

## WELCOME



Guy Lonsdale

*FocusCoE project coordinator*

” Those of you who have shared projects or otherwise interacted with me over the years will know that I fully stand behind the position about the pivotal role of HPC applications that we started in our proposal for FocusCoE: HPC Matters (borrowing a slogan used previously by the IEEE SC conference), primarily because the use of HPC to address industrial, scientific and societal challenges matters! FocusCoE has been established to support the CoEs to more effectively fulfil their role within the European HPC ecosystem and the EuroHPC initiative.

Two major strands of activities within FocusCoE concern industrial outreach (promoting CoE competences and services to industry and providing the CoEs feedback on industrial needs for such) and concerted HPC training (providing a vehicle for the promotion of user training from across the CoEs and providing appropriate cross-area training to CoEs). In addition, the more “strategic planning” activity is the creation of the EU HPC CoE General Assembly (GA): which should be a platform that allows the CoEs to collaboratively define a strategy

for contributions to the EU HPC Ecosystem and plan its implementation and should involve CoE members in addition to selected strategic partners. The “CoE GA” was a key discussion topic at our first workshop with the CoEs, which was held on February 21st in Frankfurt. We are currently working with the CoEs on the definition of the operational procedures for the CoE GA and the inaugural meeting will be held during the EuroHPC Summit Week in Poznan (on May 17th).

Looking beyond the EHPCSW '19 event, we will be helping to promote the CoEs during this year's Teratec Forum in Paris in June and we also expect to interact with many of you during the ISC'19 conference & exhibition in Frankfurt. Somewhat later in the year – the September/October time-frame is planned – FocusCoE will be organising, with support from the European Commission, an HPC education and training stakeholder workshop, which should quite naturally involve all of the HPC CoEs. We'll keep you informed through our web-site and other communication channels... and of course through future editions of the newsletter. “

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## DON'T MISS !

**Workshop on  
Machine learning  
for Weather and  
Climate Models**  
September 2-5, 2019

**Registration open until  
May 1**

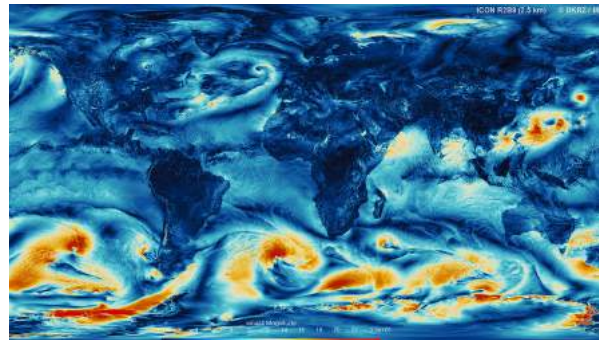
**Comp Bio Med  
Coference 2019**  
September 25-27, 2019

**Early Bird Registration  
and Abstract Submissi-  
on deadline 15th May  
2019.**

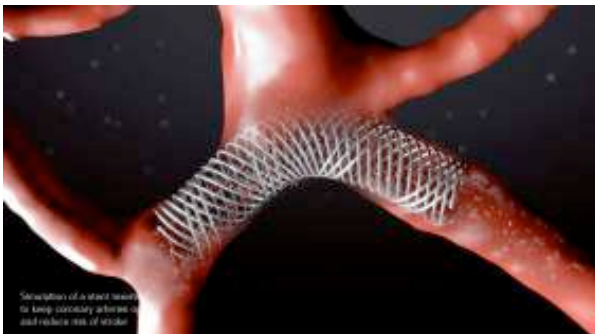
## MEETING THE CHALLENGES OF TOMORROW - AT SCALE

With the help of a multi-million funding programme for applications in High Performance Computing, the EC aims to address European societal, economic and scientific challenges.

From computing the reduction of noise and fuel for passenger airplanes to assessing the effects of climate change – Applications in High Performance Computing (HPC) help tackle some of the world's biggest societal, scientific, and economic challenges. The development of the next generation of supercomputing systems – exascale systems, with computing speeds a billion times higher than current desktop computers – targets the future needs of such applications. However, enabling these applications to effectively use ever larger (and increasingly complex) computing systems is a major milestone which has yet to be achieved, keeping in mind that the first pre-Exascale machines will be available in Europe in 2020 according to the announced EuroHPC strategy.



