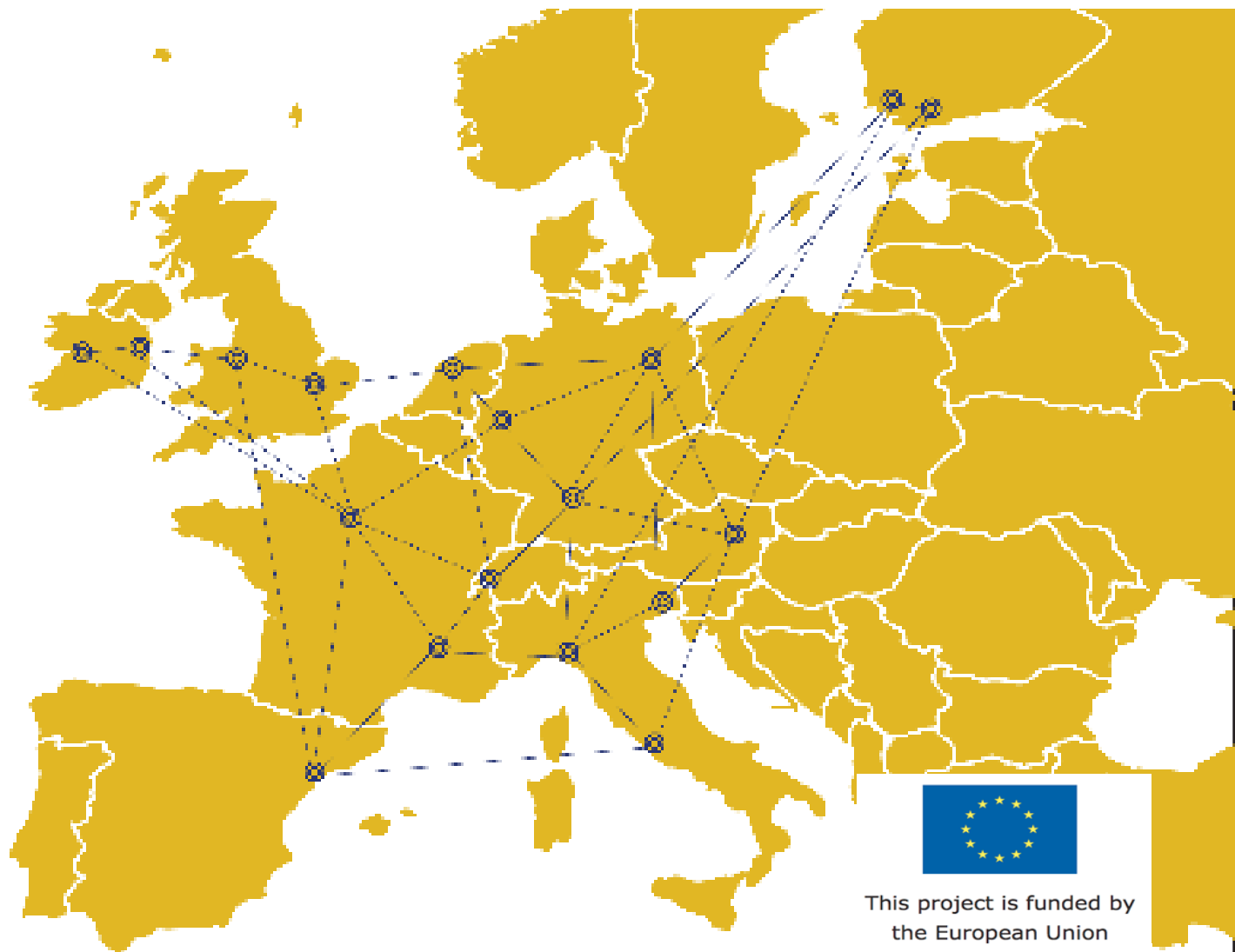




Supporting HPC
simulation in
industry and
academia

E-CAM Quarterly



June-September 2016



This project is funded by
the European Union

E-CAM Update: June- September 2016

The next E-CAM General Assembly will take place 7th - 8th November 2016 in Orsay, France at Maison de la Simulation. There will be an additional one day session for E-CAM postdoctoral fellows on 9th November 2016.

