

E-CAM Public Wiki-like pages and newsletters IV E-CAM Deliverable 9.4

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Executive Summary

This deliverable is an update of D9.3: E-*CAM Public Wiki-like pages and newsletters III* [1] and consists of: (1) an analysis of the impact of the revised dissemination strategy over the last five quarters; (2) lessons learned and actions to improve visibility; (3) a description of the key updates to the project's primary access points; and, (4) the issues of the newsletters published over this period.

Regarding (1) the analysis was performed using web-statistics of the number of visitors to the E-CAM website over the last 5 quarters. The total number of visitors to the E-CAM website since February 10, 2017 (from when we started collecting web traffic data statistics) is 175264, with 39048 visiting our pages from April 1 2019 until June 30 2020, equivalent to an average of about 90 visitors per day. A large number of pages have been consulted (measured in terms of hits or visits). In particular, the calendar of events and the software repositories, which are core E-CAM activities, are consistently attracting high interest. There has been a noticeable surge of interest in Q2 of 2020 for our technical pages such as the scientific publications page and the training portal, with a 50% increase to the scientific publications page.

Regarding (2), ongoing efforts to improve visibility include:

- the promotion of E-CAM events which will now run online (the COVID-19 pandemic and associated lock-downs starting in early March 2020 led to a postponement of all face to face events due to the closure of universities. Some of these events are now being scheduled as webinars);
- collaboration with the FocusCoE to promote E-CAM activities to the wider scientific community and enhance interactions with industry, and public awareness of HPC;
- increase focused dissemination efforts regarding recent E-CAM Software development initiatives such as: the Load balancing library, HTC library releases, and an E-CAM refactored codes with exceptional scaling on massively parallel platform; and,
- improve the accessibility of the online training portal.

Regarding (3), we made an additional effort to display on our website more results targeted to the general public and industry and engaged in the following projects:

- a Comic book about E-CAM and how it enables modelling, simulation and HPC;
- an interview with Massimo Noro, Director of Business Development at the Science and Technology Facilities Council (STFC) and former science leader of the HPC division at Unilever;
- a news piece for the EU Research Magazine targeted at all people interested in science;
- a common calendar with other HPC events running in Europe.

Finally, (4) is composed of all the issues of the E-CAM newsletter published during the period covered by this report. They were disseminated via our communication channels (e-mail, website, social networks) among our target groups. The newsletter is integrated as a News Blog in the E-CAM website, where material is continuously delivered and is web-search-able. In addition to opinion pieces, interviews and success stories, the newsletter also includes short summaries of featured software modules, case studies, scientific publications and deliverables.

In the final section of this report we summarize our dissemination activities over the last year and outline our plans for the next one. We have also developed a wish list of enhancements for the E-CAM Training Portal so as to improve user accessibility. Collaborations with other players are also being explored to ensure the sustainability of our training portal, which we believe is extremely valuable for the community, especially in a period where events are running mostly online with lectures being recorded and stored massively.

1 Introduction

This deliverable, D9.4 *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) a corresponding analysis of content that attracts more interest; (3) efforts to improve visibility; (4) updates to the E-CAM website; (5) updates to the online training portal and software library; (6) newsletters issues published since submission of D9.3[1] until April 2020; and (7) a summary of our plans for the next period. 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 and delays in reporting. As a consequence we have taken the opportunity to include in this report data from Q2 of 2020 (i.e. to report over 5 rather than the originally planned 4 quarters).

1.1 Scope of this update

The previous deliverable D9.3 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 175264, with 39048 visiting our pages from April 1 2019 till June 30 2020.

Figure 1 shows the average daily visitors to the E-CAM website over 5 quarters, from April 2019 to June 2020, 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 April 2019 to June 2020.

There are on average about 90 visitors per day to the website, with a decrease in the winter quarters presumably due to fewer events taking place at that time due to university teaching constraints. The fact that our face to face events had to be postponed due to the COVID-19 pandemic also had an impact on the number of visits to our website in Q1 and Q2 of 2020. As seen below, our calendar of events is the page on our website receiving the most visits. The fact that other events where E-CAM was planning to be present were also cancelled or postponed due to the pandemics, has probably impacted on these numbers as well.

The homepage received 31,751 visits from April 1 2019 till June 30 2020. Other technical pages receiving a large number of visits include Calendar of events (4815), Software Repositories (1882), E-CAM Partners (720), Publications (615), E-CAM Services (526), Pilot Projects (565), E-CAM News(526), Online Training Portal (502), Deliverables (487) and Case

Studies (446). There has been a noticeable surge of interest in Q2 of 2020 for our technical pages, with a 50% increase to the scientific publications page.

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. This is an important outcome, since software development and training in software development through our ESDW and transversal training events, are core E-CAM activities. Our calendar of events also include state-of-the-art and scoping workshops, targeted at academics and industry and that identify areas of mutual interest.
- There has been an increase of interest in E-CAM publications 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 deliverables and pilot projects web-pages could get further attention. However, it is worth noting a reduction might be expected as the number of postdocs employed in the pilot projects is dropping as the end of the current funding of the CoE is drawing near.
- There has been an increase of interest in Q2 of 2020 on the E-CAM online training portal page on the E-CAM website in respect to previous quarters. This is aligned with the increase of interest on E-CAM's Online Training material at https://training.e-cam2020.eu/ as given by google analytics.

