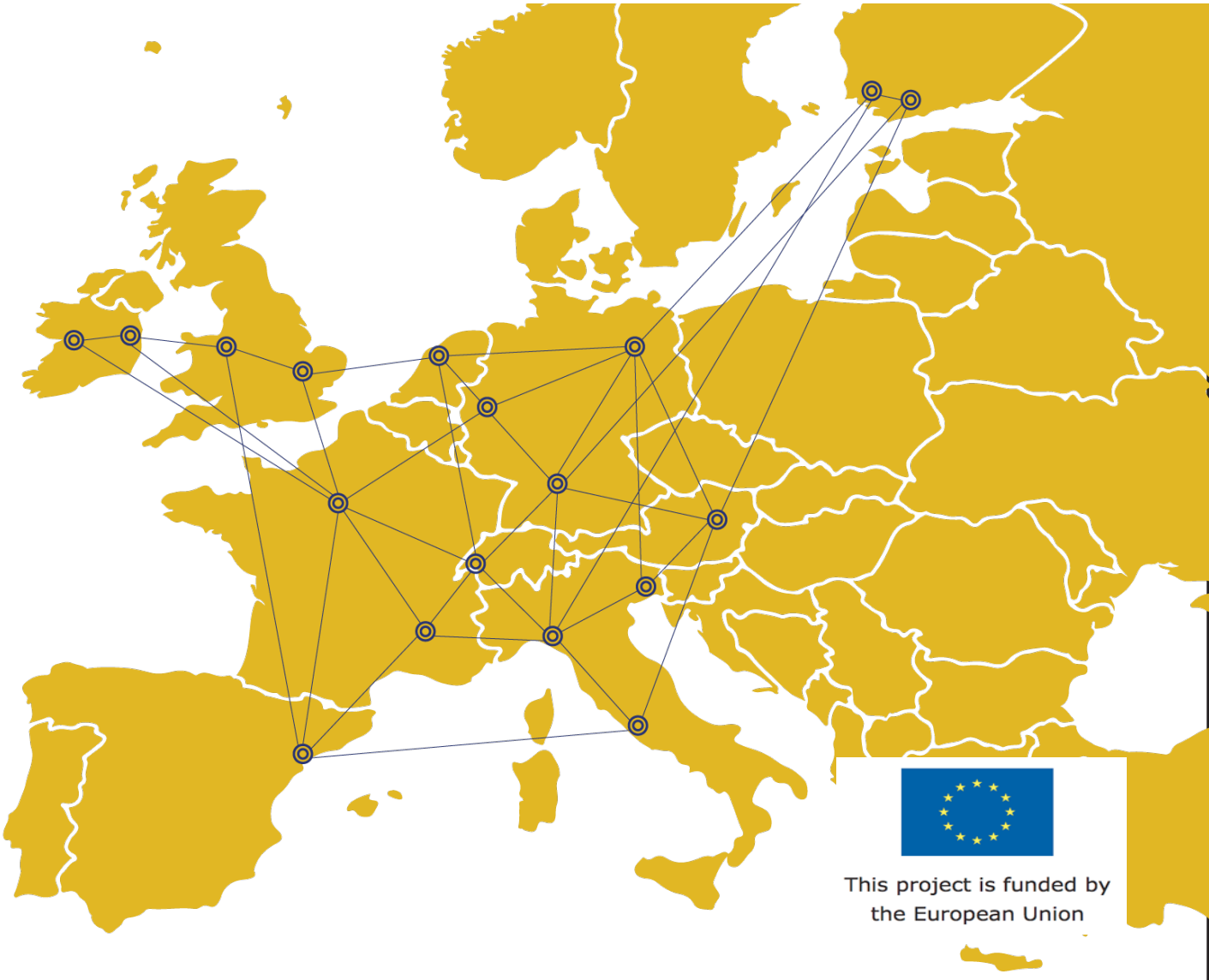
# E-CAM Quarterly

Supporting HPC simulation in industry and academia



This project is funded by the European Union

Jan-Mar 2016

**E-CAM Update**

Here are some of the things that have been happening since the last newsletter:
One of our key deliverables 6.1 ESDW Technical Software Guidelines has been submitted. Please access this document on the E-CAM website www.e-cam2020.eu

The three management groups of the project: **Software, Human Capital, and Industry** have started their monthy or quarterly meetings and are making progress towards our early deliverables on the project. You will be able to access minutes of these meetings shortly.

