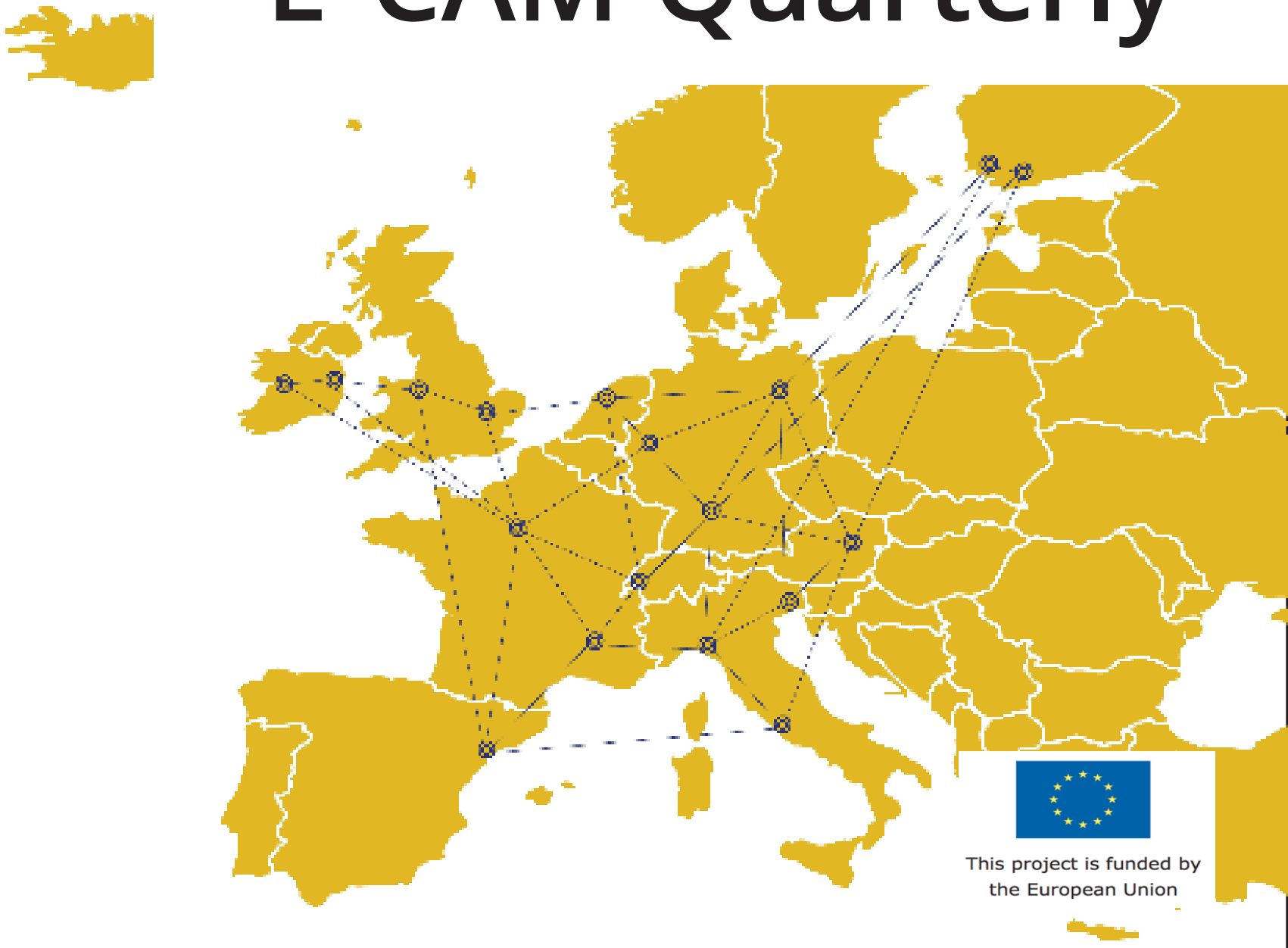
E-CAM Quarterly

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

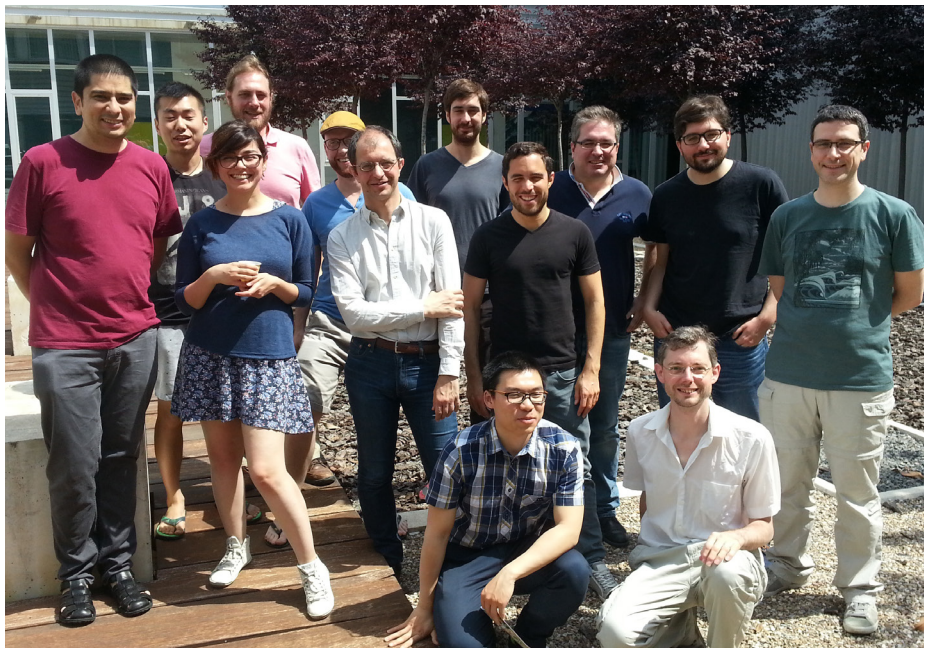
Dr. Jony Castagna received his bachelors degree in Chemical Engineer in 2004 at University of Calabria (Italy) with a thesis on the simulations of fluidized bed using the Distinct Element Method combined with Computational Fluid Dynamics. He then received a PhD at Kingston University in London in simulation 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.

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www.e-cam2020.eu