1.2.2 Actions to improve visibility

Below we highlight actions to improve project visibility, some of which are already work in progress.

- 1. Promote our events which will now run was online webinars.
 - Due to the COVID-19 pandemic, many of our events from the 2020 program had to be postponed, which impacted project visibility as can be seen in Fig. 1. Five of these events will now run online in a webinar type format. Some will be composed of several sessions. For more information on our program see https://www.e-cam2020.eu/calendar/. Efforts will be dedicated to promoting these events within our contacts, website and social media.
- 2. Collaborate with the CoE FocusCoE to promote E-CAM activities to the wider scientific community and enhance interactions with industry, and public awareness of HPC.
 - E-CAM developed a system to automatically push featured articles to the website dedicated to the CoEs at www.hpccoe.eu, which is managed by FocusCoE. We will continue to use this tool during the next period.
 - Our events are advertised on the HPC CoE website at https://www.hpccoe.eu/events/.
 - E-CAM will participate to the 3rd EMMC International Workshop scheduled for March 2-4, 2021 (online meeting), and FocusCoE is helping to promote our participation to the meeting.
- 3. Exploit E-CAM's Comic book (see sec. 2.1.1).
 - A Comics about E-CAM and how it enables simulation, modelling and HPC has been published, and is available on our website at https://www.e-cam2020.eu/e-cam-issue-of-comics-science/.
 - It has been promoted on our website, among our contacts, and on social media, and we are collecting viewing and downloading statistics which we will report on the last deliverable of this series.
 - We are currently exploring different ways to promote it, including on other websites (CECAM, hpccoe, Comics&Science, E-CAM partners websites, EU news websites, etc), at Comics fairs and at schools and universities classrooms.
- 4. Focused dissemination efforts regarding E-CAM Software development initiatives such as the Load balancing library, HTC library releases, and E-CAM refactored codes with exceptional scaling on massively parallel plat-forms.
 - This is an ongoing effort, with for example (1) the "modules of the Month" publications on our website; (2) the news items associated to our libraries such as https://www.e-cam2020.eu/e-cam-htc-library/ and (3) the case studies reporting on our software developments done in collaboration with other initiatives such as the one described here.
 - Given the increased interest in E-CAM publications (see sec. 1.2.1), stressing their relation to corresponding software modules will help to further increase the impact of both.

All of these proposed actions have been or are in the process of being done. Specific actions on the training portal are below, which will help to enhance the accessibility of this platform. More details are given in Section 2.3.1.

- Improve accessibility (i.e. readability, appeal and utility) of the training portal page on our website at https://www.e-cam2020.eu/e-cam-online-training-portal/ through a more informative page using a magazine format including short tweet-able descriptions of each key item. A video explaining how to use the portal is now present which should facilitate its exploitation considerably.
- One practical issue inhibiting usage is the very large amount of material on the portal making it difficult to sort by topic of interest. The use of suitable thematic tags will help highlight the quality of the material available on the portal to the wider simulation community. This topic is currently being addressed.
- A wish list for the training portal has been developed to enhance future user experience (see sec. 2.3.1).

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 pages² 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.

The major updates to the access points above, in respect to what was previously reported, are outlined in the subsequent sections.

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[2] 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 the last period we made an additional effort to display on our website more results targeted to the general public and engaged in the following projects:

- 1. a Comic book about E-CAM and how it enables modelling, simulation and HPC;
- 2. an interview with Massimo Noro, Director of Business Development at the STFC and former science leader of the HPC division at Unilever;
- 3. a news piece for the EU Research Magazine targeted at all people interested in science;
- 4. a video of E-CAM's online training portal that is a tour of the website;
- 5. a common calendar with other HPC events running in Europe
- 6. automatically push E-CAM featured articles to the website dedicated to the CoEs.

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

1. Comic book about E-CAM and how it enables modelling, simulation and HPC

Identifying exciting and original tools to engage the general public with advanced research is an intriguing and nontrivial 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.

The E-CAM issue of Comics&Science (Fig. 2) is freely available on our website at https://www.e-cam2020.eu/e-camissue-of-comics-science/ and is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License (CC BY-NC-SA 4.0).

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



Figure 2: Cover of the E-CAM issue of Comics&Science.

2. Interview with Massimo Noro, Director of Business Development at STFC

Particularly active in applying atomistic and coarse-grained simulations to study the interaction of nano-objects and surfactants with lipid bilayers for industrial applications (e.g. soaps, detergents, etc.), Massimo Noro has made considerable contributions to the development and application of the Dissipative Particle Dynamics (DPD) simulation technique to study soft condensed matter systems. More recently he was the science leader of the High Performance Computing division at Unilever, and currently is Director of Business Development at the Science and Technology Facilities Council (STFC), with a focus on the Daresbury Campus. In this interview intended for the general public, Massimo Noro talked about his journey from academic research, to work in Unilever and now at STFC, and shared his insights on the use of simulation and modelling in industry and the role of STFC and research in this regard. See the full interview at https://www.e-cam2020.eu/e-cam-interview-with-massimo-noro/.



