esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

Experiences with ESM Multi-model Ensembles for Educational Purposes: A report from the use of D3.1 for the 3rdE2SCMS

Deliverable D3.4

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1. Abstract /publishable summary

This document describes experiences from three summer schools, especially from the most recent one in 2016, on modelling the Earth System with a multi-model ensemble. These models have been run by the student participants at different HPC sites solving scientific assignments.
The experiences of the technical teams preparing the models for these experiments shed light on the usability of the models from different perspectives. One of the aspects of particular importance for ESiWACE is performance portability, which will be a focus for the WP in the next reporting period.

2. Conclusion & Results

From the experiences, it can be stated that adhering to best practices of software development and standard methods and data formats would probably ease the trouble of porting and performance-optimizing Earth system models considerably. This is shown e.g. by the successful introduction of the package manager of Spack (http://spack.readthedocs.io/en/latest) helping users of different levels of expertise as well as system administrators to deploy and maintain the software they need for their problem set.

3. Project objectives

This deliverable contributes directly and indirectly to the achievement of all the macro-objectives and specific goals indicated in section 1.1 of the Description of the Action:

Macro-objectives	**Contribution of this deliverable?**
Improve the efficiency and productivity of numerical weather and climate simulation on high-performance computing platforms	Yes
Support the end-to-end workflow of global Earth system modelling for weather and climate simulation in high performance computing environments	Yes
The European weather and climate science community will drive the governance structure that defines the services to be provided by ESiWACE	No
Foster the interaction between industry and the weather and climate community on the exploitation of high-end computing systems, application codes and services.	No
Increase competitiveness and growth of the European HPC industry	No

Specific goals in the workplan	Contribution of this deliverable?
Provide **services** to the user community that will impact beyond the lifetime of the project.	Yes
Improve **scalability** and shorten the time-to-solution for climate and operational weather forecasts at increased resolution and complexity to be run on future extreme-scale HPC systems.	Yes
Foster **usability** of the available tools, software, computing and data	Yes

handling infrastructures.	
Pursue **exploitability** of climate and weather model results.	No
Establish governance of common software management to avoid unnecessary and redundant development and to deliver the best available solutions to the user community.	No
Provide **open access** to research results and **open source** software at international level.	Yes
Exploit **synergies** with other relevant activities and projects and also with the global weather and climate community	Yes

4. Detailed report on the deliverable

Introduction

This Deliverable D3.4 is part of the work in ESiWACE Work Package 3 "Usability". In the ESiWACE description of activities, the work in "Task 3.1.2. Development of Use Case" and the deliverable D3.4 "Experiences with ESM Multi-model Ensembles for Educational Purposes" are described in the Description of the Action as follows:

> „Once first drafts of the white paper are circulated, a small team of scientific programmers from BSC (team lead), MPG and UREAD will start to convert the recommendations into a real life environment, our use case [D3.3]. This use case will be the workflow necessary for the ENES summer schools, planned to be held by UREAD at CSC28, Finland, – a PRACE Tier1 centre - in 2016 (3rd E2SCMS, European Earth System and Climate Modelling School). At the previous two E2SCMS, three GCMs were used to teach the students, each operated in its own framework. The use case will make it possible for students to better co-design and exploit the simulation exercises, by providing a unified framework. This way the use case shows on a somewhat smaller scale, what the system specification will be able to deliver to projects.
>
> The group will start with first framework sketches very early in the project, and iterate through further drafts. Allinea will ensure the readiness of the prototype for their methods and tools, and that the prototype is able to integrate into a modern scheduling environment. The prototype will then be handed over to T3.1.3 in time for the 3rd E2SCMS to be tested in a provisional environment at CSC. For these tests UREAD (team lead, organizer of the 3rd E2SCMS), BSC and MPG will install the software collection provided by T3.1.2 at CSC, and test it, aided by Allinea. Success metrics shall be established in advance. The ultimate test will be if the environment is usable for the 3rd E2SCMS and gets good ratings by the participants [D3.4]. The next step will then be to use the experience from the 3rd E2SCMS to develop the environment for the demonstrators. "

