E-CAM Public Wiki-like pages and newsletters V

E-CAM Deliverable 9.5
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E-CAM
The European Centre of Excellence for
Software, Training and Consultancy
in Simulation and Modelling

Project and Deliverable Information

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12th April, 2021

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Contents

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Executive Summary

This deliverable is an update of D9.4: E-*CAM Public Wiki-like pages and newsletters IV* [1]. The pandemic and associated lock-downs starting in early March 2020 led to a postponement of all face to face dissemination actions due to the closure of universities, delays in reporting. In D9.4, as a consequence we took the opportunity to include in that report data from Q2 of 2020 (i.e. to report over 5 rather than the originally planned 4 quarters). The present report D9.5 is on data collected since July 1 2020 - which is 3 quarters rather than the 5. It consists of: (1) a summary of the impact of our dissemination strategy measured in terms of web traffic statistics; (2) updates to the E-CAM website to intensify efforts to disseminate results and ensure sustainability of the website beyond the current funding;(3) newsletters issues published since the submission of D9.4, and (4) a conclusion.

Regarding (1) the total number of visitors to E-CAM website since February 10, 2017 (from when we started collecting web traffic data statistics) is 190952, with 25551 visiting our pages from July 1 2020 till March 23 2021 - and is roughly in line with the daily rate for the previous reporting period, that is, about 70 visitors per day on average. While the cancellation of face-to-face events during the COVID-19 pandemic had an impact on the number of visits to our website in Q1 and Q2 of 2020, and that has continued into 2021, nevertheless, interest in our scientific publications has continued to increase. Also the science and comics initiative has attracted significant attention.

During this last period we made an additional effort to disseminate on our website the results obtained during the project's final ramp. Consequently, the content of the E-CAM website increased considerably, mainly on the following pages on the website:

- Individual pilot project pages;
- Case studies/Success stories page
- Events calendar
- Scientific publications page
- News-blog page.

Additionally, to increase attention to successes demonstrating the increasing impact of E-CAM we have updated the website to include:

- Biosensor news-blog page;
- Highlights from the E-CAM project page.

We have developed an E-CAM web-page on the Centre Européen de Calcul Atomique et Moléculaire (CECAM) website: https://www.cecam.org/e-cam to ensure that E-CAM's most important results continue to be disseminated and communicated to the target groups even after the EU funding period, as well as the future activities that we plan to run beyond March 2021 (project end-date).

A large amount of new material has been disseminated since July 1 2020, notwithstanding the difficulties produced by the pandemic. Many of these are to be seen in the last three issues of the E-CAM newsletter. They together with recent workshops held online, software, scientific results and new IP (not described explicitly here for commercial reasons) are intensifying interest in E-CAM within the simulation community and beyond.

1 Introduction

This deliverable, D9.5 *E-CAM Public Wiki-like pages and newsletters IV* includes (1) a summary of the impact of our dissemination strategy measured in terms of web traffic statistics; (2) Updates to the E-CAM website including efforts intensify to dissemination of results, and measures taken to ensure sustainability of the website beyond the current EU funding period ;(3) newsletters issues published since submission of D9.4[2] to the end of March 2021. The pandemic and associated lock-downs starting in early March 2020 led to a postponement of all face to face dissemination actions due to the closure of universities, delays in reporting. In D9.4, as a consequence we took the opportunity to include in that report data from Q2 of 2020 (i.e. to report over 5 rather than the originally planned 4 quarters). The present report is on data collected since July 1 2020 until March 31 2021.

1.1 Scope of this update

The previous deliverable D9.4 included an overview and an analysis of our dissemination strategy. The present version builds on those largely positive findings, but also in a context where the impact of dissemination is more concrete, thereby allowing more succinct adjustments to our strategy particularly as they might serve the goal of sustainability of the CoE beyond the final period.

1.2 Analysis of impact

The visitor traffic statistics of the website allow us to see the overall number of visitors to the website, which items are attracting greater interest, and where we need to make adjustments in our dissemination strategies, either in the presentation of materials, or the use of communication channels, or both. The total number of visitors to E-CAM website since February 10, 2017 (from when we started collecting web traffic data statistics) is 190952, with 25551 visiting our pages from July 1 2020 till March 23 2021 - and is roughly in line with the daily rate for the previous reporting period.

Figure 1 shows the average daily visitors to the E-CAM website over 3 quarters, from July 2020 to March 23 2021, as collected by Wordpress. For simplicity, data is averaged per trimester, as indicated in the x-axis. Note we have not included in this measure pages which have large numbers of inexplicable spikes which are probably due to non-human visits ("automated bots"), otherwise the daily number of hits would have been far higher.
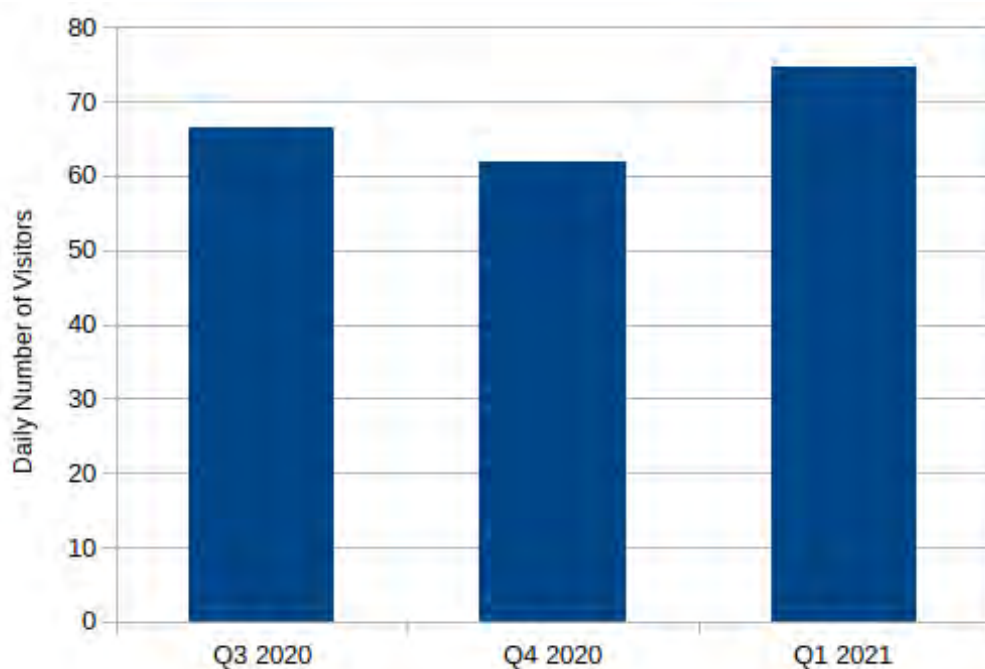
Figure 1: Daily average number of visitors to the E-CAM website per quarter, from July 2020 to March 2021.

There are on average about 70 visitors per day to the website. The cancellation of face-to-face events during the COVID-19 pandemic had an impact on the number of visits to our website in 2020, nevertheless, as seen in Fig. **??**, we recovered visitors in Q1 of 2021. As seen below, our calendar of events is the page on our website receiving the most visits.

The homepage received 44,062 visits from July 1 2020 till March 23 2021. Other technical pages receiving a large

number of visits include Calendar of events (39139), Software Repositories (1126), E-CAM Partners (399), Publications (486), E-CAM Services (526), Pilot Projects (342), LearnHPC: dynamic creation of HPC infrastructure for educational purposes (329), Deliverables (348),E-CAM News(315), Online Training Portal (295), and Case Studies (234). To highlight is the considerable number of visitors to the page dedicated to our Comics story (2104). The Comics was officially launched in October 28 2020, and had its "first outing" in October 30 with a presentation in the 2020 Lucca Comics&Games Festival. The number of downloads of our Comics available at https://www.e-cam2020.eu/e-cam-issue-of-comics-science/ is at 1223. The Comic book produced by E-CAM and the experts of Comics&Science was a unique, funny and understandable way to communicates science, simulation and HPC to the general public. Thus, these results are very important and encouraging to us, and we will continue to distribute the Comics book to different public's.