The full E-CAM consortium agreements were sent out to all beneficiaries in February 2016.

E-CAM has a new logo and the website www.e-cam2020.eu is under development.
Take a look and follow our LinkedIn page on https://www.linkedin.com/company/e-cam

E-CAM hirings are progressing well:
In addition to the appointments of Alan O'Cais (Software Manager) and Kate Collins (Project Administrator), there are 8 PDRA roles that have been advertised with 3 appointments already made for the NL, IRL and CH nodes. The roles at SNS, ES, UK-Hartree, DE-SMSM, DE-MMS (appointment brought forward) nodes have been advertised. The two programmer roles based in Daresbury and Maison de la Simulation are also being advertised. You can find some of these advertisements on the E-CAM website, on the E-CAM linkedin page, and on Indeed.com. The advertisements are also available on the individual organisation websites.

In the next issue we will provide information on E-CAM's industry projects and also provide information on our project management structures for you to access information more easily.

## IN THIS ISSUE:

# EVENTS

## E-CAM Scoping Workshops

**7th-9th September 2016, Mainz, Germany**

***Industry Partnerships***

Organisers: Burkhard Duenweg and Dominic Tildesley

http://www.cecam.org/workshop-1354.html

E-CAM scoping workshops allow industry to talk about the nature of modelling in their organisations and include scientific talks from representatives of each of the four work packages.

## E-CAM State of the Art Workshops

**6th - 11th June 2016, Lausanne, Switzerland**

***Different Routes to Quantum Molecular Dynamics***

Organisers: Basil Curchod and Michele Ceotto

http://www.cecam.org/workshop-1319.html

**29th August - 2nd September 2016, Leiden, Netherlands**

***Reaction Coordinates from Molecular Trajectories***

Organisers:Peter Bolhuis and Christoph Dellago

http://www.cecam.org/workshop-1349.html

**19th - 20th September 2016, Daresbury, United Kingdom**

***Electronic Structure***

Organisers: Leon Petit and Emilio Artacho

http://www.cecam.org/workshop-1351.html

## Extended Software Development Workshops

**6th June - 17th June 2016, Zaragoza, Spain**

***Electronic Structure Library Coding Workshop: Solvers***

Organisers: Fabiano Corsetti and Emilio Artacho

http://www.cecam.org/workshop-1274.html

**27th June - 8th July 2016, Paris, France**

***Quantum Mechanics and Electronic Structure***

Organisers: Daniel Borgis and Sara Bonella

http://www.cecam.org/workshop-0-1362.html

**14th November-25th November 2016, Traunkirchen, Austria**

***Trajectory Sampling***

Organisers: Gerhard Kahl and Christoph Dellago

http://www.cecam.org/workshop-1356.html

## Other E-CAM Events

**16th - 20th May 2016, Dublin, Ireland**

***Prace Spring School 2016 and E-CAM Tutorial on Molecular and Atomistic Modelling***

Organisers: Simon Wong and Michael Lysaght

http://www.cecam.org/workshop-1345.html

# EDITORIAL - Giovanni Ciccotti

*Prof Giovanni Ciccotti*

## High Performance Computing, Computer Simulation, and Theoretical Physics: Evolution or Revolution?

Numerical physics, i.e. numerical calculations serving the needs of traditional theoretical physics, exists at least since the times of Galileo, and probably long before. As Computer Simulation (started with solving problems in Statistical Mechanics), it exists only since the end of the second World War. It is based on the possibility of having computation speeds largely beyond human capabilities, even including speeds reachable by exploiting team work.

