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DARE [777413] “Delivering Agile Research Excellence on European e-Infrastructures”



D6.4 Pilot Tools and Services, Execution and Evaluation Report II

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Contributor(s)	M. Lindner (KIT), E. Gottschämmer (KIT), A. Rohnacher (KIT), A. Constantin (UEDIN), V. Andries (UEDIN), M. Atkinson (UEDIN)
Reviewer(s)	X. Tsilimparis (GRNET)
Document description	This deliverable will report on the implementation and execution of two new EPOS test cases within the DARE platform: the Moment

	Tensor in 3D (MT3D) test case and the Volcanology (VC) test case. It will present the set of activated DARE components and their configuration parameters. It will finally report on the pilot development evaluation phase.
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Executive Summary

This deliverable reports on the structure of a second seismological test case in the EPOS framework, the Moment Tensor in 3D (MT3D) analysis, and on its implementation in the latest DARE platform release. Moreover, structure and implementation of a new test case (VC) for the additional volcanology EPOS community are presented. The main DARE components, with corresponding configuration parameters, required for the implementation and execution, are also summarised. Finally, the deliverable reports on the training evaluation events organised by WP6 to present to the reference EPOS communities the pilots' development and execution using the DARE platform. It also focuses on the gathered feedback and suggestions in order to assess the platform usability and utility for present and future scientific applications.

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List of Terms and Abbreviations

Abbreviation	Definition
API	Application Programming Interface
CWL	Common Workflow Language
DEM	Digital Elevation Model
ECMWF	European Centre for Medium-Range Weather Forecasts
EIDA	European Integrated Data Archive
EPOS	European Plate Observing System
ES	Ensemble Simulation
FDSN	Federation of Digital Seismographic Network
MPI	Message Passing Interface
MT3D	Moment Tensor in 3D
NOAA	National Oceanic and Atmospheric Administration
P4	Protected Pervasive Persistent Provenance
PE	Processing Element
RA	Rapid Assessment
RI	Research Infrastructure
SUS	System Usability Scale
TDMT	Time Domain Moment Tensor
VC	Volcanology test case

1 Introduction

1.1 Purpose and Scope

The objective of this deliverable is to present the structure of a second seismological test case in the EPOS framework, the **Moment Tensor in 3D (MT3D) analysis**, and its implementation in the latest DARE platform release. Moreover, based on the mid-term review outcomes, a new **Volcanology test case (VC)** has been introduced to broaden the DARE platform applicability to this new EPOS community. Implementation and execution of this test case are also presented in the deliverable. Both MT3D and VC applications address typical scientific problems of the corresponding communities and are used to exemplify the platform structure and functionalities.

A description of the required DARE components is also presented in order to highlight the main advantages of using the DARE platform to ease development of scientific applications and exploitation of required RI services.

The deliverable has also the scope of reporting on the pilot evaluation trainings organised by WP6 in order to obtain feedback from the target users on the usefulness of the platform for their present work and the future developments they are planning. The first training was a volcanology school addressed to MSc students in the framework of a field course on Stromboli. The second one was a seismology training webinar mainly addressed to domain experts and research developers.

1.2 Approach and Relation to other Work Packages and Deliverables

The approach used will be to firstly describe the high level steps of both the MT3D and VC workflows and their implementation and execution in the DARE platform. Then the WP6 volcanology training school and seismology training webinar are presented focusing on the gathered user feedback.

This deliverable is closely linked to WP8, responsible for training and dissemination activities, and in particular deliverable D8.5 that describes in detail the organisation of the training events, their purposes and the chosen participants. It is also linked to WP2 that works at the architectural design and the evaluation phase, WP3 for lineage and process management, and WP4 and WP5 responsible for the platform development.

1.3 Methodology and Structure of the Deliverable

The structure of this deliverable is as follows. First, the steps of the underlying workflow of the MT3D and VC test cases are described highlighting the advantages of exploiting the platform. Then the specific DARE components used to implement both workflows in the DARE platform are presented followed by the description of the workflows' execution through a Jupyter Notebook. Finally, the organisation of the pilot evaluation events is summarised and the feedback from the target users are analysed in detail to qualitatively and quantitatively assess the achieved results.

2 EPOS Use Case Implementation

This section presents the high level structure of both MT3D and VC workflows and their implementation and execution through the latest release of the DARE platform. A summary of the main required DARE components is also given.

2.1 Moment Tensor in 3D Test Case (MT3D) Description

Following Deliverable D6.1, the second seismological test case focuses on the characterization of the earthquake source parameters and their uncertainties to study the impact on wave propagation and hazard assessment. As anticipated in Deliverable D6.2, our application considers the case in which the Earth is represented by a 3D structure and the seismic source is modelled as a point, thus its main parameters are the location and the moment tensor which describes the magnitude and mechanism of the earthquake rupture.

A typical procedure is to start from an initial solution representing the seismic source (i.e. location and moment tensor), usually routinely calculated by seismic communities using 1D wavespeed models (e.g., TDMT solutions [Scognamiglio *et al.* 2009]). Then the scope is to refine this solution by using source inversion procedures that take into account more complicated 3D wavespeed models. The adopted technique requires simulating an initial synthetic wavefield based on the starting solution, perturbing the initial source parameters and calculating the corresponding perturbed seismic wavefields called derivative synthetics (up to 10 simulations depending on the source parameters we want to invert for). Finally, the procedure finds the best perturbation to be applied to the initial solution in order to minimize the misfit between observed and synthetic wavefields. The seismology community works daily with similar inverse problems applied to the seismic source and it will greatly benefit from the possibility of executing automate, reusable and customisable workflows, such as MT3D, implemented in the DARE platform.