You can now access a range of E-CAM documents including minutes of our management group meetings on E-CAM's Redmine Project Management site <http://redmine.e-cam2020.eu> which should greatly increase internal visibility and cooperation in ongoing work on E-CAM deliverables and tasks.

We would like to draw your attention to the PADC 2016 workshop taking place 17th - 18th October 2016 at Jülich Supercomputing Centre, Germany. See page 2 for more information.

We are coming to the end of our first year of events with just one ESDW left to look forward to in 2016 for WP 1 to take place in Traunkirchen, Austria. This ESDW will be focused on trajectory sampling. Our 2017 events schedule will be announced in the next newsletter due in December 2016.

Read the reviews from some of the events that have taken place since the last newsletter such as the first E-CAM State of the Art Workshop that took place in June 2016 in Lausanne, Switzerland (see page 3), our first ESDW for WP 3 that took place in Paris in June/July 2016 (see page 5), and the first Scoping workshop that took place in September 2016 in Mainz, Germany (see page 4)

Take a look and follow our LinkedIn page on <https://www.linkedin.com/company/e-cam>; Facebook page <https://www.facebook.com/eCAMCoE/> and twitter <https://twitter.com/ecam2020>.

IN THIS ISSUE:

| | |
|----------------------------------|---|
| Events | 2 |
| E-CAM General Assembly | 2 |
| E-CAM Postdoc Workshop | 2 |
| ESDWs | 2 |
| PADC 2016 Workshops | 2 |
| State of the Art Workshop Review | 3 |
| Scoping Workshop Review | 4 |
| E-CAM Paris ESDW Review | 5 |
| E-CAM Tools | 6 |
| Deliverables to Date | 7 |

EVENTS

E-CAM General Assembly

7th - 8th November 2016, Orsay, France

E-CAM General Assembly

Organisers: Luke Drury and Daniel Borgis

All E-CAM beneficiaries, programmers, postdocs and industrial members are invited to attend the E-CAM General Assembly.

E-CAM Postdoc Workshop

9th November 2016, Orsay, France

E-CAM Postdoctoral Fellows Workshop

Organisers: Alan O'Cais, Jony Castagna, Liang, Liang

An event specifically dedicated to the E-CAM postdoctoral fellows and focused on HPC-related topics.

Extended Software Development Workshops

14th - 25th November 2016, Traunkirchen, Austria

Trajectory Sampling

Organisers: Gerhard Kahl and Christoph Dellago

<http://www.cecarn.org/workshop-1356.html>

12th - 13th December 2016, Orsay, France

Quantum Dynamics follow-up to ESDW on 27th June - 8th July 2016

Organisers: Sara Bonella and Daniel Borgis

PADC 2016 Workshops

17th - 18th October 2016, Jülich Supercomputing Centre, Germany

The "POWER Acceleration and Design Center" (PADC) was established in 2015 to facilitate joined efforts on high-performance computing based on solutions emerging in the context of the OpenPOWER Foundation. This workshop will bring together experts from different areas to present their experience on applications and new technologies.

Register to attend at <https://indico-jsc.fz-juelich.de/e/PADC16>

E-CAM State of the Art Workshops

E-CAM state of the art workshops survey new developments in simulation to regularly update the cscientific community. The outcome of these workshops will be used to transfer scientific advances to the industrial community.

The Schedule for 2017 will be confirmed in the next newsletter

E-CAM Scoping Workshops

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

The Schedule for 2017 will be confirmed in the next newsletter

Different Routes to Quantum Molecular Dynamics

E-CAM's first state of the art workshop was organised at CECAM headquarters in Lausanne, Switzerland by Ali Abedi, Guillermo Albareda, Michele Ceotto, Basile Curchod, and Philipp Marquetand, June 6-10, 2016.

Simulating the exact quantum dynamics of multi-component systems of electrons and nuclei is a task out of reach currently, except for the simplest molecules with a few degrees of freedom. Therefore, approximations are needed to surpass the exponential scaling of computational power needed to solve the time-dependent Schrödinger equation and open the possibility for reliable molecular dynamics simulations for eventual industrial applications. The main challenge in developing approximate methods is to have a balance between efficiency and accuracy, i.e., to keep the computational costs manageable and at the same time to be able to predict and interpret experiments. In this respect, the so-called quantum molecular dynamics community aims at describing more realistic molecular systems, and at taking simulations closer to experiments by improving the accuracy of available methods and developing new ones.