During the previous reporting period there had been a noticeable surge of interest in Q2 of 2020 for our technical pages, with a 50% increase to the scientific publications page. This increase in interest has been maintained in the present period (when averaged over the number of days). Two new items have attracted considerable interest: Comics & Science ? The E-CAM issue: an experiment in dissemination, which reports on the official release of the E-CAM Comics[1], and a post entitled LearnHPC: dynamic creation of HPC infrastructure for educational purposes".

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1.2.1 Lessons learned

Based on this data and other material, the following observations can be made.

- E-CAM calendar of events attracts the greatest attention, followed by our software repositories. There has been a small reduction in the number of hits pro-rata compared with the 2019-2020 figures. This is perhaps to be expected given that essentially all face-to face meetings has to be either postponed or cancelled due to the pandemic since March 2020.

- The increase of interest in E-CAM publications observed in the previous reporting period has intensified further when measured pro-rata reflecting perhaps both an increased number of publications and a more systematic effort to advertise new publications as they appear on the website and via Twitter.

- The Comics and Science part of the website which is new has attracted great interest

- The new webpage LearnHPC: dynamic creation of HPC infrastructure for educational purposes where E-CAM, FocusCoE, HPC Carpentry and EESSI join forces to bring HPC resources to the classroom in a simple, secure and scalable way has attracted significant interest.

2   E-CAM Online Documentation

E-CAM has four online access points, that serve to describe and disseminate the project activities and to interact with its users and the general public. These are:

- E-CAM Website, the public face of E-CAM, and the starting point for the Wiki-like pages[2] associated to the project (Software Library, GitLab Repositories and Training Infrastructure);

- E-CAM Software Library, a rendered documentation website divided into individual repositories for each of the current focal areas of E-CAM, hosting the documentation for all the software modules produced by the E-CAM Postdoc Research Associate (PDRA)s, the attendees of our Extended Software Development Workshop (ESDW)s and the scientists within the team;

- E-CAM GitLab Repositories, a git repository for the software modules documentation source files (produced as described in the previous item), opened to contributions from anyone in the E-CAM community;

- E-CAM Online Training Infrastructure, a data repository where we collect the content captured at our events and provide access to online training material.

Recently, we gained a new access point through the CECAM, more specifically at

- https://www.cecam.org/e-cam. This page allows accessing the main services and results from E-CAM directly through the CECAM website. CECAM is the coordinator of E-CAM and plays a critical role in its sustainability (sec. 2.2).

Since the last version of this deliverable, D9.4:E-CAM Public Wiki and newsletters IV[1], we made updates to the E-CAM website and developed a new web-page for E-CAM on the CECAM website. These efforts are reported in the subsequent sections. We didn't introduce any further updates to the other online access points since D9.4, and the changes on these websites during the last period were entirely associated to the increase of software and training content.

2.1   E-CAM website

The public face of E-CAM is the E-CAM primary landing website. We refer the reader to D9.2: E-CAM Public Wiki-like pages and newsletters II[3] for a global view of the E-CAM website look&feel and how information is structured.

2.1.1   Updates to the E-CAM website

During this last period we made an additional effort to disseminate on our website the results obtained during the project's final ramp. Results were disseminated mainly via:

- success stories reporting successful industrial-academic collaboration;

- case studies with software developed in E-CAM and their potential applications;

- the "modules of the month" category featuring our software modules;

- blog posts around the development and design of a molecular biosensor;

- the post-docs pilot project pages;

- scientific publications.

Additionally, there was also a great deal of effort in disseminating E-CAM events that happened (online) during the last phase of the project.

Consequently, the content of the E-CAM website increased considerably, mainly on the following pages on the website:

- Individual pilot project pages;

- Case studies/Success stories page

- Events calendar

- Scientific publications page

- News-blog page.

Additionally, we updated the website to include:

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

- Biosensor news-blog page;
- Highlights from the E-CAM project page.

Below we explain the nature of these updates in more detail.

1. Biosensor news-blog

The E-CAM project was built around the idea of harnessing the power of advanced simulation, software development, and massively parallel computing platforms to create new technologies able to address urgent societal problems ranging from health to novel materials.

A remarkable illustration of the potential of simulation-based approaches has been the development and optimisation of a new type of biosensor for diagnostics during the lifetime of the project. At the heart of this ongoing story is advanced simulation using massively parallel computation, rare-event methods and genetic engineering.

We have been accompanying this work through a news blog on our website at https://www.e-cam2020.eu/from-idea-to-market/ (Fig. 2). This blog aims at reporting the story of how an idea born via simulation thrived into a commercial opportunity (from idea to market). More than that, our goal is to inspire others by communicating the challenges, the expectations an the efforts of such an endeavour.
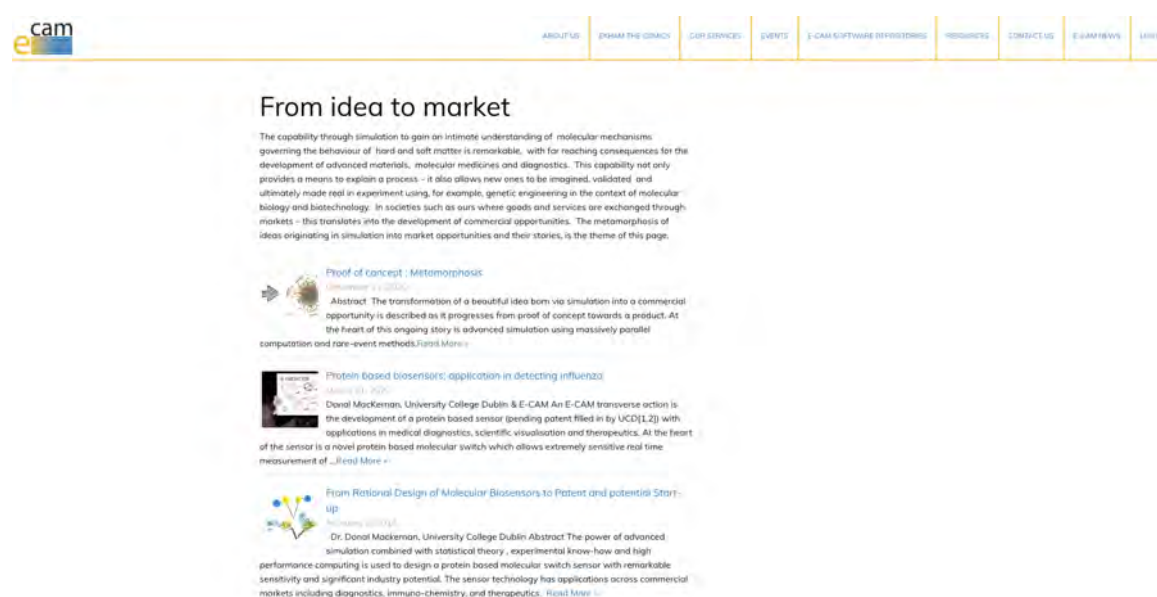

Figure 2: Snapshot of the news-blog associated to the molecular biosensor developed in E-CAM. It intends to report the story of how an idea born via simulation thrived into a commercial opportunity (from idea to market).

2. Highlights page

A new page was created on our website with some of the highlights from the E-CAM project: https://www.e-cam2020.eu/highlights-from-e-cam/.