Although D3.4 requires a report of the use of the application stack (see Fig. 1) within the 3rd E2SCMS only, the authors will take the freedom to shed some light on the experiences

made for the two pre-cursor schools:

- 1st E2SCMS held on the island of Kos, Greece https://is.enes.org/archive/events/e2scms and

- 2nd E2SCMS held in Barcelona, Spain https://is.enes.org/events/second-european-earth-system-and-climate-modeling-school-2nd-e2scms?searchterm=e2scms

For a comprehensive overview about 3rd E2SCMS the reader is referred to the ESiWACE Milestone 2 report: https://www.esiwace.eu/results/milestones/milestone-2-application-stack-running-at-fmi-csc-preparation-of-system-stack-t3-2-team/view and the ISENES2-Report for the 3rd E2SCMS, published on http://is.enes.org

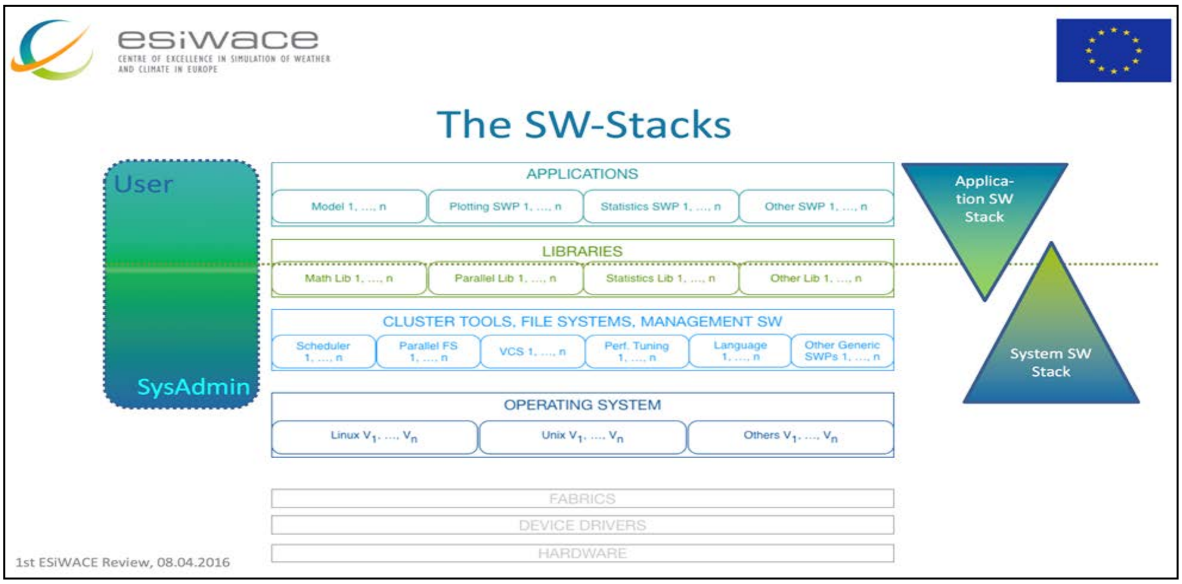

Figure 1 Application and system software stacks.

This report will assume answers to questions like “Why do we want a model to be run at a school?”, “Why do we want different models to be run at a school?” as given and part of the pedagogical concept of the school organizers. Also, “What does it take to prepare a model for a school?” and “What is the definition of a good model for a school?” will not be discussed, but only touched upon, due to lack of resources. Such questions are also related to the fundamental question “Wouldn’t it be sufficient for a school with this focus to provide data sets to the participants to answer their scientific questions?”, which organizers of such schools need to deeply consider before engaging into school preparations.

