



## ESDW guidelines and programme II

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E-CAM

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



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	Written by:	Alan Ó Cais(DE-JUELICH)
	Contributors:	Ana Mendonça (EPFL), Donal MacKernan (NUID UCD)
	Reviewed by:	Sara Bonella (EPFL)
	Approved by:	Ana Mendonça (EPFL)

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

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## Executive Summary

The present deliverable is an updated version of deliverable D5.1 on the current guidelines for Extended Software Development Workshop events. These guidelines for content, structure and output help to ensure that the workshops are run consistently across the scientific Work Packages and meet the quality standards for E- CAM software.

In addition to refining the guidelines of D5.1, this deliverable defines

- the scope of training at Extended Software Development Workshop (ESDW) events
- the online material accessible through the E-CAM software repositories and website;
- the role of the programmers;
- the concept of module in E-CAM and its acceptance criteria;
- a day-to-day set of recommendations by previous ESDW participants and the certification of workshop attendees.

The programme of ESDWs for the second year of the project is also defined within this document.

These guidelines are intended to be a living document which evolves to reflect experience gained in running the ESDWs and thus they are subject to further revision based on the outcomes of each year's activities.

# 1 Introduction

E-CAM delivers on average four Extended Software Development Workshops every year each focused on software development in one of its four core scientific areas:

- classical MD,
- electronic structure,
- quantum dynamics,
- meso and multiscale modeling.

The purpose of an ESDW is twofold. On the one hand they are a mechanism for generating software modules for inclusion in the E-CAM repository. On the other, they are an integral part of the E-CAM training programme and represent the primary “training by doing” component.

The exact composition of an ESDW is being refined year on year, with this present document being the second iteration. This iteration includes elaboration on a number of points:

- synchronising the programmer effort with ESDWs,
- incorporating performance optimisation pipelines into ESDWs,
- the preparation requirements of ESDW participants and training material,
- development of a training webpage and training infrastructure
- day to day running of ESDWs: recommendations from participants,
- what the working definition of a *module* in E-CAM is,
- how a module is submitted to E-CAM,
- the acceptance criteria for modules,
- how a module is published by E-CAM,
- certification of ESDW participants.

It is hoped that these improvements will help to significantly streamline ESDW events, with the particular goal of maximising the efficiency of instruction on core E-CAM training content.

## 2 Purpose and Structure

An Extended Software Development Workshop (ESDW) is structured such that it serves two purposes. Firstly, it is a mechanism for generating selected software modules for inclusion in the E-CAM repository. In the E-CAM context, a software module is defined as :

Any piece of software that could be of use to the E-CAM community and that encapsulates some additional functionality, enhanced performance or improved usability for people performing computational simulations in the domain areas of interest to us.

This definition is deliberately broader than the traditional concept of a module as defined in the semantics of most high-level programming languages and is intended to capture inter alia workflow scripts, analysis tools and test suites as well as traditional subroutines and functions. Because such E-CAM modules will form a heterogeneous collection we prefer to talk about the E-CAM software repositories rather than library. The modules do however share with the traditional computer science definition the concept of hiding the internal workings of a module behind simple and well-defined interfaces. It is probable that in many cases the modules will result from the abstraction and refactoring of useful ideas from existing codes rather than being written entirely de novo.

Perhaps more important than exactly what a module is, is how it is written and used. An important function of the ESDWs, where modules are produced, is to bring modern programming standards and techniques into the work practices of the participants. A final E-CAM module will adhere to current best-practice programming style conventions, be well documented and come with either regression or unit tests (and any necessary associated data). ESDWs will contain an explicit introduction session at the start explaining what an E-CAM module is, why good software style is important, and how to use modern software development tools and methods.

