Dissemination Report

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E-CAM
The European Centre of Excellence for
Software, Training and Consultancy
in Simulation and Modelling

Funded by the European Union under grant agreement 676531

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***Disclaimer**:This deliverable has been prepared by the responsible Work Package of the Project in accordance with the Consortium Agreement and the Grant Agreement. It solely reflects the opinion of the parties to such agreements on a collective basis in the context of the Project and to the extent foreseen in such agreements.*

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Contents

List of Figures

Executive Summary

The objective of the present deliverable is to report on the dissemination activities of E-CAM during the last 4 quarters regarding (a) the generation and updating of a Wiki (or equivalent) describing E-CAM's activities and, (b) E-CAM newsletters; published in previous 4 quarters, which are downloadable at the E-CAM website. The pdf version of this report includes extensive use of hyper referencing to online items, and are visible as blue clickable text.

The primary access point to E-CAM is its website E-CAM. It is rendered using WordPress. The home page includes 4 primary button links on how to:

- attend a workshop;
- become a partner;
- access the E-CAM software library;
- ask a technical question.

It's main menu bar has links for more detailed material.

General information is at the webpage about E-CAM which includes links to the 4 E-CAM scientific workpackages, brief descriptions of the E-CAM software repository, and upcoming and past E-CAM Events

Four issues of the E-CAM newsletter have been published in this reporting period. Each newsletter typically includes a list of upcoming events, an editorial or commentary on an important scientific/technical/industrial topic, a list of deliverables published in the last quarter, brief reports on E-CAM events in the last quarter, and recent news. That said, the format is not rigid, and additional items are added on occasion.

1 Introduction

This deliverable describes the E-CAM online documentation and the newsletters published in the first four quarters. The intended readers of this material include: members of E-CAM, industrial partners, and the wider simulation community.

The technical documentation of E-CAM is created and edited via a wiki[2] process using publicly accessible repositories stored on the E-CAM GitLab service. Additions to this repository can be made by anyone via *Merge Requests*[3]. Each individual modification of the repository automatically causes the associated documentation on ReadTheDocs.org to be rebuilt (this is described on our Software Repositories webpage). The use of *Merge Requests* allows E-CAM to implement a quality-control mechanism on contributed content.

The public face of E-CAM is the E-CAM primary landing website. The website is based on the WordPress blogging platform. This again allows for registered users to create editable content, a feature we plan to leverage more as the project matures.

2 E-CAM Online Documentation

The primary access point to E-CAM is the E-CAM project website seen in Fig.1. The home page includes 4 primary button links on how to:

- attend a workshop;
- become a partner;
- access the E-CAM software library;
- ask a technical question.

It's main menu bar has links for more detailed material (ABOUT US, EVENTS, E-CAM SOFTWARE REPOSITORIES, RESOURCES, CONTACT US and NEWSLETTER). General information is at the webpage about E-CAM which includes

Figure 1: E-CAM home page

[2] A website or database developed collaboratively by a community of users, allowing any user to add and edit content.

[3] Merge or pull requests are created in a git management application and ask an assigned person to merge two branches. Tools such as GitHub and Bitbucket choose the name pull request since the first manual action would be to pull the feature branch. Tools such as GitLab and Gitorious choose the name merge request since that is the final action that is requested of the assignee.

links to the 4 E-CAM scientific workpackages: Classical Molecular Dynamics; Electronic Structure; Quantum Dynamics; and, Meso- and Multi-Scale Modelling. The website also includes brief descriptions of the E-CAM software repository, and upcoming and past E-CAM training opportunities/workshops/events. Also included are links to the other H2020 Centres of Excellence. The About Us menu item contains a dropdown list with links to the history of E-CAM, the E-CAM personnel, published E-CAM deliverables, and current vacancies.

The E-CAM software repository is becoming one of the principle access points for users wishing to interact with E-CAM. There they are encouraged to download and upload software, through a structured scheme of quality control and what is effectively a support infrastructure. This is facilitated through an extensive set of E-CAM services Redmine, Etherpad, SharedLatex, and in particular Gitlab.

E-CAM also uses as much as possible community software development training - and has a detailed training page to this end.

3 E-CAM Newsletters

Four issues of the E-CAM newsletter have been published in this reporting period. Each newsletter typically includes a list of upcoming events, an editorial or commentary on an important scientific/technical/industrial topic, a list of deliverables published in the last quarter, brief reports on E-CAM events in the last quarter, and recent news. That said, the format is not rigid, and additional items are added on occasion. Tne newsletter is distributed to individuals on the E-CAM mailing lists (including all scientific members of the E-CAM consortium, industrial partners, and members of the public who have subscribed), and through a newsletter page on the E-CAM website.

3.1 Newsletter Issue1

The European Centre of Excellence for Software, Training and Consultancy in Simulation and Modelling

Supporting HPC simulation in industry and academia

E-CAM Newsletter Issue 1, January 2016

Funded by the European Union

Contents

E-CAM Calendar of Events

	JUNE 2016	
TBC	State of the Art Workshop: Electronic Structure	Daresbury
TBC	ESDW: Trajectory Sampling	Vienna
	JULY 2016	
TBC	ESDW: Quantum Mechanics and Electronic Structure	Paris
	AUGUST 2016	
29 Aug -2 Sept	State of the Art Workshop: Reaction Coordinates from Molecular Trajectories	Leiden
	SEPTEMBER 2016	
7-9 Sept	Scoping Workshop: Industry Partnerships	Mainz
	October 2016	
TBC	ESDW: Wannier Functions	London
	November 2016	
7-9 Nov	2nd General Assembly	Paris

Editors: Kate Collins & Dónal Mac Kernan Main Contributors: Luke Dury; Damien English Minister for Skills, Research and Innovation. Includes edited excerpts from recent topical publications by members of the E-CAM consortium and their collaborators.

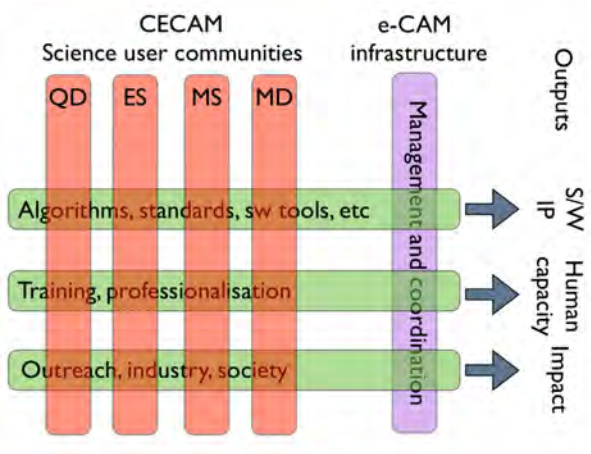
1 E-CAM in a nutshell

Luke Drury E-CAM Chair, University College Dublin & Dublin Institute for Advanced Studies, email: ld@cp.dias.ie

The E-CAM centre of excellence is based around the experience and scientific community of the extended CECAM family, established over more than four decades, as well as the computational and hardware expertise of the European partnership PRACE. Since its founding in 1969 CECAM has been at the forefront of promoting computational simulation as a powerful research tool for understanding and predicting the properties of materials, including biological systems, both at European and international level. E-CAM in partnership with PRACE and the other centres of excellence will now build on and broaden this by adding a strong infrastructural element as part of the European Union's ambitions for HPC under Horizon 2020.

At the scientific level E-CAM has chosen to prioritise four broad areas of science that are central to the interests of CECAM. These vertical scientific pillars are electronic structure calculations, classical molecular dynamics, quantum dynamics, and meso-scale and multi-scale modelling; in addition to covering most of the scientific interests of the extended CECAM community these areas were chosen because they are also of considerable interest to industrial researchers. At the institutional level E-CAM takes advantage of the distributed nodal structure of CECAM and brings together 18 institutions with a good geographic distribution across Europe including three PRACE centres. It already has twelve industrial partners and aims to significantly increase this number over the life of the project as part of its road map to long-term sustainability.

E-CAM complements the scientific focus of CECAM by emphasising three transversal activities that cut across the various scientific fields represented in CECAM and provide essential supports for the work of CECAM and PRACE (and are thus infrastructural in character). These are, first, the provision of an expert consultancy service to industry and the involvement of industrial scientists and partners in the activities of E-CAM. Cutting edge techniques and methods used in academic computational science currently take too long to transfer to industry, and conversely, interesting and significant problems and techniques thrown up by industrial research are not efficiently communicated back to the world of academic research. E-CAM will address this by building communication channels between these two worlds at both personal and at institutional level. This is a key defining characteristic of E-CAM; it is firmly industry-facing (including both SMEs and multi-nationals) and is determined to break down, or at least lower, the barriers between academic and industrial research in its areas of science. Just as the distinction between basic and applied research is at root a false dichotomy, so too is that between industrial and academic research; ultimately what matters is good and interesting science wherever it is done and excellence can be found outside the pale of academia.



The second transversal activity of E-CAM focuses on the need for new and improved algorithms and code modules. There is growing recognition that Moore's law is beginning to break down and that we can no longer expect newer and faster processors to improve the performance of our old legacy codes. Recent advances in computational power depend on either massive parallelism, or specialist hardware accelerators, or both; this means that the old legacy codes need to be rewritten to exploit these possibilities and in many cases that totally new algorithms have to be implemented. E-CAM will do this in collaboration with the other centres of excellence and the European partnership for supercomputing PRACE. In many ways it is not just a question of new software, but of finding new and more efficient ways to produce robust and well documented software that is easily ported and adapted for new challenges. At present people developing new codes waste too much time on routine aspects replicating what has been done before. Frameworks, tools and standards need to be developed to allow better use of the creativity of programmers and the extraordinary success of many free-software projects in using distributed networks of volunteer programmers needs to be replicated in the sphere of scientific software. This also throws up the difficult question important for the long-term health of the field of how the work done by scientific programmers should be adequately recognised and rewarded by career progression; we have all seen good students careers blighted by writing code and not scientific papers.

The same applies to the question of gender stereotyping and implicit biases. That said, the primary output of this activity will be the online E-CAM repository of tested and robust code modules, snippets, wrappers and tests that support modern simulation science across a range of platforms. These will be developed in association with PRACE and other FET projects to enable efficient exploitation of the current and next generation of European supercomputer facilities.

The third transversal activity is associated with the broad issue of training, mentoring and continuing professional development of the European pool of human capital available in support of computational simulation. This is crucial. The health of computational science depends on a steady influx of new people into the field and on a continuing effort to maintain the skills of its established practitioners. E-CAM recognizes this and will devote significant effort to training and up-skilling workshops. An important aspect of these workshops is that they will address a broad audience of both academic and industrial scientists and they will combine more traditional training with practical hands-on training. In particular extensive use will be made of "extended software development workshops" which will have a two-fold purpose. On the one hand they will be the primary means of generating the software modules that ultimately constitute the E-CAM repository. On the other they will have an explicit training dimension in that participants will gain direct experience of using modern software engineering techniques and open-source development tools to generate community code.

These three actions should not be seen as disjointed activities. As we have seen the extended software development workshops address both the training and the algorithmic innovation transversal themes. Equally the software repository, and especially the expertise to use it, will be the key to the success of the industrial consultancy action. And ultimately it all depends on having a good pool of human capital to draw on. Nor will E-CAM operate in a vacuum. Just as the three E-CAM actions enhance and complement each other, so too E-CAM will exploit synergies and overlaps with other centres of excellence and HPC initiatives.

2 E-CAM Kick-off Meeting

The kick-off meeting and first General Assembly was held in the historic meeting room of the Royal Irish Academy. In welcoming participants Luke Drury gave a short account of the history of the Academy from its foundation in 1785 and mentioned in particular its most distinguished scientific member, Sir William Rowan Hamilton. He then called on Christoph Dellago, President of the CECAM council to say a few words on its behalf, noting that he was seated in the chair once used by Hamilton when presiding over meetings of the Academy. Christoph Dellago replied by welcoming the establishment of E-CAM as an important development for CECAM. This was followed by a series of talks and open discussions including: the implementation of E-CAM by Dominic Tildesley Director of CECAM; consultancy moderated by Mike Payne, University of Cambridge; algorithm and software development moderated by Godehard Sutmann, Forschungszentrum Jülich; and mentoring and training moderated by Michael Lysaght, ICHEC. A pause from disussions was taken to receive an address by Minister Damien English.

2.1 Speech by Minister Damien English

Minister for Skills, Research and Innovation Damien English T.D. speaking on the launch of E-CAM

Introduction

Good afternoon to you all, I am very pleased to have the opportunity to speak to you today on the occasion of the E-CAM kick-off and first meeting of the General Assembly. I would like to thank Prof. Padraig Dunne, Head of the School of Physics in UCD and his colleagues for inviting me here today and to the Royal Irish Academy for hosting this event. I would also like to take the opportunity to welcome the E-CAM consortia members that have travelled from across Europe to be here for this inaugural meeting and to congratulate all involved in this successful Horizon 2020 project.

E-CAM Administrator Kate Collins and E-CAM consortium members and friends after the address by Minister English.