Quantum molecular dynamics is thus a rich and rapidly growing field, involving different communities in physics, chemistry, and applied mathematics. However, while the available approaches span quite a wide range of formal frameworks, common goals and unifying theoretical grounds are still missing. Comparing shortcomings and advantages, understanding the restrictions of each approach, and defining benchmarks

to assess merits and limitations of the different approaches to identify the different areas of applicability have been the main goals of the E-CAM-sponsored workshop "Different Routes to Quantum Molecular Dynamics".

A typical day of this alternative-format workshop was split into two parts. During the morning, senior lecturers were proposing an overview of their method. During the week the audience enjoyed lectures on "Quantum dynamics" by Prof. Tucker Carrington and Prof. Uwe Manthe, "Trajectory-based and trajectory-guided methods" by Prof. Dmitry Shalashilin and Prof. Joe Subotnik, "Semiclassical methods" by Prof. Kenneth Kay and Prof. Eli Pollak, and "Path integral molecular dynamics" by Prof. David Manolopoulos and Prof. Stuart Althorpe. Each set of lectures was followed by a discussion session. During the afternoons, more specialised discussions were organised, followed by a series of contributed talks. These talks – given by young researchers – offered a perspective on recent developments of the methods presented in the morning and a more detailed view of possible applications. A round table closed each day of the week for a critical assessment of each quantum dynamics method.

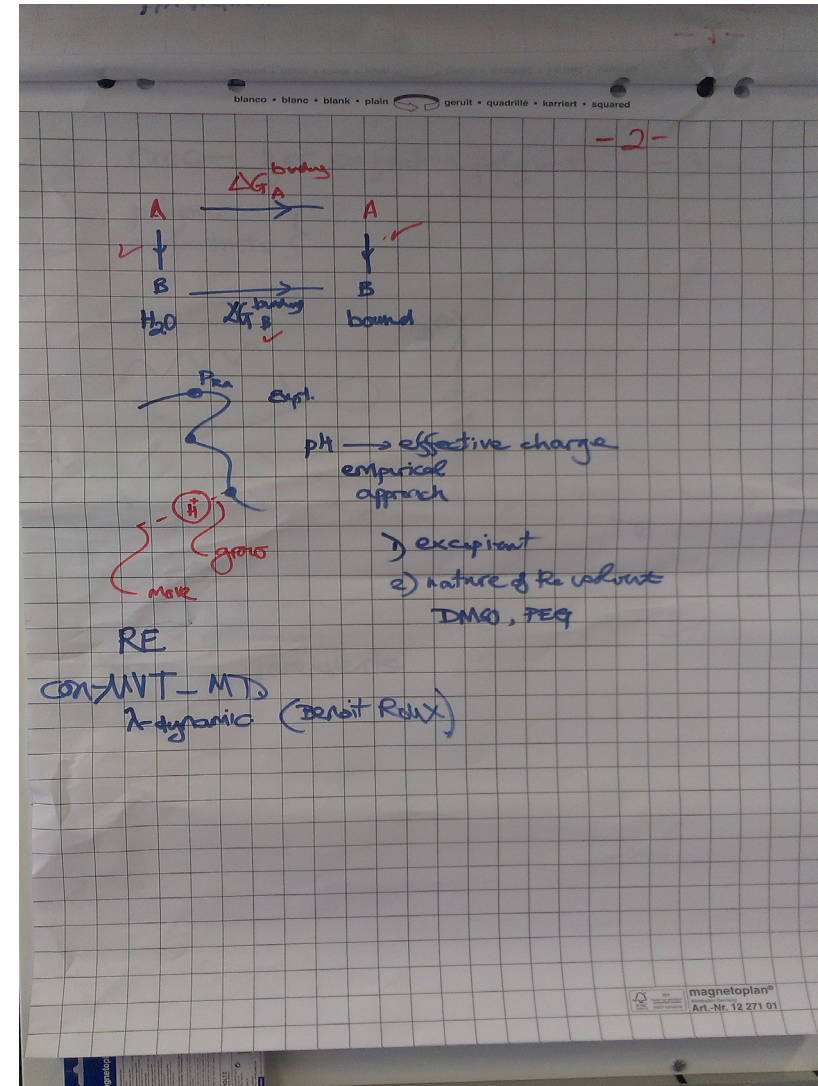
This workshop offered a unique opportunity for the quantum dynamics community to critically and open mindedly discuss the most important issues existing in the overall field, as well as to stay informed on the recent development within the different sub-domains.