Secondly, ESDWs are an integral part of the E-CAM training programme and represent the primary “training by doing” component of that programme. E-CAM modules should be written in such a way that they can potentially take advantage of anticipated hardware developments in the near future. We will use ESDWs to create a top-down approach for training for next-generation architectures. Attendees will come to the ESDW with a particular module to develop, we will advise them on a workflow and expose them to the tools that will allow them to create these modules using programming best practices and with an eye on the future of the hardware where they will run such modules.

### 2.1 Attendees

The typical size of the workshop will be 10-15 trainees plus staff.

**Trainees:** The trainees typically consist of a mixture of post-doctoral research assistants or senior PhD students, and young industrial researchers. These researchers will have already trained in simulation and modelling and, for industrial researchers, would be considered part of the companies expertise base in this field. The ESDW will extend their skill range and produce the required training boost to keep them at the leading edge of their discipline. These workshops will also be of potential value to academic staff from European institutions, in the process of changing or extending their current research fields. Trainees should come from a diverse range of backgrounds and a conscious effort will be made to avoid biases, implicit or explicit, in their selection, especially in the area of gender.

**Staff:** The workshop will be led by at least one senior academic member of the E-CAM consortium, who is an expert in the field under discussion and already familiar with the needs of industry or academic users. He or she will be supported by the project software manager, an E-CAM programmer and the PDRAs associated with the scientific area of the ESDW in that particular year of the project. We will invite other senior stakeholders and guests to lecture and mentor during the workshops when required.

All trainees must commit to the full period of the workshop both in residence and back at their home bases. In the case of industrial participants this will require the written permission of their line-managers and in the case of academics the written permission of their supervisors. We are currently trialling remote participation to a subset of the ESDW in order to facilitate increased industrial participation.

ESDWs will normally be available to European applicants but applications from the rest of the world will be considered and accommodations will be made when the non-European applicant can add high value to a workshop. Given the significant time requirement for participation in one of these workshops, early and binding commitments will need to be obtained from perspective trainees. It is important that people appreciate that the workshops are indeed “extended” in that significant amounts of work will be done outside the face-to-face meeting. Conversely, in view of this considerable commitment by participants when back at their home intuitions, organisers should ensure where practical, that modules are such that participants can tune them to their own research priorities on their return to their home bases, so as to allow and facilitate substantial further development work there.

## 2.2 Logistics

Depending on the specific subject area, the workshops will have a variable total duration. Generally, they will consist of

- Preliminary work by the attendees to ensure minimum common expertise and identify the modules to be developed
- Two-week residential workshop
- Variable period of work by participants at their home bases, off-line and on-line
- Final wrap-up residential workshop.

Trainees will normally be divided into teams to develop the software, and will need office space, with projector(s) and white-boards. A small resource library will be created of leading edge texts, reports or training material available on-line which can be used with each workshop. Code development will be performed on desktop machines at the location of the ESDW or, preferentially, on portable computers belonging to the trainees.

When necessary, remote access to massively parallel and heterogeneous platforms will be ensured, including specialised compilers, profilers and debuggers. Such access requires significant time to arrange and must be signalled months in advance of the workshop.

Specifications for the minimum requirements in terms of operating system and installed software and compilers will be detailed before each ESDW.

Assistance will be provided, as with all Centre Européen de Calcul Atomique et Moléculaire (CECAM) schools, to the attendees and staff for accommodation during the residential parts of the ESDW.

Participants will be advised of the remote collaboration tools that are used by E-CAM and that can enable the teams to continue to work on their software projects when dispersed back to their home institutions. Host institutions must provide necessary system level support to enable such remote collaboration (e.g. opening designated ports on fire-walls).

## 2.3 On-line training

E-CAM is in the process of developing an appropriate online training infrastructure. To this end it is establishing strong partnerships with PRACE and leading HPC centres in Europe in order to connect to appropriate training content that can bring the E-CAM user communities to the exa-scale.