Figure 1 shows the detailed steps of the high level workflow for MT3D:

1. Users choose a model to describe the physical properties and geometry of the wave propagation medium, i.e. a 3D wavespeed model and a mesh, as well as a list of seismic stations.
2. An initial model of the point-like seismic source is defined.
3. With inputs in 1. and 2., a waveform simulation is run to obtain the initial synthetic seismograms; the chosen numerical code is SPEC3D_CARTESIAN [Peter *et al.* 2011].
4. The initial source parameters in 2. are perturbed.
5. Perturbed synthetic seismograms (called derivative synthetics) are simulated using the inputs in 1. and 4. and SPEC3D_CARTESIAN (up to 9 simulations).
6. Corresponding raw observed seismograms for the chosen earthquake are downloaded e.g. from public European archives, such as EIDA¹.
7. All the synthetic seismograms (both initial in 3. and derivative in 5.) and observed data (in 6.) are pre-processed in the same way (e.g. filtering the traces); this prepares the seismograms for the following analyses assuring the consistency between data and synthetics.
8. Observed data and synthetics are compared and suitable time windows for the source inversion are selected using the python code pyflex² (Deliverable D6.2).

¹ <http://eida.rm.ingv.it>

² <http://krischer.github.io/pyflex>

9. New source parameters (moment tensor and location) that minimize the misfit between data and synthetics are calculated through the inversion procedure using the python code `pycmt3d`³ (Deliverable D6.2).
10. Output source parameters are finally stored with their metadata and provenance.

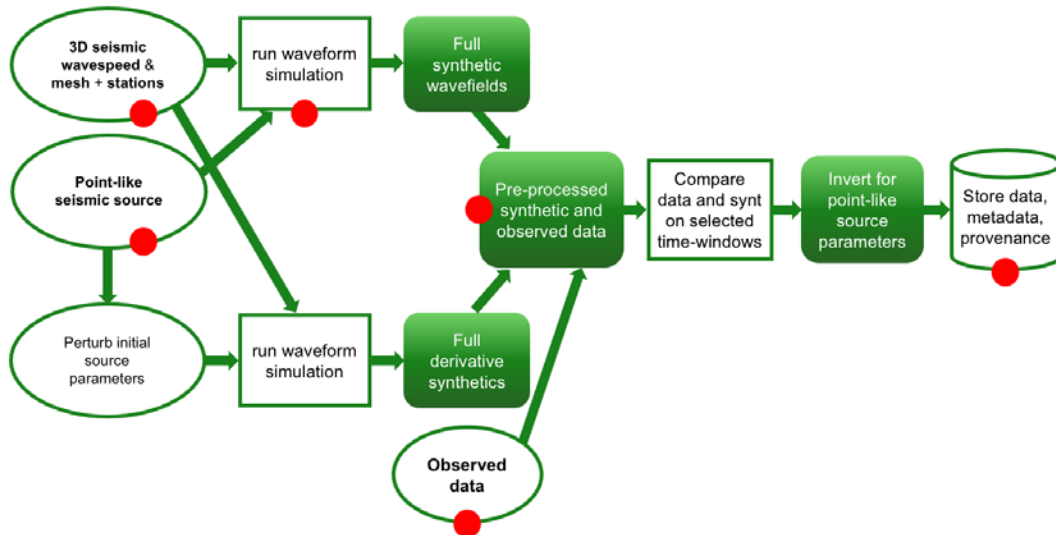


Figure 1. Steps of the workflow for the MT3D test case. The coloured dots at the edges of the boxes indicate the steps that are in common with the RA test case (compare with Figure 1 in Deliverable D6.2).

The first part of the MT3D workflow is composed by the same steps of the RA test case (Deliverable D6.3), so they can be entirely reused. This is a crucial requirement of the pilot use cases perfectly accomplished by the flexible and abstract DARE approach used to construct and implement the workflow steps (see §2.4). The RA-MT3D common steps are 1.-3.: simulate synthetic seismograms for 3D Earth models and the initial point-like seismic source, step 6.: download corresponding recorded seismograms, step 7.: pre-processing of synthetic and recorded traces, and step 8.: storage of output. The remaining steps are new and should be again implemented and executed in order to be reusable (in case with minor changes) for other more general scientific applications, also beyond seismology. Typical output obtained from the execution of MT3D describes the new source solution calculated for the chosen earthquake, see Figure 2.

Deliverable D6.2 described the remaining requirements to complete MT3D test case, among which the execution of multiple SPEC-FEM3D simulations with different input (step 5.) is crucial. All these requirements have been achieved in the last months of the project producing a comprehensive structure to execute all the developed seismology test cases, and further the volcanology test case, in a consistent way (see §2.4).