Computer simulation in Theoretical Physics is based on the idea that we can solve, by brute computing power, models of matter based on the exact laws of physics. In the case of Condensed Matter, that amounts to solving the Schroedinger equation or, possibly, justified approximations to it (often classical mechanics and a suitable model for the interactions is a sufficient substitute), and to use the mechanical information so obtained to compute the statistical mechanical properties of the system. By this token, Computer Simulation has established itself as the key tool of Theoretical Physics to which it has become an integral part. Let us refer to it as Modern Theoretical Physics. It is not an exaggeration to say that this process - still now not completely understood by some traditional practitioners - has been much more a revolution than a simple evolution of the discipline. So much so that today the predictive power of Physics has gone largely beyond its historical boundaries invading (and in part been reshaped) not only by Chemistry and its related disciplines, but also Biology, Materials Sciences, Geosciences, etc: from simple fluids to the human immune response!

The fundamental tools of this approach (Monte Carlo, Molecular Dynamics, classical and, then, Ab initio, Path Integrals, etc and, correspondingly, an entire arsenal of statistical tools) have been progressively included, but depend in a really dramatic way on the availability of potent algorithms and computer power. Indeed, it is known that the progress and development of Computer Simulation is due to the combined introduction of efficient algorithms to confront specific scientific challenges and to the exponential growth of computer power. The latter in turn is the result not only of increased speed in the transmission of signals in processing units, but also to the development of more sophisticated architectures.

From the point of view of scientific progress, it is easy to show that the development of new algorithms has been in the past much more effective in advancing the field than the bare increase in computer power. However, the situation is slowly changing and new algorithms cannot be any more easily developed without some help coming from people developing software using the new possibilities offered by the new computers: vectorization and parallelization are two typical aspects of this new trend.

Associated with this is the birth of a new profession: software engineering. Scientific progress in computer simulation will slow down if the help which can come from new software tools is neglected. The awarness of this change is already present in the US but is slow in penetrating European funding agencies. The damage induced by this delay can become indeed very serious.

At the same time, progress in computing power can saturate if not helped by the challenges offered by computational sciences, be it in the fast production of large scale dynamic data, the retrieval of large masses of stored data or their handling and high-level analysis. This new intricate field is what we encompass when speaking of High Performance Computing as proposed and apparently developed today in the European National-level Computing Centers and stimulated (although with some bias: too much attention to exascale power and too little to the scientific targets…) from the more than welcome European PRACE project which distribute to high level computationally intensive projects computer time and some software assistance.

It is a serious misfortune that the collaboration between computational and computer scientists is still in its infancy. Only a few national authorities have been able to start a close collaboration between scientists, software engineers and, possibly, full level computer scientists. Jülich is certainly one of these smart enterprises but much remains to be done at National and European levels even in Germany. To understand the reasons of this delay in joining forces let us look at the situation a bit more closely.

Computational scientists are normally under pressure to produce good scientific results, and in particular publications. The details about the way in which these results have been obtained using computers fall well outside their focus. At the same time, the management of computer centers is keen to use scientists as high level testers of the best computational facilities, largely disregarding the scientific value of their output.

The result is a confused and confusing development which doesn't help the efficiency of the entire process, with the consequence of wasted investments and progress slower than desirable and possible. To help in such a situation, one new element should be added or created, a new generation of scientifically trained software engineers to interface constructively with computational and computer scientists, not to speak of the technological environment. This profession is already largely accepted in the US and, at least for what I know, in Japan, but finds great difficulties in old Europe.

The new profile, despite being a necessity for the progress of computational science, is ignored in academic circles, while with few exceptions, it is not found in the computer centers even at high levels. A strong action is needed to change this negative trend. UCD and ICHEC in Ireland, as coordinators of the European project E-CAM, together with CECAM, the historical European hub of computational scientists in soft and hard matter, have taken a courageous initiative opening a European collaboration for software development. This is a very wise step in the right direction, and we can only wish full success to it. It has to be hoped that complementary initiatives like PRACE, computational centers scientifically oriented to HPC and academic institutions, will, sooner rather than later give due and full credit to that.