Horizon 2020

As some of you know Ireland performed well in FP7, the programme which preceded Horizon 2020. We had set ourselves a target of €600 Million and Irish researchers in academia and industry were awarded €625 Million in funding in FP7, significantly exceeding our target. Horizon 2020 is a core part of the Europe 2020 strategy, designed to deliver on priorities set out in the Innovation Union and the European Research Area. It is responding to the economic crisis to invest in future jobs and growth, addressing people's concerns about their livelihoods, safety and environment and strengthening the EU's global position in research, innovation and technology. Horizon 2020 focuses on 3 key areas – excellent science, industrial leadership and societal challenges. This approach sees a focus on innovation across the entire continuum of research from basic science moving to applied science into commercialisation via competitive industries in the interest of addressing the great societal challenges of our time. Most especially, in these times of economic challenge and austerity, the conversion of scientific effort into real and sustainable jobs for citizens is a key priority. Ireland aims to win €1.25 Billion over the lifetime of Horizon 2020. This is a doubling of the target we had under FP7. While ambitious, I feel this is an achievable target given the growing strength of our national research system which has now, in so many spheres, achieved a world class standard. E-CAM is an excellent example of success to date. We now have full year data for 2014 and we can see some very encouraging results. Irish researchers and companies have secured funding in excess of €127 million. We have surpassed our target for 2014 by 27%. Stiff competition has always existed for funding under EU framework programmes. In Horizon 2020 it is particularly intense. Our success to date is therefore a real testament to the quality of the proposals coming from Ireland. Successful participation in Horizon 2020 is valuable at any level. But where the leading role is taken on by Ireland as is the case with E-CAM, greater rewards are achieved, on all dimensions.

President of the CECAM council Christoph Dellago with Minister Damien English

E-CAM Project Success

I would like to congratulate the E-CAM consortium on its success in securing 4,8M€ of the 140M€ recently allocated by the European Union to support high performance computing applications, and in particular of course the Irish organisations involved. It is a source of pride to me that Ireland has been trusted by you to lead this consortium and I would like to congratulate all those involved, in particular Dr Dónal MacKernan, Director of the Irish node of CECAM, Professor J-C Desplat, Director of the Irish Centre for High-End Computing, and Professor Luke Drury of the Dublin Institute for Advanced Studies. As I have mentioned the government has set a very ambitious target for Irish participation in Horizon 2020 and I am delighted to see this excellent project as a great example of Irish and European success.

Deputy Director of CECAM Sara Bonella, Carlo Piereloni (University of Rome) and Carsten Harmann (Free University of Berlin)

This next generation supercomputing technologies and applications are very important as tens of thousands of researchers across Europe already use the power of massively parallel supercomputers to solve scientific problems that cannot be answered in the laboratory. Super Computing is increasingly a key tool of researchers in all fields, from genomics and ecology to medicine, engineering and education. It, and more generally large scale distributed computing, is now central to much of modern commerce and social interaction. This will only increase with the development of the "Internet of things", involving vast numbers of interacting sensors combined with GPS technology to build new capabilities. But there are obstacles to the realisation of this opportunity.

Director of IDRIS (the Super Computer and PRACE Centre) of the French CNRS Denis Girou with Minister Damien English

Many researchers in academia and industry still do not have easy access, or the skills needed to exploit Super Computers or for that matter Cloud Computing. Moreover, the ability to extract meaning from vast amounts of data, whether for scientific purposes or for commerce and societal needs, remains a challenge.

Software plays a crucial role in theefficiency of super computers, the science to be simulated on them, and the accessibility of such machines to a vastly larger potential community of users. Thus investment in algorithm and software development is essential and integral to any large-scale computation program. It is also true that computer scientists and mathematicians are only beginning to understand how to optimally use the types of highly parallel designs that computer architects are exploring.

Godehard Suttman from the German National Super Computer & PRACE Centre at Forschuncentrum Jülich with Minister Damien English

E-CAM I am told will 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 through three complementary instruments:

1. through the development, and dissemination of software targeted at end-user needs;
2. through advanced training of current and future academic and industrial researchers to exploit this software and associated underpinning software standards; and,
3. through multidisciplinary, applied consultancy to support industrial end-users (both large multinationals and SMEs) in their use of simulation and modelling.

Daniel Borgis from the Maison de Simulation with Minister Damien English

It will do this directly through 18 institutions across Europe including four national super computer centres, and industrial associates (including multi-nationals and SME's) through some 30 postdoctoral researchers, programmers and their laboratories through an initial award of nearly 5 million euro. The project will also involve the CECAM community of thousands of scientists and engineers and young researchers, and the wider community of researchers in the many tens of thousands across Europe and further afield.

Michael Lysaght from ICHEC the Irish National Super Computer & PRACE Centre with Minister Damien English

New Science and Innovation strategy

In Ireland we are currently developing our new Strategy for Science, Technology Innovation as we move into a new phase of economic growth and societal development. It is now time for us to advance fresh strategic ideas that will distinguish Ireland globally through its ability to make research work to maximum effect for the country.

E-CAM a moment of reverie and multiple discussions

In Ireland, we are proud of our achievements to date. In the past decade and a half we have made significant progress in our national innovation system which started from a very low base by international comparisons. We have successfully built up research capacity and now we have a significant reputation for research excellence along with an increasing base of RD active enterprises. Nonetheless, we now need to build on this progress made in developing Ireland's research and innovation system. As economic recovery takes hold this is not the time to stand still. Scientific and technological progress advance at rapid rates, and we are competing in an ever-growing competitive global environment. Supporting effective research that produces outputs of maximum impact for Ireland's economy and society is our goal but we now have an opportunity. The new Strategy will seek to articulate a broader and longer term vision for Ireland's Research and Innovation system and identify its defining characteristics. It will also set out strategic goals and targets, based on a robust evidence base, our own vision and an examination of international trends and good practice. We plan to bring it to fruition this year, and work is well underway to this end.

E-Cam Chair Luke Drury, Giovanni Ciccotti from the University of Rome, UCD and the Free University of Berlin with Minister Damien English

Today's meeting and the E-CAM project embody many of the strategic priorities we will be setting out in our new Strategy including: Increased collaboration between academia and industry; and between academic and research performing institutions; International collaboration, to maximise return on investment and to optimise success under EU Framework programmes; and Facilitating the translation of knowledge and the transfer of technology into jobs E-CAM with its focus on the development of expert computational science skills, support for cutting-edge research, and consultancy services to innovative industries is perfectly aligned with my portfolio and clearly has the potential to be of significant importance in the national, European and global stage.

Minister Damien English with E-CAM Chair Luke Drury, and E-CAM technical manager and Director of CECAM Dominic Tildesley

It remains for me to congratulate Dr Dónal MacKernan, Professor J-C Desplat, and Professor Luke Drury and the other consortia members for winning support for this very worthwhile project from Horizon 2020 and to wish you all every success in in bringing this vision to a reality. *Go n'éirí an bóthair libh* – which for those of you who not know Irish literally means "May the road rise with you", loosely translated as "May you rise to the challenge".

E-CAM Ignacio Pagonabarraga from the University of Barcelona, Peter Bolhuis from the University of Amsterdam, and Burkhard Dünweg from the Max Planck Soceity Polymer Research Centre in Mainz.

2.2 Actions and General Assembly

The first E-CAM General Assembly (GA) took place on 20th October 2015 at the Royal Irish Academy in Dublin, Ireland. All 18 membrs of the consortium had voting representatives present and therefore the meeting was quorate. The GA, by a unanimous vote, approved the appointment of the Executive Board (EB) consisting of Luke

Drury, Dominic Tildesley, project administrator (Kate Collins), and the software manager (Alan O'Cais) with an industrial cooption. The EB is responsible for appointing the three management support teams specified in the consortium agreement: software group, human capital group, and industry group. The GA also had a long discussion over the issue of software licensing where it was concluded that, pending further analysis and discussion, the GPL, LGPL, and FreeBSD licences could be used. This was approved by 17 votes with UCD abstaining. Under AOB the technical manager asked, and got approval by unanimous vote, that the GA agree that travel expenses of representatives attending the GA be chargeable to the project. The next meeting of the GA will take place 7-9 November 2015 and will be hosted by the *Maison de la Simulation*.

E-CAM engrossed in conversation, only Carlo Pierleoni (University of Rome) is looking at the photographer.

3 E-CAM Management Appointments

Two key full-time management positions of the E-CAM CoE are the project Administrator (based in NUID UCD), and the software manager (based at Forschuncentrum Jülich) have been filled. The E-CAM project Administrator, Dr. Kate Collins leads the administrative management activities of E-CAM and sits on the Executive Board reporting to the E-CAM chair; participates in the General Assembly, the Human Capital Group and the Industry Group. She is responsible for reporting to the European Commission on administrative issues. She is also responsible for coordination and dissemination activities as described in several of the E-CAM work packages. The Software Manager, Dr. Alan O'Cais leads the software development in the project, supporting the technical manager with specialist knowledge of software development. Alan sits on the Executive Board reporting to the E-CAM chair with an additional line to the Technical manager. He is responsible for setting up and participating in the Software Management Group. Short biographies of each post-holder follow.

3.1 E-CAM Administrator

Kate Collins is an accomplished project manager, researcher, administrator and trainer. She has worked across the public, private and not for profit sectors over the past 10 years. She has previously worked in roles such as managing editor of the Journal of Agricultural Education and Extension at Wageningen University in the Netherlands and operations manager for Worklink Partners Ltd, a not for profit company that she helped to setup in Ireland. She joined UCD in 2012, and until recently acted as PhD Training Coordinator for the PhD Simulation Science at UCD. Kate has also lectured in Scientific Writing both in the Netherlands and in Ireland. Kate holds a PhD from the Dublin Institute of Technology (DIT) in the area of workplace learning, a MSc Marketing also from DIT, and a BA from University College Dublin.

Mikko Alava from University of Aalto Finland, enjoying a provocation of Mike Payne from the University of Cambridge

3.2 E-CAM Software Manager

Dr. Alan O'Cais has been active in the field of computational research and high performance computing since receiving his bachelors degree in Theoretical Physics from Trinity College Dublin in 2001. He received a Masters Degree in High Performance Computing in 2002 and a PhD in Lattice Quantum Chromodynamics in 2005. He has held research positions at Trinity College and the University of Adelaide. In 2008 he joined the Cyprus Institute as Scientific Coordinator of the Computation-based Science and Technology Research Centre (CaSToRC) and has worked at the Jülich Supercomputing Centre since 2010 within the Application Support division. Until 2015, he was primarily focussed within the LinkSCEEM-2 project helping to develop a Virtual Research Community in Computational Science in the Eastern Mediterranean region. He has been an invited speaker for "Performance Analysis and Optimisation" lectures with PRACE Advanced Training Courses on multiple occasions and currently manages the user software and application environment on the multi-PFlop JURECA hybrid cluster system at JSC.

4 E-CAM Science View

Dónal Mac Kernan

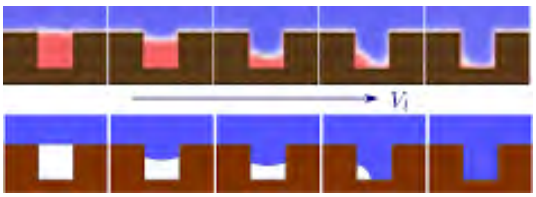
E-CAM Scientist at University College Dublin, email: Donal.MacKernan@ucd.ie

E-CAM laboratories have interests across its 4 principle scientific platform areas of molecular simulation, electronic structure, quantum dynamics and meso-scale/multi-scale simulation. In this first issue, as an indication of the capabilities of E-CAM partners just before its launch we have chosen to report only on published work in 2015-2014 in molecular simulation and meso-scale/multi-scale simulation, with a strong emphasis on results which have a reasonable direct bearing on potential industry applications, or are so general in scope that they need to be highlighted. Below is an overview, followed by longer summaries of each work. In the next issue, the focus will instead by on electronic structure, quantum dynamics, and algorithms/coding methods.

Nucleation, including crystallization has been a central topic of interest in simulation, with applications such as purification and processing in industries as disparate as advanced materials, pharmaceuticals and food. At times many have been perplexed by the apparent discrepancies in estimates of reaction rate constants between experimentalists and simulation. In a beautiful and profound molecular simulation study of a comparatively simple model, Jungblut at al have shown how changes in the structure of small crystalline seeds in undecooled melts can lead to widely different rate constants - and indeed counter-intuitive results, see 4.1 for a summary.

Continuing the theme of using simple models to investigate profound problems, Goujon et al examine, and resolve the discrepancy between experiment and simulation of liquid argon in the presence of interfaces, by demonstrating that the addition of three body interactions responsible for polarization is critically required, in addition to proper treatment of Van der Waals long range coupling. The importance of this result goes far beyond simply the case of argon. That a comparatively simple to compute correction could resolve such a serious discrepancy is particularly useful see 4.2 for a summary.

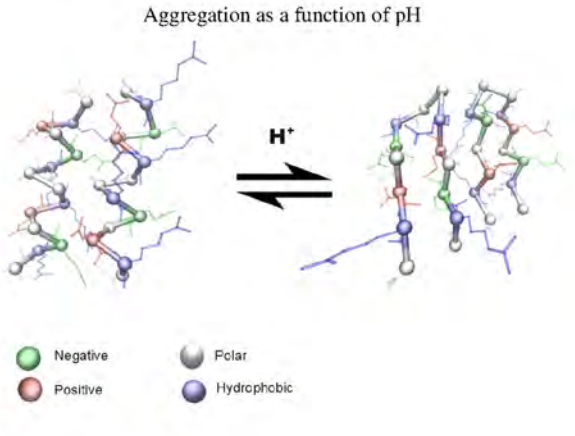
The possibility of designing anti-fouling surfaces that self-clean and minimise drag under flow conditions has a variety of industrial applications. Hydrophobic materials can be turned into superhydrophobic ones if their surfaces are decorated with micro- or nano- corrugations, and gives rise to a phenomenon, known as “lotus effect” from the properties and structure of lotus leaves. What is the effect of the shape of the surface corrugation and its size on the mechanism of stability of such superhydrophobic states is elucidated in 4.3 using molecular dynamics and rare-event based methods.