The [E-CAM software repository](#) is the principle access point for users wishing to interact with E-CAM, including training. There, they are encouraged to download and upload software, 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](#): Redmine, Etherpad, ShareLatex, and in particular Gitlab. The provision, use and further development of these services is an integral part of ESDW's, and one of the principle means by which E-CAM will deliver on-line material.

E-CAM also is making extensive use of [community-created online training infrastructure](#). In the development of its own training material, E-CAM will take the example of the [Software Carpentry Foundation](#) who are leaders in the field of developing collaboratively created, open source training content for teaching researchers computational skillsets. Software Carpentry maintains a set of core lessons that form the basic toolbox of a computational researcher, and from which they can develop more complex skills. Their webpage also contains video presentations of the core lessons, as well as links to all of the source material. In particular, given the the main E-CAM software development service is our GitLab repository, we recommend that all members of the E-CAM community are familiar with the version control system Git. Git is core content within the Software Carpentry syllabus, with the both basic and more advanced material available.

## 2.4 Funding

Funding for the ESDW is provided via the CECAM contribution to E-CAM: 2/3 funded from CECAM Headquarters, 1/3 from the local beneficiary hosting the event including possible funding from external sources and co-sponsors.

Participation is free of charge for academic participants and for industrial participants from one of the current or future industrial partners of E-CAM. An attendance fee of up to 1000 Euro may be charged to industrial trainees from outside the E-CAM partnership. Special provisions for licensing and upload to the repository of software developed by paying trainees will be made if necessary.

### 3 ESDW Program

The locations, organisers, dates and indicative contents of the workshops in the second year of the project are described in Table 1<sup>2</sup>. They are advertised on the E-CAM website under the [E-CAM event calendar](#), and on the CECAM website under the [CECAM Workshops Programme](#).

Table 1: ESDW's taking place during the second year of the project.

Number	WP	Title	Start	End	Location	Organisers
ESDW4	4	Meso and multiscale methods	17.04.17	28.04.17	UB	Ignacio Pagonabarraga
ESDW6	1	Classical Molecular Dynamics	21.08.17	01.09.17	NL	Peter Bolhuis
ESDW7	3	Quantum MD	10.07.17	22.07.17	NUID UCD	Graham A. Worth Donal Mackernan Sara Bonella
ESDW8	4	Meso and multiscale modelling	18.09.17	29.09.17	UK-MAXWELL	Carsten Hartmann Luigi Delle Site

The content and location of the workshops for the second year is established based on the activities planned in Work Packages 1-4 in the Grant Agreement. From year 3, supervised by a Industry Management Group, the ESDW topics and the software modules to be developed in each area will be selected via:

1. specific development requests emerging from the CECAM programme;
2. requests collected through the web;
3. the software development needs of the PDRAs associated to the Pilot Projects in Work Packages 1-4;
4. direct requests from current industrial partners;
5. the outputs of the E-CAM scoping workshop through the respective scientific reports;
6. the outputs from the E-CAM state-of-the-art workshops through the respective scientific reports.

The software development requests will be collected and monitored by the software manager and the technical manager and considered in detail by the ESDW organiser (the academic beneficiary responsible). These requests will be ranked in order of merit and assigned to a specific ESDW via a refereeing process. Referees will be selected by the software and technical manager according to the specific scientific areas of the proposed ESDW within WPs 1-4 and members of the Scientific Advisory Committee of CECAM. Within the spirit of modern software management methods, the teams will have significant freedom to choose or prioritise which of the code modules ranked above they wish to develop.

Although the original locations for the ESDW workshop have been decided (see Table 1), it will be possible to choose different locations defined by the beneficiaries responsible for their delivery, in agreement with the Software Management Group and CECAM.

The program for each year will be published by Dec. 20 for the following year of the project.

<sup>2</sup>Note that in 2016, two ESDWs took place for WP2, and zero for WP4. Two ESDWs in WP4 are being held in 2017 to address this imbalance.



