



## **E-CAM Software Platform I**

E-CAM Deliverable 6.3

Deliverable Type: Report

Delivered in Month 12– September 2016



E-CAM

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



Funded by the European Union under grant agreement 676531

### Project and Deliverable Information

|                              |  |
|------------------------------|--|
| Project Title                | E-CAM: An e-infrastructure for software, training and discussion in simulation and modelling   |
| Project Ref.                 | Grant Agreement 676531   |
| Project Website              | <a href="https://www.e-cam2020.eu">https://www.e-cam2020.eu</a>  |
| EC Project Officer           | Dimitrios Axiotis  |
| Deliverable ID               | D6.3   |
| Deliverable Nature           | Report   |
| Dissemination Level          | Public   |
| Contractual Date of Delivery | Project Month 12(September 2016)   |
| Actual Date of Delivery      | 01.11.2016   |
| Description of Deliverable   | On-line publication of the E-CAM web-platform. The platform will include: the E-CAM library of software modules and interfaces; end users portal (to access E-CAM's resources, make requests for software developments, register for events); web infrastructure for teaching tools. |

### Document Control Information

|            |                   |   |
|------------|-------------------|---|
| Document   | Title:            | E-CAM Software Platform I   |
|            | ID:               | D6.3  |
|            | Version:          | As of November 3, 2016  |
|            | Status:           | Accepted by WP Leader   |
|            | Available at:     | <a href="https://www.e-cam2020.eu/deliverables">https://www.e-cam2020.eu/deliverables</a> |
| Review     | Document history: | <a href="#">Internal Project Management Link</a>  |
|            | Review Status:    | Reviewed  |
| Authorship | Action Requested: | <b>Submit</b>   |
|            | Written by:       | Alan O'Cais(Juelich Supercomputing Centre)  |
|            | Contributors:     | Dominic Tildesley (EPFL),   |
|            | Reviewed by:      | D. Tildesley (EPFL)   |
|            | Approved by:      | A. O'Cais (JSC)   |

### Document Keywords

|           |   |
|-----------|---|
| Keywords: | E-CAM, <a href="#">HPC</a> , <a href="#">CECAM</a> , Materials, ... |
|-----------|---|

November 3, 2016

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

**Copyright notices:** This deliverable was co-ordinated by Alan O'Cais<sup>1</sup> (Juelich Supercomputing Centre) on behalf of the E-CAM consortium with contributions from Dominic Tildesley (EPFL), . This work is licensed under the Creative Commons Attribution 4.0 International License. To view a copy of this license, visit <http://creativecommons.org/licenses/by/4.0>.



<sup>1</sup>[a.ocais@fz-juelich.de](mailto:a.ocais@fz-juelich.de)

Contents

|                          |   |
|--------------------------|---|
| Executive Summary        | 1 |
| 1 Introduction           | 2 |
| 1.1 Delivery and Back-up | 2 |
| 2 Software Modules       | 3 |
| 3 Users Portal           | 4 |
| 3.1 Version Control      | 4 |
| 3.1.1 GitLab             | 4 |
| 3.2 Project Management   | 5 |
| 3.2.1 Redmine            | 5 |
| 3.2.2 Kanban             | 6 |
| 3.2.3 EtherPad           | 6 |
| 3.2.4 ShareLatex         | 7 |
| 4 Online Learning        | 8 |
| 4.1 Future Development   | 8 |
| References               | 9 |

List of Figures

|   |  |   |
|---|--|---|
| 1 | An example of one of the four module repositories      | 3 |
| 2 | A list of the E-CAM repositories on our GitLab service | 4 |
| 3 | A view of the E-CAM project within our Redmine service | 5 |
| 4 | An example use case for our Kanban service             | 6 |
| 5 | An example use case for our Etherpad service           | 6 |
| 6 | An example use case for our ShareLatex service         | 7 |
| 7 | A subsection of the E-CAM training page                | 8 |

List of Tables

|   |                                  |   |
|---|----------------------------------|---|
| 1 | E-CAM documentation repositories | 3 |
|---|----------------------------------|---|

## Executive Summary

This deliverable describes the provision of online services in the E-CAM project which together form the E-CAM web platform. The primary landing point for information about the resources of the project is the [E-CAM project website](#). This site alone covers the basic requirements of the E-CAM User Portal:

- *E-CAM library of software modules and interfaces*

The [software modules of E-CAM](#) are linked through the website, in addition to the rendered documentation that result from them.

- *Access to E-CAM's resources*

All of E-CAM resources are described and available through the E-CAM website. This includes our [upcoming E-CAM events](#) and the [E-CAM online services](#).