# DELIVERABLES TO DATE

We have now submitted 3 deliverables to the commission on schedule. You can access these deliverables via the E-CAM website:

**5.1: Guidelines for the Extended Software Development Workshops (ESDWs) - Delivered December 2015**

E-CAM will deliver four workshops every year, each focused on software development in one of its four core scientific areas: classical MD, electronic structure, quantum dynamics, meso and multiscale modeling. The document outlines the purpose and structure of the ESDWs, key performance indicators for each ESDW, a tentative schedule for 2016, and the duration and content of workshops.

**6.1: ESDW Technical Software Guidelines - Delivered March 2016**

The report outlines the technical framework within which the ESDWs will operate including general programming guidelines, adding contributions to the E-CAM Application libraries, and also adding contributions to the E-CAM Software libraries. E-CAM will produce 2 different types of libraries: an application library and a more traditional software library.

**11.0: Initial Data Management Plan - Delivered March 2016**

This initial DMP describes how E-CAM will manage the data relating to the project. The data will be in the form of an "Application Library" and a "Software Library". The plan goes onto describe the data set, the standards and meta data, how data will be shared, and how data will be archived and preserved.

# FUNDING AND EMPLOYMENT OPPORTUNITIES

## Scientific Programmer, Maison de la Simulation

*Maison de la Simulation*

**Principal Duties and Responsibilities**

The post holder will be required to support E-CAM's activities and collaborate with its teams:

- In the development, testing and documentation of E-CAM software and its deployment on massively parallel computation platforms (through testing and optimization of associated modules).
- To fully participate in and occasionally lead the E-CAM Extended Software Development Workshops and follow up activities.
- To support the production of E-CAM deliverables and reporting in the form and timing agreed with the European Commission.

**Contact: Daniel.borgis@ens.fr, a.ocais@fz-juelich.de**

**http://www.e-cam2020.eu/vacancies**

## Computational Software Engineer, Daresbury

*STFC*

**List of Duties / Work Programme / Responsibilities**

You will work on large-scale high-performance scientific applications targeting a range of applications for industrial and scientific end users. You will develop applications written in high level programming languages such as Fortran, C and C++ using advanced parallel and distributed programming environments. You will have access to a range of the latest hardware technologies, including IBM POWER, NVIDIA GPUs, Intel x86, Intel Xeon Phi, ARM and other novel architectures. These systems are some of the most powerful in Europe.

Contact **Dr Luke Mason 01925 603159, email luke.mason@stfc.ac.uk**

Apply by 15th April to:

**http://www.topcareer.jobs/Vacancy/irc221811_6307.aspx**

## Postdoc Software Development, Max Planck

One postdoctoral position is available at the Max Planck Institue for Polymer Research, Mainz, in the Theory Department.

The initial contract will be for one year, with possible extension for a further 11 months. Applicants should hold a PhD degree and have a strong background in theoretical physics. Exceptional candidates from physical chemistry, theoretical chemistry, chemical engineering, or applied mathematics will also be considered. Experience in programming (C++) is essential.

Contact **Burkhard Duenweg (duenweg@mpip-mainz.mpg.de).**

http://www.mpip-mainz.mpg.de/4566526/jobadpostdocecam

## Postdoc Fellowship, Nanogune CIC

One postdoctoral fellowship is available at CIC Nanogune to work in the area of computational methods for electronic structure and for materails research and optimization. The candidate will be based at Nanogune (San Sebastián, Spain).