E-CAM perspectives on Simulation, Modelling and Data in Industry

The first E-CAM scoping workshop was organised at Johannes Gutenberg University in Mainz, Germany by Burkhard Duenweg, Dominic Tildesley, and Kate Collins, September 7-9, 2016. The workshop was attended by 8 industrialists and 15 academic partners.

E-CAM Industrial partners and academics worked together to sharpen and focus the work plan for the project. E-CAM work package leaders outlined the major advances to be expected in each of the four scientific areas with an emphasis on application to industry.

The workshop consisted of an introduction by three centres of excellence with presentations from E-CAM by Prof. Dominic Tildesley, from MaX by Prof. Pablo Ordejón and from NOMAD by Prof. Alessandro de Vita. Each of E-CAM's work packages 1, 3 and 4 provided an update on progress with presentations from Dr. Donal MacKernan (WP 1), Dr Sara Bonella (WP 3), and Prof. Ignacio Pagonabarraga (WP 4). Prof Syma Khalid also provided an overview of Biomolecular Simulation. The workshop concluded with a panel discussion about what industry wants from simulation and what is possible through E-CAM. The final session involved three break-out groups with different industrial members to discuss potential projects facilitated by E-CAM that would be of interest to them.



E-CAM Scoping Workshop break-out session flip chart page on prediction of PH discussion

E-CAM ESDW Quantum Dynamics, June-July 2016

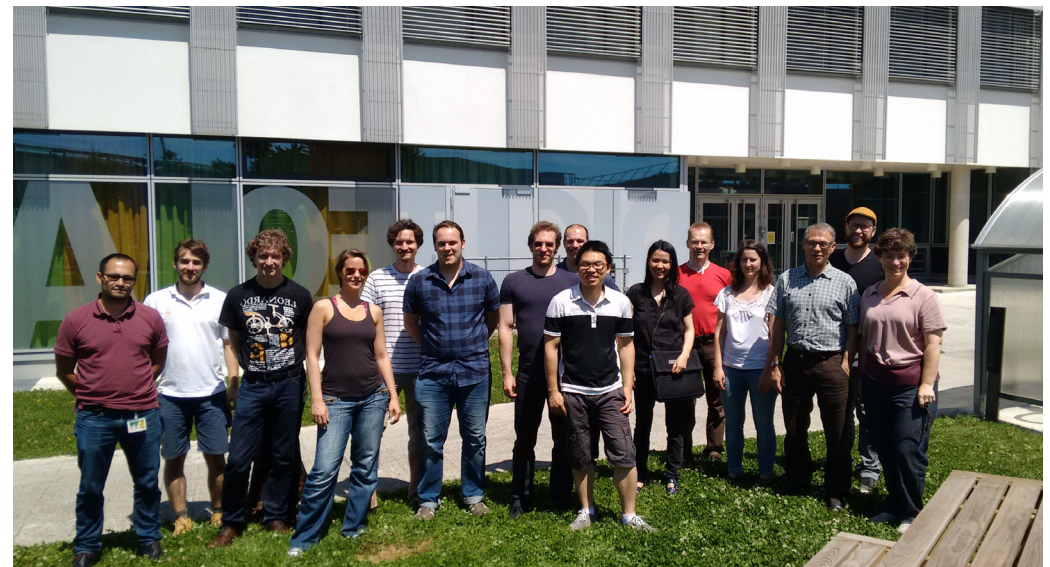
The first Extended Software Development Workshop for E-CAM WP3, Quantum Dynamics, was held at the Maison de la Simulation, Orsay, FR, from the 27th of June to the 8th of July 2016. The workshop was organised by Saran Bonella and Daniel Borgis. 10 students and 6 tutors, including Dr. Ivano Tavernelli representing the industrial partner of the Work Package, IBM, worked to develop software modules in the following areas:

- Exact quantum propagation methods for low dimensional systems to be used to provide benchmarks for approximate schemes;
- Development of a library of single and multi surface potentials for benchmark systems;
- Calculation of approximate quantum time correlation functions.