Exploring loss of superhyrophobicity: comparison of continuum and molecular simulation predictions

Biological and soft matter systems are characterized by the existence of processes with many different length and time scales. computationally treating very large systems with full molecular detail is not possible, and one needs to deal with simplified, or coarse-grained versions of the system. However, in any coarse-grained model some atomic/molecular detail is lost, which can be problematic if crucial mechanisms occurring at an atomistic or molecular level are missing. In some cases, the need for atomistic detail is confined in small regions of space, and there is hope that a hybrid scheme coupling an atomistic with coarse-grained descriptions may be a successful approach. A variety of methods have been developed over the years, many of which despite their success had practical and conceptual difficulties, including for instance, lack of energy conservation. In the publication highlighted in 4.4 the authors derive a rigorous hybrid coarse grained atomistic method termed Hamiltonian Adaptive Resolution Scheme (H-AdResS) which can be used for all of the standard ensembles of statistical mechanics.

Continuing with the coarse graining theme, a series of papers have been recently published that seek either to model very large systems, or perhaps even more ambitiously, design through simulation new systems, that can be subsequently built in the laboratory through appropriate experimental techniques. In 4.5 coarse graining is used to investigate the mechanisms involved when nanoparticles (NP) pass through cellular membranes - which is of great interest not only to nano-toxicology but also more widely, for instance in the context of complex fluids interacting with inorganic surfaces. In a similar vein, how coarse graining methods can be extended to allow simulation of constant pH conditions is highlighted 4.6 where is is used to investigate aggregation of peptides.



For many practical applications in electronics, photo-

voltaics, and biomimetic material synthesis, ordered mono- and bilayers are often needed. An approach based on coarse graining providing a novel and simple way to tune via external parameters the ordering of heterogeneously charged colloids into quasi two-dimensional structures is outlined in 4.7. Such tuning can be implemented through subtle variations of the relative charge of the system components, emerging via pH modification, and give rise to reversible changes either from extended aggregates to a monomeric phase or from triangular to square domains.

Tribology, literally, the study of rubbing, has been studied at a formal level at least as far back as Leonardo Da Vinci in work on friction. Controlling tribology interactions, including friction, wear, and adhesion, is a topic of considerable industrial importance. From antiquity if not before, lubricants have been used to reduce the detrimental effects of friction and wear. In the publication summarized in 4.8, the authors, through a model employing molecular dynamics, have focused on the properties of nematic liquid crystals (LCs) as a particularly interesting lubricant. LC systems can be characterized by the presence or absence of positional and/or orientational order of the elongated molecules, which is controllable by tuning the temperature or applying external electric or magnetic fields.

Self organization in nature exhibited, for example, in the flocking of birds, bacteria colonies tissue repair, and colloids, has fascinated many. Breakthroughs in particle synthesis have enabled the fabrication of artificial colloidal micro-swimmers that show a high potential for application, in, for instance, bio-sensing and drug delivery. In the publication summarized in 4.9 the authors show that active matter can serve as a medium to generate unexpectedly large effective interactions between large immersed objects to direct their motion and assembly, and find surprising results.

Exploring the properties of very large biological systems including explicit water is immensely difficult and indeed a major limitation on the size of system that can be simulated. Classical density functional theory is one approach to try to resolve this difficulty, but until now has had considerable problems of its own, particularly regarding accuracy. In the publication outlined in 4.10 not only are corrections to classical functional theory are derived, they are used to find that the hydration free-energies computed for a dataset of 500 organic compounds are of similar quality as those obtained from molecular dynamics free-energy perturbation simulations, with a reduced computational cost of two to three orders of magnitude.

Beauty is said to be in the eyes of the beholder, and when it comes to the notion of what can be abstracted to be a particle - this beauty can be found at many scales. In the provocative publication summarized in 4.11, the authors explore the phenomena of clogging, with examples ranging from the common experience that the pouring of salt from a salt-cellar frequently requires shaking so as to break the clogging arches, to flow interruptions in industrial conduits and silos, and at smaller scales, to provoke embolization of blood vessels in order to shrink a tumour, or at the nano-scale when electrons on the liquid helium surface pass through nano-constrictions. Despite the extraordinary range of scales, the authors show that clogging in several disparate systems is amenable to a unified treatment, including a model colloidal suspension. simulated using the Lattice Boltzmann method.

4.1 On the reaction coordinate for seeded crystallisation

Jungblut, Swetlana, and Christoph Dellago*. Molecular Physics, **113** (2015) 2735-2741.
* E-CAM Scientist at University of Vienna, email: christoph.dellago@univie.ac.at

The crystallisation of under-cooled liquids is a widely studied topic with many technological implications. Classical nucleation theory posits that a small crystalline nucleus forms within an under-cooled liquid. Due to the creation of a crystal–liquid interface surrounding the nucleus, this process is free-energetically uphill in its initial stages. Driven by thermal fluctuations, the crystalline nucleus may nevertheless grow until it reaches a critical size after which further growth is thermodynamically favourable eventually leading to the crystallisation of the entire system. While the basic perspective provided by the classical nucleation theory is essentially correct, its details are still subject of current discussions.

By introducing small seeds with various structures into the under-cooled liquid, one can modify the crystallisation mechanism by favouring the nucleation of particular arrangements and inhibiting the formation of others. Several computer simulation studies agree that the structure of the crystalline clusters formed in the course of the transition is not uniform and reorganises as the reaction proceeds. In LJ crystallisation, the body-centred cubic (bcc) structure is formed first and subsequently transforms into the face-centred cubic (fcc) structure, such that the crystalline clusters have, on average, an fcc-structured core and a bcc-structured surface. While fcc is the thermodynamically stable phase in bulk LJ crystals and the bcc phase is only metastable, the initial formation of bcc crystals is favoured kinetically by a lower free energy barrier.

In earlier studies, the same authors showed that the effect of the seed is related to its structure in the sense that the commensurability with the bulk equilibrium structure is one of the factors which influence the crystallisation rate.

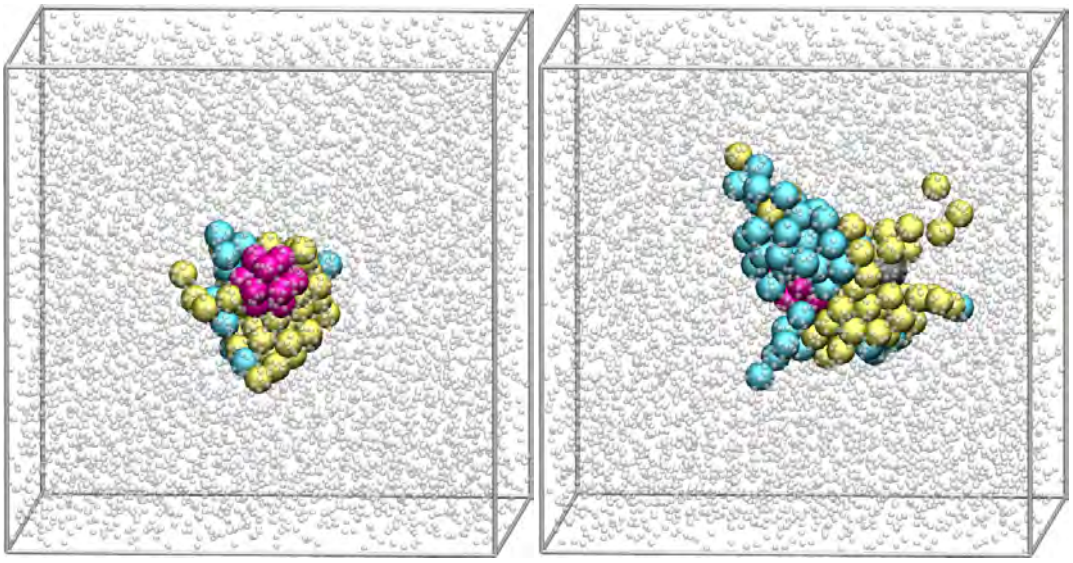


Figure 1: *Examples of seeds having body-centred cubic and face-centred cubic structure respectively.*

In particular, they found that the seeds with a regular fcc structure produced the largest increase of the reaction rate. This tendency was expected, but the increase of the reaction rate by several orders of magnitude was rather surprising considering the size of the seeds.

In the publication higlighted here, the authors study seeded crystallisation at a slightly larger under-cooling and found that, in this case, the largest increase of the crystallisation rate is obtained with bcc rather than fcc seeds. Their result, as they explain, is counter-intuitive, because in the bulk the bcc structure is only metastable. As in the case of homogeneous crystallisation, the analysis of recurrence times has revealed that the size of the largest crystalline nucleus evolves in a non-Markovian way, pointing to the necessity to include additional collective variables such as structure and shape into the description of the nucleation mechanism.

4.2 The gas-liquid surface tension of argon: A reconciliation between experiment and simulation

Florent Goujon, Patrice Malfreyt, and Dominic J. Tildesley*, J. Chem. Phys. **140** (2014), 244710
∗ E-CAM Technical Manager and CECAM HQ director at EPFL, email: dominic.tildesley@epfl.ch

The success of molecular simulations in the quantitative prediction of thermodynamic properties of bulk liquid and inter-facial systems has been achieved with the use of relatively simple effective potentials which model the van der Waals and electrostatic interactions. In most cases, the simulations use two-body Lennard-Jones site-site potentials and partial charges. These pair potentials have been shown to be successful in reproducing the temperature dependence of the surface tension of various organic liquids,water,and acid gases. Although, the surface tension, γ of the simple Lennard Jones liquid was the first to be studied,the agreement between the simulated surface tension and the experimental results for liquid argon is poor (with typical deviations greater than 20 %.

In the above article, the authors explain that the discrepancy with experiment cannot be attributed to methodological problems such as finite size-effects, long range corrections, and the intrinsic accuracy of different routes to estimating γ. A hint to the origin of the discrepancy can be gleaned from the fact that Argon has a large atomic polarizability, which is such that a the triple induced-dipole potential is likely to make a significant contribution to the surface tension. The authors, to the best of their knowledge, are the first to perform simulations including three-body potentials on argon involving an explicit interface, which allows an accurate calculation of the surface tension. In a very detailed study taking great care to incorporate long range interactions they investigated the performance of various two body potentials, combined with the triple-dipole Axilrod-Teller potential, and succeeded in reproducing the experimental values of the surface tension of Argon within about 3 %.

4.3 Mechanism of the Cassie-Wenzel transition via the atomistic and continuum string methods

Alberto Giacomello, Simone Meloni, Marcus Müller and Carlo Massimo Casciola* J. Chem. Phys. **142** (2015): 104701. ∗ E-CAM Scientist at University of Rome La Sapienza, email: carlomassimo.casciola@uniroma1.it

The possibility of designing anti-fouling surfaces that self-clean and minimise drag under flow conditions has a variety of industrial applications. In fact, hydrophobic materials can be turned into superhydrophobic ones if their surfaces are decorated with micro- or nano- corrugations, and gives rise to a phenomenon, known as the "lotus effect" from the properties and structure of lotus leaves, which results in liquid droplets forming with high contact angles that can reach almost complete de-wetting values. Superhydrophobicity is related to the trapping of gaseous pockets (air and/or vapour) inside surface roughness, which the authors refer to as as the Cassie state. However, superhydrophobicity breaks down as soon as the surface roughness becomes wet in the so-called Wenzel state. In earlier work, the authors established that the Cassie state consists of two metastable states associated with two distinct contact angles, as well as exploring the nature of the free energy barrier associated with the Cassie-Wenzel transition. One of the objectives of the present highlighted publication was to elucidate the effect of the shape of the surface corrugation and its size on the mechanism of the Cassie-Wenzel transition, and on the related free-energy barrier.

4.4 Statistical mechanics of Hamiltonian adaptive resolution simulations

P. Espagnol , R. Delgado-Buscalioni , R. Everaers* , R. Potestio , D. Donadio, and K. Kremer. J. Chem. Physics **142** (2015): 064115. ∗ E-CAM Scientist at ENS Lyon, email: ralf.everaers@ens-lyon.fr

Biological and soft matter systems are characterized by the existence of processes with many different length and time scales. These processes are usually coupled, making their theoretical, experimental, and computer simulation description a daunting task. The functioning of a protein, for example, involves chemical processes at active sites as well as the overall dynamics of the protein and its environment. Crack propagation is another example in which the atomic processes occurring at the crack tip affect crucially the overall elastic behaviour of the sample, and vice-versa. Treating such large systems computationally with full molecular detail is not possible, and one needs to deal with simplified, or coarse-grained versions of the system. By definition, in any coarse-grained model some atomic/molecular detail is lost. In some fortunate cases, the need for atomistic detail is confined in small regions of space as in the examples above, and there is hope that a hybrid scheme coupling all atom (AA) with coarse-grained (CG) descriptions may be a successful approach.