³ <https://github.com/wjlei1990/pycmt3d>

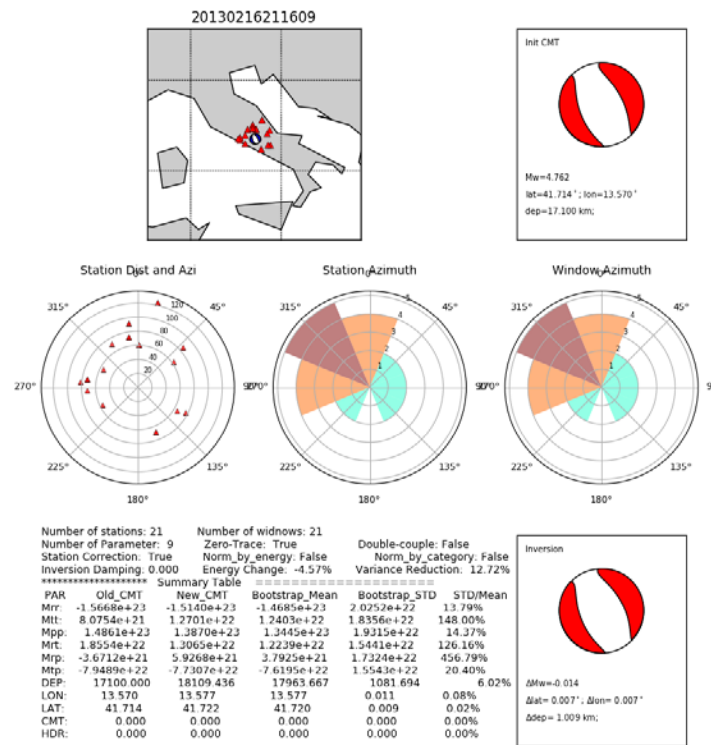


Figure 2: Example of output from the execution of MT3D test case. The top right rectangle indicates the initial source solution with corresponding parameters; the bottom right rectangle is the new source solution from the inversion.

2.2 Volcanology Test Case (VC) Description

The Volcanology (VC) test case, as described also in Deliverable D6.2, has been developed in order to extend the use of the DARE platform to the EPOS volcanology community and test the possibility of easily interacting with the platform by new users beyond seismology and climate frameworks.

The scientific purpose of the test case is to analyse ash dispersal after volcanic eruptions including distributions of deposit thickness, ground load and airborne mass. Similar to the seismological test cases, especially the RA test case, a fast and reliable simulation of the mentioned VC specific parameters and their mapping onto the affected area is an important procedure in volcanic hazard modelling. The DARE platform, together with its user friendly and platform independent execution can support domain specialists in achieving these tasks.

The high level structure of the workflow that we implemented on the DARE platform is shown in Figure 3 and can be summarised as follows.

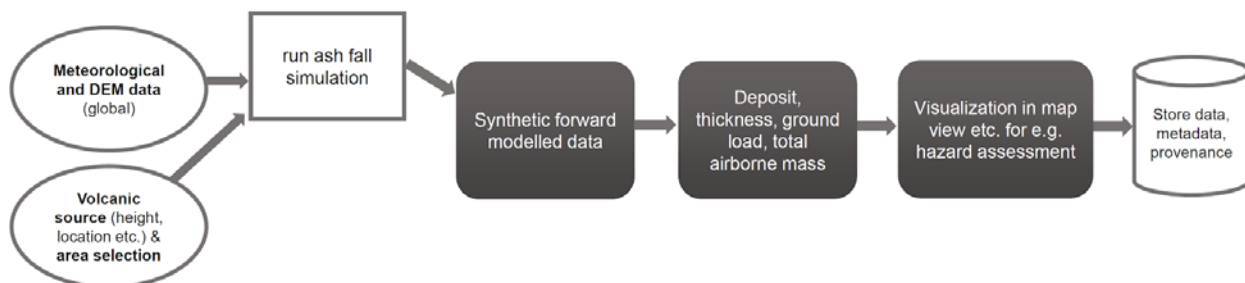


Figure 3: Steps of the workflow for the volcanology test case.

1. Basic information needed to construct a new VC test case scenario are the location information of the volcano of interest and the eruption source parameterizations like eruption time, eruption duration, erupted mass, etc. This information should be prepared by the users.
2. Based on this information, the users then prepare the required regional meteorological data for the selected eruption time, as well as the local digital elevation model (DEM) where we currently support ETOPO1. The meteorological data are freely available by downloading them from NOAA or ECMWF/ERA5 in daily or monthly means.
3. Using the inputs in 1. and 2., we run simulations with FALL3DPy, a python port of the original Fortran code FALL3D by [Folch *et al.* 2009], to obtain ash dispersal distributions.
4. In the post-processing step the content of NetCDF files together with the user input is used to generate visualisations of the individual ash distributions.
5. Outputs are stored together with their metadata and provenance information.

Figure 4 shows exemplary time steps for a simulation at Stromboli volcano in the Mediterranean Sea.