Work was performed by teams of 2-4 students, assisted by the senior participants and by E-CAM's Software Manager, Alan O'Cais, and the Software Developer associated to WP3, Dr. Liang Liang.

In addition to the software development activities, the Workshop enjoyed lively scientific discussions centered on presentations made by the students and the senior participants. The on-line E-CAM tools for software development, including the Git repository, and tools for the documentation (Doxygen) and performance analysis were presented by E-CAM staff members and participants were instructed on their use via tutorials. The program was further enriched by the interactions with experts on software

and hardware development working at La Maison de la Simulation who gave talks on topics such as architectures and programming paradigms and the use of advanced visualization tools such as the Image wall hosted by the Maison de la Simulation.



Participants at E-CAM ESDW, Paris

E-CAM TOOLS

E-CAM Search:

+ Overview Activity Issues Gantt Calendar News Documents Wiki Files Settings

Overview

European Centre of Excellence that supports Software, Training and Discussion in Simulation and Modeling. Please read the [ECAM_Wiki](#) to get further information about how to use this service correctly.

- Homepage: <http://www.e-cam2020.eu/>

Issue tracking

| | open | closed | Total |
|-----------|------|--------|-------|
| Task | 74 | 0 | 74 |
| Milestone | 0 | 0 | 0 |

Members

Manager: Alan O'Cais, Kate Collins

Spectator: Burkhard Duenweg, Carsten Hartman, Christian Krekeler, Christoph Dellago, Daniel Borgis, David Swenson, Denis Girou, Dominic Tildesley, Donal MacKernan, Emilio Artacho, Etienne Plesiat, Francesco Fracchia, Gerhard Kahl, Giordano Mancini, Godehard Sutmann, Graham Worth, Hideki Kobayashi, Ignacio Pagonabarrage Mora, Jony Castagna, Jussi Heikonen, Leon Petit, Liang Liang, Luigi Dellesite, Luke Drury, Michael Lysaght, Michael Payne, Michael Seaton, Mikko Alava, Momir Malis, Peter Bolhuis, Ralf Everaers, Sara Bonella, Vincenzo Barone

Within the E-CAM consortium we are using the following services:

<http://gitlab.e-cam2020.eu>

Our main service is an online home for git repositories and can also be used to manage build tests, bugs, support, etc.

<http://kanban.e-cam2020.eu>

A workflow management tool that links into GitLab

<http://etherpad.e-cam2020.eu>

A web-based collaborative real-time editor, allowing authors to simultaneously edit a text document. We use it for minutes and live notes in workshops, but it is freely available.

<http://sharelatex.e-cam2020.eu>

An online LaTeX editor that allows real-time collaboration and online compiling of projects to PDF format. In comparison to other LaTeX editors, ShareLaTeX is a server-based application, which is accessed through a web browser.

<http://redmine.e-cam2020.eu>

A web-based project management and issue tracking tool. It allows users to manage multiple projects and associated subprojects. It features per project wikis and forums, time tracking, and flexible role based access control.

DELIVERABLES TO DATE



Six deliverables have now been submitted to the Commission on schedule. You can access these deliverables on the E-CAM redmine site and they are also available on the E-CAM website.

Deliverables 11.0 and 4.1 were re-submitted upon request from E-CAM's reviewers on 30th September 2016.

In order to ensure deliverable quality in the future we will have an internal peer review process. The review of a deliverable should commence 6 weeks prior to submission. Each deliverable should be reviewed by at least one member of the E-CAM consortium not directly involved in the deliverable creation process (where possible). The reviewer should be nominated at a suitable time ahead of the 6-week review. There will also be a responsible author assigned to coordinate the deliverable production and others named as responsible for the deliverable should work together in its realisation from an early stage.