A particular difficulty arises in liquid systems. When a molecule crosses the interface between the AA and CG regions, its interaction with other molecules changes accordingly. The idea of interpolating AA and CG interactions through a hybrid region is not new. However, the force-based Adaptive Resolution Scheme (AdResS) and the potential based adaptive Multi-scale Molecular Dynamics (MMD) suffered various methodological difficulties associated with the conservation of energy. In the present highlighted publication, the authors have resolved many of these vexations through what they have termed a Hamiltonian Adaptive Resolution Scheme (H-AdResS), that they derived on a statistical mechanics basis, and which includes a switching field that allows for a swift interpolation between the truly microscopic Hamiltonian and a CG version of it. Several exact results concerning the local equations of state for the pressure and temperature allow for the formulation of the free energy compensation term in an iterative way. They also showed that under a local equilibrium approximation, valid when the hybrid region is wide, the iterative procedure can be simplified leading to an approximate but very efficient way for the calculation of the free energy compensation term in the Hamiltonian. They have analysed the effect of the width of the transition layer where molecules gradually change their resolution. A significant outcome is that the H-AdResS total free energy compensation is independent on the layer, even for widths of the same order of the molecular diameter. Another very important observation is that the H-AdResS total free energy correction is equal, within error bars, to the free energy difference between both fluids (atomistic and coarse-grained) evaluated from Kirkwood thermodynamic integration. Although more research is required in this direction, this would allow H-AdResS to be used as a flexible tool for estimation of free energy differences in different scenarios.

4.5 Coarse-grained model of adsorption of blood plasma proteins onto nano-particles

Hender Lopez and Vladimir Lobaskin*, J. Chem. Phys. **143** (2015): 243138
* E-CAM Scientist at University College Dublin, email: vladimir.lobaskin@ucd.ie

When uncoated nano-particles (NP) enter a living organism, they are first exposed to biological fluids, which results in a formation of stable or transient NP-biomolecule complexes. For large NPs, the biomolecular coating is referred to as the (protein) corona. The composition and structure of the corona determines the biological reactivity and toxicity of the NPs as well as the NP systemic transport including NP uptake into cells. An additional interest in such interactions is driven by applications of NPs in food, cosmetics, and medicine.

There is still much controversy about the physical picture of protein adsorption on NPs including: disagreement on whether the adsorption is reversible; whether proteins change conformation and preserve their functionality when complexed with certain particle types: whether the corona survives the NP uptake into the cell, etc. While full atomistic simulations of protein on surfaces have already proved useful to advance the understanding of molecular interactions, they are limited to systems composed of one or a few proteins at most, and give information well below the time scales relevant for the formation of the protein corona. This restriction can in principle be overcome using coarse-grained (CG) models. Some CG models to study the kinetics of the protein corona formation have already been proposed,but most lack the level of molecular detail required to study reliably adsorption kinetics.

Lopez and Lobaskin in the above publication report on a a CG model they have developed that allows calculation of adsorption energies of arbitrary globular proteins onto hydrophobic NPs of arbitrary size. Protein molecules are represented by one bead per amino-acid and the nano-particle by a homogeneous sphere that interacts with the amino-acids via a central force that depends on the nano-particle size, while water is treated implicitly. The methodology is used to predict the adsorption energies for six common human blood plasma proteins on hydrophobic charged or neutral nano-particles of different sizes as well as the preferred orientation of the molecules upon adsorption. Their approach allows proteins to be ranked by their binding affinity to the nano-particle, which can be used for predicting the composition of the NP-protein corona. The predicted ranking is in good agreement with known experimental data for protein adsorption on surfaces

4.6 Influence of pH and sequence in peptide aggregation via molecular simulation.

Marta Enciso, Christof Schütte, and Luigi Delle Site*, J. Chem. Phys **143** (2015): 243130.
* E-CAM Scientist at the Free University of Berlin, email luigi.dellesite@fu-berlin.de

Protein aggregation is a ubiquitous event that may happen to any known protein. Aggregation propensities, however, depend on the particularities of protein sequence and structure, as well as on external factors like pH, concentration, ionic strength, to cite a few. Among the latter, pH is of key importance because of its clinical relevance (it has even been suggested as a diagnosis method) and its impact in drug production and synthesis. From a computational point of view, media acidity is also a challenge, as a proper description of the system pH implies instantaneous changes in the protonation states of the involved species. Several simulation strategies have been developed over the last 2 decades. The most relevant drawback of constant-pH atomistic simulations for aggregation studies is their computational cost, which usually makes these models impractical for aggregation purposes. Coarse-grained pH-dependent methods, in contrast, are still competitive and, if a discrete protonation approach is used, do not even have a large impact on computational efficiency. Enciso et al have recently proposed a constant-pH simulation algorithm in combination with a simple but accurate coarse-grained force field wherein each amino acid of a peptide is described as a bead centre, placed at the α-carbon position, and such that each molecule is embedded in an environment described via an implicit solvent approximation. The system pH is modelled through discrete protonation states, which are allowed to fluctuate during the simulation according to a Monte Carlo scheme, where in each “pH move,” a protonable site is randomly selected and its protonation state is accepted or rejected according to the detailed balance condition, which depends on the “sensitivity” of the specific amino acid towards protonation and on the particular pH value. Overall, this approach allows for an order of magnitude increase in the systems’ size compared with molecular simulation, as well as the exploration of several pH conditions and sequence alternatives within the same study.

The present highlighted publication exploits this methodology to explore the effect of pH and peptide sequence on aggregation in a systematic way, and used realistic systems sizes, i.e., larger than the critical nucleus size. This critical size is a function of the peptide sequence and its length and it is usually set (by both experimental and computational means) to between four and ten polypeptide chains. The authors used twenty-four peptides per simulation box in replica exchange Monte Carlo and kinetic Monte Carlo pH-dependent simulations; which is, apparently, the first time that such a large scale approach has been used to take into account the effect of pH in the aggregation process. They

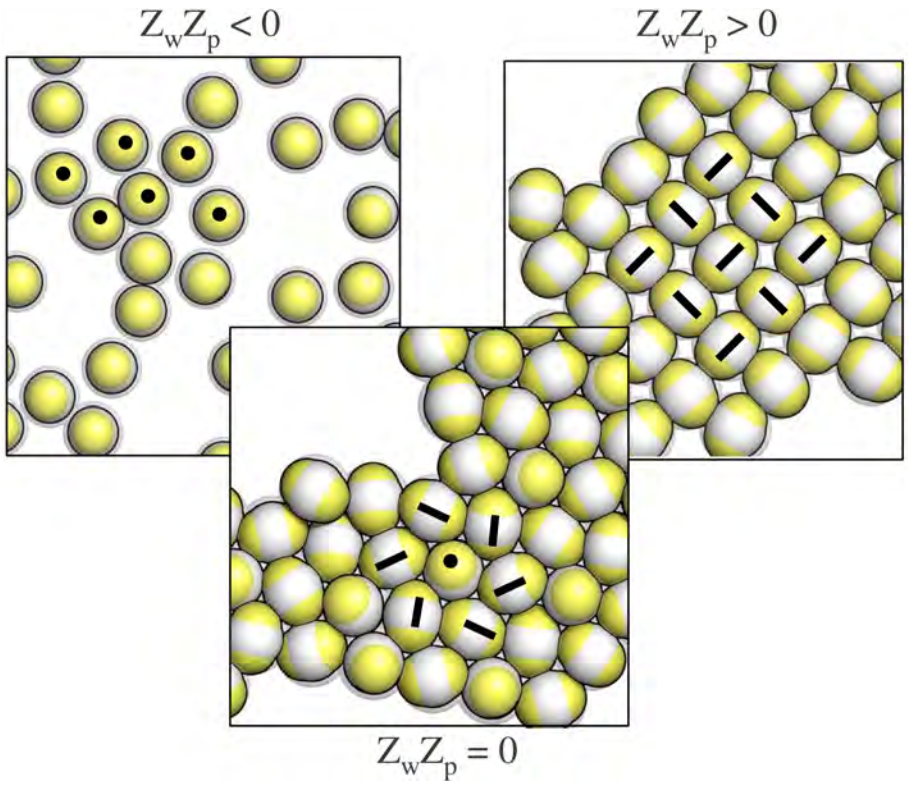
took the de novo sequence KTVIIE as a starting point, designed by de la Paz and co-workers as intrinsically amyloidogenic, and then enlarged simulation study to include other peptide sequences.

4.7 Tunable assembly of heterogeneously charged colloids

Bianchi, Emanuela, Christos N. Likos, and Gerhard Kahl*. Nano Letters **14** (2014): 3412-3418.
∗ E-CAM Scientist at University of Vienna, email: gerhard.kahl@tuwien.ac.at

Colloids, that is systems comprising one substance consisting of insoluble particles suspended in another consisting typically of a fluid, have long been exploited in applications as diverse as food, medicine, rubber production, and increasingly of late, advanced materials. For the latter, the colloidal particles, typically of micron scale but can be indeed far smaller, can have a variety of interesting electronic and optical internal properties. And, via suitable synthesis processes, the interactions between colloidal particles can be easily manipulated to give rise of structurally ordered materials at length scales ranging from nano- to micrometers, through self-assembly, with remarkable properties. Such manipulations can be made at the processing level, allowing the creating of materials with very well defined structural properties.

For many practical applications in electronics, photovoltaics, and biomimetic material synthesis, ordered mono- and bilayers are often needed. In this highlighted publication the authors present a novel and simple way to tune via external parameters the ordering of heterogeneously charged colloids into quasi two-dimensional structures. Upon subtle variations of the relative charge of the system components, emerging via pH modification, reversible changes either from extended aggregates to a monomeric phase or from triangular to square domains are observed. The authors have discovered a novel and until now unexplored route to steer in a reliable and reversible manner the self-assembly of colloidal particles possessing heterogeneously charged surfaces, so-called inverse patchy colloids (IPCs), consisting of two charged, broad polar caps and an oppositely charged equatorial region.



Typical self-assembly scenarios of IPCs (with patch charge Z_p) confined between two parallel, charged walls (with wall charge Z_c) for representative values of Z_p and Z_c. The patches of the IPCs are marked in yellow, while the body of the particles is grey.

Depending on the charge balance between the different surface regions, IPCs can be overall either neutral or charged. In their coarse grained simulation, an aqueous solution of IPCs is confined between two horizontal, parallel planes either under tight or loose confinement conditions. Experimental systems that feature in-homogeneously charged surfaces are diverse: they include, for example, PbS-Au4 nano-structures and PbS-Au4 nanocubes, synthesized spotted vesicles, viral capsids, and virus-like nano-particles. In the latter case, the overall particle charge can be controlled via pH modifications, allowing for a tuning of both their propensity to act as assembly sites for viral capsids and their

functionality as building blocks for two-dimensional self-assembly into ordered structures. Using the pH, the salinity, and the wall charge as external control parameters, the authors find that one self-assembly scenario can be transformed into another in a reversible fashion.

4.8 Friction control with nematic lubricants via external fields

W Chen, S Kulju,AS Foster,MJ Alava*,L Laurson Physical Review E**91** (2015): 012504.
∗ E-CAM Scientist at the University of Aalto, mikko.alava@aalto.fi

Tribology, literally, the study of rubbing, or more precisely, the rubbing of surfaces was studied as far back as Leonardo Da Vinci in work on friction. Controlling tribological interactions, including friction, wear, and adhesion, is a topic of considerable importance. In the absence of proper control of such effects in micro- and nano-scale mechanical devices, their lifetimes and reliability are greatly reduced, which has motivated an extensive search for strategies to control friction, ranging from electric field control of polyelectrolytes coatings or ionic liquids to applying vibrating normal forces to tuning of van der Waals forces and using magnetic nano-fluids. From the earliest times, lubricants have frequently been used to reduce the detrimental effects of friction and wear. The authors of this highlighted article have focused on the properties of nematic liquid crystals (LCs) as a particularly interesting lubricant as it has recently been shown to give rise to low friction coefficients and wear rates. LC systems can be characterized by the presence or absence of positional and/or orientational order of the elongated molecules, which is controllable, for instance, by tuning the temperature or applying external electric or magnetic fields.

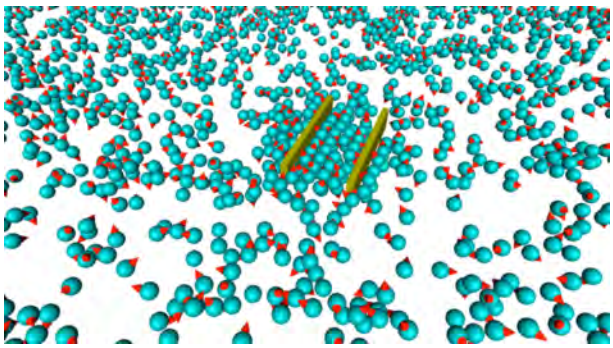
To elucidate the fundamental mechanisms via which order and orientation of a nematic lubricant affect its frictional properties, the authors have performed extensive molecular dynamics simulations of a rigid bead-necklace model of elongated molecules, confined by two rigid, parallel plates in relative sliding motion. The equilibrium system displays fluid like isotropic and layered in-plane nematic phases depending on temperature and the confining pressure. Sliding slowly the top surface gives rise to a preferred in-plane molecular orientation along the sliding direction and leads to a small perturbation of the equilibrium phase diagram. The two phases are found to be correlated with the frictional properties of the lubricant, with higher friction coefficients observed in the fluid like isotropic phase. Their detailed study of the effect of applied fields reveals that the related tunability of friction is intimately connected to the phase behaviour of the lubricant: the largest relative increase in friction is obtained when in-plane fields perpendicular to the sliding direction are applied with the system close to the nematic-isotropic transition boundary; and, the largest relative friction reduction occurs in the isotropic phase with applied fields along the sliding direction.