- *Make requests for software developments*

We would like to deal with development requests directly on a case-by-case basis with the relevant Work Package (WP) leader and the Software Manager being in direct contact with the person making the request. For this reason we have created a very simple [technical first contact page](#) in order to channel users to the correct WP.

- *Register for events*

All E-CAM events are managed through Centre Européen de Calcul Atomique et Moléculaire (CECAM) with registration for events happening through them. On the E-CAM website we provide [detailed descriptions of the E-CAM events](#) and links to the registration process of CECAM.

- *Web infrastructure for teaching tools*

An [E-CAM training page](#) is under development to provide a list of training tools for the project beneficiaries, participants and the wider community in the High Performance Computing skills space. More complex teaching infrastructures are planned but will take considerable time to reach maturity.

However, E-CAM has delivered a number of additional online resources and capabilities that include:

- Software modules are contributed to E-CAM through the documentation repository of the relevant research-related Work Package. The sources for the documentation are stored on the [E-CAM GitLab service](#) with rendered documentation available through [ReadTheDocs.org](#).
- A [Kanban service](#) has been made available to facilitate a lower setup overhead and direct interaction with the issue reporting features of GitLab.
- The [Redmine service](#) is used to manage larger software projects and track related issues. It allows users to manage multiple projects and associated sub-projects. It features project wikis and forums, issue tracking, time tracking, and flexible, role-based access control.
- An [Etherpad service](#) has been provided for a number of participants to simultaneously add to meeting notes and minutes during an online collaborative meeting.
- A [ShareLatex service](#) has been added to facilitate the collaborative production of publication-quality papers using  $\LaTeX$ .

Over the lifetime of the project these online services will mature and expand, particularly in the case of online learning.

# 1 Introduction

In its role as an e-infrastructure for the wider E-CAM community, a number of services have been made available to facilitate the creation of, collaboration on and publication of software projects.

This report highlights the services that are currently available to E-CAM users and outlines the purpose of each service. These services include

- Online software repositories and associated services,
- A number of project management services effective collaboration on software projects and to streamline the creation of associated publications,
- An initial set of training material relative to the exascale efforts of the E-CAM community.

Over the lifetime of the project these online services will mature and expand, particularly in the case of online learning.

## 1.1 Delivery and Back-up

Each E-CAM service is delivered as a Docker container<sup>2</sup> and is run on a special purpose server at [CECAM](#) headquarters. This approach makes the backup of E-CAM services efficient and straightforward. It also facilitates easy migration of services to either a new server or a new site in the future.

---

<sup>2</sup>Docker is an open-source project that automates the deployment of Linux applications inside software containers.

## 2 Software Modules

One of the primary outputs of E-CAM are the software modules produced by the postdoctoral researchers of the project and the participants of E-CAM Extended Software Development Workshop (ESDW) events.

Software modules are contributed to E-CAM through the documentation repository of the relevant research-related WP. The sources for the documentation are stored on the E-CAM [GitLab service](#) (see Section 3.1.1). Contributions to the repositories are made through *Merge Requests*<sup>3</sup>. Each individual modification of the repository automatically causes the associated documentation on [ReadTheDocs.org](#) to be rebuilt.