## 4 ESDW Content

### 4.1 Scientific Content

Funding for ESDW events is provided by CECAM and are the CECAM contribution to the E-CAM project. Every ESDW event must follow the normal CECAM [procedures and guidelines for submitting a workshop proposal](#). Therefore, E-CAM is not directly responsible for the scientific evaluation of ESDW proposals but can only shape the scientific content of proposals based on the guideline parameters listed in Section 3. ESDW proposals submitted to CECAM must, in addition to these guideline parameters, ensure that they align themselves with the stated goals of CECAM flagship programme in each calendar year. For this reason, we do not discuss scientific content here but focus instead on the technical training components present in ESDW events. Coherence between the E-CAM and CECAM requirements is ensured by the E-CAM's Technical Manager, who is also the Director of CECAM.

### 4.2 Technical Training Content

Each ESDW event must contain training components relating to

- general computing competencies,
- parallel computing competencies and
- training beyond state-of-the-art,

which are discussed in more detail in this section.

We further categorise training components at three different proficiency levels:

- *awareness*, where a presentation is considered the appropriate medium
- *working knowledge*, where a tutorial with hands-on components are appropriate
- *specialist knowledge*, where a dedicated workshop is required.

Given that, for typical ESDW events, technical training forms only part of the overall program, here we only consider training at the *awareness* or *working knowledge* level. If *specialist knowledge* technical training is required, then a specific ESDW event can be considered in cases where such specialised training is not already provided elsewhere (for example, as part of the PATC programme of training events) or where there is particularly high demand within the community for tailored content.

A brief overview of some of the tools used within the expected context of technical training can be found in [Deliverable 6.2](#).

#### 4.2.1 General Computing Competencies

The ESDWs will teach skills to ensure that the E-CAM repository embodies long term coding best practices. Software development methods will be close to the approach successfully used in open-source projects, and a description of the general software standards that we strive for the workshops is contained in [Deliverable 6.1](#). This deliverable will be migrated to a living document and expanded to include content relevant to Subsections 4.2.2 and 4.2.3.

It is expected that software will normally be written in C or C++, modern versions of FORTRAN (e.g Fortran 2008) and Python. The interoperability of the software in each language will be an important component of the development. All code will contain extensive on-line documentation. Subroutines and functions will be stored collectively in modules, with the ultimate goal to construct a variety of programs in a common application space from the same building blocks. Each module developed should come with appropriate test cases and including specimen results where necessary.

A more detailed description of the available tools and the recommended workflow is given in [Deliverable 6.2](#). The tools are hosted on the E-CAM server at [CECAM](#).

It is mandatory for each ESDW to include a session by the Software Manager or the Programmers that will cover the workflow necessary for the participants to submit their modules to the E-CAM repository (as described in Subsection 5.1). This content has been designed in such a way that it also simultaneously touches on many aspects of the recommended workflow (version control, source code documentation, code review,...).

Examples of the appropriate type of training content for this topic includes:

- version control using Git (this is a mandatory inclusion for an ESDW),
- introduction to Python,
- source code documentation,
- technical skills specific to the ESDW.

If training content in this category is required, then it **must** be provided at the *working knowledge* level. Any necessary material at the *awareness* level should be provided to the participants well in advance. See Section 4.3 for more details.

#### 4.2.2 Parallel Computing Competencies

In addition to coding sessions, the typical workshop will consist of training lectures in parallel computing such as: techniques in parallel software development; lectures on computer hardware and advances in new architecture relevant to the applications being developed; parallel programming techniques (MPI, OpenMP, OpenACC, CUDA,...); and accessing large-scale High Performance Computing (HPC) resources.

Access to HPC resources will be provided where necessary, subject to notification well in advance. See Section 4.3.2 for the E-CAM approach to performance analysis with the applications under development.

Each ESDW event must include training content that covers some aspects of the topic of Parallel Computing, though the material given can be at either the *working knowledge* or *awareness* level as appropriate for the audience and the topic of the ESDW.