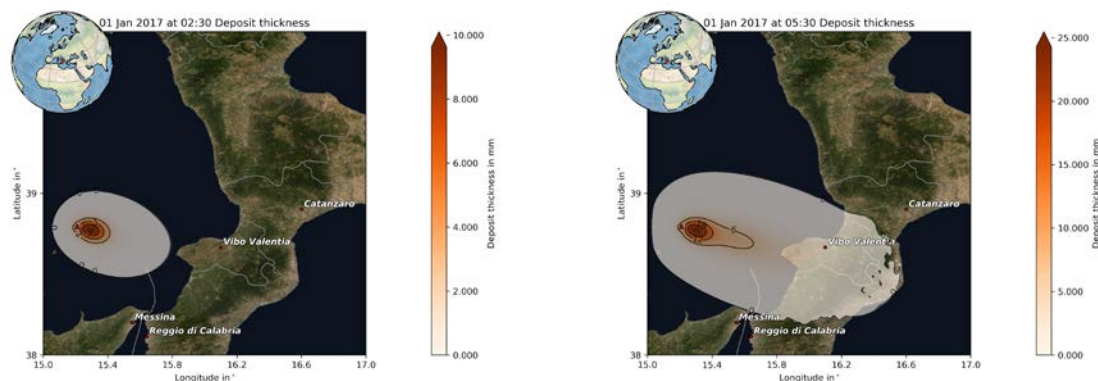


Figure 4: Simulation results for the VC test case. They show the deposit thickness in mm 2:30 h (left) and 5:30 h (right) after the eruption started for a scenario at Stromboli volcano on 01. January 2017.

As the seismological test cases, this workflow has been implemented into the DARE platform and is executable via a Jupyter Notebook interface, as introduced in Deliverable D6.2 and detailed in §2.4.

2.3 Overview and updates of DARE API

The implementation and execution of the described test cases within the DARE platform is based on the exploitation of the DARE API and its main components.

More specifically, the DARE API is a grouping of exposed web APIs of individual components that are part of the DARE platform. These components are largely described in the online material (see §6), in [Klampanos *et al.* 2020], and in previous (D6.3, D6.2) and latest deliverables (D4.8, D5.2) which detail also the recent updates. To summarise, the main components of the DARE platform exploited for the execution of workflows are:

- **DARE Login Service**
- **Execution API**
- **dispel4py registry** (also referenced as Processing Elements Library)
- **CWL workflow registry**
- **sProv-api & sProv-viewer** (both composing the Provenance Management component)
- **dispel4py** and **CWL**

An important update introduced in the second phase of the project is a general reorganisation of the DARE shared file system which benefited all the implemented workflows (see also Deliverable D5.2). The file system is interactable via the API and it is useful when executing workflows in order to list and retrieve files, as well as to perform other file-based actions.

The new file system has a specific structure with a base path `/home/mpiuser/sfs/`. In the `sfs` folder, each user owns a directory named with his/her username. All user folders contain three directories, namely *debug* (for the debug functionality of the platform), *uploads* (typically for the input files uploaded to the platform), and *runs* (for the output results of a workflow execution). Thanks to this change on the file system, all the test cases work within a consistent structure seen by all the dispel4py and CWL workflows. In order to handle the files in the platform, i.e. upload/download/list files, the Execution API of the DARE platform is used. A thorough description can be found in the online documentation and tutorials (see §6), and in Deliverable D4.8.

Details on how the described DARE components are exploited for the workflow execution are in §2.4.

2.4 Implementation and Execution of the Test Cases

All the seismology and volcanology test cases are implemented and executed in the DARE platform exploiting the components described in §2.3.

Regarding **MT3D**, the applied strategy is summarized in Figure 5 (updated from Deliverable D6.2):

- The initial input (like parameter files, mesh and wavespeed models) are uploaded by the users in the shared file system of the DARE platform to make them available for the workflows. A suitable upload function is used (see below).
- The simulation of the initial synthetic seismograms is performed using the dockerized version of the code SPECFEM3D as for the RA test case (Deliverable D6.3) and the approach has been extended to manage the multiple simulations for the derivative synthetics. The specific steps to run a SPECFEM3D simulation are described by a CWL workflow summarised in Figure 6 (see also Deliverable D4.3). Through a specific API call, now common to all the test cases (including volcanology), the SPECFEM3D docker is executed in the DARE cluster and in turn the CWL workflow is called. The multiple simulations with different input are handled through the same Kubernetes pod that runs all simulations.
- All the other steps of MT3D are implemented as dispel4py workflows and executed in the platform via appropriate API calls. The steps of downloading the recorded data and of their pre-processing together with the synthetics are implemented by using the same dispel4py workflows as for RA (just extending the pre-processing to the derivative synthetics) and launched through the same API calls. Then, a new dispel4py workflow has been created to produce the input files describing both the initial seismic source and the perturbed ones. Finally, a unique dispel4py workflow has been constructed to describe the last two steps of MT3D (steps 8. and 9. §2.1): the step that uses pyflex to select the time windows on the seismograms suitable for the source inversion, and the step that uses pycmt3d to do the source inversion and calculate the new source solution that minimizes the misfit.

The API calls to launch the dispel4py workflows in the DARE platform have always the same structure with different set up of the parameters (see below).

Metadata and provenance have been implemented and refined for all the dispel4py and SPECFEM3D CWL workflows of MT3D, following the approach described in Deliverable D6.2, and they are fully explorable and customisable.