The deliverable production schedule is as follows (D-day = last day of the due month):

D-day – 6 weeks: advance information to authors and internal reviewer(s)

D-day – 19 working days: version for internal review made available via ShareLaTeX

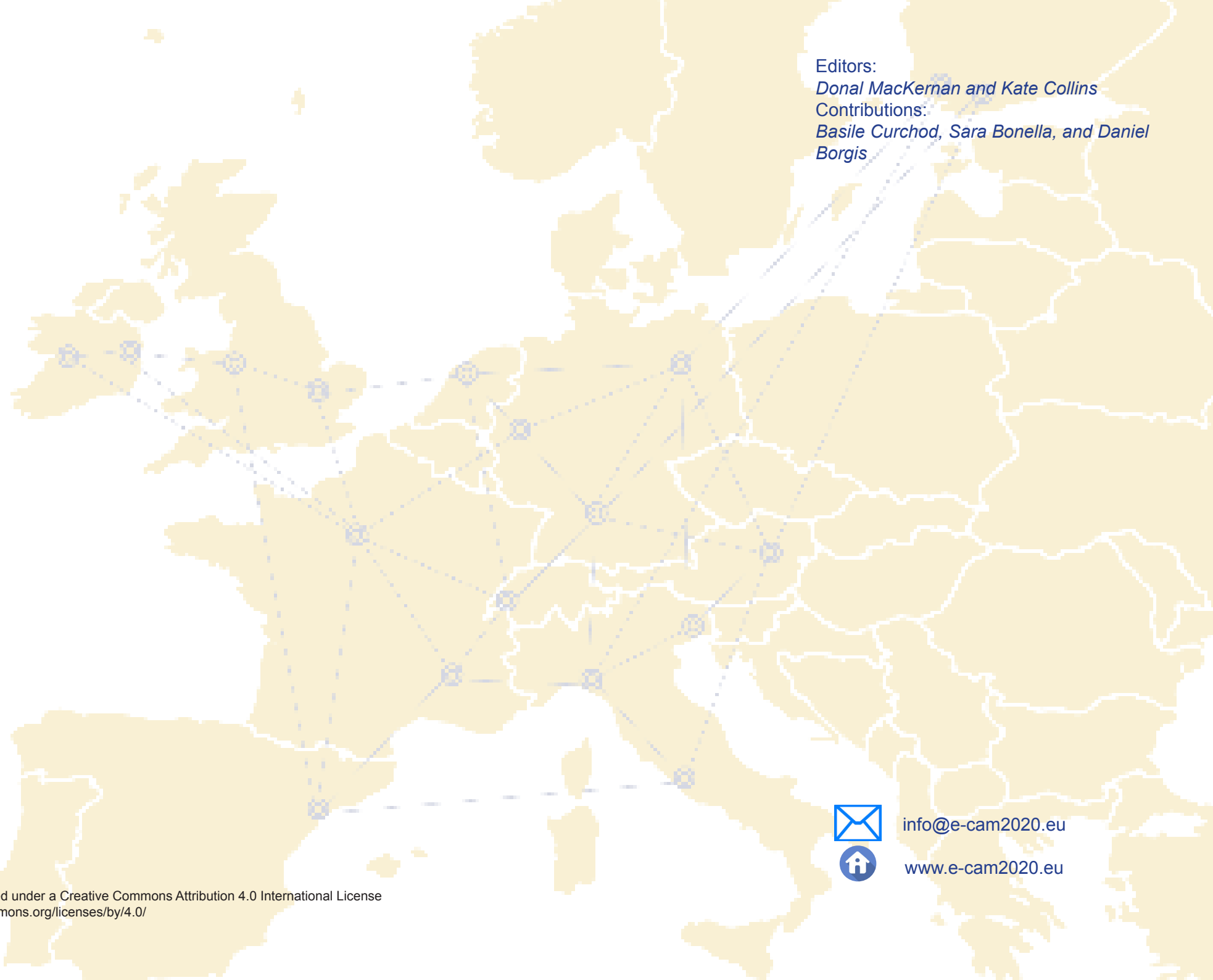
D-day – 14 working days: internal review completed

D-day – 9 working days: final version for approval by WP leader

D-day – 4 working day: request for approval by EB

D-day: Deliverables approved by EB and submitted to EC by project coordinator

Editors:
Donal MacKernan and Kate Collins
Contributions:
*Basile Curchod, Sara Bonella, and Daniel
Borgis*



info@e-cam2020.eu



www.e-cam2020.eu