. The reactivity of each of the studied sugars was compared by simulating all of the possible reaction pathways, with more than 500 quantum chemical calculations being performed overall using the local HPC cluster at the University of Miskolc and additional resources from the KIFÜ HPC infrastructure in Hungary.

Based on the results, it was shown that a fructose-based PU was the most promising candidate. Fiser and his group have now gone one step further and actually synthesised this new polymer, which is now being tested for its functional properties. His graduate student, Min-Yen Lu, performed most of the synthetic work with the help of department engineer Attila Surányi. As long as the functional properties of these materials are not drastically changed by the use of bio-polyols in synthesis, they represent new eco-friendly alternatives to conventional PUs for a number of applications.

Phoretic active matter and micromachines

The directed motion of colloidal particles in the presence of a temperature gradient can be used to build spontaneously moving micro-structures. **Marisol Ripoll** has been using HPC to explore the possibilities of these micromachines, which could be useful in such applications as energy harvesting.

In the 1966 film Fantastic Voyage, a submarine crew are shrunk to microscopic size so that they can venture inside the body of an injured scientist and repair damage to his brain. As with all the best sci-fi, it turns out that fantasy is now taking its first steps into reality.

Marisol Ripoll of Forschungszentrum Juelich has been using HPC to investigate what is known as active matter. Active matter is composed of large numbers of active "agents", each of which consumes energy in order to move and drive the whole group to behave in very complex ways. Due to the energy consumption, these systems are intrinsically out of thermal equilibrium. Examples of active matter in nature are schools of fish, flocks of birds, and bacteria colonies. In fact, most examples of active matter are biological in origin, but a great deal of current experimental work is devoted to synthetic systems, which is where Ripoll has been focusing her attention.

"Micromachines could have a huge economic impact, as they are able to transform waste heat energy into kinetic motion"

Synthetic versions of active matter have the potential to be very useful in a number of fields. By harnessing the behaviour of synthetic active matter, it is possible to use it for many applications, including harvesting energy using tiny microscale machines (or micromachines).

Ripoll explained how a concept called thermophoresis is used to power such machines. Thermophoresis refers to the directed motion of colloidal particles in the presence of a temperature gradient, which can occur towards cold or warm areas. Together with the colloid motion, the temperature gradient also induces a thermo-osmotic flow of the surrounding solvent. This flow can eventually translate into the formation of thermophoretic crystals, or be used to generate diverse flow patterns in microfluidic environments.

Marisoll Ripoll

This thermophoretic effect can be exploited to build micromachines, which Ripoll and her team have been investigating using a mesoscopic simulation technique known as multiparticle collision dynamics simulations (MPC). Asymmetric micro-gears locally heated in a cooled surrounding solvent can be shown to rotate spontaneously and unidirectionally. The resulting temperature gradient along the edges of the gear teeth translates into a directed thermophoretic force, which exerts a net torque on the gear.

Microscale turbines rotating in the presence of external fields can be constructed by assembling anisotropic blades in a chiral manner based on the so-called anisotropic thermophoretic effect, characteristic of elongated objects.

These devices could potentially have a huge economic impact, since they are able to transform waste heat energy into kinetic motion. Although these micromachines are not yet at the stage of development where they can provide these benefits, Ripoll's research is surely just the beginning of another fantastic voyage into the very reaches of scientific possibility.

Binary neutrons stars

Last year's conference saw Minna Palmroth of the University of Helsinki, present her spectacular visuals of near-Earth space weather, and continuing in the same astrophysics vein this year was **Luciano Rezzolla** of the Goethe University Frankfurt, who gave a keynote speech about his work on binary neutron stars.

Black holes represent one of the most fascinating implications of Einstein's theory of gravity, but Luciano Rezzolla's aim in this talk was to convince the gathered delegates that neutrons stars in binary systems are of equal interest, where gravity blends with astrophysics and particle physics.

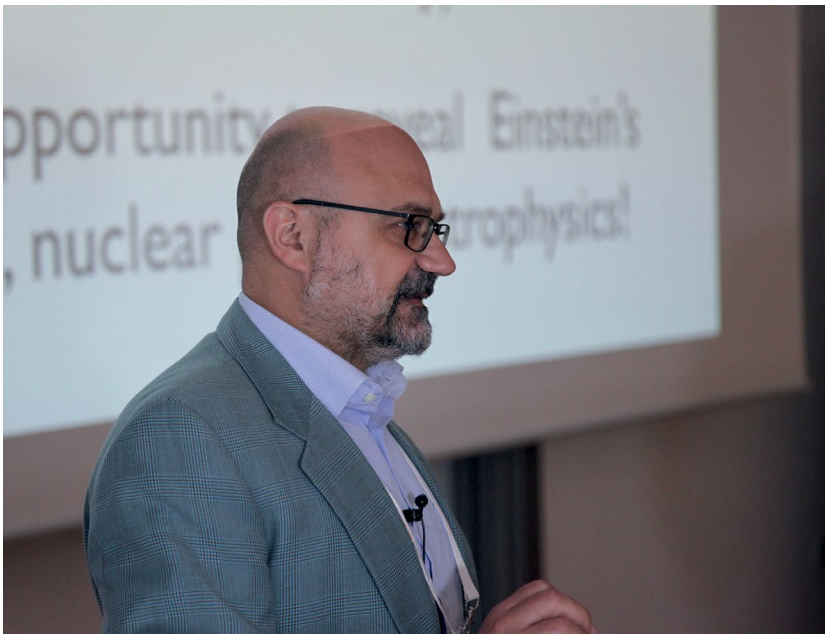
Neutron stars are for many reasons among the most intriguing astrophysical objects. The most extreme regimes of physics are combined in essentially perfect spheres of a dozen kilometres in radius. These objects have enormous densities, ultra-strong magnetic fields and produce large curvatures in spacetime. Rezzolla and his colleagues study these objects and have developed a fully three dimensional numerical code, Whisky, for carrying out simulations of general relativistic hydrodynamics.