In the chapter “**Settings**” following this introduction it will be explained, why it was not possible to install the planned framework and run all three models at CSC in Finland, what was done instead and after the school.
The chapter “**Lessons Learned**” will describe what the authors think are the most important observations and key issues in preparing, executing and evaluating the schools.
From this, “**Recommendations**” are formulated in the next chapter, followed by a chapter “**Conclusions**”.

Settings

For an introduction and background as well as technical and organizational information the reader is referred to MS2, giving details on the preparations and execution of the 2016 school.

The setting can be summarized as follows: Whereas it was planned to install all three models in question at CSC in the framework newly established according to the recommendations provided by the ESiWACE software stack handbooks, it turned out to be possible for only one of the models, which was ready to be executed by the time the school started. But the ease of use / usability was still so much higher “at home” for even this one model, that the school organizers decided to run the model “at home”. Nevertheless, it should be mentioned that CSC substantially supported our efforts as in-kind contribution.

3rd E2SCMS was the third in a series of international Earth System Modelling Schools. While the first school was run with two models (FAMOUS .= UK, and MPI-ESM1 := DE), three models were used in schools #2 and 3 (UK, DE, EC-Earth := EC). UK and DE had been used in educational context before, and sported something like a "school-configuration", model #3 was taken directly from the production version and not re-engineered for the school.

In the first school UK and DE could be installed and run on the DKRZ super computer and operated remotely from the school location in Greece. Already by then ideas surfaced to execute and evaluate those two models within a common framework.

The second school saw a mixed setup at the BSC in Barcelona: DE and EC were run in Barcelona, whilst for UK the installation from the first school at DKRZ was re-used remotely. For time and resource constraints and from the experiences from the first schools, in school #3 the organizers, decided very early and before ESiWACE actually started, to rather run the models "at home": UK@STFC, DE@DKRZ and EC @BSC. For instance, EC was previously deployed at CSC by FMI scientists, but in order to be able to run the assignments, it was less effort to use the model version available at BSC facilities. Only DE could successfully be ported to CSC in time for the 2016 school, but was decided not to be used for practical reasons: The HPC- and model evaluation-, i.e. post-processing-, environment in Hamburg was more apt for the job. This proves that not only model deployment needs consideration, but also the post-processing environment. Analysing models in comparison is made difficult by many model specifics in their data treatment. But in practice it turned out that even the lack of a common data format would have necessitated the installation of an extra layer of software to enable the use of common data analysis tools. I.e., a common software to put data into the CMOR http://www-pcmdi.llnl.gov/software/cmor/cmor_users_guide.pdf format would have been helpful, but was not available at the time. The same applies e.g. to ESMvalTool https://www.esmvaltool.org

Lessons Learned

Whereas porting to and running at a common site using similar Application and System Software Stacks seemed possible after the first two schools, when ESiWACE was planned, things turned out completely different for the third school. Given the boundary conditions at the time – like the employment and project load situation at the different institutions involved - , the implications of the porting effort were estimated to be so costly, and anyway the timing was so unfortunate, that neither the UK team nor the EU team could imagine to cope with it.

E.g., installing FAMOUS on any new machine typically takes several weeks of effort by an engineer with strong expertise in the software infrastructure. Setting up FAMOUS for “automatic” installation on any machine would take several months and is even then still likely to require expert assistance to manage inevitable unforeseen issues at the time of installation. Similar estimates apply for EC-Earth. To prepare MPI-ESM1 for a completely new architecture is estimated to also take weeks to months. So, the porting proved to be very difficult to impossible.

Currently our only conclusion is, that Earth system modelling, and especially extra-curricular activities above and beyond institutional means, is underfunded and understaffed, to different degrees in different countries. And an extra-effort in portability is not sufficient – it needs adherence to standards, see below.