Highlights are divided into four categories: Software developments, training, industrial interactions and outreach. This page is accessible from the homepage, and also from the main menu "ABOUT US" (see Fig. 3).
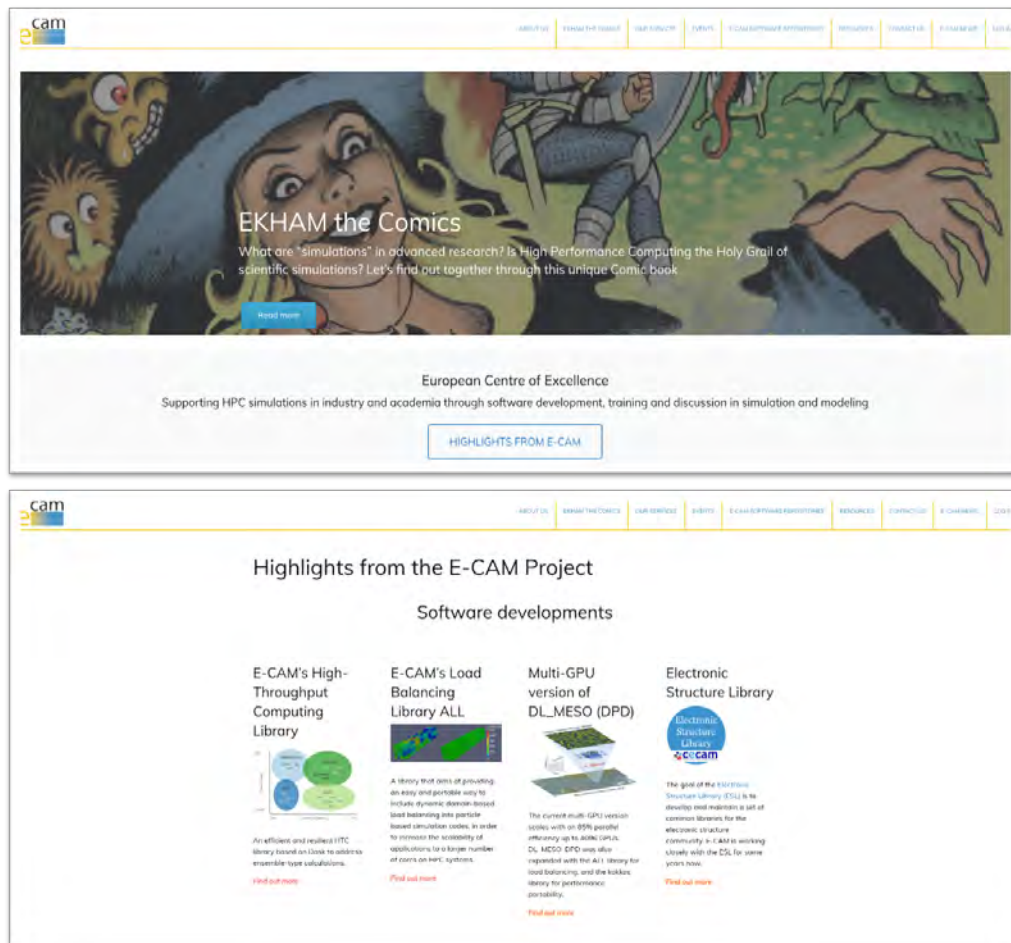
Figure 3: Upper image: Snapshot of the home page evidencing the highlights from the E-CAM project page. Lower image: snapshot of the highlights page, showing only the category "software developments".

2.2   E-CAM webpage on the CECAM website

In view of expanding the access points to E-CAM we have developed an E-CAM web-page on the CECAM website: https://www.cecam.org/e-cam . CECAM is the coordinator of E-CAM and plays a critical role in E-CAM's sustainability. This initiative ensures that E-CAM's most important results continue to be disseminated and communicated to the target groups even after the EU funding period, as well as the future activities that we plan to run beyond March 2021 (project end-date). A snapshot of this page is in Fig. 4.

The page was built using elements of the CECAM home page itself. It contains quick access points to our services and most important results so far. More specifically, it features highlights from the project (sec. 3), our repositories (software and training portal), success stories and events. Furthermore, it explains our goals and features our latest news.

Figure 4: Snapshot of the E-CAM webpage on the CECAM website.

3   E-CAM Newsletters

Three issues of the E-CAM newsletter were published. As reported previously, we use a continuous mode of dissemination. That is, news are reported as they come in, and Newsletters contain the most important items published in the months preceding its release. All the newsletters submitted during the project are located here.

Issue 14 - September 2020 (section 3.1) - The newsletter included the following items.

1. An introduction to E-CAM's HTC library addressing interactive HTC workloads with HPC characteristics.

2. A success story on a collaboration between the EU H2020 E-CAM and MaX Centres of Excellence, and the Swiss NCCR MARVEL entitled "Accelerating the design and discovery of materials with tailored properties using first principles high-throughput calculations and automated generation of Wannier functions"

3. An E-CAM Industrial Case Study: Calculations for Applications in Photovoltaic Devices

4. Two featured Software Modules: "An extendable Python toolbox to compute scattering of electrons with a given kinetic energy in liquids and amorphous solids", and "Minimal distance segment to segment with Karush-Kuhn-Tucker conditions"

5. Five new scientific publications: " Gap variability upon packing in organic photovoltaics", "Automated high-throughput Wannierisation", "PANNA: Properties from Artificial Neural Network Architectures", "The CECAM Electronic Structure Library and the modular software development paradigm", and, "Unfolding the prospects of computational (bio)materials modelling".

6. Submitted deliverable: D7.9: on hardware developments that will affect the scientific areas of interest to E-CAM and detailed feedback to the project software developers including: discussion of project software needs with hardware and software vendors; completion of survey of what is already available for particular hardware platforms; and, detailed output from direct face-to-face session between the project end-users, developers and hardware vendors.

Issue 15 - December 2020 (section 3.2) - The newsletter included the following items.

1. A report on a ongoing successful PRACE-ICEI proposal involving E-CAM, FocusCoE, HPC Carpentry and EESSI join forces to bring HPC resources to the classroom in a simple, secure and scalable way entitled "LearnHPC: dynamic creation of HPC infrastructure for educational purposes"

2. A report on a Load Balancing Library (ALL) developed within E-CAM at the Julich Supercomputing Center that aims to provide an easy and portable way to include dynamic domain-based load balancing into particle based simulation codes.

3. Identifying exciting and original tools to engage the general public with advanced research is an intriguing and non-trivial challenge for the scientific community. E-CAM decided to try something unusual, and embarked on an interesting and slightly bizarre experience: collaborating with experts and artists to use comics to talk about HPC and simulation and modelling. Three additional articles have been produced: "Comics & Science ? The E-CAM issue: an experiment in dissemination", "Conversation with the authors of Ekham the Wise", and, "The E-CAM Issue of Comics & Science presented at the international comics festival of Lucca 2020".

4. An article about E-CAM was released with the Autumn edition of the EU Research Magazine. The piece describing E-CAM's work in software development,training and interactions with industry.

5. Three Featured Software Modules: "Dask-traj", PerGauss, Periodic Boundary Conditions for gaussian bases", and, "Load balancing for multi-GPU DL_MESO".

6. Two new scientific publications "Quantum Monte Carlo determination of the principal Hugoniot of deuterium", and "Towards blood flow in the virtual human: efficient self- coupling of HemeLB"

7. Two upcoming events:"High throughput Computing with Dask", and, "an Extended Software Development Workshop in HPC for mesoscale Simulation"

Issue 16 - April 2021 (section 3.3) - The newsletter included the following items.

1. An E-CAM interview on the Implementation of High-Dimensional Neural Network Potentials for coarse-grained models with Andreas Singraber, and the ensemble of his work to improve user accessibility to the code via the LAMMPS package and new tools that he developed during his E-CAM pilot project.

2. Computation based methods play a growing role in all stages of accelerated medicine pipelines responding to industry challenges of drug substance development as explained by Dr. Jacek Zeglinski in this E-CAM interview

based on his experience working with APC, an Irish based company founded in 2011. APC has grown organically partnering with companies across the world, large and small, to bring medicines to market at unprecedented speed.

3. Technical success story on the development of an HTC-based, scalable committor analysis tool in OpenPath-Sampling opens avenues to investigate enzymatic mechanisms linked to Covid-19

4. Recognition of an E-CAM developed Molecular Switch as a disruptive technology, with initial applications as a diagnostic sensor for COVID 19 and influenza. The sensor was developed using using massively parallel computation, rare-event methods, and genetic engineering.