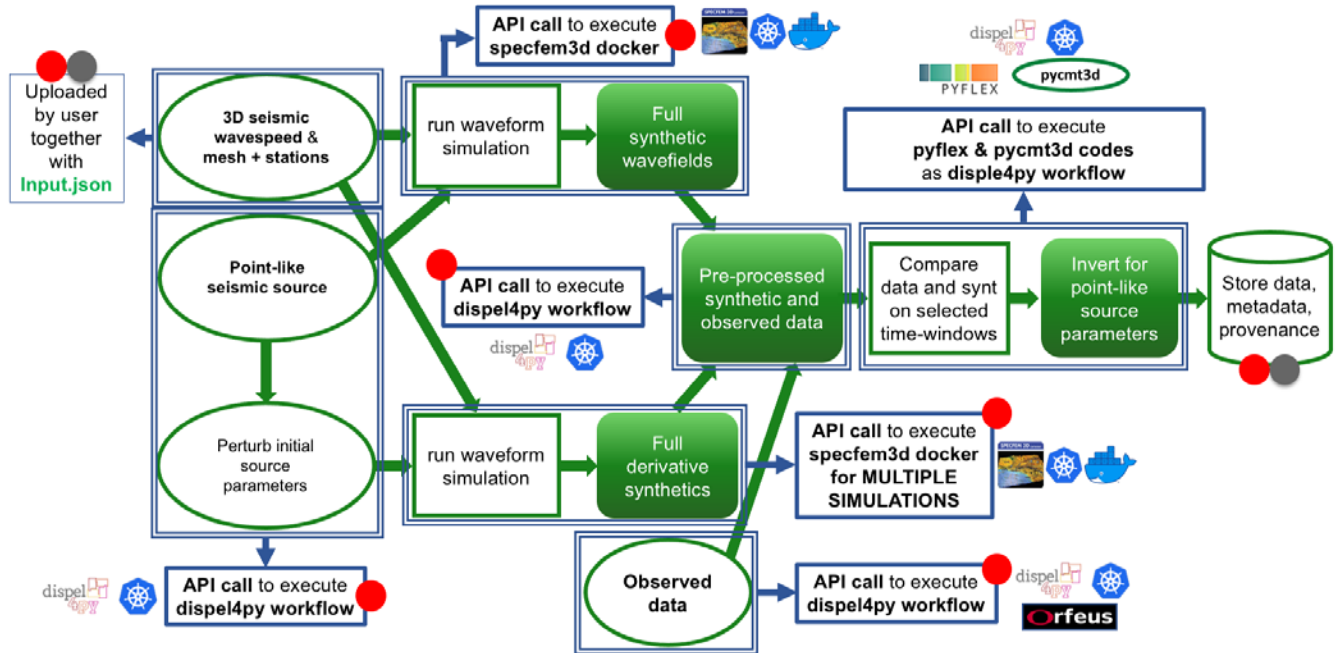


Figure 5: Implementation of the MT3D test case in the DARE platform. Steps with red dots are in common with RA, those with grey dots are in common with VC.

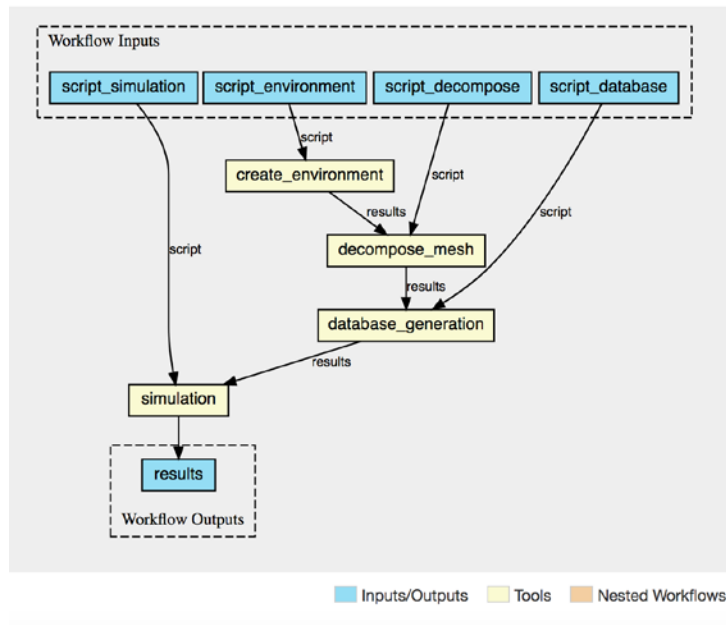


Figure 6: SPECFEM3D CWL workflow.

Based on the above description, three main updates are evident for MT3D with respect to the initial approach used to implement the RA test case (described in Deliverable D6.3):

- A general input file (Input.json) has been introduced and contains the input parameters for all the dispel4py sub-workflows and also for the SPECFEM3D simulation management. Now only this file and those for the mesh, wavespeed model and seismic stations are prepared and uploaded by the user.

- The input file describing the initial seismic source can be now created by using a new displ4py workflow instead of being uploaded by the users. This workflow is the first executed and can create both the file for the initial source and all the files for the perturbed source parameters.
- The SPECSEM3D docker is now executed using the CWL endpoint homogenizing the API call to the one already used in the VC test case (Deliverable D6.2).

In order to have a consistent implementation of all the seismological test cases (also in agreement with volcanology and climate applications in DARE), the updates introduced for the MT3D test case have been in turn applied to the **RA test case**. Figure 7 summarises the updated implementation and execution of RA with respect to the initial prototype described in Deliverable D6.3.