#### 4.2.3 Training Beyond State-of-the-Art

Work Package (WP) 7 of E-CAM connects the project to the overall development of HPC hardware/software and the people/projects in Europe that operate in this space. Given that "beyond state-of-the-art" is by definition unavailable hardware, WP 7 will create *awareness* level training content that can be presented at all ESDW events. This content will be updated annually and presented by the programmer assigned to the ESDW and will cover

- European HPC hardware available within a 5 year horizon
- Programming methods, models and tools to leverage this hardware
- Algorithm considerations for efficient scalability.

If additional training content in this space is required it needs to be requested months in advance to ensure that appropriate instructors for training at this level can be found.

### 4.3 Preparation

The impact of an ESDW to a participant critically depends on an appropriate level of preparation prior to the meeting. For this reason it is essential that the scientific and technical content of the ESDW is confirmed *a minimum of 3 months in advance*. This is to ensure that the organisers, participants and programmers will have adequate time to prepare and that there is sufficient time to request external trainers where necessary.

Trainees will be provided with training material sufficiently in advance of the workshop. Any necessary assistance with this material will be provided through the organisers and programming team as appropriate. Contents of the such training material may include: basic parallel programming (MPI, OpenMP); version Control; scientific background material....

#### 4.3.1 Recommendations on the day to day running of an ESDW

Using the output of surveys from past ESDWs, a set of guidelines will be provided to the organisers to ensure optimal management of the event. From the participant feedback from the 2016 programme, there have been some very noteworthy points.

There is always a risk that organisers eagerness to cover as much material as possible during workshops may be counter-productive, and exhaust participants so much that they cannot learn additional material. The fact that ESDW's may cover material that is very new to a participant and also require that the participant simultaneously codes new modules is intellectually very demanding. It is therefore essential to give participants time to assimilate

what they have learned, by not over-charging the number of hours of work/lectures each day or presenting too many different topics within a short period, and including a long break between the morning and afternoon session (or the equivalent).

Ideally, participants should arrive the day before the beginning of ESDW's, particularly if travelling to a training site takes very long. If a session is required on the day of the arrival, it should be kept short and not be essential for the rest of the meeting.

It is also advisable to record, where possible, audio/video with slides, allowing participants to revisit lectures or demonstrations in their own time, both during and after the meeting. Such material also can be used by people who did not have the opportunity to attend the ESDW in person, thereby increasing the potential number of future users, and the impact of the ESDW.

Where a substantial amount of software already exists, to which the participants are adding modules, it is critically important that such software be fully documented, with a legible glossary of terms and definitions. Organisers should liaise with programmers and the software manager to ensure that appropriate documentation is prepared and communicated to participants at least two months before the meeting. Modules should be identified such that participants can tune them to their own research priorities on their return to their home bases, so as to allow and facilitate substantial further work there.

#### **4.3.2 The role of the *Programmers***

Typically applications within an ESDW will not be developed from scratch and so, prior to the workshop, the programmers role is to gain some familiarity with these applications. The applications to be used must therefore be decided at the time the programme is finalised. The programmers will implement a Performance Analysis workflow for the applications which includes:

- Integrate the application into [EasyBuild](#),
- Scaling analysis with [JUBE](#),
- Performance analysis with [Scalasca](#).

During the workshop, the programmers are there to provide instruction and support in the tools used by the ESDW and assist the participants where necessary with these tools. They can also leverage the performance analysis workflow that they have prepared to help analyse the performance impact of the work undertaken during the ESDW on the Partnership for Advanced Computing in Europe (PRACE) HPC resources to which E-CAM has access.

## 5 ESDW Outputs

The core output of these workshops is a number of software modules, skills acquisition by the trainees and, where relevant, a performance analysis workflow for the applications considered during the event.

