

## E-CAM Public Wiki-like pages and newsletters III E-CAM Deliverable 9.3

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



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## **Executive Summary**

This deliverable is an update of D9.2: E-CAM Public Wiki-like pages and newsletters II [1] and consists of: (1) an analysis of the impact of the revised dissemination strategy[2] over the last 12 months; (2) a description of the key updates to the project's primary access points; and, (3) the issues of the newsletter over twelve months. The revised strategy in a "nut shell" is to (a) disseminate continuously, systematically seizing opportunities as they appear; and (b) leverage the work that is being done across all of the WPs within E-CAM, and with those who engage with it externally via its many software, training and industry workshop activities. The effects of that approach have been most visible in the increased production and interest in E-CAM software output available in the E-CAM public repositories, their highlights as feature news items; and in E-CAM case studies, and success stories.

Regarding (1) the analysis was performed using web-statistics of the number of visitors to the E-CAM website over the last 4 quarters.

The total number of visitors to E-CAM website since February 10, 2017 (from when we started collecting web traffic data statistics) is 131'704, with 47'289 visiting our pages during the last twelve months. A large number of pages have been consulted (measured in terms of hits or visits) in the last 4 quarters. In particular, the software repositories which are core to E-CAM are consistently attracting high interest. Success stories, case-studies and interviews attract great attention when they appear. The analysis also allows us to pin-point areas where more dissemination effort is needed, and joint collaborative projects with the Coe FocusCoe to engage the wider scientific community, the public, and industry.

Regarding (2), a report of the key updates to the project's primary access points: the Web-portal, the Software Library, the GitLab Repositories and the Training Infrastructure, are presented. These updates are as follows:

- the project website has been updated to include key output from the project in its front page. Content pages have been added to increase visibility;
- the Software library and GitLab repositories now integrate the software developed in all of the scientific areas of interest for E-CAM;
- the training portal is online since December 2017. E-CAM has expanded the capabilities of Clowder from NSA to include new filetypes that cover the scope of the content to be included by E-CAM: video presentations, PDFs and URLs. Content of all types collected during the Extended Software Development Workshop (ESDW) program of 2017 and 2018 has been added to the E-CAM Training Portal. This content is being widely leveraged in the 2019 program.

Finally, (3) is composed of all the issues of the E-CAM newsletter released during the past twelve months. 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 websearch-able. In addition to opinion pieces and interviews, the newsletter also now includes items on software modules and case studies.

In the final section of this report we summarize our dissemination activities over the last year and outline our plans for the next one. The former include continuing to do that which already works well, such as the promotion of E-CAM software, the build-up of case studies reporting successful industrial/academic collaboration, interviews, and their proper dissemination to the target groups; The latter include intensifying our dissemination of the E-CAM training portal; intensifying our participation to non-E-CAM events where our infrastructure is likely to be useful; and actions towards increasing the interest of the general public as reported in the second iteration of the additional deliverable on "dissemination strategy, training strategy and cross WP collaboration", submitted to the European Commission in June 2019[3].

## 1 Introduction

In the previous version of this deliverable, D9.2: E-CAM Public Wiki-like pages and newsletters II[1], we analyzed the impact of E-CAM's revised strategy for dissemination defined in the additional deliverable "Dissemination strategy, training strategy and cross WP-collaboration" (August 2017)[2]. The revised strategy in a "nut shell" is to: (a)disseminate continuously, systematically seizing opportunities as they appear; and (b)leverage the work that is being done across all of the WPs within E-CAM, and with those who engage with it externally via its many software, training and industry workshop activities. Since the implementation of that approach, the effects have been most visible in the increased production and interest for the E-CAM software output available in the E-CAM public repositories, their highlights as feature news items; and in E-CAM case studies, and success stories. At the same time, the more lengthy interviews continue to identify and probe issues of future importance to the community.

## 1.1 Scope of this update

This update includes an overview of our dissemination strategy; a summary of its impact measured in terms of web traffic statistics; a corresponding analysis of content that attracts more interest; lessons learned and recommendations; updates to the E-CAM website; updates to the online training portal; newsletters issues in the previous twelve months; and a summary of our plans for the next year. Final drafting of the present dissemination report coincided with preparation of the second iteration of the additional deliverable on dissemination strategy, training strategy and cross WP collaboration, submitted to the EC in June 2019[3].