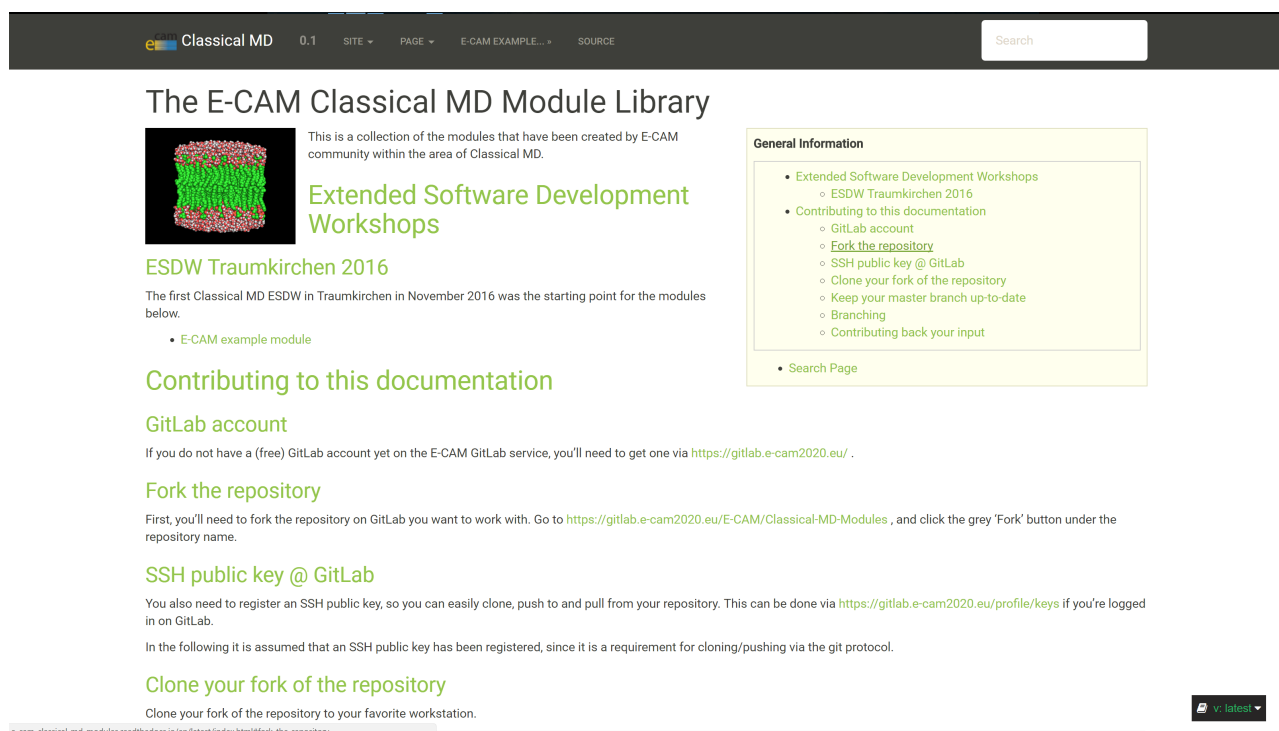


Figure 1: An example of one of the four module repositories

An example of the landing page for the Classical MD WP can be seen in Fig. 1. The individual repositories for each research WP and the location of the resultant documentation page can be found in Table 1.

Table 1: E-CAM documentation repositories

|                                 |  |  |
|---------------------------------|--|--|
| Classical MD                    | <a href="#">WP1 Documentation Repository</a> | <a href="#">WP1 Rendered Documentation</a> |
| Electronic Structure            | <a href="#">WP2 Documentation Repository</a> | <a href="#">WP2 Rendered Documentation</a> |
| Quantum Dynamics                | <a href="#">WP3 Documentation Repository</a> | <a href="#">WP3 Rendered Documentation</a> |
| Meso- and Multi-scale Modelling | <a href="#">WP4 Documentation Repository</a> | <a href="#">WP4 Rendered Documentation</a> |

<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.

### 3 Users Portal

The primary landing point for information about the resources of the project is the [E-CAM project website](#). This site alone covers the basic requirements of the User Portal:

- *Access to E-CAM's resources*

All of E-CAM resources are described and available through the E-CAM website. This includes our [upcoming E-CAM events](#) and the [E-CAM online services](#).

- *Make requests for software developments*

We would like to deal with development requests directly on a case-by-case basis with the relevant [WP](#) leader and the Software Manager being in direct contact with the person making the request. For this reason we have created a very simple [technical first contact page](#) in order to channel users to the correct [WP](#).

- *Register for events*

All E-CAM events are managed through [CECAM](#) with registration for events happening through them. On the E-CAM website we provide [detailed descriptions of the E-CAM events](#) and links to the registration process of [CECAM](#).

However, E-CAM has delivered a number of additional online resources and capabilities that are described in the following section.

#### 3.1 Version Control

The primary software development tool that E-CAM provides is a version-control system. Git is ubiquitous in modern software development and is the obvious choice as the main version control system.

##### 3.1.1 GitLab

We have chosen to create a [GitLab service](#) as our online git repository management system. This provides us with the possibility of creating unlimited private repositories, something that is essential when considering either licensing or the Intellectual Property (IP) requirements of our partners (particularly those in industry).