5. Five Featured Software Modules: "ALL Load Balancing Library", "DL_MESO (DPD) on Kokkos for enhanced performance portability", "HemeLB, a CoE collaboration", "n2p2 - Improved link to HPC MD software", and, "MaZe, Mass-Zero Constrained Dynamics for Orbital Free Density Functional Theory".

6. A new scientific publication "Transition Path Sampling as Markov Chain Monte Carlo of Trajectories: Recent Algorithms, Software, Applications, and Future Outlook".

7. Two Upcoming Extended Software Development Workshops to be held in October 2021: "Improving bundle libraries", and, "HPC for simulation of complex phenomena".

8. Three E-CAM deliverables: "D2.6: Electronic structure E-CAM modules Nine software modules delivered to the E-CAM repository in the area of Electronic Structure", D3.6: Quantum dynamics E-CAM modules - Six software modules delivered to the E-CAM repository in the area of Quantum Dynamics", and " D4.6: Meso- and multi-scale modelling E-CAM modules - Nine software modules delivered to the E-CAM repository in the area of Meso- and Multi-scale modelling".

3.1   Newsletter September 2020

Display problems? Open this email in your [web browser](#).

Newsletter

September 2020

[Addressing interactive HTC workloads with HPC characteristics: introduction to E-CAM's HTC library](#)

Traditionally high-throughput computing (HTC) workloads are looked down upon in the HPC space, however the scientific use case for extreme-scale resources required by coordinated HTC workflows exists. For such cases where there may be thousands of tasks each requiring peta-scale computing, E-CAM has extended the data-analytics framework [Dask](#) with a capable and [efficient library](#) to handle such workloads.

Read more

[Accelerating the design and discovery of materials with tailored properties using first principles high-throughput calculations and automated generation of Wannier functions](#)
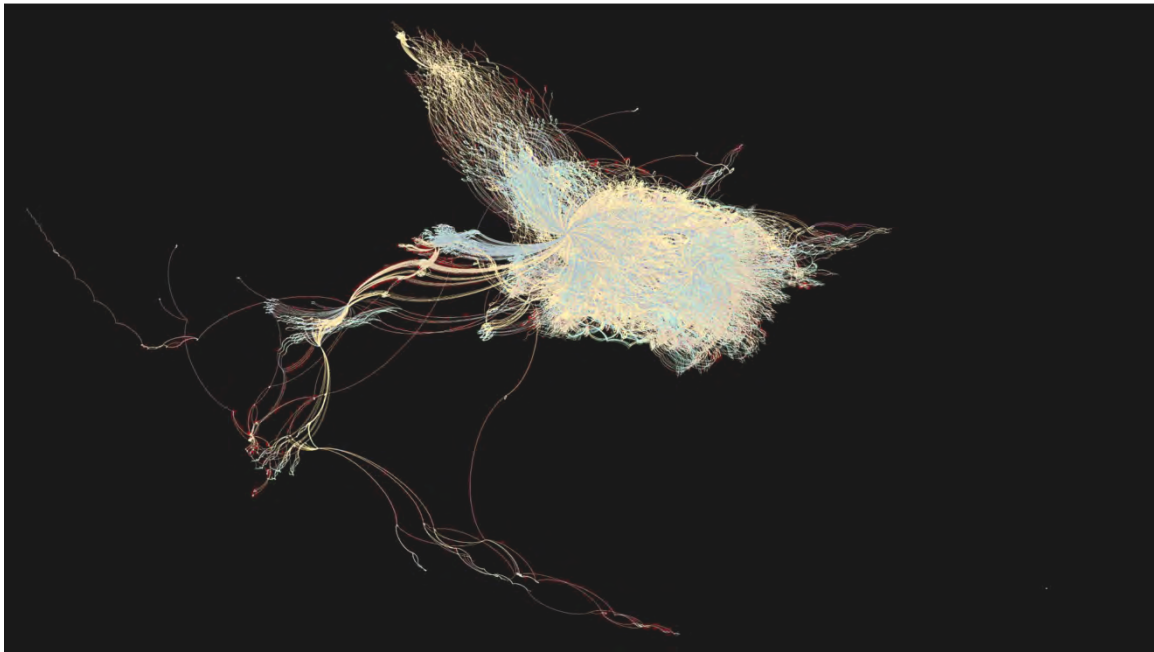

In a recent paper[https://doi.org/10.1038/s41524-020-0312-y], researchers from the Centres of Excellence [E-CAM](#) and [MaX](#), and the centre for Computational Design and Discovery of Novel Materials [NCCR MARVEL](#), have proposed a new procedure for automatically generating Maximally-Localised Wannier functions for high-throughput frameworks. The methodology and associated software can be used for hitherto difficult cases of entangled bands, and allows the electronic properties of a wide variety of materials to be obtained starting only from the specification of the initial crystal structure, including insulators, semiconductors and metals. Industrial applications that this work will facilitate include the development of novel superconductors, multiferroics, topological insulators, as well as more traditional electronic applications.

Read more

[E-CAM Industrial Case Study: Calculations for](#)

Applications in Photovoltaic Devices
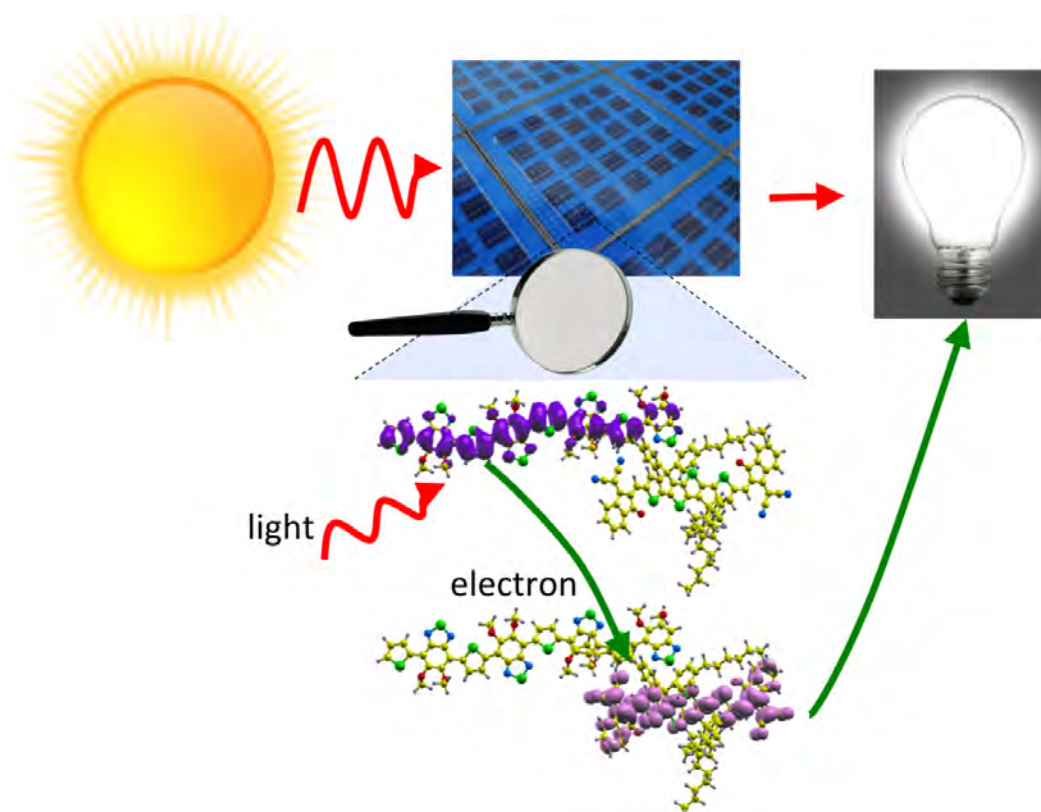
The need to find easily renewable and environmentally friendly energy sources alternative to the traditional fossil fuels is nowadays a global quest. The solar energy is a promising candidate and Organic Solar Cells have attracted attention. In this collaboration with Merck, E-CAM scientists have used electronic structure calculations to study how a key magnitude – the HOMO-LUMO band gap – changes with respect to the molecular disposition of the donor-acceptor molecule pair.