## 1.2 Dissemination instruments and strategies - overview

For clarity, it is useful to recall the current dissemination instruments and strategies.

- 1. The format of newsletter is now integrated as a News Blog in the E-CAM website, where material is continuously delivered and is web-searchable.
- 2. The project's website includes the most recent news items, success stories, case studies, opinion pieces, interviews and upcoming E-CAM events. This mapping more accurately reflects the dissemination strategy of the project. Project results are now communicated through these items and through the new category "Modules of the Month" where every month we publicize the best certified modules and their potential applications.
- 3. Results specific to each pilot project in collaboration with industry are also communicated through pages dedicated to pilot projects.
- 4. The website contains a page summarizing our services.
- 5. Software modules associated with pilot projects and those produced via E-CAM Extended Software Development Workshops now each have a public abstract which is easy to read for non-experts, and facilitates dissemination via email and the news blog, Twitter, and presentation to industrialists. This change has also been enforced for deliverables and scientific publications.
- 6. Lectures at E-CAM events are now recorded and made available online through an online training infrastructure.
- 7. Success stories documenting fruitful industrial and academic collaboration within E-CAM are now being produced, and disseminated to our industrial partners via the most appropriate communication channels. Case studies are also being produced, focused on the software modules produced and their potential applications, and properly disseminated to industry. They are stored on our website and are downloadable.
- 8. Our activities now involve extreme-scale computing through a set of activities throughout the WPs. The output generated is being disseminated through workshops, the online training platform, software modules, success stories and case studies, helping to build a path to extreme-scale computing for industry and academia.
- 9. All of the content generated by E-CAM is being disseminated via social networks Twitter and LinkedIn.

#### 1.2.1 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 131'704, with 47'289

visiting our pages during the last twelve months. Figure 1 shows the average daily visitors to the E-CAM website over the last 4 quarters, from April 2018 to March 2019, as collected by Wordpress. For simplicity, data is averaged per trimester, as indicated in the x-axis. Another measure is visits – (i.e. hits) which is useful as it can show which pages are most frequently viewed by visitor. We can identify a reduction in the number of visitors to the website in the last



Figure 1: Daily average number of visitors to the E-CAM website per quarter over the last year

year, while the number of visits to technically specialized web pages, such as for example software module pages has either increased, or remained steady. The reduction in visitor numbers to about one hundred visitors per day may be due to the novelty factor of E-CAM having dissipated, but in any case is typical stakeholders behavior during a project life cycle. As reported in ref. [4], stakeholders interest throughout the different phases of a project follows a "U-shaped" curve, reflecting initial enthusiasm, lower levels of interest during development phases, and renewed interest as the project nears completion.

In reporting the number of visits we have not included hits to specific pages which could have been affected by bots. Figure 2 shows that the one year "h-index" of E-CAM web-pages is 65. While a few pages have hits in excess of several thousands during the last twelve months, the figure reveals the breadth and depth of community interest in a large number of pages (over 65), most of them highly technical in nature. Additionally, 4 is the average the number of pages seen by each visitor to the E-CAM website.



Number of visits for top ranked E-CAM pages in last 12 months

Figure 2: Distribution of top 65 E-CAM web pages ranked by number of visits over the last year (log-lin plot)

Figure 3 (left) shows that over the last year the E-CAM software repositories has attracted by far the greatest interest in respect to the other pages, and that the interest is growing.



Figure 3: Number of visits per quarter for the last year to the E-CAM Software Repository (left) web-page and deliverables web-page respectively (right)

Visits to the deliverables project web-page on the other hand has reduced somewhat. Fig. 4 shows a more nuanced trend regarding visits to the E-CAM pilot project and training portal web pages.



Figure 4: Number of visits per quarter for the last year to the E-CAM pilot project web-page (left) and the Training Portal web page respectively (right)

#### 1.2.2 Lessons learned

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

- 1. The total number of visitors to the E-CAM web site has reduced
- 2. The community interest in the E-CAM site is deep in the sense that over the last 4 quarters more than 65 individual web pages have each been visited more than 65 times of visits (it has a one year h-index of over 65). Given the very technical/specialized nature of most of these pages, that is significant.
- 3. E-CAM software attracts the greatest attention
- 4. The training portal is still under utilized
- 5. The deliverables and pilot projects web-pages could get further attention.