It is known that when two black holes interact they merge together to create a larger black hole and give off gravitational waves. This was first predicted by numerical simulations and then later proven through the detection of the gravitational waves. In the case of binary neutrons stars, a similar situation arises with the formation of a black hole, but through a longer process.

When two neutron stars collide, they first form what is known as a hyper mass neutron star. They want to form a black hole, but cannot. It is this hyper-massive neutron star phase – where matter as heavy as the sun is squashed into the size of a small city – that can provide clear information on the equation of state.

Eventually, a black hole with a toroidal accretion disc forms, after which gravitational waves are released. This phase can explain much of the phenomenology of short gamma ray bursts, while the ejection of matter during the merging of the two neutron stars can shed light on chemical enrichment of the universe. Rezzolla believes that almost all of the gold in the universe may have been created from such phenomena.

Rezzolla briefly showed the audience the numerical methods he has used in his research. As he put it himself, "the equations of numerical relativity are as beautiful as they are analytically intractable". The slide presenting this sea of equations was soon swapped out, however, for a much more aesthetically pleasing demonstration of his work: a visualisation of the highly accurate and self-consistent simulation of the merging of two neutron stars.

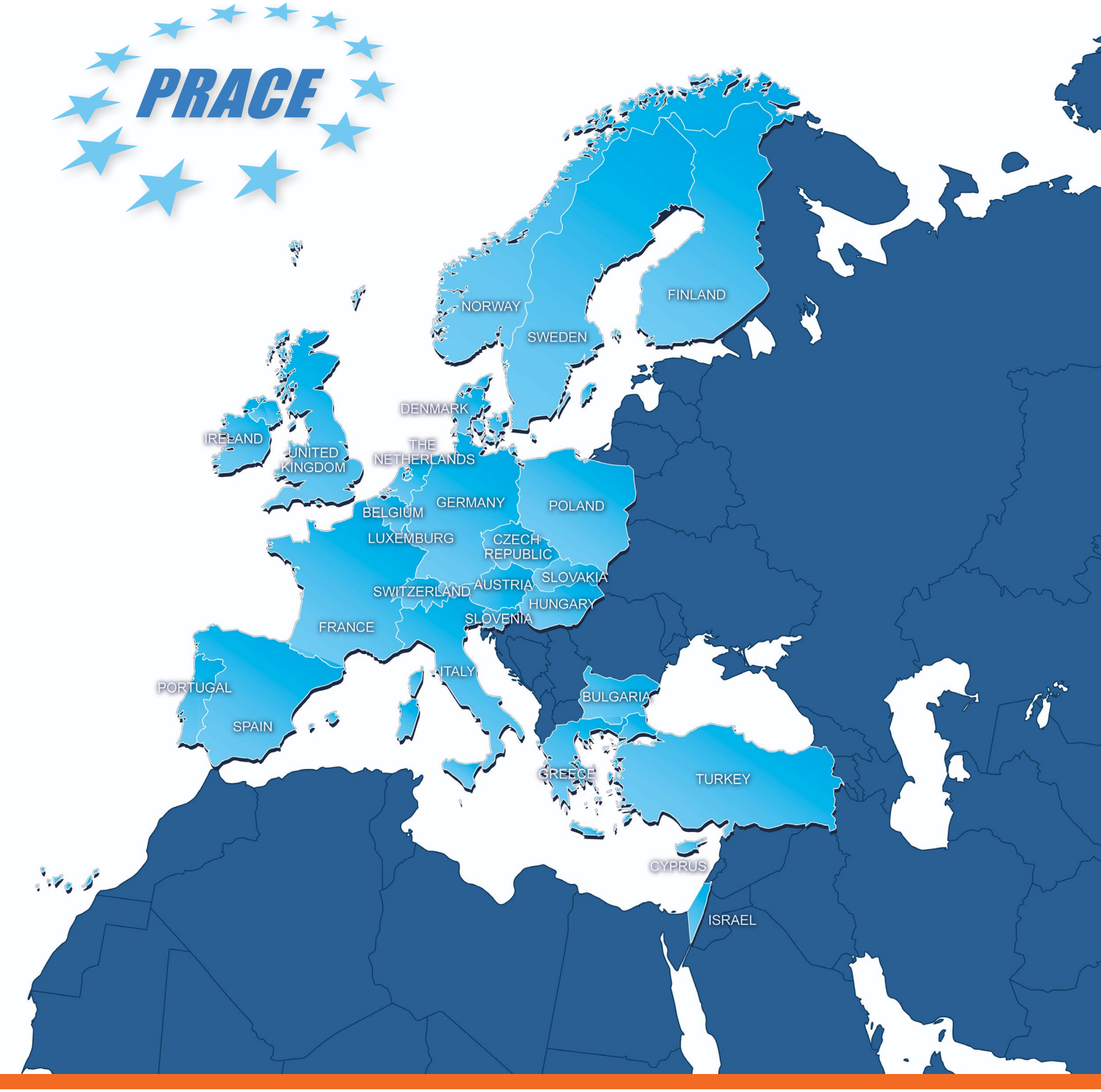


Luciano Rezzolla

> *"Almost all of the gold in the universe may have been created during the merging of neutron stars"*

Supercomputers have come on leaps and bounds in their ability to model gravitational wave signal frequencies with numerical simulations of different binary systems. Gravitational wave spectroscopy is now possible. "We can look at the peaks and tell things about the makeup of each system," Rezzolla explained. "There are frequencies associated with different stages of merging, with large peaks showing the different parts of the process."

Executive Summary



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