Simulation of wind magnitude at 10 m high at a global horizontal resolution of 2.5 km. © ESIWACE / DKRZ



Simulation of a stent inserted to keep coronary arteries open and reduce risk of stroke. © CompBioMed / Barcelona Supercomputing Center

After an investment of 42 M€ in 2015, the European Commission confirmed its support with an additional budget of 74 M€ in December 2018 resulting in 10 operational European HPC Centres of Excellence (CoEs) for computing applications. Achieving excellence in HPC Applications takes a pivotal place – it is the applications that deliver solutions to the aforementioned challenges – in the European HPC Ecosystem alongside the development of Exascale technologies and provision of access to extreme-scale infrastructure. Simultaneously, FocusCoE has been selected as a Coordination and Support Action (CSA) in order to support these CoEs in their mission to contribute to a globally competitive HPC ecosystem. The launch of the new HPC Centres of Excellence continues to support the key role of applications and this is expected to be a crucial element within the EuroHPC Programme.

## GENERAL ASSEMBLY TO SUPPORT

### STRATEGIC COLLABORATION

In a Workshop organized by FocusCoE on 21st February in Frankfurt, all European HPC CoEs came together to discuss cross-community collaboration, common training activities and concerted outreach to support industry. As one of the main outcomes of the workshop, the establishment of the EU HPC CoE General Assembly was initiated, a body comprising CoE members and other strategic partners. The General Assembly will allow EU HPC CoEs to collaboratively define a strategy for contributions to the EU HPC Ecosystem and plan its implementation.

FocusCoE aims to channel information on CoE contributions to important societal, scientific, and economic challenges across Europe and thus give EU HPC CoEs a unified voice, creating a common understanding of the importance of HPC applications across public, academic, and industrial stakeholders. Additional support services of FocusCoE therefore comprise promotion, support for industrial outreach and business development, and providing cross-area training to the CoEs.

“ We aim to bring these competences together and support the CoEs to find synergies that help them more effectively fulfill their pivotal role within a globally competitive EU HPC ecosystem “

Identifying these cross-area intersections was one of the main objectives of the first EU HPC CoE workshop in Frankfurt. Many CoEs address specific HPC application areas such as Life Sciences, Earth Sciences, Material Sciences, and Engineering. However, other CoEs focus on computational approaches as tools to address challenges across multiple application areas, such as Machine Learning, Code Performance Optimization, and Data Analytics. “With the help of the GA and other support activities”, project coordinator Guy Lonsdale states, “we aim to bring these competences together and support the CoEs to find synergies that help them more effectively fulfill their pivotal role within a globally competitive EU HPC ecosystem”. In the coming months, the CoEs will work together towards their common goal to make today’s largest-scale applications fit for tomorrow’s challenges.



Stuttgart-based company RECOM Services uses HPC for computational process optimization and problem analysis in industrial combustion. © RECOM Services

# EVENT HIGHLIGHTS



## PATC POP 32th VI-HPS Tuning Workshop

POP experts will give an overview of the VI-HPS programming tools suite, explain the functionality of individual tools, and how to use them effectively, and offer hands-on experience and expert assistance using the tools at the 32th VI-HPS Tuning Workshop at the University of Bristol, UK. This workshop is a PRACE Training Centre (PTC) course.

Bristol, UK

## EuroHPC Summit Week

The inaugural meeting of the European HPC CoE General Assembly (GA) will take place during EHPSCSW19 on Friday, May 17th – preceded by a GA discussion meeting held on May 13th. Multiple sessions – organised by EuroHPC, EXDCI-2 and PRACE-5IP – address interactions within the European HPC Ecosystem where the role of applications has a high significance and an active participation of the CoEs is sought.

Poznan, Poland



## Teratec Forum 2019

The TERATEC Forum brings together international experts in HPC, Simulation and Big Data to promote the strategic importance of these technologies for developing industrial competitiveness and innovation capacity. Visit the European HPC Centres of Excellence at booth #19 and speak with HPC application experts from POP2, ESIWACE, and EXCELLERAT.

Palaiseau, France

## 2nd DYAMOND-ESIWACE Hackathon

Global high-resolution weather and climate simulations are of interest for scalability and performance investigations, as well as the analysis workflow. In this Hackathon, ESIWACE provides computational performance expertise to participants and enables them explore large amounts of data provided by the DYAMOND initiative resulting from global high-resolution atmospheric simulations.