#### 1.2.3 Recommendations and remedies

The actions for next period needed to strengthen dissemination effort for 1 to 5 above, are as follows. More details are given in Section 4.

- Increase visibility of E-CAM results such as deliverables, case studies, publications, material in our online training portal.
- Ensure that every deliverable and scientific publication has a very well written summary.
- Where possible, strengthen the connection between software generation in pilot projects and industry testcases.
- Improve accessibility (i.e. readability, appeal and utility) of the training portal
- Participate to selected external events where the E-CAM infrastructure is likely to be of interest, including joint dissemination actions with other EU CoE's and consortia.
- 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
- Create an E-CAM "comic" narrative explaining the role of simulation and modelling and HPC to the general public
- Increase focused dissemination efforts regarding recent E-CAM Software development initiatives: Load balancing library, HTC library releases, E-CAM refactored codes with exceptional scaling on massively parallel platform
- Discussions with industry: new set of activities in connection to industry training events for industrialists, as mentioned in our revised E-CAM business plan, submitted to the EC in March 2019[5].

## 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<sup>2</sup> 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 ESDWs 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. Following our dissemination strategy reassessment (section 1.2), the webpage front page was rebuilt and new pages were added describing E-CAM's activities in a language appropriate for the general public. While the content of the website has increased substantially since the last dissemination report and improvements have been made (see 2.1.1), the high-level structure is essentially the same, and we redirect the reader to D9.2: E-CAM Public Wiki-like pages and newsletters II[1] 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

The following improvements where made to the E-CAM website during the last period:

- 1. Direct links to main project results are now given on the website front page
- 2. Short synopsis are being added to the scientific publications page
- 3. A page dedicated to the online training portal was created
- 4. Events calendar view was improved to allow for a more attractive user experience
- 5. We have created a page to store case studies
- 6. All workshop reports have now an abstract, in a language easy to read for non-experts.

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

#### 1. Direct links to main project results are now given on the website front page

With the goal to generate more interest for our results, we now have primary access icons on the website front page, to the following important outputs resulting from training and software development activities and relationship with industry:

- Online Training Portal;
- Scientific Workshop Reports;
- Scientific Publications;
- Case Studies;
- Attend an event;
- Software Repository.

<sup>&</sup>lt;sup>2</sup>A website or database developed collaboratively by a community of users, allowing any user to add and edit content.

Below each icon there is a short description to what the reader should expect to find at each of these pages.

#### 2. Short synopsis are being added to scientific publications page

In the page "scientific publications" besides providing a list of publications connected to E-CAM, we also add a synopsis of each publication, that is easy to read for non-experts.

#### 3. A page dedicated to the online training portal was created

A page describing the online training portal explained in 2.3 was added to the project website. It explains how to access the portal, what is the terminology used, and it gives instructions to ESDW participants.

Additionally, public lectures have been uploaded to this page. These lectures have the permission by the presenters to be stored at our website. Further lectures are available if the user creates an account at our online training portal and request access to these lectures. Currently, public lectures on our website are on the areas of Quantum Dynamics, Classical MD, and on software development best practices. The upload of public lectures will continue in the future. Furthermore, the user can also search for other lectures tagged under a topic of their choice. This is facilitated by the addition of tags to the lectures, on the training portal.

#### 4. Events calendar view was improved to allow for a more attractive user experience

The Calendar view was improved using the Timely Calendar plugin (see Fig. 5). The new Calendar catches the eyes of website visitors with a variety of displays. Furthermore, it also allows to set up automatic newsletters to notify visitors about upcoming events.



Figure 5: E-CAM Calendar View

#### 5. We have created a page to store case studies

A webpage was created on our website, which stores cases studies emerging from our pilot projects focused on industrially oriented problems, and that report on successful industrial/academic collaboration. These case studies are

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focused on software development and point to other potential applications of the software. Case studies are maximum 3 pages long, and are in pdf format to allow the reader to easily download the document.

#### 6. All workshop reports have now an abstract, in a language easy to read for non-experts

To support an effective dissemination of our workshop reports, each report is now associated with an abstract targeted to the general public.