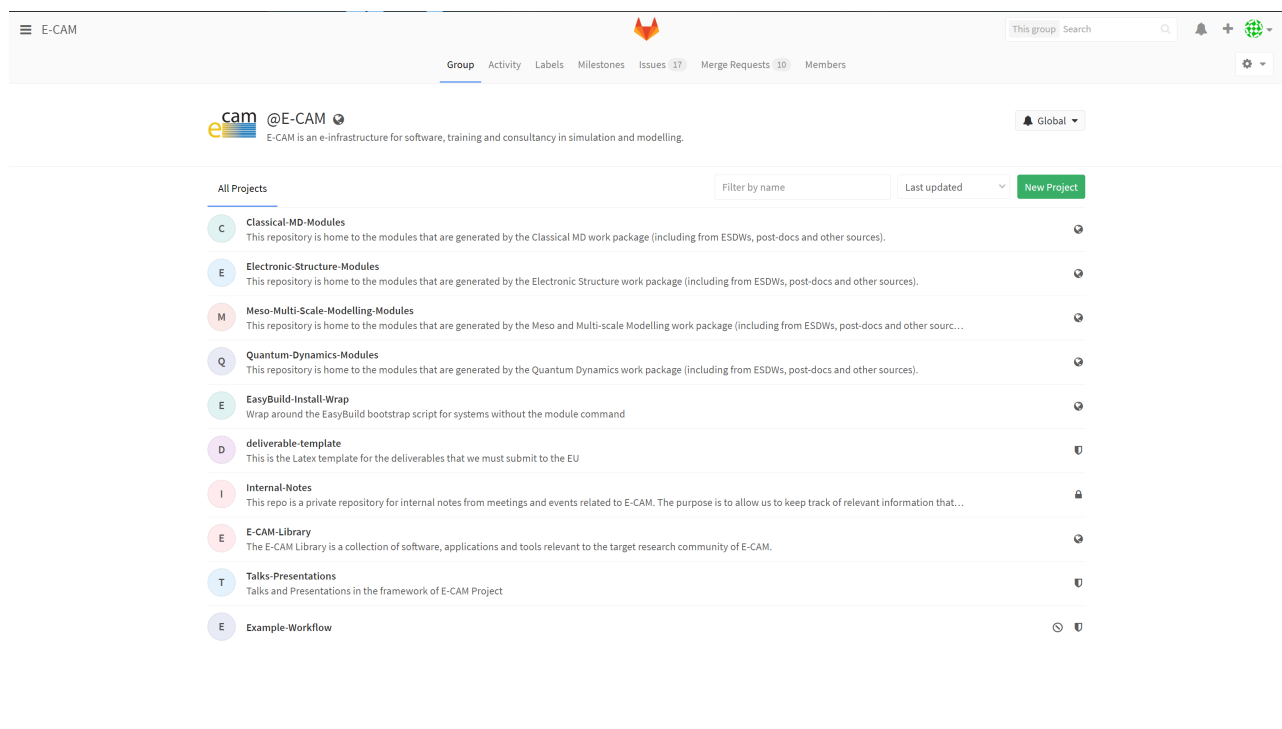


Figure 2: A list of the E-CAM repositories on our [GitLab service](#)

A screen shot of the direct repositories of the E-CAM software group can be seen in Fig. 2. Some of these repositories have already been discussed in Section 2. The actual number of software repositories is far greater than this. On our main project website we also provide a link to [all publicly accessible repositories of E-CAM](#).

**Continuous Integration** Continuous Integration is a software development practice in which a developer builds and tests software every time that they create new code in an application. GitLab provides a method of implementing continuous integration and we in turn make it available to our community.

**Authentication** Where possible we leverage the OAuth<sup>4</sup> features of GitLab in order to have single-sign-on capabilities for all E-CAM services.

## 3.2 Project Management

Supporting and streamlining the management of software projects, including bug-tracking and feature requests, is another area where E-CAM can be of service to the community. Many of these capabilities already exist in our GitLab service, however we have enabled a number of additional services that seek to make remote collaboration on software projects as straightforward as possible.

### 3.2.1 Redmine

[Redmine](#) is a free and open source, web-based project management and issue tracking tool. It allows users to manage multiple projects and associated sub-projects. It features project wikis and forums, time tracking, and flexible, role-based access control. It includes a calendar and Gantt charts to aid visual representation of projects and their deadlines. Redmine integrates with various version control systems and includes a repository browser and a diff viewer.