4.9 Tunable long range forces mediated by self-propelled colloidal hard spheres.

Ni, Ran, Martien A. Cohen Stuart, and Peter G. Bolhuis*. Physical review letters**114** (2015): 018302. ∗ E-CAM Scientist at University of Amsterdam, email: p.g.bolhuis@uva.nl

Self organization in nature exhibited, for example, in the flocking of birds, bacteria colonies tissue repair, and colloids, has fascinated many, and indeed been also the subject of a number of CECAM workshops. Developments in particle synthesis have enabled the fabrication of artificial colloidal micro-swimmers wit applications such as biosensing and drug delivery. A number of different active colloidal systems have been realized in experiments, such as colloids with magnetic beads acting as artificial flagella, catalytic Janus particles, laser-heated metal-capped particles, light-activated catalytic colloidal surfers, and platinum-loaded stomatocytes. In contrast to passive colloids undergoing Brownian motion due to random thermal fluctuations of the solvent, active self-propelled colloids experience an additional force due to internal energy conversion.

In this highlighted work, the authors address the question whether active matter can serve as a medium to generate large effective interactions between large immersed objects to direct their motion and assembly. In their model study, they explore the effective interaction between two parallel hard walls immersed in suspensions of self-propelled colloidal hard spheres, and find that that when the density of particles is relatively high, a dynamic crystalline bridge forms between the two walls, which induces a strongly oscillating repulsive dynamic wetting force, with a range depending on the size of the dynamic clusters. With decreasing density of particles, this dynamic crystalline bridge becomes smaller, and the effective force between the two walls develops a long attractive tail. remarkably, in the limit of zero density, the effective interaction turns into a long range dynamic depletion force, with a range depending on the persistence length of the mean free path of the particles, which can be tuned by varying the self-propulsion on the particle.



Snapshot two parallel hard walls immersed in a of suspension of self-propelled colloidal hard spheres

Their results suggest a novel way to tune the interaction between large objects by immersing them in suspensions of small self-propelled colloids. The sign of interaction can be tuned from long range repulsive to long range attractive by changing the density of particles, and the range of interaction can be controlled by varying the magnitude of self-propulsion of the particles.

4.10 Fast computation of solvation free energies with molecular density functional theory: Thermodynamic-ensemble partial molar volume corrections

Volodymyr P. Sergiievskyi, Guillaume Jeanmairet, Maximilien Levesque, and Daniel Borgis* The Journal of Physical Chemistry Letters **5** (2014): 1935-1942.
∗ E-CAM Scientist ENS Paris & CNRS, email: daniel.borgis@ens.fr

Solvation Free Energy (SFE) is one of the main physical quantities of interest in solution chemistry. Many important characteristics, such as dissociation constants, partition coefficients, which are necessary for describing most of the processes in physical chemistry and biochemistry are expressed through the SFE. Unfortunately, the determination of SFE is often problematic. Experimentally, it can require very significant time and resources, especially if SFE is calculated for low soluble and low volatile substances, and underlies the importance of estimating SFE computationally. Molecular Density Functional Theory (MDFT) offers an efficient implicit solvent method to estimate molecule solvation free-energies while retaining a molecular representation of the solvent. Even within a second order approximation for the free-energy functional, the so-called homogeneous reference fluid approximation, the authors find that the hydration free-energies computed for a dataset of 500 organic compounds are of similar quality as those obtained from molecular dynamics free-energy perturbation simulations, with a reduced computational cost of two to three orders of magnitude. The high quality results entailed the introduction of a proper partial volume corrections to account for a value of the pressure on the solute that is pertinent to experiments. In addition, the author established that this correction can be extended to 3D-RISM calculations, giving a sound theoretical justification to empirical partial molar volume corrections that have been proposed recently.

4.11 Clogging transition of many-particle systems flowing through bottlenecks

Iker Zuriguel Daniel Ricardo Parisi ,Raúl Cruz Hidalgo, Celia Lozano,Alvaro Janda,Paula Alejandra Gago, Juan Pablo Peralta, Luis Miguel Ferrer,Luis Ariel Pugnaloni, Eric Clḿent, Diego Maza, Ignacio Pagonabarraga*, Angel Garcimartín, Scientific reports**4** (2014).
∗ E-CAM Scientist at University of Barcelona, email: ipagonabarraga@ub.edu

In this provocative article the authors ask if it be taken for granted that an enclosure filled with particles could be emptied through a small opening in a finite time, with examples ranging from the mudane everyday experience that the pouring of salt from a salt-cellar frequently requires shaking so as to to break the clogging arches, to flow interruptions in industrial conduits and silos, and at smaller scales, to provoke embolization of blood vessels in order to shrink a tumour, or at the nano-scale when electrons on the liquid helium surface pass through nano-constrictions. And at its most dramatic, in human stampedes frequently leading to a clog in narrow passages.

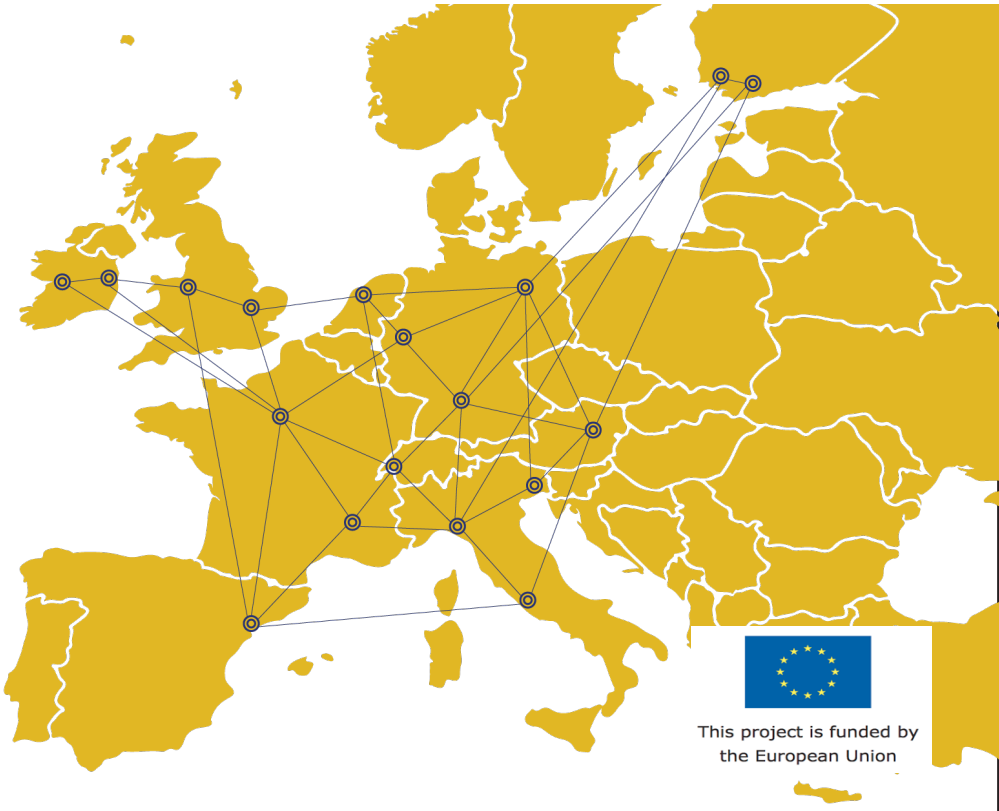
Despite the extraordinary range of scales, the authors show that clogging in several disparate systems is amenable to a unified treatment, including that it can be analysed through a model colloidal suspension, simulated using the Lattice Boltzmann method. Previous studies in colloids have focused on the mechanisms leading to the development of permanent clogs. Instead, the approach taken by the authors above is conceptually different, and focuses on the the

statistical analysis of the flow intermittencies, without the necessity of observing permanent clogs. In particular, they find that time lapse distributions display power-law tails while the burst size distributions remain exponential, that is the approach to complete obstruction in colloidal suspensions obeys the same universal scenario that is observed in the human models and granular materials, demonstrating that the transition to clogging is not very sensitive to the microscopic details of the system.

3.2 Newsletter issue2

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

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

Prof Giovanni Ciccotti

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

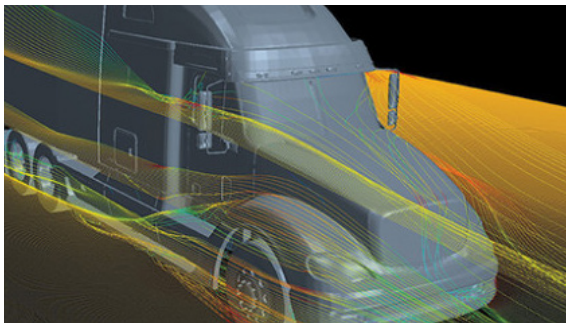


Image from HPCWire.com

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".

Developing a skills network to make the most of HPC

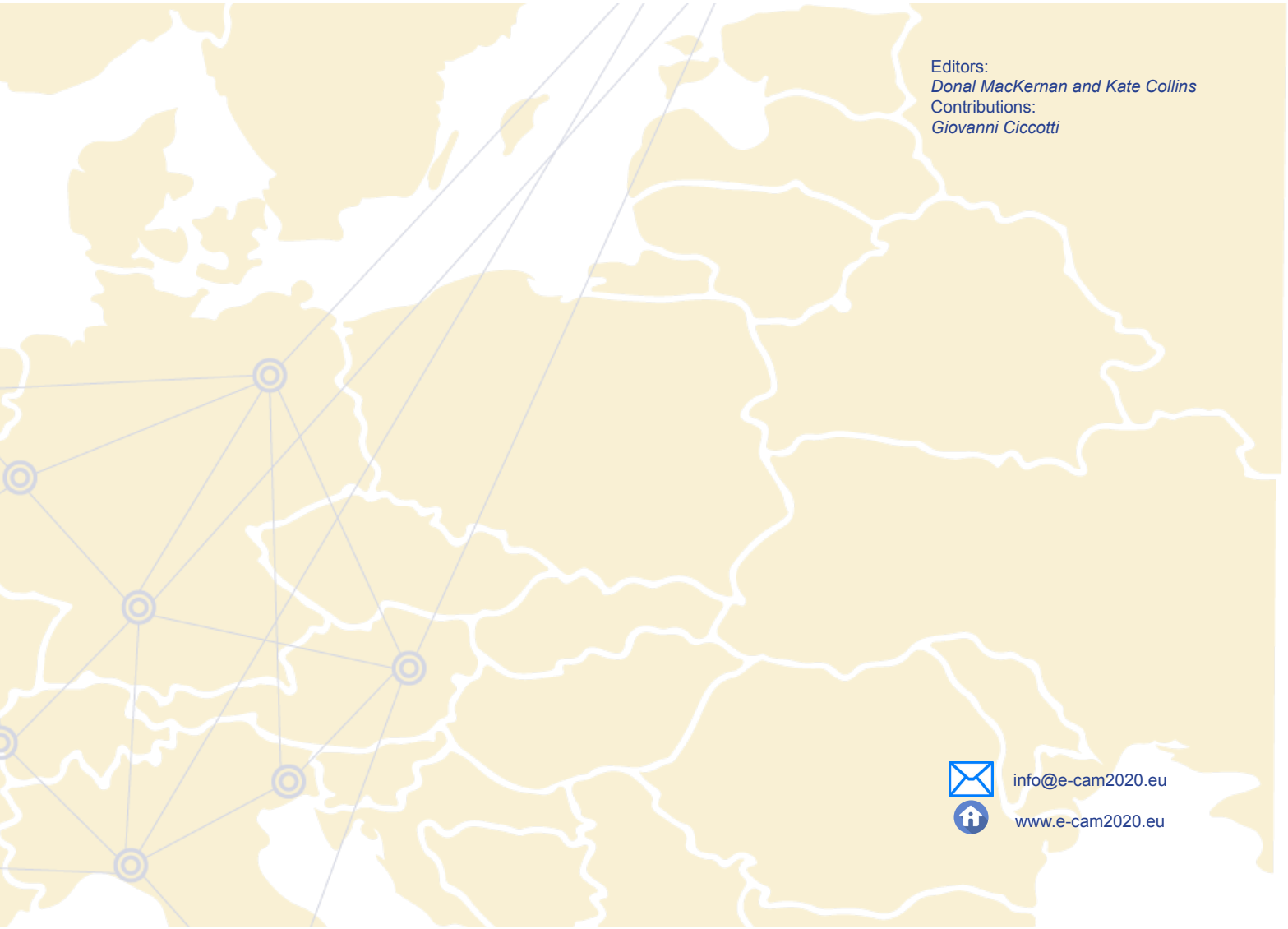
Image from stfc.ac.uk

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

15th June 2016, Birmingham, UK
H2020 European Brokerage Event "Materials & Nanotechnology, Process Industries & Manufacturing"
https://www.b2match.eu/h2020nmp2016