## 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, Etherpad, SharedLatex, 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*<sup>3</sup>. 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 D6.6: E-CAM Software Platform IV[6] for a more comprehensive description of the E-CAM library.

#### 2.2.1 Updates to the Software Repositories

The Software Development Best Practices defined in WP6 are now incorporated directly into 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 D6.6: E-CAM Software Platform IV [6].

The goals of our training infrastructure haven't changed. These are:

- **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.

 $<sup>^{3}</sup>$ 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.

Relevant portions of the entire ESDW program of 2018 and the first part of 2019, as well as other relevant training events have been captured, and stored in the portal. Public lectures have been uploaded to the E-CAM website, as mentioned in 2.1.1. Tags are added to the lectures, allowing to gather content by topic.

Before each ESDW, organizers and the software manager upload preparatory material to the collection dedicated to the ESDW, to share with the participants. This material is focused on tools that can assist the participants and other interested groups to develop software for extreme-scale hardware. The contents of the online training modules are outlined in D5.4: ESDW guidelines and programme IV[7].

We have also a capture and remote participation methodology in place for our training events. This methodology was successfully demonstrated for the 2nd EasyBuild User Meeting that E-CAM co-organised.

Five ESDW's will take place during 2019 (see D5.4[7]), which will highly leverage the content already captured and stored during the 2017 and 2018 programs.

The system upon which our service 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 include new filetypes that cover the scope of the content to be included by E-CAM: video presentations, PDFs and URLs. The platform is under continuous development by E-CAM, to improve the end-user experience.

## 3 E-CAM Newsletters

Three issues of the E-CAM newsletter were published during the period, rather than 4 as originally planned. The reason for the change, reported already in 2018 is that we have moved to a continuous mode of dissemination, rather than one determined by quarters. That is, news are reported as they come in, rather than delaying items for later publication in a block. The newsletter consists of a structured collection of items published in the corresponding period in a single output used for targeted distribution.

The newsletter issues published during this period were as follows.

- Issue 8 (section 3.1) Consists of news items including the open call for CECAM flagship events 2019; upcoming events with a focus on a transversal E-CAM ESDW "High Throughput Computing Workshop"; and the launch of the E-CAM onlione training portal. A industrial case study is presented on a "hierarchical equilibration strategy for polymer melts", and two featured software modules emerging from our pilot projects are highlighted. We point to the workshop scientific reports from State-of-the-Art and Scoping Workshops 2017 stored on our website, and the deliverables submitted in the last quarter. This issue can be consulted online here.
- Issue 9 (section 3.2) It includes an interview with Professor Tim Conrad on "The Curse of Dimensionality in Data-Intensive Modeling in Medicine, Biology, and Diagnostics". The issue also includes an E-CAM industrial Case Study "Designing control pulses for superconducting qubit systems with local control theory"; an overview of a new E-CAM scientific publication on multiscale method and algorithm entitled "Adaptive Resolution Molecular Dynamics Technique: Down to the Essential"; and descriptions of two featured software modules from the "modules of the month" category on our website. The newsletter also promotes: an upcoming ESDW on "Scaling Electronic Structure Applications"; the workshop scientific reports from scoping workshops in "Dissipative particle dynamics" and "solubility prediction" stored on our website; and the deliverables submitted in the last quarter. This issue can be consulted online at here.
- Issue 10 (section 3.3) The newsletter included news items on the E-CAM programme of events 2019, focusing on the "ESDW in Topics in Classical MD"; two papers introducing OpenPathSampling, a software package to study rare events; workshop scientific reports from the two State-of-the-Art workshops in 2018 "Improving ab initio prediction for materials" and "Large scale activated event simulations". An E-CAM industrial Case Study was featured, entitled "Mesoscale models for polarisable solvents: application to oil-water interfaces"; as well as three E-CAM software modules. The deliverables submitted in the last quarter were also featured in this issue. Issue 10 can be consulted online at here.

## 3.1 Newsletter May 2018

Display problems? Open this email in your web browser.



# Open call for CECAM flagship event proposals 2019



The CECAM CALL for workshops and schools that will run from April 2019 to March 2020 is now open! The text for the call and information on how to submit a proposal can be found at

https://www.cecam.org/submitting.html. Deadline for submissions is 16 July 2018.