Figure 3: Snapshot of the interview with Massimo Noro, Director of Business Development at STFC.

3. News piece for the EU Research Magazine

An article about E-CAM intended for all public interested in science was released with the Autumn edition of the EU Research Magazine.

The piece consists on an interview to Prof. Ignacio Pagonabarraga, E-CAM technical manager, Dr. Sara Bonella, leader of our work-package focused on quantum dynamics and also of the work-package that deals with the interactions with industry; Dr. Donal Mackernan, leader of our dissemination work-package and Dr. Jony Castagna, programmer in E-CAM.



Figure 4: First page of the E-CAM news piece on the Autumn edition of the EU Research Magazine.

4. Video of E-CAM's online training portal

We generated a video tour of our online training portal, and added it to the dedicated page on our website at https://www.e-cam2020.eu/e-cam-online-training-portal/. This video is intended to show the functionalities of the portal and work as a supporting tool on how to use it.



Online Training Portal

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How to access

Terminology

Figure 5: Training portal page on the E-CAM website.

5. Common calendar with other HPC events running in Europe

We have added to our calendar at https://www.e-cam2020.eu/calendar/ a tab "Other EuroHPC Events" dedicated to showing other events being organized in the context of EuroHPC so that users can browse through a wider range of HPC events.



Figure 6: E-CAM Calendar of events now offers the possibility to browse through a wider range of HPC events.

6. Automatically push E-CAM featured articles to the website dedicated to the CoEs

E-CAM collaborated with the CoE FocusCoE, to automatically push featured articles to the website dedicated to the CoEs at www.hpccoe.eu/. This procedure will be used for the next period, facilitating exchange of information.

2.2 E-CAM Software Library

The E-CAM Software Library is one of the principle access points for users interacting with E-CAM, as shown by the number of visitors it has compared to other contents. There, visitors are encouraged to access and contribute software developments, 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 such as Redmine, CodiMD, ShareLatex, and in particular GitLab.

This set of technical documentation of E-CAM is created and edited via a wiki 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. Final inclusion in the published software library follows screening from E-CAM's software manager. Each individual modification of the repository automatically causes the associated documentation on the E-CAM Software Library to be rebuilt. The use of *Merge Requests* allows E-CAM to implement a quality-control mechanism on contributed content. See Deliverable D6.7: E-CAM Software Platform V[3] for a more comprehensive description of E-CAM's software library and the latest updates to our software tools and platforms.

2.2.1 Updates to the Software Repositories

During the last period, the E-CAM Software Library underwent a cosmetic redesign to ensure it remained modern looking and attractive to read on devices with large resolutions.

 $^{^{3}}$ 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.



Figure 7: The homepage of the E-CAM Software Library.

2.3 E-CAM Training Infrastructure

The E-CAM Training Portal is publicly available since December 2017. The extent of the development efforts to create the platform, as well as the organisational structure we adopt to leverage it, are described in detail on deliverable D6.7: E-CAM Software Platform V[3].

The goals of our training infrastructure are to:

- **Collect the content captured at our training events (ESDWs)**, allowing participants to revisit lectures or demonstrations in their own time, both during and after the meeting. Such material can also be used by people who did not have the opportunity to attend the ESDW in person (in particular our industrial partners),
- Generate online training modules for each ESDW, which will be a set of preparatory material shared with the participants and that will allow everyone to acquire the same basic knowledge before the meeting.
- Be a repository for the data associated to our other events (captured lectures, lecture materials, reading materials, tutorial content and software requirements).
- Build tutorials on programming best practices to develop software for extreme-scale hardware, that we can propose them to the extended CECAM community that has active means to transfer this knowledge to industrial contacts, multiplying E-CAM's impact.
- Associate with other groups and projects with similar training scope such as PRACE, other CoEs and MolSSI, to cover for different and broader training material.

2.3.1 Updates to the Training Infrastructure

The system upon which our online training portal is built is Clowder, which is developed at NCSA. Clowder is a research data management system designed to support any data format and multiple research domains. E-CAM has expanded the capabilities of Clowder to be able to, among other things:

- shrink the input video to just 1.2MB per minute for full HD video (roughly the same size as simple stereo audio files)
- extract the slides from the captured presentation and prepare them for the previewer
- create a navigation panel for the video allowing the user to easily jump between slides in the video (and allowing slide navigation to be auto-synchronised with the video)
- When URLs are giving as teaching material, display previews of target URL (as well as some additional site information)

• change the file format for the slide metadata images, saving up to 70% of the space required for these images.

During the last period, we worked on maintaining the developments above. Additionally, we worked on a white paper for the portal. We have also developed a wish list for the E-CAM Training Portal, which hints at future developments towards:

- Improving the user interface;
- Controlling the metadata that is used;
- Managing lecture tags;
- Developing a user guide.

Collaborations with other players are also being explored to ensure the sustainability of our training portal, which we believe is extremely valuable for the community, especially in a period where events are running mostly online with lectures being recorded and stored massively. Concerted actions to store this material in an sustainable way is urgently needed.

3 E-CAM Newsletters

Three issues of the E-CAM newsletter were published. As reported already in 2018, we have moved to 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.

Issue 11 (section 3.1) - The newsletter included the following items.