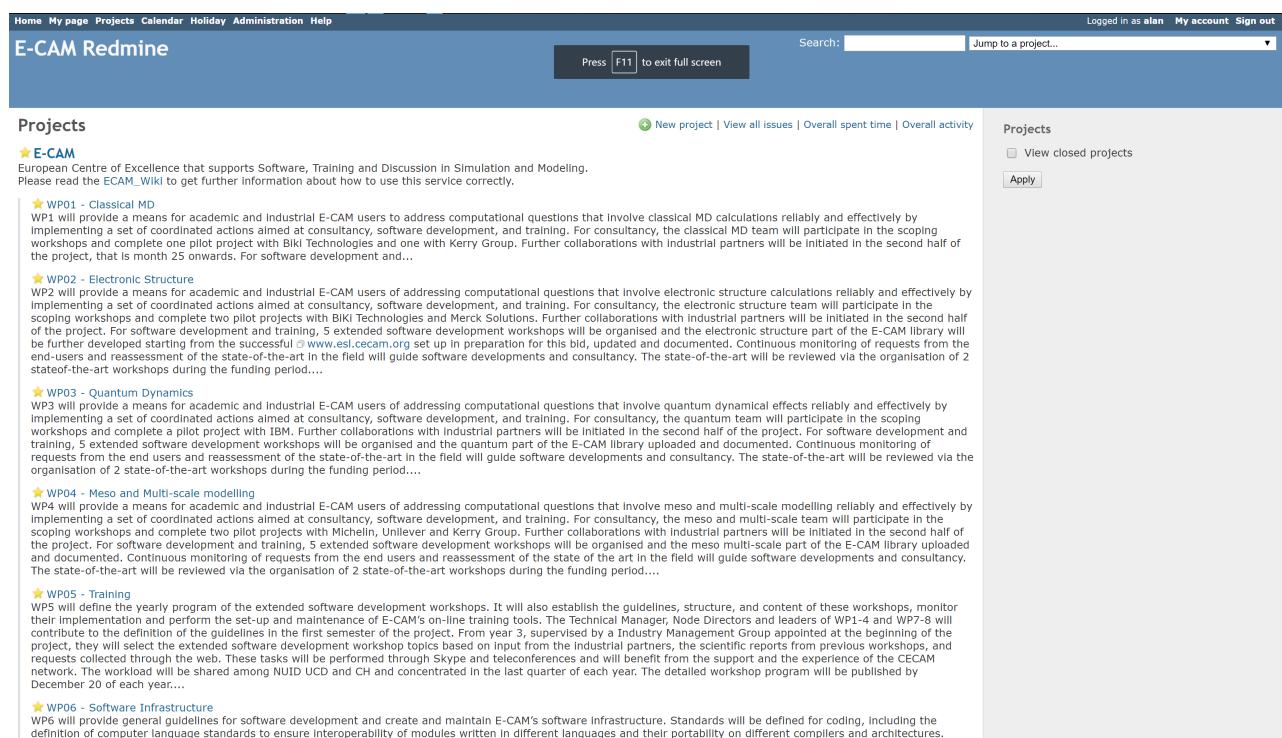


Figure 3: A view of the E-CAM project within our [Redmine service](#)

We also use the [Redmine service](#) to manage the overall E-CAM project and this example of Redmine usage can be seen in Fig. 3

<sup>4</sup>OAuth is an open standard for authorization, commonly used as a way for Internet users to authorize websites or applications to access their information on other websites but without giving them the passwords.



### 3.2.2 Kanban

In order to facilitate a lower setup overhead and direct interaction with the issue reporting features of GitLab, we have also made a Kanban<sup>5</sup> service available that connects directly to the GitLab repositories.

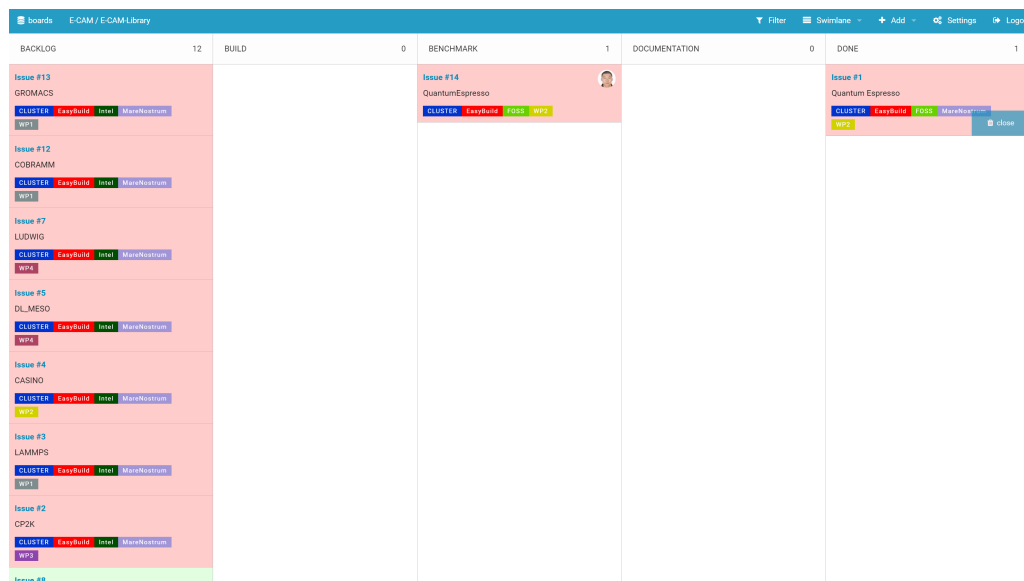


Figure 4: An example use case for our [Kanban service](#)

An example of its use in the case of one of the E-CAM repositories can be seen in Fig. 4

### 3.2.3 EtherPad

In geographically distributed collaborative projects, regular meetings are essential. To facilitate taking minutes in such meetings we have created an [Etherpad service](#). Etherpad is a web-based collaborative real-time editor, allowing authors to simultaneously edit a text document, and see all of the participants' edits in real-time, with the ability to display each author's text in their own color.