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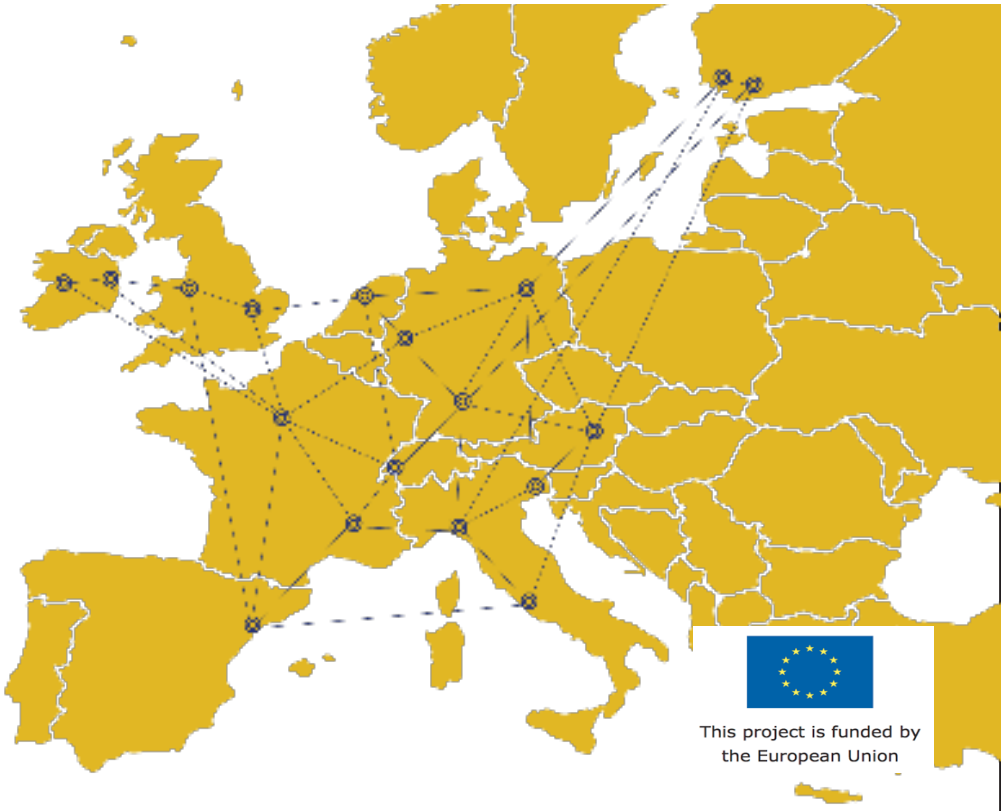
www.e-cam2020.eu

3.3 Newsletter issue3

E-CAM Quarterly

Supporting HPC simulation in industry and academia



This project is funded by the European Union

April-June 2016

E-CAM Update: March - June 2016

The next E-CAM General Assembly will take place 7th - 9th November 2016 in Orsay, France at IDRIS and Maison de la Simulation. Please keep these dates free.

E-CAM was requested to attend a Commission Review on 17th May 2016 where two expert reviewers: Prof Sabrina Pricl and Prof Stefan Wesner provided the project with constructive feedback on progress to date. Updates are currently underway in response to this feedback.

You can now access a range of E-CAM documents including minutes of our management group meetings on E-CAM's googlesite https://sites.google.com/site/ecamh2020/home. You can view all documents without having to login, however, if you need to edit documents or upload documents you will need to login with a google account. The E-CAM project is now using the redmine a project management tool http://redmine.e-cam2020.eu which should greatly increase internal visibility and cooperation in ongoing work on E-CAM deliverables and tasks.

The synergy between E-CAM and PRACE was marked by a PRACE E-CAM CECAM spring school May 16-20 2016 supported by PRACE and CECAM-IRL, and organised locally by ICHEC – see page 11 for more details.

We also had strong E-CAM representation at the PRACEDays that took place in Prague in May 2016 with Luke Drury (E-CAM Chair), Alan O'Cais (Software Manager), Dominic Tildesley (Technical Manager), and Michael Lysaght (ICHEC) amongst others.

We have commenced our programme of events with the first E-CAM State of the Art Workshops and Extended Software Development Workshops taking place in June 2016. Read about our first ESDW on the Electronic Structure Library on page 11.

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**.

All of E-CAM's Programmers and Postdoctoral students have now been recruited. You can read profiles of new staff members on pp. 7-10.

Also in this issue find a very interesting article by Prof Mike Payne, University of Cambridge, on technology transfer between academia and industry.

IN THIS ISSUE:

EVENTS

E-CAM Scoping Workshops

7th-9th September 2016, Mainz, Germany

Simulation and Modelling in Industry

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 modeling in their organisations and include scientific talks from representatives of each of the four

E-CAM State of the Art Workshops

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

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

Extended Software Development Workshops

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

12th - 16th September 2016, San Sebastian, Spain

Wannier90 Software Development Workshop

Organisers: Mike Payne and Arash Mostofi

http://www.cecam.org/workshop-1357.html

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

Trajectory Sampling

Organisers: Gerhard Kahl and Christoph Dellago

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

E-CAM General Assembly

7th - 9th 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.

EDITORIAL - Mike Payne

Prof Mike Payne

Technology Transfer from the Academic World to Industry is a Difficult Process in all Scientific Fields

In many countries there is increasing demand for measurable socio-economic impact from academic research. Perhaps the UK is furthest down this path with a significant fraction of the funding for Universities dependent on the 'Impact' (defined as impact outside of academia) of the research performed [1]. However much we might wish to ignore this trend, I am convinced that it will only increase, at least over the short to medium term. I also believe that, as a community, we should try to engage with this process and we must not pretend that this task is straightforward. For instance, some of the questions that industry might ask when assessing a computational methodology are:

1. Is it relevant - does it determine quantities of interest to me?
2. Is it accurate/predictive?
3. Is it easy to use?
4. What is the cost compared to present methodology/other solutions?

Addressing these questions is not straightforward, some of them differ markedly from the academic world view and there is a degree of conflict between them. For instance, in relation to the first question, the topics and problems that academics think are interesting are not necessarily those of most importance to industry. If academics are to engage with industry then they do need to be aware of what issues are of concern to industry. A further complication is that planning horizons in industry tend to be shorter than in academia and priorities can shift rapidly. It is not uncommon for an academic to work on a project that is believed to be relevant to industry only to find that industry's priorities have changed before the project comes to fruition. Similarly, it can be difficult to get industry interest, let alone engagement, for long term academic research that may take a decade to complete no matter how large a potential benefit is claimed for the work.

On the second question, the electronic structure community is, perhaps, guilty of suggesting that if a computed result does not come directly from quantum mechanics or some equally rigorous underlying model then it cannot be accurate or predictive. In contrast, industry only cares about whether a method gives useful results and is happy to accept a certain fraction of failures as long as this fraction is sufficiently small. The rapid adoption of machine learning methods throughout industry clearly shows the acceptance of this more pragmatic approach to problem solving. The amount of theoretical or modelling work carried out in many companies, particularly in materials, is currently generally small. This is in stark contrast to many branches of engineering where the entire design cycle is performed computationally. However, we should be prepared to admit that at present and for the foreseeable future we are not capable of virtual

design, testing and certification of real world materials. Until this point is reached, modelling will be a somewhat niche activity for most companies.

Often a small group of modellers provide services to a whole company and, as a result, constantly shift from one problem to another, each one requiring different methods of solution. Not surprisingly, the ease of use of each modelling method then becomes paramount as the modellers do not have the time to become expert in each method they use – hence the importance of the third question.

The final issue of cost is superficially easily understood by academics. However, for industry to change methodologies there usually has to be a significant cost advantage to justify the disruption and risk associated with any change of process. While it is difficult to quantify when any company would change approaches it is much more likely to occur when there is a factor of 10 cost advantage than a factor of 2 and, unless it concerned a methodology that was used very widely by the company, then any cost advantage of less than a of 2 would probably not be sufficient to persuade the company to change. Here, computation has a significant advantage over experimental methods as the costs of compute decrease significantly over time whereas experiment tends to either increase in cost or reduce at a much slower rate. However, the computer is only one part of the cost of the 'modelling' effort for a company and the other costs, such as personnel costs, will not reduce with time.

So far, we have concentrated on the potential disconnect between industrial use of academic software and some of the challenges to industry and academia working together. There are, of course, many examples of long term successful collaborations between companies and academic researchers which prove that these challenges are not insurmountable. Indeed, one of the simplest ways of overcoming some of the difficulties is simply for industry to fund projects in academic groups and there is evidence for very wide use of this model in the electronic structure field [1].

Technology transfer from the academic world to industry is a difficult process in all scientific fields. Software has some particular advantages that make the process somewhat easier. In principle, it is possible for academic research software to be sold commercially. In the terminology of Technology Readiness Levels - TRLs [2], it is possible for the exactly the same piece of software that is used to develop novel scientific functionality (TRL1) to be sold commercially (TRL9). This contrasts markedly with a commercialisation of a new material discovered in the laboratory. This might involve a continuous move through the TRLs starting from the one-off academic research experiment at TRL1 all the way to industrial scale production with tight quality controls and certification at TRL9. This is a very expensive process and slow process. In the case of materials, the time to market is typically 20 years or more. Speeding up this process is a major driver of the Materials Genome Initiative [3]. So why is not far more academic software used in industry? Often the reason is that it fails under the initial questioning of relevance, accuracy, ease of use or cost. If it passes these tests, there may be other reasons for lack of adoption associated with the software itself. There may by questions of code ownership that will prevent commercialisation or the code itself may be of poor quality and/or lack documentation and/or lack a suitable test

suite. The author feels that the over-emphasis on Open Source software did little to address these problems. While there are many examples of excellent quality Open Source software, unfortunately, Open Source on its own is no guarantee of quality. It is often said that research funders do not understand the intellectual challenges of software development and do not properly fund this process. Certainly, such arguments can be further extended to their inability to differentiate between good quality and poor quality software. The UK can be rather proud of recent changes in this area and, in particular, EPSRC (Engineering and Physical Sciences Research Council) have recognised the importance of Research Software Engineers (RSE) and have introduced funding for RSE Fellowships – at the same time the RSE community in the UK is organising itself into a self-help and self-support community [4]. Other countries are also responding to the challenges of scientific software, such as the US with its recently launched Computational Materials Sciences Centres [5]. If these initiatives are successful and are copied elsewhere then this will significantly enhance the degree of industrial adoption of academic software in the future.

One of the goals of E-CAM is to strengthen interactions between academic research and industry. This will be a difficult challenge and one that all the members of E-CAM must take responsibility for and make efforts to address. Over the years, I have commissioned reports from Goldbeck Consulting on the economic impact of molecular modelling [6], industry interactions of the electronic structure research community in Europe [1] and I contributed funding for a report on the economic impact of materials modelling [7] prepared for the European Materials Modelling Council [8]. These reports provide useful background information to those of us who wish to interact with industry. For those who are interested in commercialisation of software, there are a series of reports prepared by the Software Taskforce of UK E-Infrastructure Leadership Council [9] which provide guidance and advice along the whole of the technology transfer path. Copies of these reports have can be found on the E-CAM Website [10].

References

[1] Industry interactions of the electronic structure research community in Europe, G. Goldbeck, 2014 (available from https://zenodo.org/collection/user-emmc).
[2] https://en.wikipedia.org/wiki/Technology_readiness_level
[3] https://www.whitehouse.gov/mgi
[4] http://www.rse.ac.uk/who.html
[5] http://science.energy.gov/bes/funding-opportunities/closed-foas/computational-materials-sciences-awards/
[6] The economic impact of molecular modelling, G. Goldbeck, 2012 (available from https://zenodo.org/collection/user-emmc).
[7] The Economic Impact of Materials Modelling, G. Goldbeck and C. Court, 2016 (available from https://zenodo.org/collection/user-emmc).
[8] https://emmc.info/
[9] https://www.gov.uk/government/groups/e-infrastructure-leadership-council
[10] *** Software Taskforce Reports will be made availabe on e-cam website www.e-cam2020.eu ****

DELIVERABLES TO DATE

Five deliverables have now been submitted to the Commission on schedule. You can access these deliverables on the E-CAM googlesite.

On 17th May 2016 Prof Luke Drury (E-CAM Chair) and Prof Dominic Tildesley (E-CAM Technical Manager) attended a Commission Review of all Centres of Excellence in Brussels. In that meeting E-CAM's two project reviewers provided feedback on the progress of the project to date. The reviewers emphasised that deliverables are a contractual obligation that must be fulfilled exactly as stated in the deliverable description. As such, the project coordinator is preparing an amendment to the grant agreement to ensure that deliverables reflect what can be achieved by E-CAM in a realistic time- frame.

The following deliverables have been completed and submitted:

D 5.1: ***ESDW Guidelines and Programme I*** (December 2015)

D 6.1: ESDW Technical Software Guidelines I (March 2016)

D 11.0: Data Management Plan (March 2016)

D 4.1: Identification/Selection of E-CAM Meso and Multi-Scale Modeling Codes for Development (April 2016)

D 6.2 E-CAM Software Development Tools (May 2016)

D 7.1 Hardware Developments I (June 2016)

E-CAM POSTDOCS

Dr Momir Mališ, Postdoc at EPFL (WP 3)

Dr. Momir Mališ has entered the field of theoretical chemistry during his university days by studying systematic approaches for construction of reaction coordinates necessary for the description of large amplitude motions under the supervision of Dr. Nađa Došlić. After obtaining his diploma in chemistry from the University of Zagreb in 2009, he switched his interest towards computational photochemistry. During his PhD under the supervision of Dr. Došlić at the Ruđer Bošković Institute in Zagreb he wrote his own computer code for simulating nonadiabatic molecular dynamics using Tully's trajectory surface hopping approach. He used it to elucidate the nonradiative deactivation mechanisms of electronically excited model peptides and formic acid at the time dependent density functional theory level, while later the code was upgraded and used for calculating excited state lifetimes in pyrrole also at the ADC(2) level. He obtained his PhD from the University of Zagreb in 2015 with the thesis Nonradiative relaxation mechanisms of electronically excited phenylalanine in model peptides, and continued to work at the Ruđer Bošković Institute on mapping the accessibility of the whole conical intersection seam and on examining new potential nonradiative deactivation mechanisms of retinal in solution. In 2016 he started his postdoc at CECAM, EPFL in Lausanne on development and testing of wave and trajectory based methods relevant for studying open quantum system as part of the Work Package 3 "Quantum Dynamics" project within the E-INFRA5 Centre of Excellence ECAM. He is the author and coauthor of eleven scientific papers and has collaborated on a few international projects.