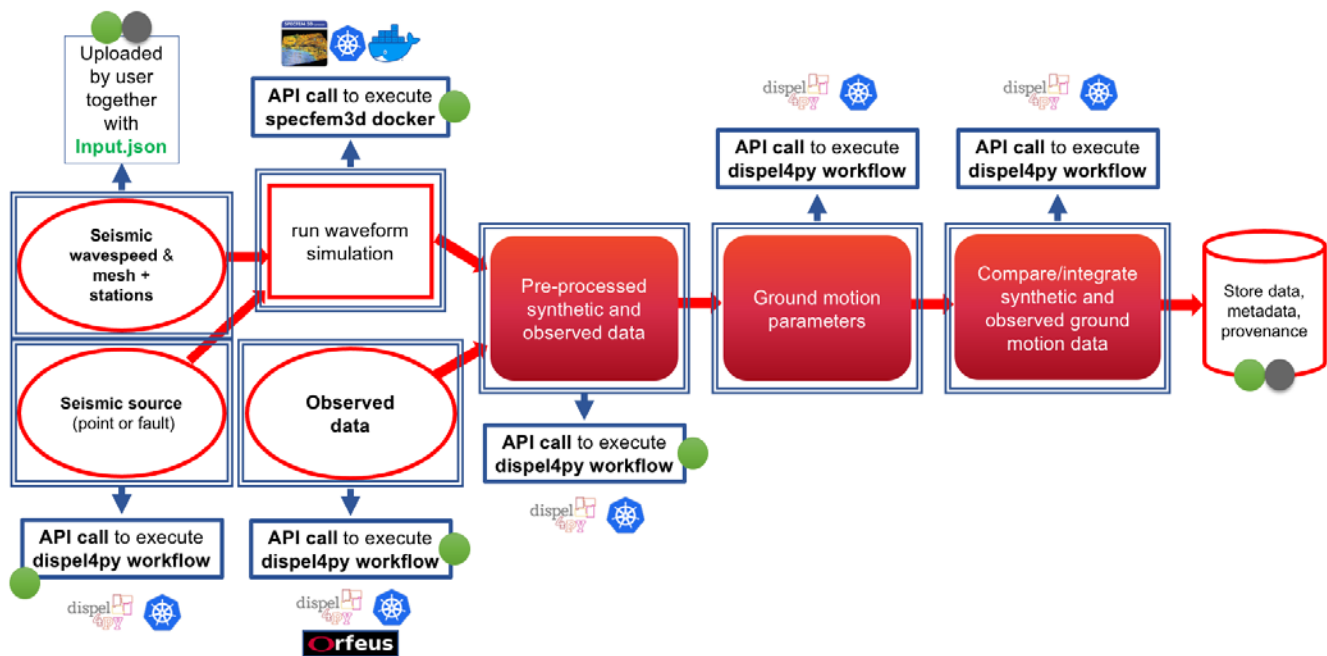


Figure 7: Implementation of the RA test case in the DARE platform. Steps with green dots are in common with MT3D, those with grey dots are in common with VC.

The implementation of the **VC workflow** in the DARE platform has followed the same strategy as for the seismology test cases above and the key steps are shown in Figure 8:

- The input file, which specifies the eruption parameters (volcanic source, area, time), is uploaded by the users. This is an Input.json file, similar to the seismological test cases, which will be used as general input files to the workflow.
- Meteorological data for the selected time is downloaded from NOAA or ECMWF/ERA5 by a displ4py workflow, which is activated by a specific API call. The notebook features a data access wrapper PE, which allows the users to directly download these data from the external archives. Optional, if the required files are already stored locally, the download step can be skipped if not explicitly required.
- For the simulation step, the dockerized version of FALL3DPy is executed through a specific API call that creates in Kubernetes an MPI cluster to run the code.
- All the other steps of the VC test case (post-processing including plotting of the results) are described by displ4py workflows, made by several displ4py PEs and launched through specific API calls with the same structure and different parameter set up.

Metadata and provenance are again captured and stored through dispel4py and CWL (Deliverable D6.2).