Considering the three models involved, the following can be stated:

- **FAMOUS,** while providing a model which can run multi-year simulations in short wall clock times, is ideal for a summer school environment, it nevertheless relies on a computational infrastructure which is very out-dated. The model is configured through a user interface, hosted on a machine at Reading, which communicates information about the desired workflow to the chosen HPC system (ARCHER in this case) in a semi-manual fashion. Job submission on the HPC system requires further user intervention. Porting the user interface system to the HPC would alleviate many manual steps by eliminating the extra communications. However, to do so would mean devoting further effort in support of an archaic workflow management system and runs counter to modern modelling and workflow developments so was not considered appropriate. New versions of the Unified Model can be expected to be more apt for the job. The Rose/Cylc workflow management infrastructure coupled with central model configuration and code repositories solves the problem. FAMOUS post-processing took place on an ARCHER virtual machine dedicated for that purpose, loaded with a comprehensive analysis software stack complied by JASMIN http://www.jasmin.ac.uk/services/jasmin-analysis-platform, along the lines considered here with respect to Spack developments. We note that there was no additional funding available neither for the preparation of codes, their porting nor for the tutors on-site in Helsinki.
- **MPI-ESM1**: There was always the idea that it should be possible to run the model at different sites, and for educational purposes - MPI-M would like to have a scientifically proven model in a configuration, a PhD student can start his thesis with, without too heavy support burden from experienced staff necessary. This partially influenced the technical solutions that have been implemented by the model's developers, which led to the possibility of configuring and running the model's workflows not only on DKRZ's Bull/ATOS machine, but also on Cray HPC at CSC, and even on desktops. In terms of governance this does not mean that it is always easy for the maintainers to get the full support for this approach, especially in a time when the development focus at MPI-M switched to a new model - but it is agreed upon that this approach is a good idea. Similar approaches will indeed be taken for MPI-ESM2.
- **EC-Earth** was never meant to be serving as an educational model. It is in fact developed by a consortium for scientific purposes, and as a model to be used for CMIP experiments. So, the educational view has not been an objective in the model's development so far. Architecture-wise, EC-Earth is a coupled model using different components developed by different institutions. This heritage impedes setup and execution of the model. Moreover, there is no coarse resolution version of EC-Earth, which would be especially suitable for educational runs: The computational resources

needed for a typical summer school assignment are not negligible. Finally, EC-Earth is employing IFS code by ECMWF, a licensed code with very restrictive distribution rules. To this end, future work by SMHI to replace IFS by OpenIFS, the open version of the IFS code, in the next version of EC-Earth (support by ESiWACE WP2) will make distribution easier. OpenIFS shows code quite different from IFS, and was developed i.A. for an educational purpose. So, two impediments will be eased. After the school, without the pressure of time and assignments, the model has been ported to DKRZ facilities. Even with an experienced team, this took a few days.

The three ESMs under consideration are so diverse with such distinctly different infrastructure and runtime requirements that shaping them to fit a common structure for installation and job submission proved to be rather hard, at least not possible in the time and with the resources given.

Recommendations

From these lessons learned, we draw some recommendations, which are summed up in ESiWACE MS2 report:

- Models and other applications should be built with standard tools. The standard tools should be those targeting as broad a community as possible. This helps to develop solutions for specific situations more easily, and dramatically reduces the effort required in software deployment.
- Scripts that implement model workflows should be flexible enough to easily adjust to different scheduling systems and policies in force across different HPC facilities.
- Model workflows should be kept clean of applications which duplicate functionality.
- Installation of comprehensive system software required to satisfy model dependencies is amenable to package management
- Installation of the models themselves is less amenable to package management given the maturity and diversity in current model infrastructures. It will be advantageous in development of new models to include at the outset consideration of installation procedures for maximum portability and hence maximum usability.
- Models should come with a detailed and comprehensive user guide. Describing the installation procedure and the model itself is mandatory to speed up the deployment time.