At the end of the second meeting associated with each ESDW, the software manager and senior E-CAM scientists leading it will prepare a report on the contents of the workshop and related actions. These reports will be used to monitor and improve the structure and planning of future ESDWs, as anticipated in WP 5 (Training) and in WP 6 (Software Infrastructure).

### 5.1 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 ESDW events. The number of expected modules from each ESDW will be established during the event planning, leading also to the definition of its contents. This will contribute to meet the projected number of modules for each year in each scientific area.

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](#). 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.

The individual repositories for each research WP and the location of the resultant documentation page can be found in Table 2.

Table 2: 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>

The E-CAM Classical MD Module Library

This is a collection of the modules that have been created by E-CAM community within the area of Classical MD.

**Extended Software Development Workshops**

ESDW Traumkirchen 2016

The first Classical MD ESDW in Traumkirchen in November 2016 was the starting point for the modules below.

- E-CAM example module

**Contributing to this documentation**

**GitLab account**

If you do not have a (free) GitLab account yet on the E-CAM GitLab service, you'll need to get one via <https://gitlab.e-cam2020.eu/>.

**Fork the repository**

First, you'll need to fork the repository on GitLab you want to work with. Go to <https://gitlab.e-cam2020.eu/E-CAM/Classical-MD-Modules>, and click the grey 'Fork' button under the repository name.

**SSH public key @ GitLab**

You also need to register an SSH public key, so you can easily clone, push to and pull from your repository. This can be done via <https://gitlab.e-cam2020.eu/profile/keys> if you're logged in on GitLab.

In the following it is assumed that an SSH public key has been registered, since it is a requirement for cloning/pushing via the git protocol.

**Clone your fork of the repository**

Clone your fork of the repository to your favorite workstation.

**General Information**

- Extended Software Development Workshops
  - ESDW Traumkirchen 2016
- Contributing to this documentation
  - GitLab account
  - Fork the repository
  - SSH public key @ GitLab
  - Clone your fork of the repository
  - Keep your master branch up-to-date
  - Branching
  - Contributing back your input
- Search Page

Figure 1: Example of one of the four module repositories.

<sup>3</sup>Merge or pull requests are created in a git management application and ask an assigned person to merge two branches.

An example of the landing page for the Classical MD WP can be seen in Fig. 1. The current [template format for the submission of modules](#) is available through the documentation pages as well as a [description of how the software module is submitted](#).

### 5.1.1 Acceptance Criteria

The software manager (together with the programmers) is responsible for the evaluation of the software quality of the modules and their upload to the E-CAM repository under the appropriate software licence conditions.

An acceptance criteria checklist is applied to the submitted modules before accepting the merge request. This list covers aspects including:

- Coding style and naming conventions
- Sufficient source code documentation
- Passing unit and/or regression tests

## 5.2 Key Performance Indicators

The output of the ESDWs will also be measured via a set of Key Performance Indicators (KPI):

- Number of software modules developed
- The training impact of the ESDWs, measured both in terms of the number of people trained and the level of technical skill acquired through the ESDWs and associated activities before and after (see Subsection 5.2.1 below)
- Impact in increasing diversity within the training programme, both in terms of gender, and academic background/discipline. The baseline for this measure will be the initial diversity levels in the first set of ESDWs
- Degree of industrial engagement in the ESDWs.

### 5.2.1 Certification

The project has decided on 2 levels of certification stemming from participation at ESDW events. The first is a general certificate of participation in the event.

The second is a certification of the acceptance of a software module generated by the participant into the repositories of E-CAM. This certification requires that the participant will have achieved a *working knowledge* of the approach to software development taken by E-CAM.

### 5.2.2 Attendee Feedback

Attendees are provided with a feedback form to allow us to improve the organisation of ESDW events in future years.

## 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

**KPI** Key Performance Indicators

**WP** Work Package

**PATC** PRACE Advanced Training Centre

### URLs referenced

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Internal Project Management Link ... <https://redmine.e-cam2020.eu/issues/9>

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

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**Citations**