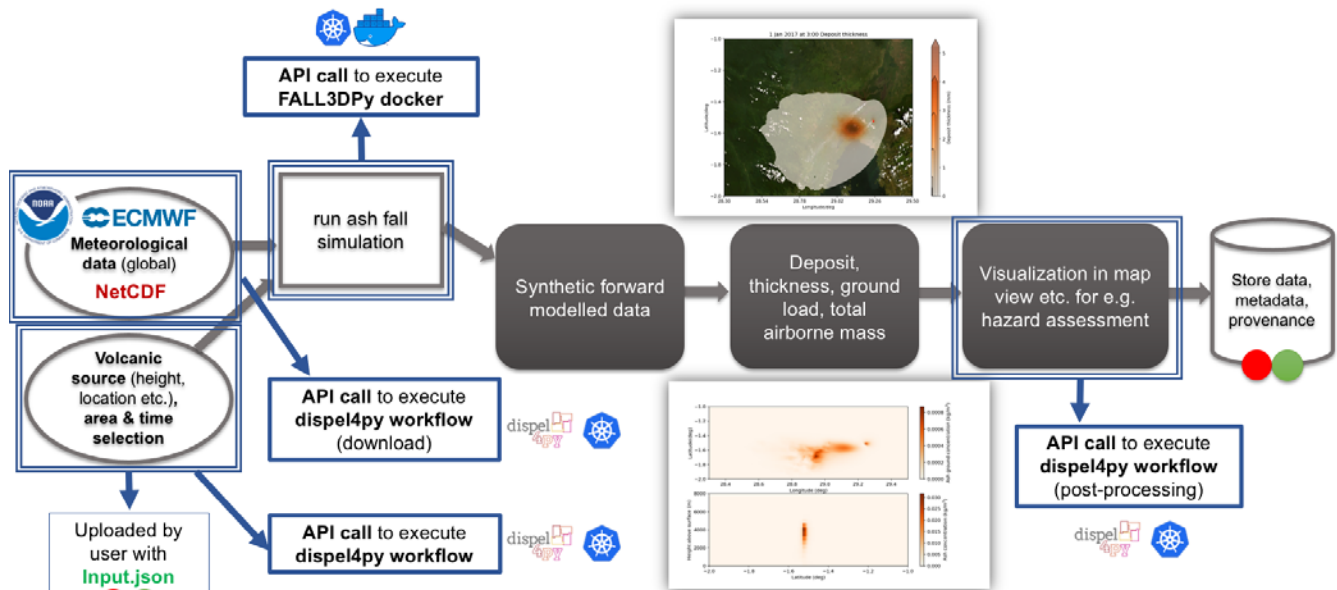


Figure 8: Implementation of the VC test case in the DARE platform. Steps with green dots are in common with MT3D, those with red dots are in common with RA.

As anticipated in Deliverables D6.3 and D6.2, the interface used to execute all the described workflows in the DARE platform is a Jupyter Notebook. In particular, the notebook created for each test case can be uploaded and executed in the development environment of the DARE Jupyter Lab⁴ (Deliverable D5.2).

Thanks to the commonality of the steps between the test cases, and the abstract and flexible structure of the API calls, the notebooks are simply constituted of an initial part common to all the test cases and of following cells containing the API calls to execute the specific workflows' steps, with same structure but different parameter set up. The main steps of the notebooks are presented in the following and are updated with respect to Deliverables D6.2 and D6.3 to increase the abstraction and applicability for general and multidisciplinary applications.

- Register to the dispel4py registry and get a token for following authorization:


```
dm=DareManager(dare_platform_url=BASE_URL,config_file=credentials_file)
token=dm.token
```
- Upload required input files:


```
dm.upload_file(remote_path=remote_path,filename=filename,
               local_path=local_path)
```
- CWL workflows as SPECSEM3D and FALL3DPy runs:
 - register docker


```
docker_params={"docker_name":docker_name,"docker_tag":docker_tag,
                "url":docker_url,"script_names":script_names,"path":
                docker_folder}
```

⁴ <https://jupyter.dare.scai.fraunhofer.de>

```

response=dm.register_docker(docker_params)
response=json.loads(response[1])
dm.provide_docker_image_url(docker_params)

```

- register CWL workflows

```

cwl_params={"workflow_name":workflow_name,"workflow_version":
            workflow_version,"spec_name":spec_name,"path_to_cwls":cwl_folder}
workflow=dm.register_cwl(cwl_params=cwl_params,docker_params=
                        docker_params,register_docker=False)
workflow=json.loads(workflow[1])

```
- execute CWL workflows with the suitable API call

```

dm.exec_cwl(nodes=nodes,input_data={input_data},
            workflow_name=workflow_name,workflow_version=workflow_version)

```

where `input_data` is a dictionary specifying the input files.

- dispel4py workflows:

- Register the PE/workflow to the dispel4py PE registry:

```

workspace_id,impl_id=dm.register_d4p_workflow(name=wf_name,code=code)

```
- Execute the PE/workflow with the dispel4py API call specifying requirements and input:

```

dm.exec_d4p(impl_id=impl_id,workspace_id=workspace_id,pe_name=wf_name,
            nodes=nodes,no_processes=no_processes,iterations=iterations,
            target=d4p_model,prev_run_id=prev_run_id,
            reqs="requirements",inputdata=input_data)

```

Additional functions are also available to download files, monitor the runs and explore output directories and files. A detailed description of all the mentioned functions for the latest release of the DARE platform can be found in Deliverable D4.8 and in the online documentation⁵ (see §6).

The test cases implemented in the framework of the DARE project steered the platform development and, above all, highlight that the platform is enough flexible to allow users to implement their own workflows by reusing sub-workflows already developed and registered in the platform, or writing and implementing new workflows following a common, ready-to-use and robust approach.

To summarise, the main advantages of exploiting the DARE platform for the developed test cases but also for more general scientific applications are:

- use of dockers that handle all the details and requirements needed for execution, hiding them from the users;
- transparent use of computing and storage resources without the need to deal with environment specificity;
- possibility of exploiting external RI services (as FDSN web services for data download) by including them in the workflow itself;
- full customisation and storage of metadata and provenance to ease investigation of results and errors as well as reproducibility and shareability of science;
- easy customisation of workflows benefiting from the large flexibility and abstraction of pipelines which allow to reuse the same steps in different workflows with small changes;
- thus finally ease domain researchers and research developers to implement and execute scientific workflows hiding the technical details and letting them focusing on their work.

⁵ <https://project-dare.gitlab.io/dare-platform/api/>

In the very last period interesting work is in progress to exploit the functionalities of the general-purpose element of the DARE Knowledge Base (DKB) in collaboration with WP2. This will further ease the structure of the Notebooks used for workflow execution by hiding additional details from the users. Above all, the general-purpose DKB will greatly enhance the reusability, reproducibility and shareability of scientific methods and results by storing in a common database the developed workflows and all related IDs and information. See Deliverable D2.2 §4.2.5 for additional details and for a practical example.