From this series of schools, and from observations not only in the EU ESM community, the authors would also like to highlight the following statements:

- Only very few models are portable in the sense that young scientists could download a software package, install it on an arbitrary system of their choice, and start experimenting with it.
- Especially, performance portability is not given for the European models the authors have knowledge of.
- Models are not usable in the sense that codes are written in a comprehendible manner, come with extensive and comprehensive documentation, and could be started and run with reasonable error treatment.
- Adapting the student assignments to perturb the models and see the impacts on changing behaviour and parametrization of the models is not always straightforward.

Some parts of the models are not well documented and modifications are hard to implement.

- Even the model probably closest to the ideas above can only be kept in a state like that for two reasons:
  - The maintainers of the model understand that successful PhD programs and early career scientist support depend on the availability of usable models.
  - The owner institute is aware that a model that is good in the sense defined above is the best signboard for an institute doing ES model development and application.

Running multiple ESMs with full model installation remains a complex task requiring significant domain expertise principally to ensure correct model set up. Nevertheless, we conclude that running 3 models at the same school site would have been possible if the recommendations above would have been sufficiently considered.

Models

The authors do not have any own experiences with modelling in other schools, but from our observations, porting a model is always avoided due to expected difficulties. And experiences in porting for other purposes is supporting this statement. This is mainly due to incompatibilities between operating systems, and sites: The System Software Stack does not sufficiently support the application software stack. This should now be remedied by the existence of the ESiWACE "Handbook for System Administrators: Specification of a standard recommendation for an ESM System Software Stack", available as ESiWACE deliverable D3.5 https://www.esiwace.eu/results/deliverables/d3-5-how-to-select-configure-and-install-esm-software-stacks/view

The question "What models should be used for a school?" we recommend to keep the setup as simple as possible. In a case like this, where model comparison was the focus of the school, the question "Do we do model, or do we do model data comparison?" needs to be answered first. If it is the former, the same assignments need to done with the different models, and the answers of the models needs to be compared. So, some research is necessary upfront, if the models involved can cope with the perturbations introduced by the assignments, and if it is clear why the models behave the way they behave, especially comparatively.

From an educational point of view, it is very interesting for the students to have a close look at the model and follow the installation procedure, and the configuration. To understand the difficulty and the technical challenge of this work is a very valuable experience for future scientific careers and helps to appreciate the work of technical teams.

On the other hand, the easier the models are to port and use, and the more reduced their complexity is, the less work it is for the technical team running the school – and the more time the participants can spend on the scientific questions instead of tedious technical problems. Furthermore, such schools have the function to advertise and disseminate the models involved. Participants will compare their usability, and their portability. Some students obviously used the school to compare models for the selection of their research tool.

So, from this and from the observations mentioned above, it can only be recommended to avoid specialized solutions and stick to standards wherever possible.

Facilities

Most of the HPC-centres nowadays offer training and support for their customers, oftentimes even in a research-field-specific manner. The teams offering such services are natural contact points if an ESM school is planned at a general-purpose compute center, since they know their facilities best. It is a good idea to establish good working relations to these people well in advance of the school, possibly by visits at the site. In every case, not only the HPC-part of the site under consideration needs to be thoroughly checked, but also the post-processing (PP-)facilities as well as the equipment in and the training rooms themselves need to be tested beforehand, including workstations (or possibly laptops), presentation means etc. . Especially, if one of the models is run off-site, network connections need to be checked, and working relationships established to their maintainers.

For obvious reasons, the team made very good experience running the models for all assignments well in advance of the school. Only then it is possible to ensure the current model versions can give answers to the current versions of the assignments. Also, realistic estimates for the resource requirements are possible only this way. The data from these runs need to be available, as backup, on-site for the school, independent of where the model runs.

Resources necessary to run and store the models and their output obviously depends on the number of models, of assignments, and the numbers of model years to get conclusive answers for the assignments – this can be up to some hundred model years. The resources should be applied for at the site of choice, but possibly also at a reserve facility, if possible, given sufficient model portability.