Applicants should have a PhD in Physics or Chemistry. A strong background in quantum mechanics and computer simulation of quantum systems of condensed matter, materials or molecules are required. Experience and proficiency in coding are essential. Applications should be sent to **Emilio Artacho (e.artacho@nanogune.eu**) providing an up-to-date CV, a letter of motivation, and the names and contact details of at least two academic referees.

http://www.e-cam2020.eu/vacancies

## Funding News

**$300K Supercomputing Grants for Manufacturers from the US Department of Energy through the High Performance Computing for Manufacturing (HPC4Mfg) programme.**

In the United States grants worth $300,000 are up for grabs for manufacturers giving year-long access to national lab supercomputing cycles and half the staff hours of computer scientists with domain expertise. The program, which is led by Lawrence Livermore National Laboratory (LLNL) and includes Lawrence Berkeley (LBNL) and Oak Ridge National Laboratories (ORNL), gives manufacturers access to some of the most powerful HPC systems in the world.

See the project website https://hpc4mfg.llnl.gov/index.php

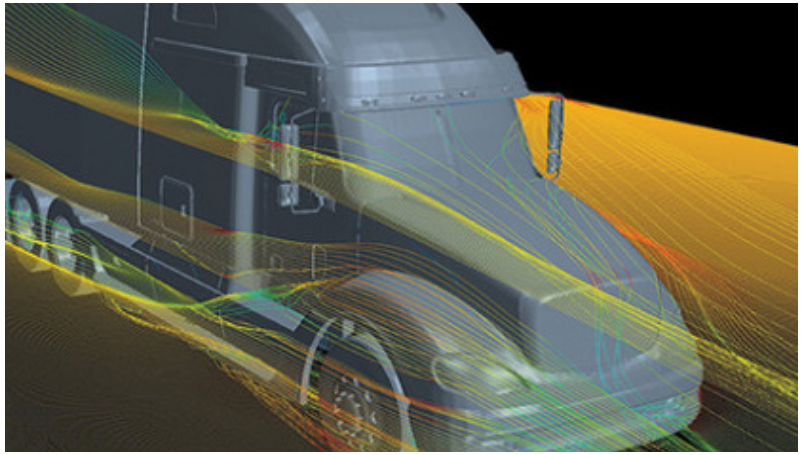


*Image from HPCWire.com*

# ITEMS OF INTEREST

The **Digital4Science Platform** was launched in September 2015 and encourages conversations on Excellence in Science and its activities around Open Science, e-infrastructures, Future & Emerging Technologies and the FET flagships. The platform is available at the following address: **http://ec.europa.eu/d4science.**

The **Digital4Science Platform** have launched an open consultation in the context of preparation of the next Horizon 2020 e-infrastructure Work Programme 2018-2020. The objective of this consultation is to gather input from e-infrastructure stakeholders on the challenges they face and that the future work programme should address.

The UK Science & Technology Facilities Council posted an article on the E-CAM project entitled “Developing a skills network to make the most of HPC”, read the full article at: **bit.ly/1MdskKL.**

E-CAM’s Software Manager, Alan O’Cais, was asked to provide a short contribution to the EC’s Communication on ICT Standardisation in the context of advancing the Digital Single Market at the beginning of February. You can read his contribution on E-CAM’s website under “News”.