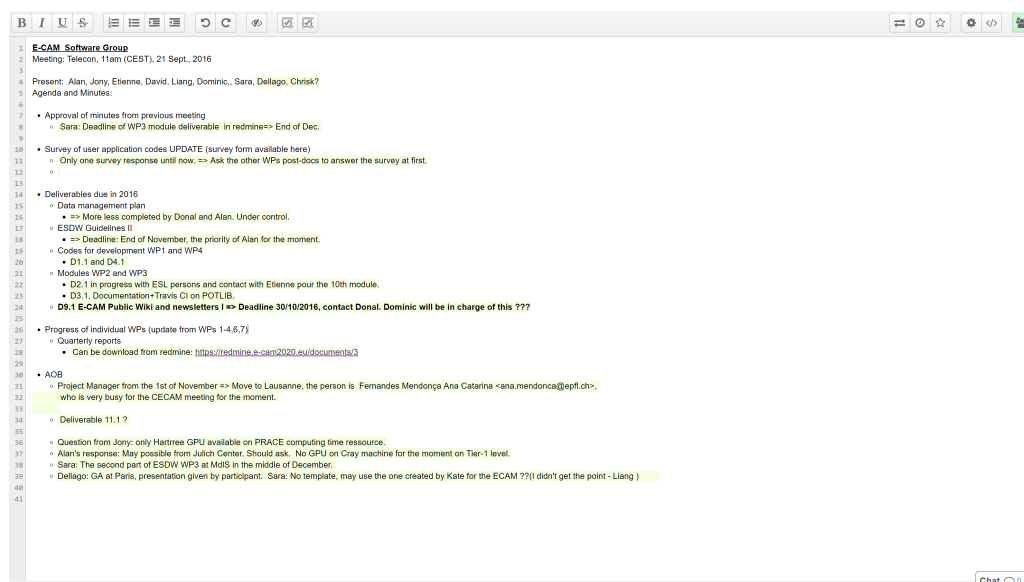


Figure 5: An example use case for our [Etherpad service](#)

An example use of an etherpad is given in Fig. 5.

<sup>5</sup>[Kanban](#) in the context of software development provides a visual process-management system that aids decision-making about what to produce, when to produce it, and how much to produce.

### 3.2.4 ShareLatex

Many of the E-CAM beneficiaries are academic researchers, who use Latex to produce technical documents and papers. ShareLaTeX is an online LaTeX editor that allows real-time collaboration and online compiling of projects to PDF