Furthermore, measures must be taken to ensure that model runs are finished within strict time constraints during the school: within the first 24 to 36 hours the experiments should be finished to be able to start the extensive analysis. This problem can be solved with the introduction of a high priority queue for the school.

Experiences show, that difficulties with creating various user accounts for the participants (for desktops, for HPC facility) can occur. Different sites have different policies on this, and it can take unexpectedly long to get accounts. Finally, the organizers of the school often don't know in advance which participants will work in a group with whom, with which model, and thus, on which HPC facility; sometimes they don't even know well in advance the full list of participants. For this, one needs anonymous ("functional") accounts, which are not allowed at some sites. This issue needs to be settled in advance, since it can influence the course of the school.

People

Apart from the lecturers, for hands-on modelling sessions at schools employing complex ESMs with interesting assignments a 5:1 ratio students: tutors per model seems like a good value. The tutors not only have to know the models quite well, but even more important the

PP system. Additionally, support staff from the center needs to be available on demand, should things fail on the system side.

Assignments

For the number of students per assignment and model, 2-4 seems like an advisable number, mostly depending upon the number of terminals available. Examples for assignments are given in the appendix.

From a technical point of view, assignments can be a challenge, depending on the model. Some assignments can be solved by changing only one parameter, whereas others may need a lot of changes in the source code. If in such a case the code is not well document and there is a lack of knowledge, assignments can be difficult to implement. The implementation of the "eyeball" assignment in EC-Earth can serve as an example here. This assignment could not be completed with this model due to the difficulty to find out where the parameters affecting the rotation speed in the IFS and NEMO models are located. Even after finding them, the model was simulating values lying outside of a "security threshold": So the simulation was automatically stopped, and the assignment could not be solved with this model.

Work after the 3rd E2SCMS

To amend the work accomplished for the school, the WP team decided to provide the team working on the Task 3.2 with additional ideas on possible solutions for application and software stacks maintenance. The result of these efforts and the analysis not only of the experiences made during the work for the school, but also from other porting efforts, was the adaptation and application of Spack – a package manager that helps users of different levels of expertise to deploy and maintain the software stacks they need for their experiments. The tool has been tested thoroughly by now on different platforms. It has shown good results in terms of time-to-solution, ergonomics, and stability on four different HPC environments:

- Mistral@DKRZ https://www.dkrz.de/Klimarechner-en/hpc
- Archer@EPCC https://www.epcc.ed.ac.uk/facilities/archer
- Mare Nostrum@BSC https://www.bsc.es/discover-bsc/the-centre/marenostrum
- Altamira@University of Cantabria (Spanish only) https://www.bsc.es/news/bsc-in-the-media/presentado-el-supercomputador-altamira

As well as on desktops operated by different Unix systems (for details see MS2 report).

Conclusions

The WP3 team suggests, that better usability of Earth system models for the purposes of early career scientists means to design models from the start with the idea, that they should adhere to best practices in software engineering and standards in formats and languages, that they should be made with performance portability as a target by reducing the last bit of optimization in favour of portability and ensuring conformance to standards across architectures, and that they need to be well documented and comprehendible. The team hopes to help these issues with the handbooks. Unfortunately, it also seems clear, that scientific ambition impedes such measures. As technology is progressing, virtualization and containerization seem to offer increasingly realistic solutions to training challenges and demand further investigation.

It is not foreseeable that the E2SCMS series will be continued due to lack of funding and missing support by the institutions involved. But building portable, comprehendible, well performing and well documented models which can be used by well-educated early career scientists on HPC platforms of their choice/which are available to them, will remain a goal of ENES, and, such, of ESiWACE and its planned successors.

Appendix

Some assignments from 3rd E2SCMS:

Soil respiration
In this experiment, the consequences of an abrupt increase of slowly decomposable leaf litter is analyzed. One can think of this as if the litter had been somehow poisoned so that only extremely specialized bacteria or fungi are able to consume the litter.