- 1. An industry success story involving the Mesoscale simulation of billion atom complex systems using thousands of GPGPU's.
- 2. A short description of an Extended Software Development Workshop in Mesoscopic simulation models and HPC to be held in Finland
- 3. An open call for E-CAM focused proposal submissions for the 2020 CECAM flagship programme.
- 4. A scientific report from the workshop "Software vendor SMEs as a boost for technology transfer in industrial simulation pipelines".
- 5. Featured Software Modules: Abrupt GC-AdResS: a new and more general implementation of the Grand Canonical Adaptive Resolution Scheme; Module DBCSR MatrixSwitch - an optimised library to deal with sparse matrices; and, Porting of electrostatics to the GPU version of DL-MESO.
- 6. New Publications: Molecular Dynamics of Open Systems Construction of a Mean-Field Particle Reservoir; and, the Fluctuation-Dissipation Theorem as a Diagnosis and Cure for Zero-Point Energy Leakage in Quantum Thermal Bath Simulations.
- 7. Submitted deliverables: D5.4: ESDW Guidelines and Programme IV; and, D7.6: E-CAM Software Porting and Bench-marking Data a report on the results of porting and optimisation of E-CAM modules to massively parallel machines and their bench-marking and scaling.

Issue 12 (section 3.2) - The newsletter included the following items.

- 1. A Conversation on The Fourth Industrial Revolution: Opportunities & Trends for Particle Based Simulation (interview).
- 2. An E-CAM Case Study: The development of the CG-AdResS scheme from smooth coupling to an abrupt interface.
- 3. Two upcoming events: a State of the Art Workshop: Challenges in Multi-phase Flows; and An Extended Software Development Workshop: Integration of the Electronic Structure Library modules into electronic structure codes.
- 4. Three Featured Software Modules: Extension of the ParaDiS code to include precipitate interactions, and code optimisation to run on HPC environment; Multi-GPU version of DL_MESO_DPD Mesoscale Simulation Package, with multiple NVidia Graphical Processing Units (GPUs); and, Pyscal- a python module for structural analysis of atomic environments.
- 5. Brief descriptions of two new E-CAM Scientific Publications: Local control theory for super-computing qubits; and, Atomistic insight into the kinetic pathways for Watson-Crick to Hoogsteen transitions in DNA.
- 6. A short description of an E-CAM deliverable: D7.7: including detailed studies on Hardware developments, Software Needs, and interactions between end-users, developers, and vendors.

Issue 13 (section 3.3) - The newsletter included the following items.

- 1. An E-CAM interview with Massimo Noro, Director of Business Development at STFC and former science leader of the HPC division at Unilever.
- 2. Some useful tips to help moving to online training built from a collection of useful information to help our community, other Centres of Excellence and interested groups, on the transition to online training.
- 3. A description of an E-CAM transverse action regarding the development of a protein based sensor with applications in medical diagnostics, scientific visualisation and therapeutics including applications for COVID 19 and influenza A & B.
- 4. Two Featured Software Modules. The first, PANNA: Properties from Artificial Neural Network Architectures -a package for training and validating neural networks to represent atomic potentials. It implements configurable all-to-all connected deep neural network architectures which allow for the exploration of training dynamics.

The second, Automated high-throughput Wannierisation, emerged from a a successful collaboration between E-CAM, the MaX Centre of Excellence and the NCCR MARVEL.

- 5. Brief descriptions of two new E-CAM Scientific Publications. The first, entitled "Towards extreme scale dissipative particle dynamics simulations using multiple GPGPUs", and reports on an extension of the DL_MESO package to MPI+CUDA in order to exploit the computational power of the latest NVIDIA cards on hybrid CPU–GPU architectures. The second publication, Adiabatic motion and statistical mechanics via mass-zero constrained dynamics describes a new algorithm to solve numerically the dynamics of the shell model for polarization.
- 6. A short description of two E-CAM deliverable. The first, D5.5: Hardware developments included E-CAM's Extended Software Development Workshop (ESDW) programme for 2020/2021, and the most recent guidelines for the organisation of these events; an analysis of the profile of the participants to our ESDWs, and the results of our satisfaction surveys. The second, D6.7: E-CAM Software Platform V report described the updates made to the online services in the E-CAM project, including the E-CAM library of software modules, the end users portal, and the online training portal.

3.1 Newsletter June 2019

Display problems? Open this email in your web browser.





Industry Success Story

<u>Mesoscale simulation of billion atom complex</u> <u>systems using thousands of GPGPU's</u>



By Dr. Jony Castagna, Science and Technology Facilities Council, UK

Jony Castagna recounts his transition from industry scientist to research software developer at the <u>STFC</u>; his E-CAM rewrite of DL_MESO, an industrially useful package for DPD Dissipative Particle Dynamics simulations, allowing the simulation of billion atom systems on thousands of GPGPUs; and his latest role as Nvidia ambassador focused on machine learning.



Upcoming event

Extended Software Development Workshop in Mesoscopic simulation models and HPC







E-CAM partners at Aalto University (CECAM Finish Node) in collaboration with the HPC training experts from the CSC Supercomputing Centre, are organizing a joint Extended Software Development Workshop from 15-19 October 2019, aimed at people interested in particle based methods, such as the Discrete Element and Lattice Boltzmann Methods, and on their massive parallelization using GPU architectures. The workshop will mix three different ingredients: (1) workshop on state-of-the-art challenges in computational science and software, (2) CSC -run school, and (3) coding sessions with the aid of CSC facilities and expertise.