**Read more**

Featured Software Modules

[An extendable Python toolbox to compute scattering of electrons with a given kinetic energy in liquids and amorphous solids](#)

CLstunfti is an extendable Python toolbox to compute scattering of electrons with a given kinetic energy in liquids. It uses a continuum trajectory model with differential ionization and scattering cross sections as input to simulate the motion of the electrons through the medium.

Read more

[Minimal distance segment to segment with Karush-Kuhn-Tucker conditions](#)
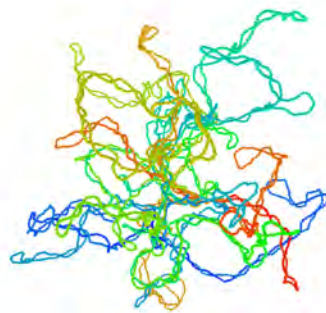
To preserve topology in systems of entangled polymers the minimal distance between two bonds needs to be determined. Once that is done, one can apply either a soft potential or a hard potential to avoid the crossing of two bonds. With this module we propose to determine the minimal distance between two segments with the help of the Karush-Kuhn-Tucker conditions.

Read more

Recent Publications

Gap variability upon packing in organic photovoltaics

D. López-Durán , Etienne Plésiat, Michal Krompiec and Emilio Artacho, *PLoS ONE* 2020, 15(6): e0234115 DOI:

https://doi.org/10.1371/journal.pone.0234115

Automated high-throughput Wannierisation

Valerio Vitale, Giovanni Pizzi, Antimo Marrazzo, Jonathan R. Yates, Nicola Marzari and Arash A. Mostofi, *npj Comput Mater* 2020, 6, 66
DOI:
https://doi.org/10.1038/s41524-020-0312-y

PANNA: Properties from Artificial Neural Network Architectures

Ruggero Lot, Franco Pellegrini, Yusuf Shaidu, Emine Küçükbenli *Comput. Phys. Commun.* 2020, 256, 107402
DOI:
https://doi.org/10.1016/j.cpc.2020.107402

The CECAM Electronic Structure Library and the modular software development paradigm

J. Chem. Phys. 2020, 153, 024117
DOI: 10.1063/5.0012901
Open access version

The electronic structure library project is an initiative to stimulate, coordinate and amplify the efforts in library sharing already started within the electronic

structure community. It was initiated by CECAM, which continues its support together with E-CAM, spearheading a push within the community for a better model of electronic structure software development which, it is hoped, will enhance dynamism, versatility, maintainability and optimisation of electronic structure codes. It is believed it will also allow the re-engineering efforts needed for deployment of electronic codes on novel computer architectures to be carried out more efficiently, widely, and by professionals close to hardware companies and HPC centres.

Unfolding the prospects of computational (bio)materials modelling

G. J. Agur Sevink, Jozef Adam Liwo, Pietro Asinari, Donal MacKernan, Giuseppe Milano, and Ignacio Pagonabarraga
J. Chem. Phys. 2020, 153, 100901
DOI: https://doi.org/10.1063/5.0019773
Open access version

Community-driven review on the history, developments, and challenges facing coarse graining and multiscale simulation and a set of recommendations on how the latter may be addressed was recently published. The perspective emerged in part from a two-week school and workshop including some 35 experts in this area hosted by the Lorenz Center in the Netherlands.

Read more

Submitted deliverables

D7.9: Hardware Developments V*

Update on the hardware developments that will affect the scientific areas of interest to E-CAM and discussion of project software needs with hardware and software vendors.

*This is a draft document delivered to the European Commission but not yet

approved

[ALL DELIVERABLES](#)

Access our software repository	**Online Training Portal**	**Ask a technical question**

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 676531

Legal notice

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MailPoet

3.2 Newsletter December 2020

Newsletter

December 2020

[LearnHPC: dynamic creation of HPC infrastructure for educational purposes](#)


In a newly successful [PRACE-ICEI](#) proposal, [E-CAM](#), [FocusCoE](#), [HPC Carpentry](#) and [EESSI](#) join forces to bring HPC resources to the classroom in a simple, secure and scalable way. Our plan is to reproduce the model developed by the Canadian open-source software project [Magic Castle](#). The proposed solution creates virtual HPC infrastructure(s) in a public cloud, in this case on the [Fenix Research Infrastructure](#), and generates temporary event-specific HPC clusters for training purposes, including a complete scientific software stack. The scientific software stack is fully optimised for the

available hardware and will be provided by the European Environment for Scientific Software Installations (EESSI).

Read more

The ALL Load Balancing Library
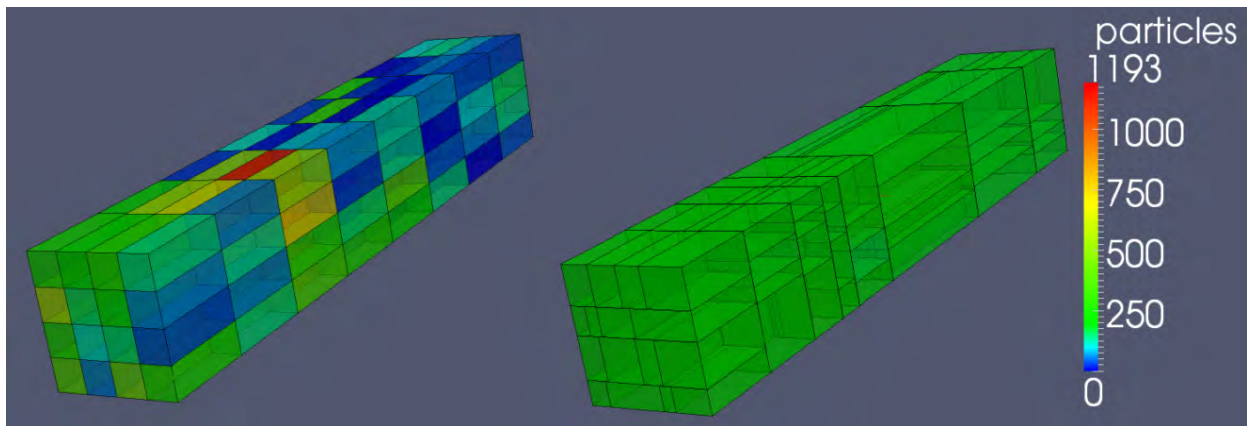
Scalability of parallel applications depends on a number of characteristics, among which is efficient communication, equal distribution of work or efficient data lay-out. Especially for methods based on domain decomposition, as it is standard for, e.g., molecular dynamics, dissipative particle dynamics or particle-in-cell methods, unequal load is to be expected for cases where particles are not distributed homogeneously, different costs of interaction calculations are present or heterogeneous architectures are invoked, to name a few. For these scenarios the code has to decide how to redistribute the work among processes according to a work sharing protocol or to dynamically adjust computational domains, to balance the workload. The A Load Balancing Library (ALL) developed within E-CAM at the Julich Supercomputing Center aims to provide an easy and portable way to include dynamic domain-based load balancing into particle based simulation codes.
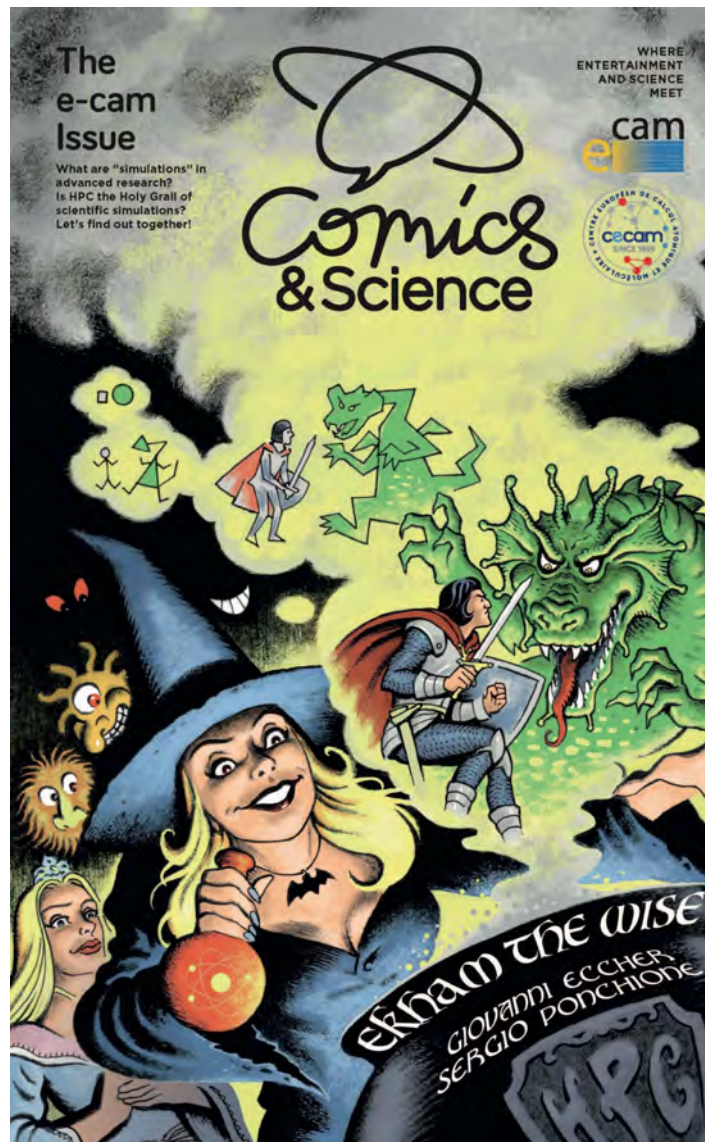
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EKHAM the Comics