# Upcoming events

# High Throughput Computing Workshop



E-CAM is organising a one week (16-20 July 2018) Extended Software Development Workshop in Turin, Italy that will focus on intelligent high throughput computing (HTC) as a technique that crosses many domains within the molecular simulation community in general and the E-CAM community in particular. The workshop will be a hybrid learning/coding event targeted at scientists with particular problems to solve. There will be 3 days of tutorial content presenting 3 different task management frameworks and 2 days code development time with the framework developers to help you integrate them into your application. <u>Read more</u>

Extended Software Development Workshop: Quantum Dynamics

June 18-29, 2018

Organizers: Federica Agostini Basile Curchod Ari Paavo Seitsonen

CECAM-FR-MOSER

Read more

Extended Software Development Workshop: Atomistic, Meso- and Multiscale Methods on HPC Systems

September 3-4, 2018

Organizers: Ignacio Pagonabarraga Burkhard Duenweg Godehard Sutmann

CECAM-DE-JUELICH

## Read more

State-of-the-Art Workshop: Improving the accuracy of abinitio predictions for materials

September 17-20, 2018

Organizers: Carlo Pierleoni Dario Alfè David Ceperley

CECAM-FR-MOSER

Read more

## E-CAM events

E-CAM Case Study: The implementation of a

# hierarchical equilibration strategy for polymer melts, to help studying the rheological properties of new composite materials



## By Dr. Hideki Kobayashi, Max Planck Institut für Polymerforschung

## Abstract

The ability to accurately determine and predict properties of newly developed polymer materials is highly important to researchers and industry, but at the same time represents a significant theoretical and computational challenge. We have developed a novel multiscale simulation method based on the hierarchical equilibration strategy, which significantly decreases the equilibrium properties calculation time while satisfying the thermodynamic consistency. A number of E-CAM modules was developed and implemented in the ESPResSo++ software package.

**Read more** 

# The launch of the E-CAM Online Training Portal

4/1/2019

E-CAM Newsletter - May 2018



Our E-CAM training portal is now online. The goals and expected impacts for our online training infrastructure are to: (i) collect the content captured at our Extended Software Development Workshops (ESDWs); (ii) generate online training modules for each ESDW; (iii) be a repository for the data associated to our events; (iv) build tutorials on programming best practices to develop software for extreme-scale hardware; (v) Associate with other groups and projects with similar training scope. The content of the training portal is freely available upon registration, but we also keep a selection of publicly available lectures accessible directly from the E-CAM website.

Read more

<u>Scientific reports from State-of-the-Art and Scoping</u> <u>Workshops 2017 are now available on our website</u>



The scientific reports from the following workshops of the project E-CAM running in (2017):

- E-CAM Scoping Workshop: "From the Atom to the Material", 18-20 September 2017, University of Cambridge (UK)
- E-CAM State-of-the-Art Workshop WP4: "Meso and Multiscale Modelling", 29 May 1 June 2017, University College Dublin (Ireland)

**Read more** 

# Featured Software Modules



## <u>Contact Map - a package for</u> analyzing and exploring contacts from a trajectory generated by MD

Contacts can be an important tool for defining (meta)stable states in processes involving biomolecules. For example, an analysis of contacts can be particularly useful when defining bound states during a binding processes between proteins, DNA, and small molecules (such as potential drugs). The contacts analyzed by the **contact\_map** package can be either intermolecular or intramolecular, and can be analyzed ... LocConQubit - a module for the construction of controlled pulses on isolated qubit systems using the Local Control Theory



The **LocConQubit** module implements the Local Control Theory, an algorithm for onthe-fly construction of a time-dependent potential that drives the evolution of a Hamiltonian towards one of its eigenstates. The algorithm is applicable to any Hamiltonian that is separable into a timedependent and into a time-independent part, where the first part is directly incorporated into the algorithm, while the ...

#### Read more

Read more

All featured modules

# Submitted deliverables

## D2.2: Identification/Selection of E-CAM Electronic Structure Codes for Development



A review of current algorithms for electronic structure calculations and an overview of the software modules to be developed within the Electronic Structure WP (WP2) of E-CAM.