Dr Momir Malis, EPFL (WP 3)

Dr David Swenson, Postdoc at UvA (WP 1)

Dr. David W.H. Swenson received his bachelor's degree from Colorado College in 2003, completing majors in Chemistry, French Literature, and Physics. He followed that with a second undergraduate degree in Mathematics/Computer Science from Université Louis Pasteur (Strasbourg) in 2005. His PhD in Chemistry, which he received from the University of California, Berkeley in 2011, involved developing methods for semiclassical approximations to quantum dynamics, and applying them to models of nanoscale electronics. He has held visiting researcher positions at D.E. Shaw Research, at Tel Aviv University, and at Memorial Sloan Kettering Cancer Center. His primary postdoctoral work, at the University of Amsterdam, has involved the development of methods for path sampling simulations of rare events, as well as applications of those methods to problems of biological interest, and the development of reusable software to enable others to apply those methods.

Dr David Swenson, UvA (WP 1)

E-CAM POSTDOCS

Dr Christian Krekeler, Postdoc at FU Berlin (WP 3)

Dr. Christian Krekeler studied chemistry at the Georg-August University Göttingen, and finished with a diploma in Chemistry (2004) with a study of small molecules using coupled cluster methods and computational chemistry. For the PhD thesis (2008) at the Max Planck Institute for Polymer Research (MPIP) in Mainz, he studied electrostatic interactions of small ion-water clusters up to ions in solution and ionic liquids utilizing ab initio molecular dynamics simulations in a multiscale approach. After that he worked for several years as a PostDoc at Frankfurt Institute for Advanced Studies (FIAS, Frankfurt (M)) and TU Darmstadt. The topic was to study small heavy metal clusters with respect to chirality violation (via relativistic quantum chemistry) and more efficient ways to predict those. Then in 2012 he moved back into the field of condensed systems again, in particular simulations of thin films for organic electronics, at the TU Braunschweig with close cooperation with the Innovationlab GmbH (in Heidelberg). The first part of the work was to understand the molecular build-up of thin films, which included the development of a reasonable molecular deposition scheme. The second part was to understand the electronic interactions of molecules within the films, for which an effective QM/MM scheme was developed.

Dr Étienne Plésiat, Postdoc at CIC NanoGUNE (WP 2)

Dr Étienne Plésiat received a Bachelor degree in Physics in the Université de Franche-Comté (France) in 2004, a Master degree in “Condensed matter and Nanophysics” at the Université de Strasbourg (France) in 2006, and a European Master degree in “Theoretical Chemistry and Computational Modelling” at the Universidad Autónoma de Madrid in 2010. Following this master degree, he pursued a PhD in Chemistry at the Universidad Autónoma de Madrid. The work aimed at describing theoretically the single photoionization of polyatomic molecules in the weak field regime by using a DFT method. After his PhD (obtained in 2012), he has held a postdoctoral position in the Modern optics group of the Humboldt Universität zu Berlin as part of the Marie-Curie Initial Training Network ``CORINF'' network (Correlated Multielectron Dynamics in Intense Light Fields). This position gave him the opportunity to extend the scope of his former PhD research to the strong field regime. In 2016, he joined the Theory group of the CIC NanoGUNE research center in San Sebastián (Spain) as part of the E-CAM project.

Dr Christian Krekeler, FU Berlin (WP 3)

Dr Étienne Plésiat, Nanogune (WP 2)

E-CAM POSTDOCS

Dr Hideki Kobayashi, Postdoc at Max Planck Institue for Polymer Research (WP 4)

Dr. Hideki Kobayashi is an experienced researcher who has been active in the field of computational physics and soft-matter physics. Particularly, he focussed on the development of mesoscale methods taking into account hydrodynamic interactions since receiving his Bachelor's degree in Physics from Tokyo University of Science in 1998. He received a Master's degree in Mathematics and Science Education from Tokyo University of Science in 2008 and a Ph.D. in Chemical Engineering from Kyoto University in 2011. As part of his graduate studies, he developed a general methodology to perform direct numerical simulations of particle dispersions in a shear flow. Using this method, he revealed the relationship between dynamics of a single polymer and rheological properties of the dilute polymer system. In recognition of these results, he received the symposium award for a presentation from The Society of Chemical Engineers Japan. In 2011 he joined the National Institute of Advanced Industrial Science and Technology (AIST) and expanded their method to the calculation of non-equilibrium structure formation processes of polymer blend melts containing colloidal dispersions. In 2012, he moved to the Theoretical Soft Matter and Biophysics group within the Institute for Advanced Simulation at Forschungszentrum Juelich (FZJ). There he worked on a project funded by the Deutsche Forschungsgemeinschaft within SFB 985 "Functional Microgels and Microgel Systems" until 2016. In this project, he elucidated a novel mechanism of the swelling of nanogels with cross-linked polyelectrolytes, as well as the internal dynamics of nanogels, using a mesoscale method taking into account hydrodynamic interactions. Within E-CAM, he plans to work on a project that attempts to generalize existing coarse-graining strategies for polymer melts to the more challenging case of block copolymers, aiming mainly at interfacial and mechanical properties of such materials.

Dr Hideki Kobayashi, Max Planck (WP 4)

Future Post Docs

Dr Francesco Fracchia, Postdoc at SNS Pisa (WP 2)

Dr Silvia Chiacchera, Postdoc at STFC (WP 4)

E-CAM PROGRAMMERS

Dr Liang Liang, Programmer at IDRIS

Dr. Liang LIANG received a Bachelor Degree in Applied Physics from the Harbin Institute of Technology in China in 2010. He participated an exchange program during 2009-2010 at Université Lille 1 in France. He continued his masters studies at Université Paris-Sud and received a ParisTech Masters Degree in Material Science in 2012. He started his PhD thesis at Ecole Polytechnique with CEA support, and graduated in March 2016. His PhD research subject was part of the French ANR project FluTi. The main tasks of his PhD thesis were the simulation of interactions between twin boundaries, dislocation cores with interstitial atoms H & O in hcp titanium using DFT based ab initio calculations. He used the resources of the French supercomputing centre GENCI, and participated at the Ecole Polytechnique's Inter-labo computer resource sharing project. He is working as a scientific programmer as part of the E-CAM project within the User Support Team of the French CNRS' Supercomputing center IDRIS.

Dr Jony Castagna, Programmer at STFC

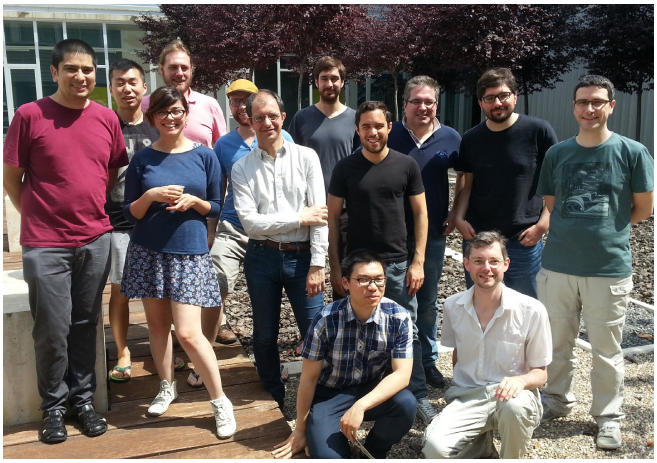
Dr. Jony Castagna received his bachelors degree in Chemical Engineer in 2004 at University of Calabria (Italy) with a thesis on the simulations of fluidized bed using the Distinct Element Method combined with Computational Fluid Dynamics. He then received a PhD at Kingston University in London in simulation of turbulent flow around complex geometries using massive parallel simulations. In 2009 he moved to Southampton University holding a research position mainly focussed on the development of a multi block code for parallel simulations of a jet in a turbulent cross flow, sponsored by the European project LAPCAT II. He then was employed by Multiphase Simulation Ltd in 2010 to developed the parallel version of their commercial software using different High Performance Computing architectures, especially for GPU accelerators. He fully developed and maintained the code since then. In 2015 he started a collaboration with the University of West England for studies on the direct numerical simulation of wall bounded turbulence using the latest UK supercomputer Archer.


Dr Liang Liang, IDRIS


Dr Jony Castagna, STFC

FIRST E-CAM ESDW AND PRACE SPRING SCHOOL

The first of the E-CAM Extended Software Development workshops was held in Zaragoza in Spain between the 8th and the 17th of June 2016. The workshop was particularly centred around solvers: eigen-solvers, poisson solvers and atomic solvers. The group involved included CECAM (and E-CAM) members from across Europe as well as contributors from the US. In addition to collaboration to create the solvers, the group also discussed methodologies that help make producing software easier and more robust. After this discussion, there has been some development of the services that E-CAM provides, including using our GitLab service (available at http://www.e-cam2020.eu:10080) more extensively, and building other services on top of it (like Kanban boards available at http://www.e-cam2020.eu:8282 which are used as a method to manage knowledge-based work).

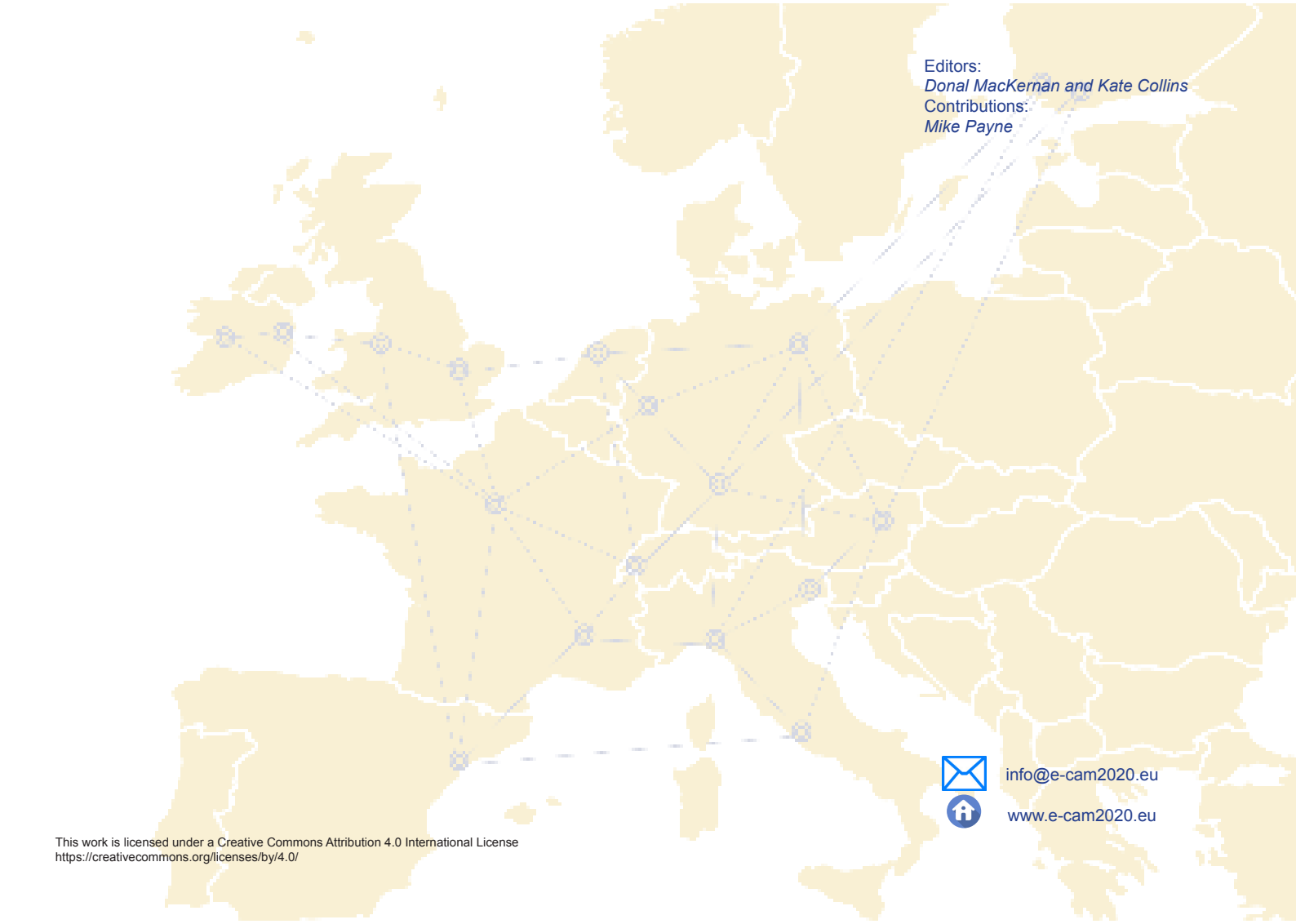


Participants at E-CAM ESDW, Zaragoza

A joint PRACE E-CAM Spring School and flagship CECAM Tutorial on Molecular and Atomic Modelling took place on 16-20 May 2016 at University College Dublin, Ireland. It was funded by PRACE and CECAM-IRL, and organised locally by ICHEC. The school was aimed at researchers needing a better understanding of methodologies and best practices in exploiting molecular and atomic modelling applications on HPC systems.