Identifying exciting and original tools to engage the general public with advanced research is an intriguing and non-trivial challenge for the scientific

community. E-CAM decided to try something unusual, and embarked on an interesting and slightly bizarre experience: collaborating with experts and artists to use comics to talk about HPC and simulation and modelling!

Read more

Join us in disseminating the story of EKHAM The Wise, to pursue together our mission to promote modelling, simulation and HPC among students of all ages and interested public!

Related Articles

[Comics & Science ? The E-CAM issue: an experiment in dissemination](#)

[Conversation with the authors of *Ekham the Wise*](#)

[The E-CAM Issue of Comics&Science presented at the international comics festival of Lucca 2020](#)

[E-CAM article on the EU Research Magazine](#)

An article about E-CAM was released with the Autumn edition of the EU Research Magazine. The piece consists on an interview to Ignacio Pagonabarraga, Sara Bonella, Donal Mackernan and Jony Castagna, and describes E-CAM's work in software development, training and interactions with industry.

Read more

Featured Software Modules

Dask-traj

For analysis of MD simulations [MDTraj](#) is a fast and commonly used analysis. However MDTraj has limitations, such as the requirement that the whole trajectory and result of the computation fits into memory. [Dask-traj](#) rewrites part of MDTraj to work with [Dask](#) in order to achieve out-of-memory computations, and combined with [dask-distributed](#) results in possible out-of-machine parallelisation, essential for HPCs and a (surprising) speed-up even on a single machine.

Read more

PerGauss, Periodic Boundary Conditions for gaussian bases

The module PerGauss (**Per**iodic **Gauss**ians) consists on an implementation of periodic boundary conditions for gaussian bases for the [Quantics](#) program package. In quantum dynamics, the choice of coordinates is crucial to obtain meaningful results. While xyz or normal mode coordinates are linear and do not need a periodical treatment, particular angles, such as dihedrals, must be included to describe accurately the (photo-)chemistry of the system under consideration. In these cases, periodicity can be taken into account, since the value of the wave function and hamiltonian repeats itself after certain intervals.

Read more

Load balancing for multi-GPU DL_MESO
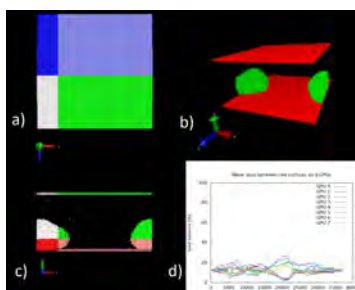
This module concerns the implementation of the E-CAM Load Balancing Library (ALL) in the multi-GPU version of DL_MESO_DPD code. The intention is to allow for better performance when modelling complex systems with DL_MESO_DPD, like large proteins or lipid bilayers, redistributing the work load across the GPUs.

<div align="center">

Read more

</div>

ALL FEATURED MODULES

<div align="center">

Recent Publications

</div>

<div align="center">

Quantum Monte Carlo determination of the principal Hugoniot of deuterium

Michele Ruggeri, Markus Holzmann, David M. Ceperley, and Carlo Pierleoni
Phys. Rev. B **102**, 144108
DOI: https://doi.org/10.1103/PhysRevB.102.144108
Open access version

Towards blood flow in the virtual human: efficient self-coupling of HemeLB

J. W. S. McCullough, R. A. Richardson, A. Patronis, R. Halver, R. Marshall, M. Ruefenacht, B. J. N. Wylie, T. Odaker, M. Wiedemann, B. Lloyd, E. Neufeld, G. Sutmann, A. Skjellum, D. Kranzlmüller and P. V. Coveney

</div>

Interface Focus **11**: 20190119

DOI: http://dx.doi.org/10.1098/rsfs.2019.0119 (open access)

E-CAM PUBLICATIONS

Upcoming Online Events

High Throughput Computing with Dask

Location: ONLINE / CECAM-FR-MOSER
Organisers: Alan O'Cais, David Swenson
Dates: 21st January, 4th and 11th February 2021

Read more

E-CAM EVENTS CALENDAR

Extended Software Development Workshop in HPC for mesoscale simulation

Location: ONLINE / CECAM-UK-DARESBURY
Organisers: Jony Castagna, Michael Seaton, Silvia Chiacchiera, Leon Petit
Dates: 18th - 22nd January 2021

Read more

All the best for 2021 !!

Characters from the story of *Ekham the wise.*
[*https://www.e-cam2020.eu/e-cam-issue-of-comics-science/*]

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This project has received funding from the European Union's Horizon 2020
research and innovation programme under grant agreement No 676531

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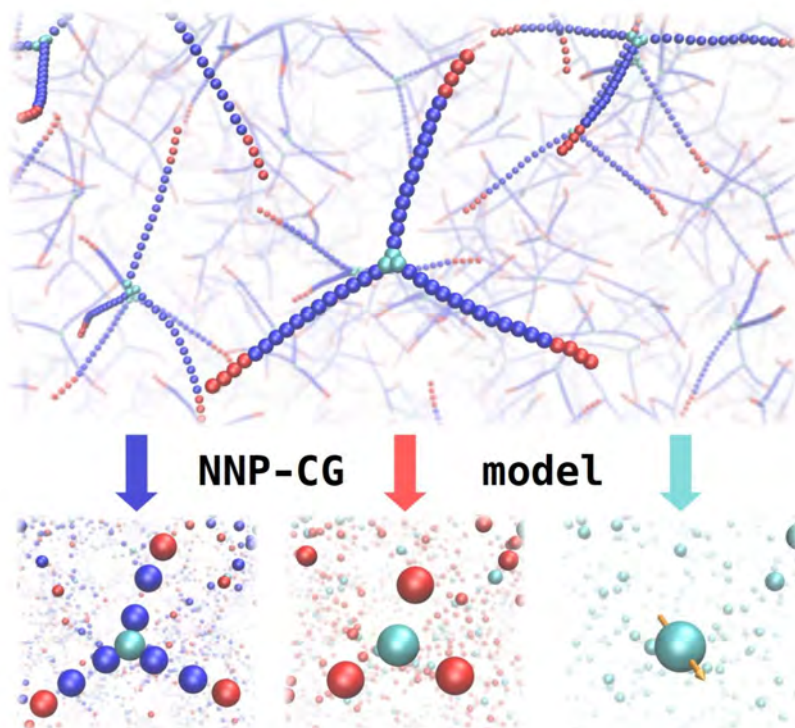
MailPoet

3.3 Newsletter April 2021

# Implementation of High-Dimensional Neural Network Potentials

In this conversation with Andreas Singraber, post-doc in E-CAM until last month, we will discover the ensemble of his work to expand the Neural Network Potential (NNP) Package n2p2 and to improve user accessibility to the code via the LAMMPS package. Andreas will talk about new tools that he developed during his E-CAM pilot project, that can provide valuable input for future developments of NNP based coarse-grained models. He will describe how E-CAM has impacted his career and led him to recently integrate a software company as a scientific software engineer.