Mainz, Germany



PATC: Introduction to OpenACC (PRACE Training)	4-5 April	Barcelona, Spain	PATC: Heterogeneous Programming on GPUs with MPI & OmpSs (PRACE Training)	22-23 May	Barcelona, Spain
PATC: Introduction to CUDA Programming (PRACE Training)	8-11 April	Barcelona, Spain	PATC: Heterogeneous Programming on FPGAs with OmpSs@FPGA (PRACE Training)	24 May	Barcelona, Spain
Emerging Technology Conference 2019 (EMIT 2019)	9-11 April	Huddersfield, UK	Alchemical Free Energy Workshop	27-28 May	Göttingen, Germany
European Open Science Cloud (EOSC) Hub Week 2019	10-12 April	Prague, Czech Republic	BioExcel / PRACE Seasonal School 2019, Sweden – HPC for Life Sciences	10-13 June	Stockholm, Sweden
Introduction to Arm SVE and gem5 simulator	16 April	Webinar	TERATEC 2019 Forum	11-12 June	Palaiseau, France
Introduction to Arm Instruction Emulator (ArmlE)	18 April	Webinar	E-CAM Workshop 'Electrochemical energy storage: Theory meets industry'	12-14 June	Saclay, France
Spring Computing Systems Week 2019 (SCW 2019)	16-18 April	Edinburgh, UK	PASC 2019	12-14 June	Zurich, Switzerland
PATC POP 32th VI-HPS Tuning Workshop	24-26 April	Bristol, UK	TERENA Networking Conference 2019 (TNC19) – Forging Digital Societies	16-20 June	Tallin, Estonia
EuroHPC Summit Week 2019	13-17 May	Poznan, Poland	International Supercomputing Conference 2019 (ISC2019)	16-20 June	Frankfurt, Germany
PATC: Performance Analysis and Tools (PRACE Training)	20-21 May	Barcelona, Spain	2nd DYAMOND-ESIWACE Hackathon	19-21 June	Mainz, Germany

# CODES

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## Quantum Espresso

With the help of QE, material scientists are able to study the electronic and modelling properties of materials at the nanoscale – representing everything that has dimensions between 1 and 100 nanometres, so from the atom to the size of a virus.

Version 6.4 released in March 2019



## Nek5000

Nek5000 is an open-source flow solver based on the spectral element method. The code solves the incompressible Navier-Stokes equations, together with a number of additional physics (heat transfer, magneto-hydrodynamics, low Mach number, electrostatics), on general hexahedral spectral elements.

Version 19.0 released in January 2019



## OpenPathSampling

OpenPathSampling (OPS) is a software package to perform path sampling simulations and other trajectory-based approaches to study rare events. Much of the development of OPS has been sponsored by E-CAM. The methods implemented in OPS can be used to study many kinds of problems, including drug binding and unbinding, self-assembly processes, conformational changes in biomolecules, and chemical reactions.



# PUBLICATIONS

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## CompBioMed

Pérez-Benito, L., Casajuana Martin, N., Jiménez-Rosés, M., Van Vlijmen, H., & Tresadern, G. (2019). Predicting Activity Cliffs with Free Energy Perturbation. *Journal of chemical theory and computation*. DOI: 10.1021/acs.jctc.8b01290

Llinas del Torrent, C., Pérez-Benito, L., & Tresadern, G. (2019). Computational Drug Design Applied to the Study of Metabotropic Glutamate Receptors. *Molecules*, 24(6), 1098. DOI: 10.3390/molecules24061098

Llinas del Torrent, C., Casajuana-Martin, N., Pardo, L., Tresadern, G., & Pérez-Benito, L. (2019). Mechanisms Underlying Allosteric Molecular Switches of Metabotropic Glutamate Receptor 5. *Journal of chemical information and modeling*. DOI: 10.1021/acs.jcim.8b00711

Skalic, M., Jiménez Luna, J., Sabbadin, D., & De Fabritiis, G. (2019). Shape-Based Generative Modeling for de-novo Drug Design. *Journal of chemical information and modeling*. DOI: 10.1021/acs.jcim.8b00706

Závodszy, G., van Rooij, B., Czaja, B., Azizi, V., de Kanter, D., & Hoekstra, A. G. (2019). Red blood cell and platelet diffusivity and margination in the presence of cross-stream gradients in blood flows. *Physics of Fluids*, 31(3), 031903. DOI: 10.1063/1.5085881

## BioExcel:

Soiland-Reyes, Stian, and Marcos Cáceres. The Archive and Package (arcp) URI scheme. 2018 IEEE 14th International Conference on e-Science (e-Science). IEEE, 2018. DOI: 10.1109/eScience.2018.00018

## E-CAM:

Luigi Delle Site, Christian Krekeler, John Whittaker, Animesh Agarwal, Rupert Klein, Felix Höfling. Molecular Dynamics of Open Systems: Construction of a MeanField Particle Reservoir. *Adv. Theory Simul.* 2019, DOI: 10.1002/adts.201900014

David W. H. Swenson, Jan-Hendrik Prinz, Frank Noe, John D. Chodera, and Peter G. Bolhuis. OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. *J. Chem. Theory Comput.* 2019, 15, 813-836, DOI: 10.1021/acs.jctc.8b00626