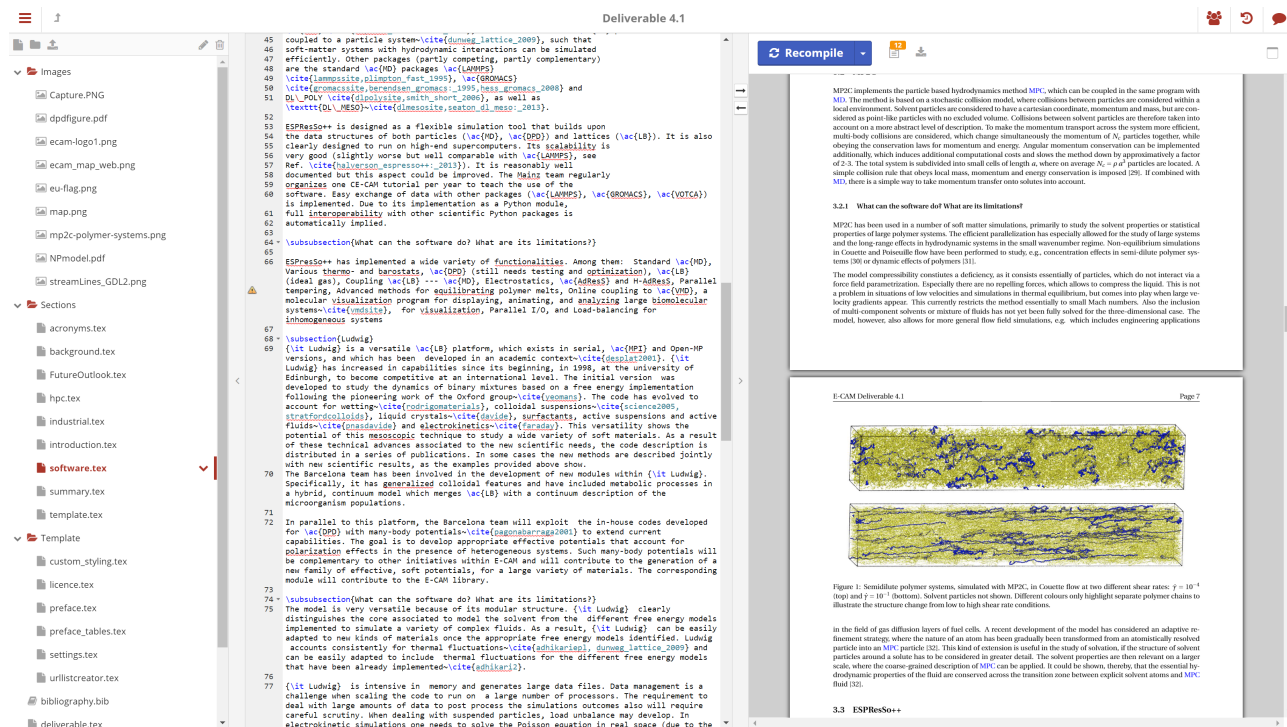


Figure 6: An example use case for our [ShareLatex service](#)

format. In comparison to other LaTeX editors, ShareLaTeX is a server-based application, which is accessed through a web browser. We have created a [ShareLatex service](#) for use by the E-CAM community to facilitate easier collaboration on project-related papers and deliverables. An example can be seen in Fig. 6

## 4 Online Learning

E-CAM wishes to develop an appropriate online training infrastructure over the course of the project. To this end, it is establishing strong partnerships with PRACE and leading HPC centres in Europe in order to provide appropriate training content that can bring the E-CAM user communities to the exa-scale.

This infrastructure is still under development however. Until we are providing a suitable platform for an online training infrastructure that would provide some information regarding existing (online) training opportunities relevant to our community.

### List of online HPC training repositories

|   |   |
|---|---|
| NERSC Training Page   | <a href="https://www.nersc.gov/users/training/">https://www.nersc.gov/users/training/</a>   |
| University of Illinois College of Engineering Computational Science and Engineering | <a href="http://cse.illinois.edu/training">http://cse.illinois.edu/training</a>   |
| HPC University  | <a href="http://hpcuniversity.org">hpcuniversity.org</a>  |
| OU Supercomputing Center for Education & Research (OSCER)                           | <a href="http://www.oscer.ou.edu/education.php">http://www.oscer.ou.edu/education.php</a>   |
| LinkSCEEM   | <a href="http://supercomputing.cyi.ac.cy/index.php">http://supercomputing.cyi.ac.cy/index.php</a>   |
| Institute for Advanced Simulation (IAS) Jülich Supercomputing Centre (JSC)          | <a href="http://www.fz-juelich.de/ias/jsc/EN/Expertise/Workshops/workshops_node.html">http://www.fz-juelich.de/ias/jsc/EN/Expertise/Workshops/workshops_node.html</a> |
| CINECA – SuperComputing Applications and Innovation                                 | <a href="http://www.hpc.cineca.it/content/training-2015">http://www.hpc.cineca.it/content/training-2015</a>   |
| ARCHER – UK National Supercomputing Service   | <a href="http://www.archer.ac.uk/training/">http://www.archer.ac.uk/training/</a>   |
| Pawsey Supercomputing   |   |

Figure 7: A subsection of the [E-CAM training page](#)

We have created an [E-CAM training page](#) to highlight some of the existing training opportunities for E-CAM users. In particular, in Fig. 7 we highlight here the training sites that are especially relevant to a High Performance Computing (HPC) environment.

### 4.1 Future Development

Given the resources attributed to the online training component of E-CAM, the services that E-CAM can potentially provide are limited. Among the list of possibilities are:

- **HPC services** - this service would provide an HPC environment to train users and to test modules before moving the testing onto larger Partnership for Advanced Computing in Europe (PRACE) machines. There is a possibility to create a pseudo-HPC-cluster using Docker containers and provide access to this over the internet. This would have significant development overhead as no such drop-in service currently exists, and we are carefully weighing the benefit of this service against the cost of provision.
- **Multimedia data repository** - Rich metadata can be created from training content such as video captures, audio, slides, URLs and source code. There is software such as [Clowder](#) that can automatically create such meta-data (given the right plugins to digest each data-object).

In the near term, E-CAM will focus on streaming portions of the training events that it is associated with. The goal is to allow remote participation for E-CAM members, and in particular for industrial partners who cannot commit to the allocated time for our [ESDW](#) events.