[**Read more**]

## Challenges to Industry of drug substance development
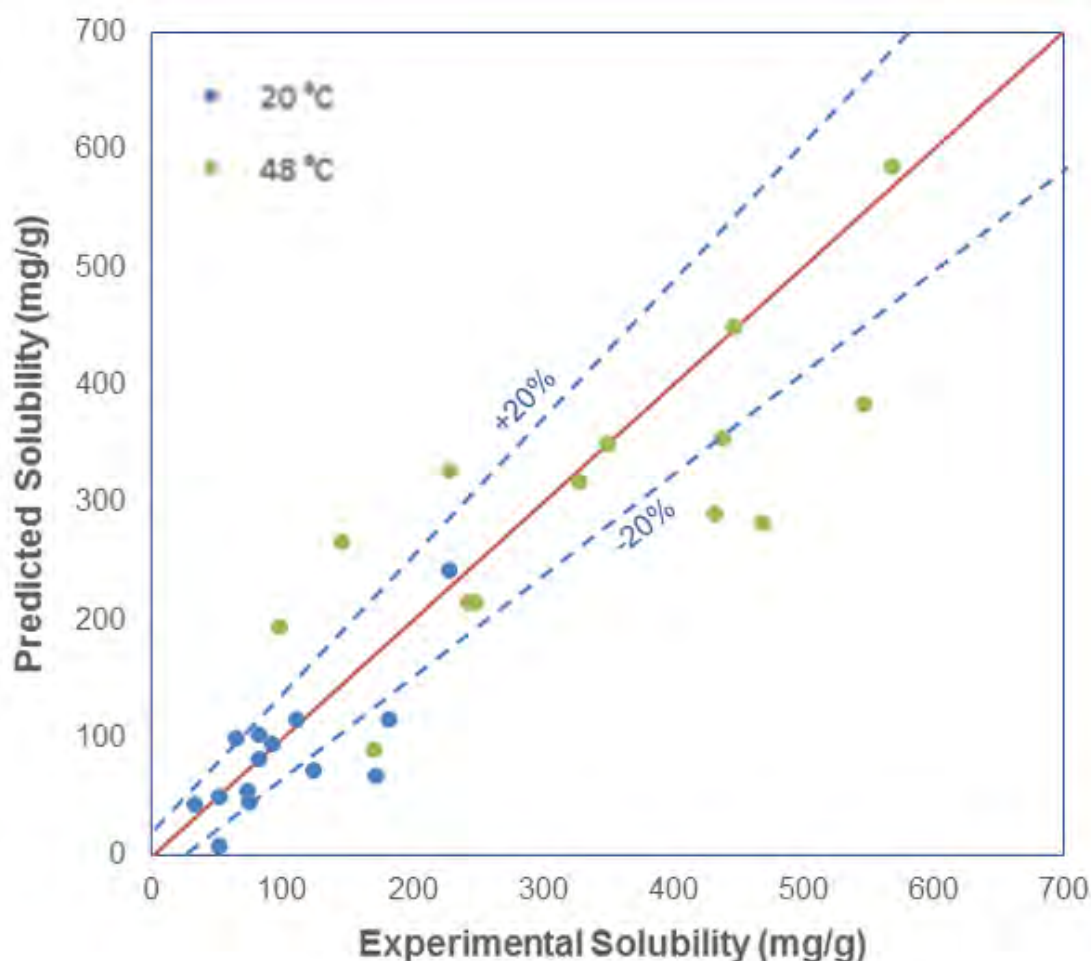
APC was created in 2011 by Dr. Mark Barrett and Prof. Brian Glennon of the University College Dublin School of Chemical and Bioprocess Engineering with a mission to harness state-of-the-art research methods & know-how to accelerate drug process development. Since then it has grown organically partnering with companies across the world, large and small, to bring medicines to market at unprecedented speed. Computation-based methods play a growing role in all stages of its medicine pipeline as explained by Dr. Jacek Zeglinski in this E-CAM interview on challenges to Industry of drug substance development.

Read more

Development of an HTC-based, scalable committor analysis tool in OpenPathSampling opens avenues to investigate enzymatic mechanisms linked to Covid-19
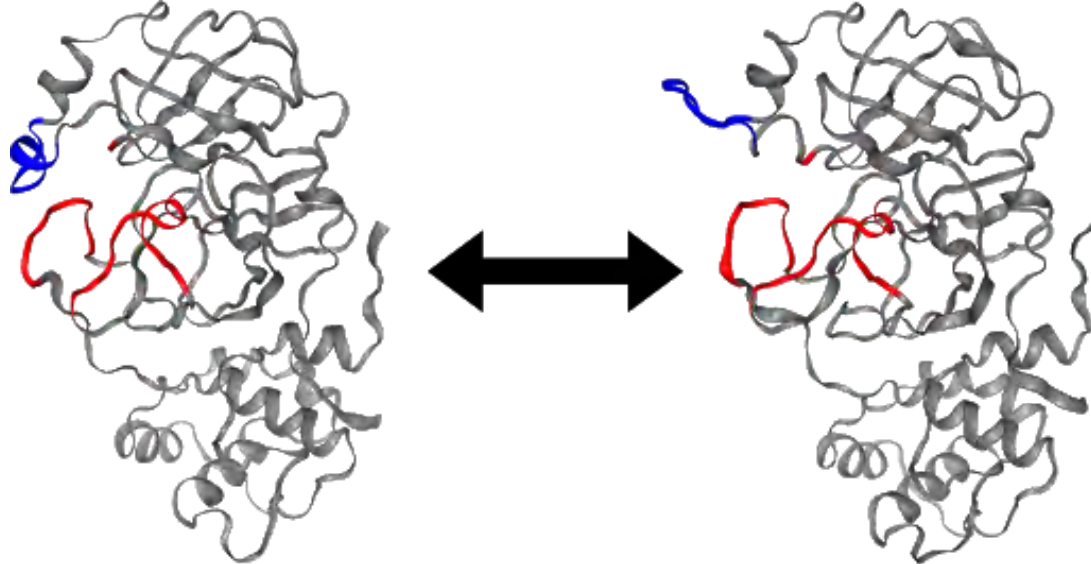
The E-CAM HPC Centre of Excellence and a PRACE team in Wroclaw have teamed up to develop High Throughput Computing (HTC)-based tools to enable the computational investigation of reaction mechanisms in complex systems. Committor analysis is a computationally expensive tool, but allows for powerful simulations. In this project, the main goal was to integrate the committor analysis methodology with the existing software application OpenPathSampling (OPS), which is performance portable across a range of HPC hardware and hosting sites. Integrating OPS and the HTC library resulted in an unprecedented parallelised committor simulation capability. These tools are now being implemented for a committor simulation of the SARS-CoV-2 main protease. The data will provide insight into the dynamics of the protease loop region and the mechanism of its gate-like activity.