Open call for CECAM flagship programme 2020

The CECAM CALL for workshops and schools that will run from April 2020 to March 2021 is now open! This is also the opportunity to submit an E-CAM proposal. The text of the call and information on how to submit a proposal can be found at https://www.cecam.org/submitting/. Deadline for submission is 16 July 2019.



Reau more

Workshop Scientific report



<u>Software vendor SMEs as a boost for technology</u> <u>transfer in industrial simulative pipelines</u>

This E-CAM workshop brought together top-level scientists of the E-CAM community, and representatives of pharmaceutical and material industries, with the objective to identify the major gaps which still hamper a systematic exploitation of accurate computer simulations in industrial R&D. Special attention was given to the role of SMEs devoted to simulative software development. The meeting highlighted the role of software vendor SMEs as a key link for the uptake of modelling in industry. They can play an increasingly important role not only in translating the science developed in academia into a proper technological transfer process, but also in building a scientific bridge between the industry requirements in terms of automation and the new theories and algorithms developed at an academic level. There was also a consensus that EU funded Centers of Excellence for Computing Applications, such as

E-CAM, can provide an opportunity to enhance the expertise and scope of software vendors SMEs.

Read more

Featured Software Modules



Abrupt GC-AdResS: A new and more general implementation of the Grand Canonical Adaptive Resolution Scheme



The Grand Canonical Adaptive resolution scheme (GC-AdResS) aives а methodological description to partition a simulation box into different regions with different degrees of accuracy. For more details on the theory see Refs. [1,2,3]. In the context of an E-CAM pilot project focused on the development of the GC-AdResS scheme, an updated version of GC-AdResS was built and implemented in GROMACS, as reported in [4]. The main goal of the project was to develop a library or recipe with which GC-AdResS can be implemented in any Classical MD Code.

Read more

Module DBCSR@MatrixSwitch: an optimised library to deal with sparse matrices

MatrixSwitch is a module which acts as an intermediary interface layer between highlevel and low-level routines dealing with matrix storage and manipulation. It allows a seamlessly switch between different software implementations of the matrix operations. DBCSR is an optimised library to deal with sparse matrices, which appear frequently in many kind of numerical simulations. In DBCSR@MatrixSwitch, DBCSR capabilities have been added to MatrixSwitch as an optional library dependency.

Read more

Porting of electrostatics to the GPU version of DL MESO

The porting of DL_MESO to graphic cards (GPUs) was reported in deliverables D4.2 of E-CAM (for a single GPU) and deliverable D4.3 (for multiple GPUs), and has now been extended to include electrostatics, with two alternative schemes: Standard Ewald and Smooth Particle Mesh Ewald (SPME) methods. This work was recently reported on deliverable D4.4.



ALL FEATURED MODULES

New Publications

Molecular Dynamics of Open Systems: Construction of a Mean-Field Particle Reservoir

E-CAM Newsletter - June 2019



L. Delle Site, C. Krekeler, J. Whittaker, A. Agarwal, R. Klein, F. Höfling *Adv. Theory Simul.* **2019**, 1900014 DOI: <u>10.1002/adts.201900014</u> (Open access)

The simulation of open molecular systems requires explicit or implicit reservoirs of energy and particles. Whereas full atomistic resolution is desired in the region of interest, there is some freedom in the implementation of the reservoirs. Here, a combined, explicit reservoir is constructed by interfacing the atomistic region with regions of point-like, non-interacting particles (tracers) embedded in a thermodynamic mean field. The tracer molecules acquire atomistic resolution upon entering the atomistic region and equilibrate with this environment, while atomistic molecules become tracers governed by an effective mean-field potential after crossing the atomistic boundary. The approach is extensively tested on thermodynamic, structural, and dynamic properties of liquid water. Conceptual and numerical advantages of the procedure as well as new perspectives are highlighted and discussed.



The Fluctuation–Dissipation Theorem as a Diagnosis and Cure for Zero-Point Energy Leakage in Quantum Thermal Bath Simulations

E. Mangaud, S. Huppert, T. Plé, P. Depondt, S. Bonella, F. Finocchi, J. Chem. Theory Comput. 2019, 15, 2863-2880, DOI: <u>10.1021/acs.jctc.8b01164</u>



Quantum thermal bath (QTB) simulations reproduce statistical nuclear quantum effects via a Langevin equation with a coloured random force. Although this approach has proven efficient for a variety of chemical and condensed-matter problems, the QTB, as many other semiclassical methods, suffers from zero-point energy leakage (ZPEL). The absence of a reliable criterion to quantify the ZPEL without resorting to demanding comparisons with path integral based calculations has so far hindered the use of the QTB for the simulation of real systems. In this work, we establish a quantitative connection between ZPEL in the QTB framework and deviations from the quantum fluctuation-dissipation theorem (FDT) that can be monitored along the simulation. This provides a rigorous general criterion to detect and quantify the ZPEL without any *a priori* knowledge of the system under study.