## D3.2: Identification/Selection of E-CAM Quantum Dynamics Codes for Development



A review of current algorithms for the simulation of quantum dynamics and an overview of the software modules to be developed within the Quantum Dynamics WP (WP3) of E-CAM.

## D7.4: E-CAM Software Porting and Benchmarking Data II



Report on results of the initial porting and optimisation of 8 new E-CAM modules to massively parallel machines and their benchmarking and scaling on a variety of architectures.

## All deliverables

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This project has received funding from the European Union's Horizon 2020 research and

#### E-CAM Newsletter - May 2018

## innovation programme under grant agreement No 676531

MailPoet
Iviain Oct

## 3.2 Newsletter Oct 2018

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<u>The Curse of Dimensionality in Data-Intensive</u> <u>Modeling in Medicine, Biology, and Diagnostics</u>



With Prof. Tim Conrad (TC), Free University of Berlin, and Dr. Donal Mackernan (DM), University College Dublin.

In this E-CAM interview with Prof. Tim Conrad, the growing importance of diagnostics in medicine and biology is discussed, including concepts rooted in signal analysis relevant to systematic dimensional reduction, and pattern recognition, and the possibilities of their

application to systematic coarse-graining. The opportunities and challenges for scientists of start-up companies are also discussed based on experience.

## Read more

# Upcoming event

# Extended Software Development Workshop: Scaling Electronic Structure <u>Applications</u>

## 7-18 January 2019, CECAM-IRL

**Organisers:** Nick Papior, Yann Pouillon, Micael Oliveira, Fabiano Corsetti, Volker Blum, Emilio Artacho, David D. O'Regan, Charles Patterson, Stefano Sanvito, Donal MacKernan

E-CAM is organising a two week (7-18 January 2019) <u>Extended Software Development</u> <u>Workshop in Dublin</u>, Irland that will focus on training of latest parallelization paradigms for scaling of electronic structure applications, implementation of the best strategies for parallelizing and optimizing, with an emphasis on the scalability of the <u>Electronic Structure</u> <u>Library (ESL)</u> applications.

Read more

E-CAM Case Study: Designing control pulses for superconducting qubit systems with local control

theory



## By Dr. Momir Mališ, École Polytechnique Fédérale de Lausanne

## Abstract

A quantum logic gate is one of the key components of the quantum computer, and designing an effective quantum universal gate is one of the major goals in the development of quantum computers. We have developed a software based on local control theory to design efficient state preparation control pulses for universal quantum gates which drive full population transfer between qubit states.

## Read more

## **New Publication**

Adaptive Resolution Molecular Dynamics Technique: Down to the Essential



A new publication by the *Theoretical and Mathematical Physics in Molecular Simulation* group of the Freie Universität Berlin, lead by Prof. Luigi Delle Site, E-CAM partner, was published in the Journal of Chemical Physics. In it, the authors study the application of the thermodynamic force in the coupling region of an adaptive resolution molecular dynamics simulation (AdResS) approach which assures thermodynamic equilibrium and proper exchange of molecules between atomistically resolved and coarse-grained regions.



# Scientific reports from the 2018 E-CAM workshops

## are now available on our website



The scientific reports from the following E-CAM workshops held in 2018 are available for download:

- E-CAM Scoping Workshop: "<u>Solubility prediction</u>", 14 15 May 2018, Ecole Normale Supérieure de Lyon (France)
- E-CAM Scoping Workshop: "<u>Dissipative particle dynamics: Where do we stand on</u> predictive application?", 24 - 26 April 2018, Daresbury Laboratory (United Kingdom)

**Read more** 

## Featured Software Modules



## Improving I/O of DL\_MESO\_DPD files using SIONlib

This module implements the SIONlib library to optimize the I/O (reading/writing) of the trajectory files generated by DL\_MESO\_DPD, the Dissipative Particle Dynamics (DPD) code from the DL MESO package. SIONlib is a library for writing and reading binary data to/from several thousands of processors into one or a small number of physical files. For parallel access to files, only the ...

Read more

## PaPIM: A code for Quantum Time Correlation Functions



**PaPIM** code is a package to study the (quantum) properties of materials, and in particular time correlation functions, via the so-called mixed quantum-classical methods. In these schemes, quantum evolution is approximated by appropriately combining a set of classical trajectories for the system. Several quantum effects, for example, the possibility to find atoms in classically forbidden regions (tunneling), are reproduced ...