*Image from stfc.ac.uk*

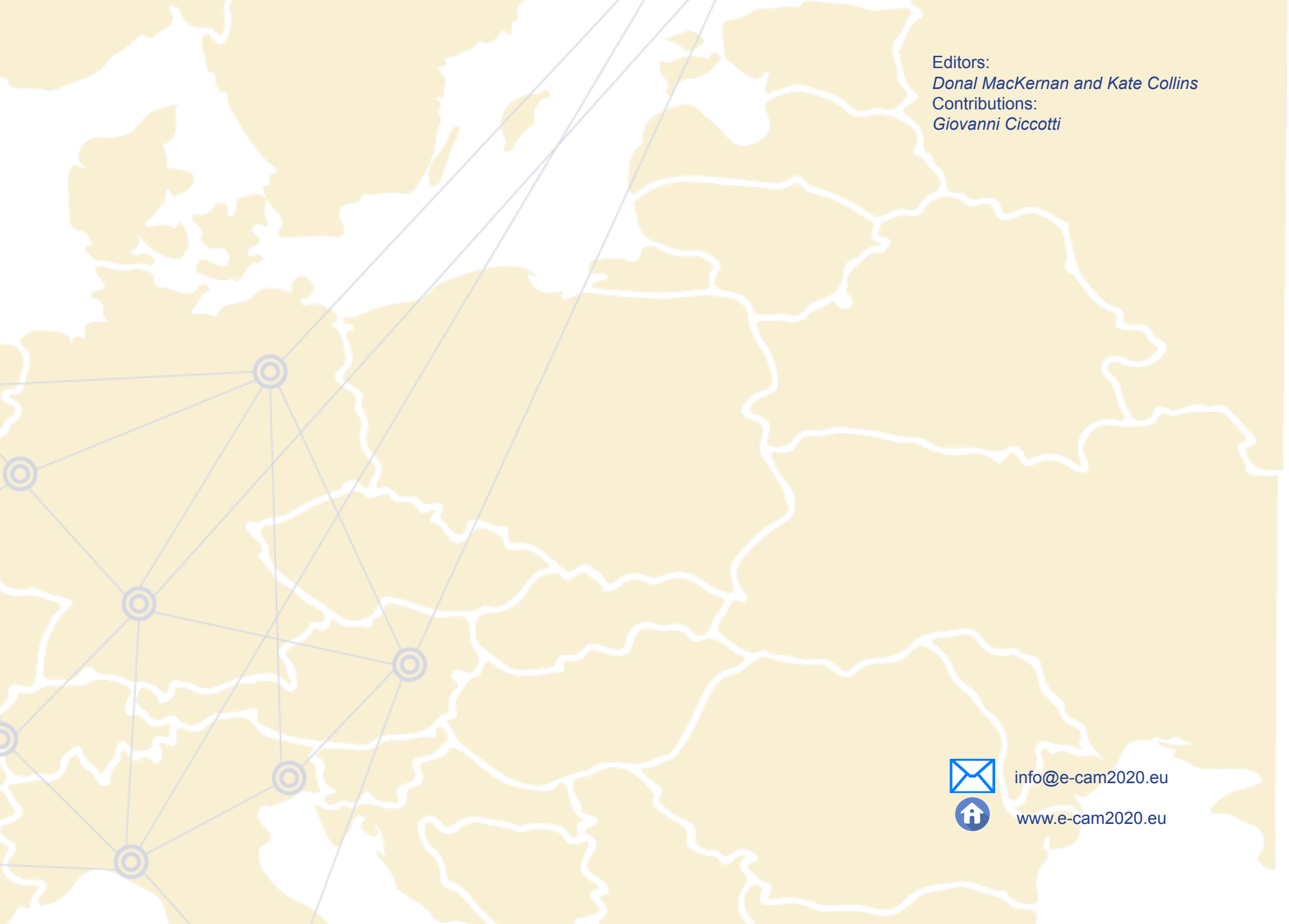
**9th - 13th May 2016, Prague, Czech Republic**
EXCDI Workshop at the HPC Summit Week
https://exdci.eu/events/hpc-summit-week-exdci-workshop

**10th - 12th May 2016, Prague, Czech Republic**
PRACEdays16
https://events.prace-ri.eu/event/488/

**12th - 13th May 2016, Prague, Czech Republic**
ETP4HPC workshop on exascale prototypes
www.etp4hpc.eu

1**5th June 2016, Birmingham, UK**
H2020 European Brokerage Event “Materials & Nanotechnology, Process Industries & Manufacturing”
https://www.b2match.eu/h2020nmp2016

Editors:
*Donal MacKernan and Kate Collins*
Contributions:
*Giovanni Ciccotti*




info@e-cam2020.eu


www.e-cam2020.eu