Submitted deliverables

D5.4: ESDW Guidelines and Programme IV*

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Interna Holecular Design & Informace holding a Molecular Foundry	ESRY: Messengie simulation model and Figh. Performance Computing	State of the art workshop: Challenges in Haltiphize Rows	Integration of ES. markings into electronic- structure cales Biectronic Structure Postero Reserver

Updated guidelines for format, content and coding styles in the Extended Software Development Workshops (ESDWs), and E-CAM program of events running in 2020/2021.

D7.6: E-CAM Software Porting and Benchmarking Data III*

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Technical report on the results of porting and optimisation of E-CAM modules to massively parallel machines and their benchmarking and scaling. The development of the modules was done in the context of E-CAM ESDWs.

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

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3.2 Newsletter December 2019



Newsletter December 2019



<u>A Conversation on The Fourth Industrial</u> <u>Revolution: Opportunities & Trends for Particle</u> <u>Based Simulation</u>



Abstract

In the margins of a recent multiscale simulation workshop a discussion began between a prominent pharmaceutical industry scientist, and <u>E-CAM</u> and <u>EMMC</u> regarding the unfolding Fourth Industrial Revolution and the role of particle based simulation and statistical methods there. The impact of simulation is predicted to become very significant. This discussion is intended to create awareness of the general public, of how industry 4.0 is initiating in companies, and how academic research will support that transformation.

Authors: Prof. Pietro Asinari (EMMC and Politecnico di Torino), Dr. Donal MacKernan (E-CAM and University College Dublin), and a prominent pharmaceutical industry scientist. E-CAM Case Study: The development of the

CG-AdResS scheme:

from smooth coupling



to a direct interface (abrupt)



Abstract

GC-AdResS is a technique that speeds up computations without loss of accuracy for key system properties by dividing the simulation box into two or more regions having different levels of resolution, for instance a high resolution region where the molecules of the system are treated at an atomistic level of detail, and other regions where molecules are treated at a coarse grained level, and transition regions where a weighted average of the two resolutions is used. The goal of the E-CAM GC-AdResS pilot project was to eliminate the need of a transition region so as to significantly improve performance, and to allow much greater flexibility. For example, the low resolution region can be a particle reservoir (ranging in detail from coarse grained to ideal gas particles) and a high resolution atomistic region with no transition region, as was needed hitherto. The only requirement is that the regions can exchange particles, and that a corresponding two "thermodynamic" force is computed self-consistently, which it turns out is very simple to implement.

Upcoming events

State of the Art Workshop: CHALLENGES IN MULTIPHASE FLOWS



Monash University Prato Center, Italy 9-12 December 2019 Organizers: Burkhard Duenweg (MPIP Mainz), Ignacio Pagonabarraga (EPFL), Ravi Prakash Jagadeeshan (Monash U.)

ESDW: Integration of ESL modules into electronicstructure codes Newsletter - December 2019



CECAM HQ, EPFL, Switzerland 17-28 February 2020 Organizers: Nick Papior (DTU), Micael Oliveira (MPSD Hamburg), Yann Pouillon(UNICAN), Volker Blum (Duke U.), Fabiano Corsetti (Synopys QuantumWise), Emilio Artacho (UPV/EHU)

Featured Software Modules



Extension of the ParaDiS code to include precipitate interactions, and code optimisation to run on HPC environment

Here present two featured software modules of the month: ParaDiS with precipitatesParaDiS with precipitates optimized to HPC environment that provide extensions to the ParaDIS Discrete dislocation dynamics (DDD) code (LLNL, http://paradis.stanford.edu/) where dislocation/precipitate interactions are included. Module 2 was built to run the code on an HPC environment, by optimizing the original code for the Cray XC40 cluster at CSC in Finland.

ALL FEATURED MODULES

Multi-GPU version of DL_MESO_DPD



This module implements the first version of the <u>DL_MESO_DPD</u> Mesoscale Simulation Package, with multiple NVidia Graphical Processing Units (GPUs).

> Pyscal- A python module for structural analysis of atomic environments

* pyscal

pyscal is a python module for the calculation of local atomic structural environments including Steinhardt's bond orientational order parameters during post-processing of atomistic simulation data. The core functionality of pyscal is written in C++ with python wrappers using pybind11 which allows for fast calculations and easy extensions in python.

New Publications

Local control theory for supercomputing qubits



M. Mališ, P. KI. Barkoutsos, M. Ganzhorn, S. Filipp, D. J. Egger, S. Bonella and I. Tavernelli, *Phys. Rev. A* 99, 052316 DOI: <u>10.1103/PhysRevA.99.052316</u> (open access)

In this work, a method is developed to design control pulses for fixedfrequency superconducting qubits coupled via tunable couplers based on local control theory, an approach commonly employed to steer chemical reactions. Local control theory provides an algorithm for the monotonic population transfer from a selected initial state to a desired final state of a quantum system through the on-the-fly shaping of an external pulse. The method, which only requires a unique forward time-propagation of the system wavefunction, can serve as starting point for additional refinements that lead to new pulses with improved properties. Among others, an algorithm for the design of pulses is proposed in this study, that can transfer population in a reversible manner between given initial and final states of coupled fixedfrequency superconducting qubits.