David W. H. Swenson, Jan-Hendrik Prinz, Frank Noe, John D. Chodera, and Peter G. Bolhuis. OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes, *J. Chem. Theory Comput.* 2019, 15, 837-856, DOI: 10.1021/acs.jctc.8b00627

## ESiWACE

Lüttgau, J., & Kunkel, J. (2018, June). Cost and Performance Modeling for Earth System Data Management and Beyond. In International Conference on High Performance Computing (pp. 23-35). Springer, Cham. DOI: 10.1007/978-3-030-02465-9\_2

Chantry, M., Thornes, T., Palmer, T., & Düben, P. (2019). Scale-selective precision for weather and climate forecasting. *Monthly Weather Review*, 147(2), 645-655. DOI: <https://doi.org/10.1175/MWR-D-18-0308.1>

Szmelter, J., Smolarkiewicz, P. K., Zhang, Z., & Cao, Z. (2019). Non-oscillatory forward-in-time integrators for viscous incompressible flows past a sphere. *Journal of Computational Physics*, 386, 365-383. DOI: <https://doi.org/10.1016/j.jcp.2019.02.010>

Smolarkiewicz, P. K., Kühnlein, C., & Wedi, N. P. (2019). Semi-implicit integrations of perturbation equations for all-scale atmospheric dynamics. *Journal of Computational Physics*, 376, 145-159. DOI: <https://doi.org/10.1016/j.jcp.2018.09.032>

Neumann, P., Düben, P., Adamidis, P., Bauer, P., Brüch, M., Kornbluh, L., ... & Biercamp, J. (2019). Assessing the scales in numerical weather and climate predictions: will exascale be the rescue?. *Philosophical Transactions of the Royal Society A*, 377(2142), 20180148. DOI: <https://doi.org/10.1098/rsta.2018.0148>

## COE'S OVERVIEW

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### BioExcel 2 Biomolecular Research

BioExcel is operating towards advancement and support of the HPC software ecosystem in the life science domain. Research and expertise covers structural and functional studies of the main building blocks of living organisms (proteins, DNA, membranes etc.) and techniques for modelling their interactions ranging from quantum to coarse-grained models up to the level of a single cell.



### ChEESE Solid Earth

In ChEESE, leading European HPC centers, academia, hardware developers, as well as SMEs, industry and public governance bodies such as civil protection are working together to prepare European flagship codes for upcoming pre-Exascale and Exascale supercomputing systems to tackle global challenges in the domain of solid earth.



### CompBioMed Biomedicine

CompBioMed is a user-driven Centre of Excellence in Computational Biomedicine, to nurture and promote the uptake and exploitation of high performance computing within the biomedical modelling community, supporting users in academia, industry and clinical practice.



### E-CAM Quantum Dynamics

The overall objective of E-CAM is to create, develop and sustain a European infrastructure for computational science applied to simulation and modelling of materials and of biological processes of industrial and societal interest.



### EoCoE-II Energy

EoCoE will use the prodigious potential offered by the ever-growing computing infrastructure to foster and accelerate the European transition to a reliable and low carbon energy supply via targeted support to four carbon-free energy pillars: Meteorology, Materials, Water and Fusion, each with a heavy reliance on numerical modeling.



## ESiWACE2 Weather & Climate

ESiWACE2 aims to link, organise and enhance Europe's excellence in weather and climate modelling to enable leading European weather and climate models to leverage the performance of pre-exascale systems as soon as possible and prepare the weather and climate community to be able to make use of exascale systems when they become available.



## EXCELLERAT Engineering

EXCELLERAT's goal is to facilitate the development of important codes for high-tech engineering, including maximizing their scalability to ever larger computing architectures and supporting the technology transfer that will enable their uptake within the industrial environment.



## HiDALGO Global Challenges

HiDALGO enables the assessment of Global Challenges problem statements by enabling highly accurate simulations, data analytics, artificial intelligence and data visualisation, but also by providing knowledge on how to integrate the various workflows and the corresponding data.



## MaX Materials Design

MaX aims to disenthral the EU leadership in materials modelling, simulations, discovery and design by creating an ecosystem of capabilities, software applications and data workflows and analysis on HPC-oriented material simulations, designed for present and future HPC architectures.



## POP-2 Performance optimization & productivity

POP-CoE assesses the performance of computing applications, identifying issues affecting code performance as well as the best ways to address them.

For more information on the European HPC Centres of Excellence visit us online:



[www.focus-coe.eu](http://www.focus-coe.eu)



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With the help of



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