Read more

## All featured modules

## Submitted deliverables

## D1.4: Classical MD E-CAM Modules III



Software modules delivered to the E-CAM repository in the area of Classical Mechanics.

## D2.4: Electronic structure E-CAM modules III

E-CAM Newsletter - Oct 2018



Software modules delivered to the E-CAM repository in the area of Electronic Structure.

## D7.5: Hardware developments III



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.

## All deliverables

Access our software repository

Ask a technical question

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## 3.3 Newsletter March 2019

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# E-CAM program of events 2019



Check out our program of events for this year, running from April 2019 to February 2020. E-CAM events are part of the <u>CECAM</u> annual flagship program, and are hosted at different CECAM Nodes locations. 4/1/2019

E-CAM Newsletter - March 2019



# E-CAM Case Study: Mesoscale models for polarisable solvents: application to oil-water

interfaces



## By Dr. Silvia Chiacchiera, Science and Technology Facilities Council, UK

Water is a polar liquid and has a dielectric permittivity much higher than typical apolar liquids, such as light oils. This strong dielectric contrast at water-oil interfaces affects electrostatics and is important, for example, to include these effects to describe biomolecular processes and water-oil mixtures involving surfactants, as detergents. In this <u>pilot project</u>, developed in collaboration with <u>Unilever</u> and <u>Manchester University</u>, we have proposed and analysed a class of polarisable solvent models to be used in Dissipative Particle Dynamics (DPD), a coarse-grained particle-based simulation method commonly used in various industrial sectors. Related software modules for the DL\_MESO package have also been developed.

E-CAM Newsletter - March 2019

## **Read more**

# Upcoming event



E-CAM is organising an Extended Software Development Workshop in Topics in Classical MD from 3 to 12 April 2019, which is a major coding initiative that will combine lectures; coding sessions and hands-on training. Topics at this workshop will include using and extending modern MD software in the domains of: advanced path sampling methods (and the software package OpenPathSampling) metadynamics ...



Two papers introducing OpenPathSampling, a software package to study rare events

Two papers introducing to <u>OpenPathSampling</u> (OPS) were recently published :

OpenPathSampling: A Python Framework for Path Sampling Simulations. <u>1.</u>
 Basics

 OpenPathSampling: A Python Framework for Path Sampling Simulations. <u>2.</u> <u>Building and Customizing Path Ensembles and Sample Schemes</u>

OPS is a software package to perform path sampling simulations and other trajectory-based approaches to study rare events. Much of the development of OPS has been sponsored by E-CAM.

Read more

# Scientific reports from E-CAM State-of-the-art workshops 2018, are now available on our website



The scientific reports from the following E-CAM State-of-the-Art workshops held in 2018 are available for download:

- Improving the accuracy of ab-initio predictions for materials @ CECAM-FR-MOSER, 17 - 20 September 2018
- Large scale activated event simulations @ CECAM-AT, 1 3 October 2018

# **Featured Software Modules**



# Module SCDM\_WFs



# <u>Quantics-QChem-</u> Interface (QQ-Interface)



The QQ-Interface module connects the full quantum nonadiabatic wavefunction propagation code Quantics to the timedependent density functional theory (TDDFT) module of the electronic structure program Q-Chem. Q-Chem provides analytic gradients, Hessians and derivative couplings at TDDFT level. With this module, it is possible to use the Q-Chem TDDFT module for excited state direct dynamics calculations. Quantics will start Q-Chem calculations whenever needed, prepare ...

Read more

## ALL FEATURED MODULES

Module SCDM\_WFs implements the selected columns of the density matrix (SCDM) method for building localized Wannier Functions (WFs). Wannier90 is a post-processing tool for the computation of the Maximally Localised Wannier Functions (MLWFs) , which have been increasingly adopted by the electronic structure community for different purposes. The reasons are manifold: MLWFs provide an insightful chemical analysis of the nature of bonding, and ...