Read more

Atomistic insight into the kinetic pathways for Watson-Crick to Hoogsteen transitions in DNA

Vreede J, Pérez de Alba Ortíz A, Bolhuis PG, and Swenson DWH, *Nucleic Acids Research* **2019**, Vol. 47, No. 21, 11069–11076 DOI: <u>10.1093/nar/gkz837</u> (open access)



DNA predominantly contains Watson–Crick (WC) base pairs, but a nonnegligible fraction of base pairs are in the Hoogsteen (HG) hydrogen bonding motif at any time. In the HG motif, the purine is "upside down" compared to the WC motif. Two classes of mechanism have been proposed for the transition between these motifs: one where the base pair stays inside the confines of the helical backbone, and one where one base flips outside of the

Newsletter - December 2019

helical backbone before returning in the "upside down" HG conformation. The transitions between WC and HG may play a role in recognition and replication, but are difficult to investigate because they occur quickly, but only rarely. To gain insight into the mechanisms for this process, researchers performed transition path sampling simulations on a model nucleotide sequence in which an adenine-thymine base pair changes from WC to HG, and found that the outside transition was strongly preferred. Simulated rates and free energy differences agree with experiments, the simulations provide highly detailed insights into the mechanisms of this process.

Read more

Submitted deliverables

D7.7: Hardware developments IV*

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

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3.3 Newsletter April 2020





E-CAM interview with Massimo Noro, Director of Business Development at STFC



Massimo Noro is the Director of Business Development at the Science & Technology Facilities Council (STFC), with a focus on the Daresbury Campus. Massimo joined STFC in February 2018, following a successful industrial R&D career at Unilever. His scientific interests focus on applying atomistic and coarse-grained simulations to study the interaction of nano-objects and surfactants with lipid bilayers for industrial applications (e.g. soaps, detergents, etc.). In this interview, he will talk about his journey from academic research, to work in Unilever and now at STFC, and will share his insights on the use of simulation and modelling in industry and the role of STFC and research in this regard.

Read more

Some useful tips to help moving to online training



E-CAM has built up a collection of (hopefully) useful information to help our community, other Centres of Excellence, and interested groups, transition to online training. The information originates from community-contributed sources and by directly sharing our experience in capturing and broadcasting E-CAM training events.

Read more

Protein based biosensors: potential application in detecting COVID-19



An E-CAM transverse action is the development of a protein based sensor with applications in medical diagnostics, scientific visualisation and therapeutics. At the heart of the sensor is a novel protein based molecular switch which allows extremely sensitive real time measurement of molecular targets, and to turn on or off protein functions and other processes accordingly. Provided that the amino acid sequences of antibody -epitope pairs specific to this coronavirus are known, the sensor can be modified to quickly detect the COVID19.

Read more



Featured Software Modules

<u>The development of QMCPack Interfaces for</u> <u>Electronic Structure Computations</u>



Quantum Monte Carlo (QMC) methods are a class of ab initio, stochastic techniques for the study of quantum systems. While QMC simulations are computationally expensive, they have the advantage of being accurate, fully ab initio and scalable to a large number of cores with limited memory requirements. Trial wave functions for electronic QMC computations commonly require the use of single electrons orbitals, typically computed by DFT. The aim of the **E-CAM pilot project** described <u>here</u> is to build interfaces between the free package for QMC simulations QMCPack and other softwares for electronic structure computations, e.g. the DFT code Quantum Espresso.

Read more

PANNA: Properties from Artificial Neural Network Architectures



PANNA is a package for training and validating neural networks to represent atomic potentials. It implements configurable all-to-all connected deep neural network architectures which allow for the exploration of training dynamics. A common way to use PANNA in its current implementation is to train a neural network in order to estimate the total energy of a molecule or crystal, as a sum of atomic contributions, by learning from the data of reference total energy calculations for similar structures (usually ab-initio calculations).

Read more

Automated high-throughput Wannierisation

a successful collaboration between E-CAM and the <u>MaX Centre of Excellence</u>



Maximally-localised Wannier functions (MLWFs) are routinely used to compute from first- principles advanced materials properties that require very dense Brillouin zone integration and to build accurate tight-binding models for scale-bridging simulations. At the same time, high-thoughput (HT) computational materials design is an emergent field that promises to accelerate the reliable and cost-effective design and optimisation of new materials with target properties. The use of MLWFs in HT workflows has been hampered by the fact that generating MLWFs automatically and robustly without any user intervention and for arbitrary materials is, in general, very challenging. We address this problem directly by proposing a procedure for automatically generating MLWFs for HT frameworks. Our approach is based on the selected columns of the density matrix method (SCDM, see <u>SCDM</u> Wannier Functions) and is implemented in an AiiDA workflow.