Ocean Mixing
In this experiment, the effect of an increased vertical mixing in the ocean mixing in the ocean is examined.

Ocean albedo
In this experiment, the effect of an increased sea water albedo is examined

Flat Earth
This experiment tests the effect of of surface elevations, e.g. mountains, high plateaus etc., on the climate. Surface elevations are represented by the surface geopotential, which is seen by the resolved flow, and by surface parameters describing the sub grid-scale surface features. In this experiment the geopotential and the parameters describing the unresolved topography are set to zero, resulting in a "flat Earth" (though the surface roughness remains unchanged).

Increase of GHG concentration
This experiment explores the effects of an increase of CO_2 concentration in the atmosphere, following a rate of 1% annually from pre-industrial levels.

5. References (Bibliography)

- MS2 report from ESiWACE https://www.esiwace.eu/results/milestones/milestone-2-application-stack-running-at-fmi-csc-preparation-of-system-stack-t3-2-team/view
- ISENES2-Report for the 3rd E2SCMS: http://is.enes.org
- D3.1, D3.3 und D3.5 deliverables can be found here: https://www.esiwace.eu/results/deliverables

6. Dissemination and uptake

6.1 Dissemination

We will present these findings as part of a presentation "Software stack deployment for Earth System Modelling using SPACK" at the Pracedays17 http://www.prace-ri.eu/pracedays17

These results have also flown into the two handbooks presented by ESiWACE:

- "The Application Software Framework" https://www.esiwace.eu/results/misc/the-application-software-framework/view and
- The "Handbook for System Administrators: Specification of a standard recommendation for an ESM System Software Stack" https://www.esiwace.eu/results/deliverables/d3-5-how-to-select-configure-and-install-esm-software-stacks/view

6.2 Uptake by the targeted audience

As indicated in the Description of the Action, the audience for this deliverable is:

X	The general public (PU)
	The project partners, including the Commission services (PP)
	A group specified by the consortium, including the Commission services (RE)
	This report is confidential, only for members of the consortium, including the Commission services (CO)

We will now start to plan for our dissemination activities. A first step is the presentation mentioned under 6.1.

7. The delivery is delayed: ☒ Yes ☐No

The experiences described here were made preparing and running the summer school, and shortly thereafter. The document is uploaded in the Participant Portal only now.

8. Changes made and/or difficulties encountered, if any

As explained under 4.), due to time and (perceived) resource constraints only one model was ported in time for the 3rd E2SCMS. During the preparation of the school, ESiWACE was in the process of re-focussing to the Extreme Scale Demonstrators.

The WP3 team will now apply the ideas concerning the software stacks to issues like performance portability, stable standard system environments, or documentation of solutions for test, performance and scalability issues.

9. Efforts for this deliverable

Person-months spent on this deliverable:

Beneficiary	Person-months	Period covered	Names of scientists involved, including third parties (if appropriate) and their gender (f/m)
DKRZ			
ECMWF			
CNRS-IPSL			
MPG	1	1 September 2015 to 28 February 2017	R. Budich (m), S. Kosukhin (m)
CERFACS			
BSC			
STFC			
MET O			
UREAD			
SMHI			
ICHEC			
CMCC			
DWD			
SEAGATE			
BULL			
ALLINEA			
Total	1		

10. Sustainability

10.1. Lessons learnt: both positive and negative that can be drawn from the experiences of the work to date

The interaction between partners in this work package was very positive and enlightening. For the work in WP4, dependency on external decisions was too large, and the time schedule for the deliverables too ambitious. All WP3 partners contributed actively to the tasks, and to the collection and writing processes for the handbooks. The topic meta-scheduling is a bit less interactive with the other partners, but even more involved with projects partners and a world-wide community of cylc-users.

10.2 Links built with other deliverables, WPs, and synergies created with other projects

The handbooks are planned to be used to serve installations of the EsDs on other platforms, experiences with these codes on different machines will flow back into the handbooks.