Read more

Proof of concept : recognition as a disruptive technology
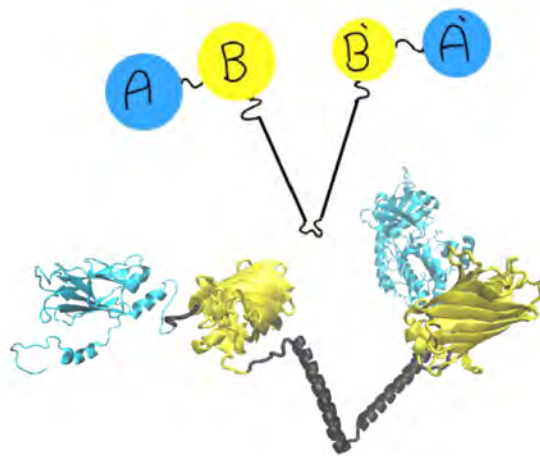
The transformation of a beautiful idea born via simulation into a commercial opportunity is recognised as a disruptive technology. At the heart of this ongoing story is advanced simulation using massively parallel computation, rare-event methods, genetic engineering, and a molecular switch developed during an E-CAM pilot project, with an initial application as a point-of-care medical diagnostic for COVID-19 and influenza. This work has recently received an award by NovaUCD.
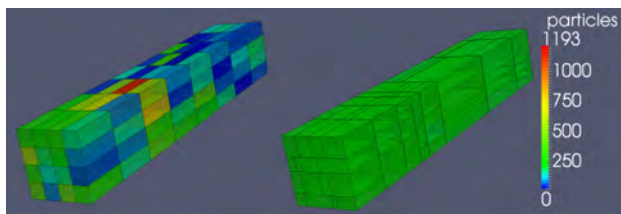
Read more

Featured Software Modules

ALL library implementation in HemeLB, a CoE collaboration

DL_MESO (DPD) on Kokkos for enhanced performance portability

This work relates to the implementation of a performance portable version of DL_MESO (DPD) using the Kokkos library. This allows to run DL_MESO on NVidia GPUs as well as on other GPUs or architectures (many-core hardware like KNL), allowing performance portability as well as

This module describes the work done in E-CAM in cooperation with the CompBioMed Centre of Excellence, on the integration of the load balancing library ALL on the HemeLB code.
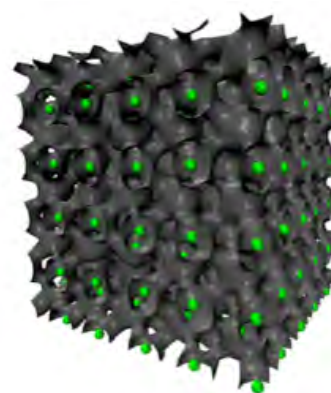
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separation of concern between computational science and HPC.

Read more

MaZe, Mass-Zero Constrained Dynamics for Orbital Free Density Functional Theory

This program performs Orbital-Free Density Functional Theory Molecular Dynamics using the Mass-Zero (MaZe) constrained molecular dynamics approach described in Phys. Chem. Chem. Phys., 2020, 22, 10775-10785.

Read more

n2p2 - Improved link to HPC MD software

This module improves the connection of *n2p2* to HPC software, in particular to LAMMPS, by creating a pull request to the official LAMMPS repository. Furthermore, the build process for the *n2p2* interface library is enhanced to allow for a selective activation of different interfaces.

Read more

Recent publication

Transition Path Sampling as Markov Chain Monte Carlo of Trajectories: Recent

Algorithms, Software, Applications, and Future Outlook

Synopsis: The development of enhanced sampling methods to investigate rare but important events has always been a focal point in the molecular simulation field. Such methods often rely on prior knowledge of the reaction coordinate. However, the search for this reaction coordinate is at the heart of the rare event problem. Transition path sampling (TPS) circumvents this problem by generating an ensemble of dynamical trajectories undergoing the activated event.

Read more

Upcoming Extended Software Development Workshops
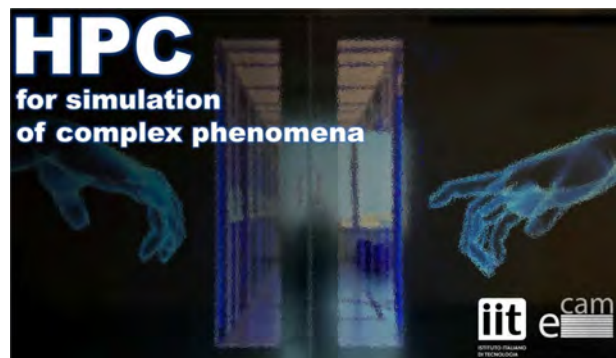
Improving bundle libraries

Organisers:

Emilio Artacho, Volker Blum, Fabiano Corsetti, Micael Oliveira, Nick Papior,Yann Pouillon

Dates: Oct 11-22, 2021

Info and registration:

https://www.cecam.org/workshop-details/23

HPC for simulation of complex phenomena

Organisers:

Andrea Cavalli, Sergio Decherchi, Marco Ferrarotti, Walter Rocchia

Dates: Oct.11-15, 2021

Info and registration :

https://www.cecam.org/workshop-details/1069

Submitted deliverables

D1.6: Classical MD E-CAM Modules V*

Nine software modules delivered to the E-CAM repository in the area of Classical Molecular Dynamics

D2.6: Electronic structure E-CAM modules V*

Nine software modules delivered to the E-CAM repository in the area of Electronic Structure

D3.6: Quantum dynamics E-CAM modules V*

Six software modules delivered to the E-CAM repository in the area of Quantum Dynamics

D4.6: Meso- and multi-scale modelling E-CAM modules V*

Nine software modules delivered to the E-CAM repository in the area of Meso- and Multi-scale modelling

*This is a draft document delivered to the European Commission but not yet approved

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4 Conclusions

This deliverable, D9.5 included a summary of the impact of our dissemination strategy measured in terms of web traffic statistics; updates to the E-CAM website to intensify efforts to disseminate results and ensure sustainability of the website beyond the current funding; and, newsletters issues published since the submission of D9.4.

During this last period we made an additional effort to disseminate on our website the results obtained during the project's final ramp. Consequently, the content of the E-CAM website increased considerably, mainly on the following pages on the website:

- Individual pilot project pages;
- Case studies/Success stories page
- Events calendar
- Scientific publications page
- News-blog page.

Additionally, we updated the website to include:

- Biosensor news-blog page;
- Highlights from the E-CAM project page.

We have developed an E-CAM web-page on the CECAM website: https://www.cecam.org/e-cam to ensure that E-CAM's most important results continue to be disseminated and communicated to the target groups even after the EU funding period, as well as the future activities that we plan to run beyond March 2021 (project end-date).

We noted that a very large amount of new material has been disseminated since July 1 2020, notwithstanding the difficulties produced by the pandemic. Many of these are to be seen in the last three issues of the E-CAM newsletter. They together with recent workshops held online, software, scientific results and new IP (not described explicitly here for commercial reasons) are intensifying interest in E-CAM within the simulation community and beyond.

Finally, although the current EU funding will close end of March 2021, a significant number of dissemination related actions will continue including the following.

- At least four workshops are planned to be held during the latter part of 2021 when the health constraints due to the pandemic are lightened including two E-CAM ESDW's: High performance computing for simulation of complex phenomena; Improving Bundle Libraries; a face-to-face follow-up ESDW "Inverse Molecular Design & Inference: building a Molecular Foundry"; and, the follow-up face-to-face SCOW Simulation of open systems in Chemistry, Pharma, Food Science and Immuno-diagnostics: Rare-event methods at constant chemical potentials including constant pH.

- The sensor development work associated with one pilot project is intensifying including software development, simulation on HPC systems, as well as experimental and commercial activities. This has included hiring of software engineers in part trained at E-CAM ESDW's. There is a good chance that this work will contribute to E-CAM dissemination and sustainability into the future, given the success that it is already having.

- At least 4 undergraduate thesis projects having a strong E-CAM training component are ongoing.

References

Acronyms Used

CECAM Centre Européen de Calcul Atomique et Moléculaire
ESDW Extended Software Development Workshop
PDRA Postdoc Research Associate
CoE   Centres of Excellence

URLs referenced

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