Read more

New Publications

<u>Towards extreme scale dissipative particle</u> <u>dynamics simulations using multiple GPGPUs</u>



J. Castagna, X. Guo, M. Seaton and A. O'Cais, *Computer Physics Communications* **2020**, 251, 107159 DOI: <u>10.1016/j.cpc.2020.107159</u> (open access)

A multi-GPGPU development for Mesoscale Simulations using the Dissipative Particle Dynamics method is presented. This distributed GPU acceleration development is an extension of the DL_MESO package to MPI+CUDA in order to exploit the computational power of the latest NVIDIA cards on hybrid CPU–GPU architectures. Details about the extensively applicable algorithm implementation and memory coalescing data structures are presented. The key algorithms' optimizations for the nearest-neighbour list searching of particle pairs for short range forces, exchange of data and overlapping between computation and communications are also given. We have carried out strong and weak scaling performance analyses with up to 4096 GPUs. A

two phase mixture separation test case with 1.8 billion particles has been run on the Piz Daint supercomputer from the Swiss National Supercomputer Center. With CUDA aware MPI, proper GPU affinity, communication and computation overlap optimizations for multi-GPU version, the final optimization results demonstrated more than 94% efficiency for weak scaling and more than 80% efficiency for strong scaling. As far as we know, this is the first report in the literature of DPD simulations being run on this large number of GPUs.



Adiabatic motion and statistical mechanics via mass-zero constrained dynamics



Sara Bonella, Alessandro Coretti, Rodolphe Vuilleumier and Giovanni Ciccotti, *Phys. Chem. Chem. Phys.* **2020**, Advance Article DOI: 10.1039/D0CP00163E

In recent work [Coretti et al., J. Chem. Phys., 2018, 149, 191102], a new algorithm to solve numerically the dynamics of the shell model for polarization was presented. The approach, broadly applicable to systems involving adiabatically separated dynamical variables, employs constrained molecular dynamics to strictly enforce the condition that the force on the fast degrees of freedom, modeled as having zero mass, is null at each time step. The algorithm is symplectic and fully time reversible, and results in stable and efficient propagation. In this paper we complete the discussion of the mechanics of mass-zero constrained dynamics by showing how to adapt it to problems where the fast degrees of freedom must satisfy additional conditions. This extension includes, in particular, the important case of first principles molecular dynamics. We then consider the statistical mechanics of the mass-zero constrained dynamical system demonstrating that the marginal probability sampled by the dynamics in the physical phase space recovers the form of the Born-Oppenheimer probability density. The effectiveness of the approach and the favorable scaling of the algorithm with system size are illustrated in test calculations of solid Na via orbital-free density functional dynamics.

Postponed event

Simulation of open systems in Chemistry, Pharma, Food Science and Immuno-diagnostics: Rare-event

methods at constant chemical potentials including constant pH - an E-CAM Industry Scoping Workshop



Organizers:

Fernando Luís Barroso da Silva (USP) Brian Glennon (UCD & SSPC), Donal MacKernan (UCD), Erik Santiso (NC State University)

Link to webpage: https://www.cecam.org/workshop-details/10

We are closely monitoring the situation to assess if more events will be affected by the crisis. Alternative options, such as virtual meetings, are also being considered. Information will be promptly updated on the <u>E-CAM</u> and <u>CECAM</u> websites.

Submitted deliverables

D5.5: Hardware developments IV*

E-CAM's Extended Software Development Workshop (ESDW) programme for 2020/2021, and most recent guidelines for the organisation of these events. Analysis of the profile of the participants to our ESDWs and the results of our satisfaction surveys.

D6.7: E-CAM Software Platform V*

Report on the updates made to the online services in the E-CAM project, including the E-CAM library of software modules, the end users portal, and the online training portal.

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

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4 Conclusions and plan for next period

This deliverable, D9.4, included a summary of the impact of our dissemination strategy measured in terms of web traffic statistics; a corresponding analysis; lessons learned and actions to improve visibility; updates to the E-CAM website and to the online training portal; and, newsletters issues published since the submission of D9.3 until April 2020.

Within the E-CAM website we note that our calendar of events attracts the greatest attention, followed by our software repositories, confirming a trend that has also been seen in previous versions of this deliverable. There has been a increase of interest in E-CAM publications and online training portal during Q2 of 2020.

Our efforts to disseminate to and engage with the public and industry included:

- a Comic book about E-CAM and how it enables modelling, simulation and HPC;
- an interview with Massimo Noro, Director of Business Development at the STFC and former science leader of the HPC division at Unilever;
- a news piece for the EU Research Magazine targeted at all people interested in science;
- a video of E-CAM's online training portal that is a tour of the website;
- a common calendar with other HPC events running in Europe.

During the last period, additionally, we worked on a white paper for the E-CAM Online Training Portal. We have also developed a wish list of enhancements for it so as to improve user accessibility. Collaborations with other players are also being explored to ensure the sustainability of our training portal, which we believe is extremely valuable for the community, especially in a period where events are running mostly online with lectures being recorded and stored massively.

Efforts to improve project visibility in the next period (some of which are already ongoing) include:

- the promotion of our events, which will now run online;
- collaboration with the CoE FocusCoE to promote E-CAM activities to the wider scientific community and enhance interactions with industry, and public awareness of HPC;
- exploitation of E-CAM's Comic book;
- focused dissemination efforts regarding E-CAM Software development initiatives.

References

Acronyms Used

CECAM Centre Européen de Calcul Atomique et Moléculaire

HPC High Performance Computing

PRACE Partnership for Advanced Computing in Europe

ESDW Extended Software Development Workshop

PDRA Postdoc Research Associate

CoE Centres of Excellence

MolSSI Molecular Sciences Software Institute

URLs referenced

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