The programme consisted of a mixture of scientific talks (HPC challenges in the field), sessions on HPC skills (parallel programming, numerical libraries) as well as application-oriented sessions with a large emphasis on hands-on practical exercises (e.g. classic molecular dynamics packages such as DL_POLY and Gromacs, electronic structure calculation packages such as CP2K and Quantum Espresso, covering example calculations, scalability and performance considerations, suggestions for development such as implementing custom functions and the Python-based Atomic Simulation Environment). Recordings of the lectures will be made available shortly on E-CAM's website at www.e-cam2020.eu.

Editors:
Donal MacKernan and Kate Collins
Contributions:
Mike Payne



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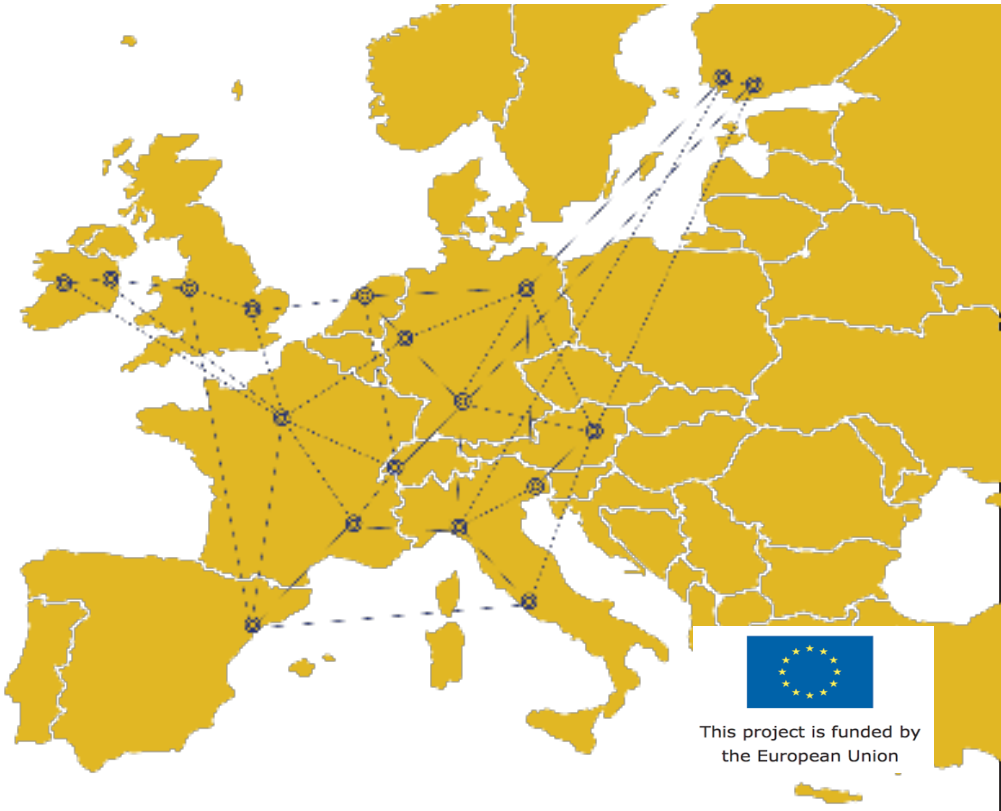
3.4 Newsletter issue4

E-CAM Quarterly

Supporting HPC simulation in industry and academia



This project is funded by the European Union

June-September 2016

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

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.cecam.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.

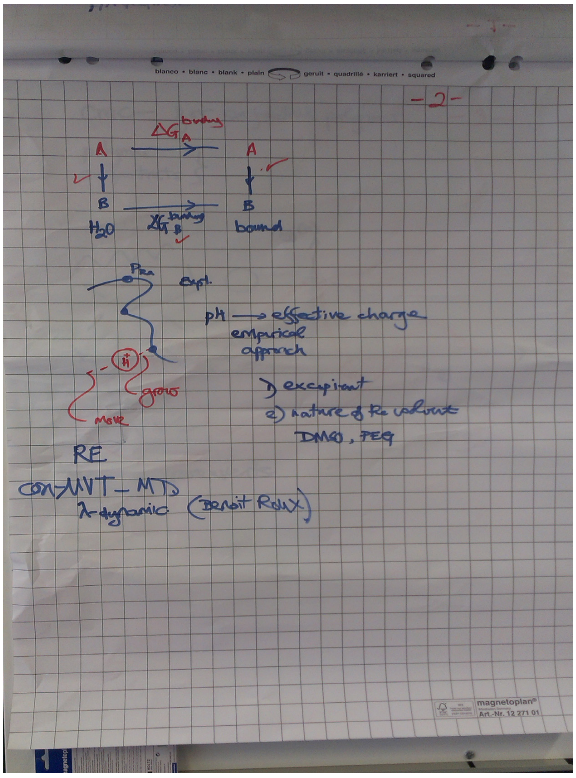
This workshop offered a unique opportunity for the quantum dynamics community to critically and open mindedly discuss the most important issues existing in the overall field, as well as to stay informed on the recent development within the different sub-domains.

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

The first E-CAM scoping workshop was organised at Johannes Gutenburg 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 faciliated 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

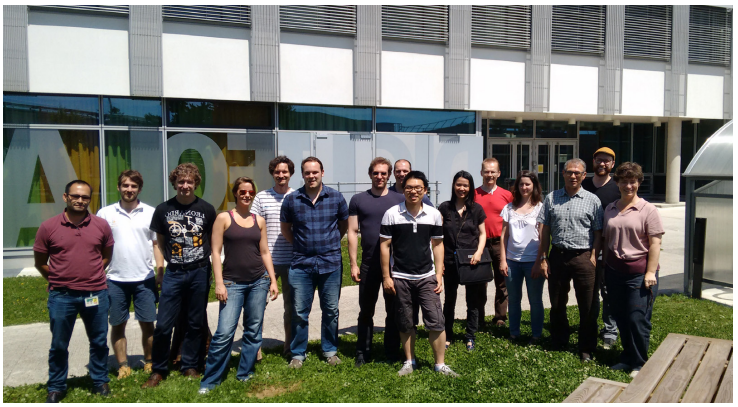
E-CAM ESDW Quantum Dynamics, June-July 2016

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.

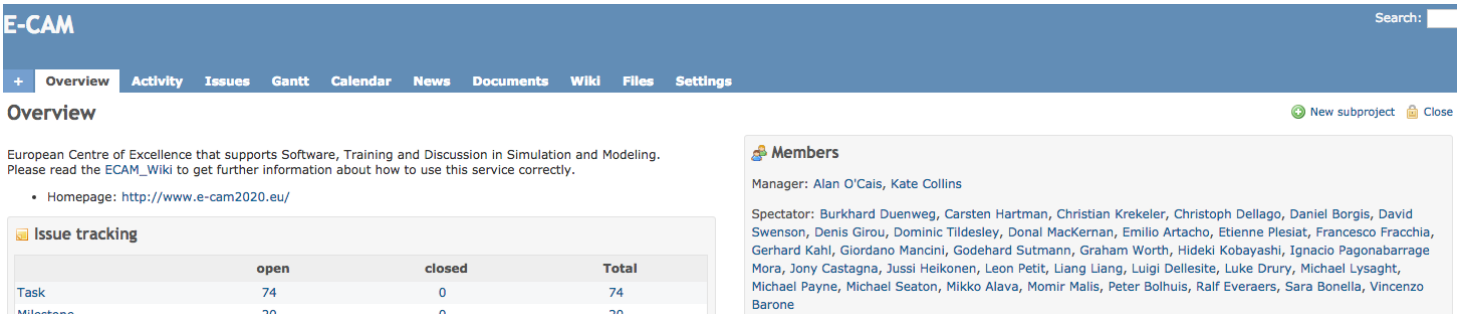
Work was performed by teams of 2-4 students, assisted by the senior participants and by E-CAM's Software Manager, Alan O'Cais, and the Software Developer associated to WP3, Dr. Liang Liang.

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



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

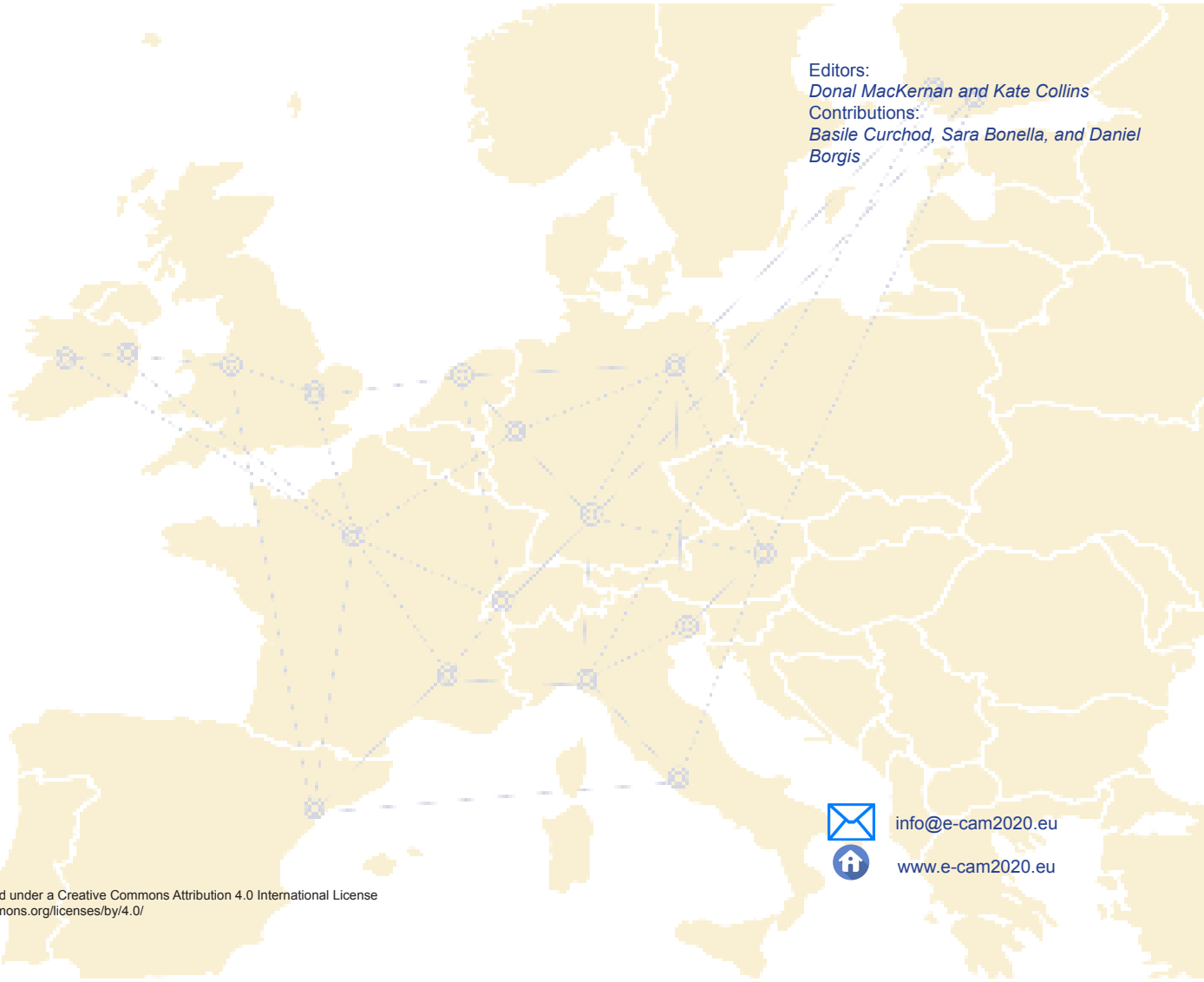
A web-based project management and issue tracking tool. It allows users to manage multiple projects and associated subprojects. It features per project wikis and forums, time tracking, and flexible role based access control.

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

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References

Acronyms Used

CECAM Centre Européen de Calcul Atomique et Moléculaire

HPC High Performance Computing

URLs referenced

Page ii

https://www.e-cam2020.eu ... https://www.e-cam2020.eu
https://www.e-cam2020.eu/deliverables ... https://www.e-cam2020.eu/deliverables
Internal Project Management Link ... https://redmine.e-cam2020.eu/issues/94
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Page 1

E-CAM website ... https://www.e-cam2020.eu/wp-content/uploads/2016/05/D6.1-Guidelines-for-web-1.pdf
E-CAM ... https://www.e-cam2020.eu
WordPress ... https://wordpress.com/
about E-CAM ... https://www.e-cam2020.eu/about-us/
E-CAM software repository ... https://www.e-cam2020.eu/software-library/
E-CAM Events ... http://www.e-cam2020.eu/?post_type=tribe_events

Page 2

GitLab service ... https://gitlab.e-cam2020.eu/
ReadTheDocs.org ... https://readthedocs.org/
Software Repositories webpage ... https://www.e-cam2020.eu/software-library/
E-CAM primary landing website ... https://www.e-cam2020.eu
WordPress ... https://wordpress.com/
E-CAM project website ... https://www.e-cam2020.eu
about E-CAM ... https://www.e-cam2020.eu/about-us/

Page 3

Classical Molecular Dynamics ... https://www.e-cam2020.eu/classical-molecular-dynamics/
Electronic Structure ... https://www.e-cam2020.eu/electronic-structure/
Quantum Dynamics ... https://www.e-cam2020.eu/quantum-dynamics/
Meso- and Multi-Scale Modelling ... https://www.e-cam2020.eu/meso-and-multi-scale-modelling/
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