Read more

# PLUMED wrapper for OpenPathSampling



PLUMED is a widely used and versatile rare-event sampling and analysis code that can be used with various Molecular Dynamics (MD) engines. It has a very intuitive and versatile syntax for the definition of Collective Variables (CVs), and a wide variety of sampling methods, which accounts for its widespread use. The present module allows PLUMED and OPS to be used ...

Read more

# Submitted deliverables

## D3.4: Quantum dynamics E-CAM modules III



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

## D4.4: Meso- and multi-scale modelling E-CAM modules III



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

## D6.6: E-CAM Software Platform IV



Update on E-CAM software tools and three main platforms <u>E-CAM Software library;</u> <u>E-CAM Website</u> and <u>E-CAM Online</u> <u>Training Portal</u>.

## ALL DELIVERABLES



Ask a technical question

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## 4 Conclusions and plan for next year

Our dissemination activities over the last year continue to build on the completely revised strategy reported in D9.2 where material is continuously delivered and includes recent news items, success stories, case studies, opinion pieces, interviews and upcoming E-CAM events. Project results are now communicated through these items and through the new category "Modules of the Month" where every month we publicize the best certified modules and their potential applications. The case studies focus on the software modules produced and their potential applications and are disseminated to industry. Results specific to each pilot project in collaboration with industry are also communicated through pages dedicated to pilot projects. Software modules associated with pilot projects and those produced via E-CAM Extended Software Development Workshops now each have a public abstract which is easy to read for non-experts, and facilitates dissemination via email and the news blog, Twitter, and presentation to industrialists. This focus on having readable summaries accessible to the public is also being enforced where possible on output, such as deliverables and publications. Lectures at E-CAM events are now recorded and made available online through an online training infrastructure. In addition to ESDW's, industry Scoping and state of the art workshops we have also organised tutorials in Ireland in partnership with PRACE and software carpentry focused on the usage of simulation software on HPC platforms aimed at a non-expert coding audience (i.e. to non-software developers). These have attracted students and people from industry relatively new to simulation.

Our web statistics have revealed that while the interest in, for example, E-CAM software has increased over the last year, there has nevertheless been a reduction in the number of visitors to the E-CAM website. This may be due to the novelty factor of E-CAM having dissipated, typical of stakeholders behavior during a project life cycle. As reported in ref. [4], stakeholders interest throughout the different phases of a project follows a "U-shaped" curve, reflecting initial enthusiasm, lower levels of interest during development phases, and renewed interest as the project nears completion. Our plans for next year have been developed in this context and are as follows.

- 1. Continue to publish via the web: special articles/interviews as they attract a great deal of interest and attention to the website; software modules of the month as they also are of great interest to a wide readership; E-CAM success stories aimed at the wider community including industry; short pieces highlighting recent E-CAM scientific publications and deliverable output.
- 2. The very large number and scope of E-CAM events in 2019 represent an extraordinary opportunity for E-CAM and will be met by intensified dissemination follow through.
- 3. Participation to non-E-CAM events which have a strong interest in exploiting the E-CAM infrastructure and identifying new collaborations.
- 4. Intensify our dissemination of the E-CAM training portal (more details in [3]).
- 5. Organise in partnership with PRACE E-CAM tutorials focused on the usage of E-CAM software and know how aimed at a non-expert coding audience (i.e. to non-software developers).
- 6. We are engaged in exploiting the natural synergy between the new CoE FocusCoE and E-CAM so as to promote the CoEs activities to the general public and to help enhance connections with industry. This will include collaborating with FocusCoE for an E-CAM website to target the general public. Further details are presented in the second iteration of the additional deliverable on dissemination strategy, training strategy and cross WP-collaboration[3].
- 7. A Comic focused on E-CAM and how it enables modelling and simulation for HPC is planned with expected delivery date in the last quarter of 2019. The objective is to have an innovative brochure, where Comics will be used to explain the CoE, its goals, and connection to HPC in a storytelling fashion. Further details of this are also presented in the fore-mentioned additional deliverable.

## References

#### **Acronyms Used**

CECAM Centre Européen de Calcul Atomique et Moléculaire

PRACE Partnership for Advanced Computing in Europe

ESDW Extended Software Development Workshop

- WP Work Package
- WP Work-package
- PDRA Postdoc Research Associate
- CoEs Centres of Excellence

MolSSI Molecular Sciences Software Institute

EC European Commission

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