## 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

**WP** Work Package

**IP** Intellectual Property

### URLs referenced

#### Page ii

<https://www.e-cam2020.eu> ... <https://www.e-cam2020.eu>  
<https://www.e-cam2020.eu/deliverables> ... <https://www.e-cam2020.eu/deliverables>  
 Internal Project Management Link ... <https://redmine.e-cam2020.eu/issues/35>  
[a.ocais@fz-juelich.de](mailto:a.ocais@fz-juelich.de) ... <mailto:a.ocais@fz-juelich.de>  
<http://creativecommons.org/licenses/by/4.0> ... <http://creativecommons.org/licenses/by/4.0>

#### Page iii

GitLab service ... <https://gitlab.e-cam2020.eu/>  
 Redmine service ... <https://redmine.e-cam2020.eu/>  
 Kanban service ... <https://kanban.e-cam2020.eu/>  
 Etherpad service ... <https://etherpad.e-cam2020.eu/>  
 ShareLatex service ... <https://sharelatex.e-cam2020.eu/>  
 E-CAM training page ... <https://www.e-cam2020.eu/resources/training/>

#### Page 1

E-CAM project website ... <https://www.e-cam2020.eu/>  
 software modules of E-CAM ... <https://www.e-cam2020.eu/software-library/>  
 upcoming E-CAM events ... <https://www.e-cam2020.eu/events>  
 E-CAM online services ... <https://www.e-cam2020.eu/resources/>  
 technical first contact page ... <https://www.e-cam2020.eu/technical-questions/>  
 detailed descriptions of the E-CAM events ... [https://www.e-cam2020.eu/events/list/?tribe\\_paged=1&tribe\\_event\\_display=past](https://www.e-cam2020.eu/events/list/?tribe_paged=1&tribe_event_display=past)  
 E-CAM training page ... <https://www.e-cam2020.eu/resources/training/>  
 E-CAM GitLab service ... <https://gitlab.e-cam2020.eu/>  
 ReadTheDocs.org ... <https://readthedocs.org/>  
 Kanban service ... <https://kanban.e-cam2020.eu/>  
 Redmine service ... <https://redmine.e-cam2020.eu/>  
 Etherpad service ... <https://etherpad.e-cam2020.eu/>  
 ShareLatex service ... <https://sharelatex.e-cam2020.eu/>

#### Page 3

GitLab service ... <https://gitlab.e-cam2020.eu/>  
 ReadTheDocs.org ... <https://readthedocs.org/>  
 WP1 Documentation Repository ... <https://gitlab.e-cam2020.eu/E-CAM/Classical-MD-Modules>  
 WP1 Rendered Documentation ... <http://e-cam-classical-md-modules.readthedocs.io/en/latest/index.html>  
 WP2 Documentation Repository ... <https://gitlab.e-cam2020.eu/E-CAM/Electronic-Structure-Modules>  
 WP2 Rendered Documentation ... <http://e-cam-electronic-structure-modules.readthedocs.io/en/latest/>  
 WP3 Documentation Repository ... <https://gitlab.e-cam2020.eu/E-CAM/Quantum-Dynamics-Modules>  
 WP3 Rendered Documentation ... <http://e-cam-quantum-dynamics-modules.readthedocs.io/en/latest/>  
 WP4 Documentation Repository ... <https://gitlab.e-cam2020.eu/E-CAM/Meso-Multi-Scale-Modelling-Modules>  
 WP4 Rendered Documentation ... <http://e-cam-meso-and-multi-scale-modelling-modules.readthedocs.io/en/latest/>

**Page 4**

E-CAM project website ... <https://www.e-cam2020.eu/>  
upcoming E-CAM events ... <https://www.e-cam2020.eu/events>  
E-CAM online services ... <https://www.e-cam2020.eu/resources/>  
technical first contact page ... <https://www.e-cam2020.eu/technical-questions/>  
detailed descriptions of the E-CAM events ... [https://www.e-cam2020.eu/events/list/?tribe\\_paged=1&tribe\\_event\\_display=past](https://www.e-cam2020.eu/events/list/?tribe_paged=1&tribe_event_display=past)  
GitLab service ... <https://gitlab.e-cam2020.eu/>  
GitLab service ... <https://gitlab.e-cam2020.eu/>

**Page 5**

all publicly accessible repositories of E-CAM ... <https://www.e-cam2020.eu/software-library/>  
Redmine ... <http://www.redmine.org/>  
Redmine service ... <https://redmine.e-cam2020.eu/>  
Redmine service ... <https://redmine.e-cam2020.eu/>

**Page 6**

Kanban ... <http://kanbanblog.com/explained/>  
Kanban service ... <https://kanban.e-cam2020.eu/>  
Etherpad service ... <https://etherpad.e-cam2020.eu/>  
Etherpad service ... <https://etherpad.e-cam2020.eu/>

**Page 7**

ShareLatex service ... <https://sharelatex.e-cam2020.eu/>  
ShareLatex service ... <https://sharelatex.e-cam2020.eu/>

**Page 8**

E-CAM training page ... <https://www.e-cam2020.eu/resources/training/>  
E-CAM training page ... <https://www.e-cam2020.eu/resources/training/>  
Clowder ... <https://clowder.ncsa.illinois.edu/clowder/>

**Citations**