3 Training Events and Evaluation Results

This section summarises the pilot training events organised by WP6 and focuses on the gathered results in order to assess the utility of the DARE platform for applications on the reference scientific communities. More details on the trainings' organisation are reported in Deliverable D8.5.

3.1 Volcanological School

3.1.1 Purposes and Development

The VC test case, in addition to validation tests, was used in a training school for students and other users during the exercises associated with a lecture about volcanic hazard in the Mediterranean area occurred on July 24th, 2020, at KIT.

The purpose of the school was to introduce the DARE platform to the volcanology community to enlarge the audience of possible future users. Moreover, we wanted to test how easily they can play with the platform interacting with its components and customising the experiments.

All participants were inexperienced with the test case (they only had some background in general volcanology and numerical modelling) and the 10 students who participated were part of the Master's degree program in Geophysics at KIT.

During the school the attendees worked with the Jupyter Notebook that was prepared to execute the VC test case in the DARE platform and was provided via JupyterHub. This allowed the users to analyse ash dispersal after volcanic eruptions including distributions of deposit thickness, ground load and airborne mass for different scenarios at Vesuvius, Stromboli, Vulcano and Etna.

The trainers included two members of WP6 with DARE partners from NCSR D and Fraunhofer on permanent standby to permit quick mending in case of bug occurrences and to monitor the server performance. An evaluation analysis was also conducted by Aurora Constantin (WP2 – UEDIN) after the school and the results are summarised in §3.1.2.

After the onsite training event had concluded, the students were able to perform further simulations from any place. This was a necessity given for the elaboration phase of the students to produce case reports of the examined volcanological studies. The deadline of the report was set to early November 2020 and the students presented the results of their joint analysis in a poster session.

More details on this event can be found in Deliverable D8.5.

3.1.2 Evaluation Results

This section also appears in Deliverable D2.2 (§5.3.1). We advise readers who have already read it to skip to §3.2.

Study Design

Aims

In this evaluation study we aimed to:

1. investigate the usability of the platform
2. collect suggestions for improving the platform.

Participants

The participants in this study were 10 BSc and MSc (in Geophysics) students from KIT.

Methods

We used a questionnaire to capture the users' perception of usability (mainly user satisfaction) and also suggestions for improving the platform regarding both usability and functionality. The questionnaire included the System Usability Scale (SUS) which consists of 10 five-point Likert scale questions [Sauro 2011]. The rest of the questions were open ended and aimed to find out what the participants like, dislike and what suggestions they have for improving the system.

Procedure

The study got ethical approval (No 34039) from the School of Informatics (UEDIN). It took place at KIT and followed up a session of student training which included using a free exploration of the DARE platform. The course's main aim was to train students in volcanic hazard assessment. At the end of the course all the students agreed to answer the questionnaire, after reading the information sheet and signed the consent form.

Data Collection and Analysis

The data from the SUS questionnaire were used to obtain the SUS score. This was calculated by combining the ten scores for each question according to [Bangor *et al.* 2009]. This score ranges from 0 to 100, with a score of 68 being considered as an average score. In order to be excellent, a system should score over 80.3. Data analysis of the answers in the open-ended questions was inspired by thematic analysis, top-down approach [Brown & Clarke 2006]. We set up three predefined themes: *likes*, *dislikes* and *suggestions*.

Results and Discussion

After analysing the data, we excluded the data from one participant as we found that their scores in the SUS questionnaire were in contradiction with their answers in the open-ended questions. Particularly, the student was very positive in appreciating the platform, but scored the platform extremely low (i.e. 15). Therefore, we only considered the results from nine participants to this study.

SUS scores on usability

The SUS scores for the nine participants ranged between 50 and 82.5 (see Figure 9 left) with an average of 65. Looking at Figure 9 right, we can see that the maximum score is very close to excellent on the adjective scale [Bangor *et al.* 2009], whereas the minimum is still OK. The average SUS score falls within the upper band of OK and is very close to what is considered the average score which puts the project at 50th percent.

Likes

parts, an initial introductory part on the DARE platform and the MT3D test case, and a second more technical part. The aim was to:

- give the participants a general overview of the project and its main goals;
- describe the main components of the DARE platform (API, provenance, dispel4py and CWL workflows);
- present the scientific problem behind the MT3D test case and the main advantages in using the DARE platform to reduce the difficulties that research developers and domain specific researchers usually face developing and executing workflows;
- show a live demo of the MT3D workflow execution using the DARE platform via Jupyter Lab;
- give more technical details on workflow implementation and platform deployment;
- gather participants' feedback through anonymous questionnaires and interviews.

During the week after the webinar, temporary accounts were created for the participants interested in trying the platform and the workflow execution, and a Slack channel for support was activated.

The trainers included two members of WP4 from NCSR D for the introduction of the DARE project and components, one trainer of WP6 from INGV to introduce the test case and perform the demo, and two members of WP2 from UEDIN to present the evaluation strategy.

The event was largely advertised through invitation emails and DARE social media channels in order to involve as many participants as possible from the reference seismological community of EPOS, INGV, KIT and DARE. This guaranteed an heterogeneous group of participants with multidisciplinary expertise who can evaluate multiple aspects of the platform development and test case implementation providing comprehensive feedback. This is shown in Figure 10, which includes DARE partners and trainers, and in question #1 in §3.2.2 referred to the participants who filled in the evaluation questionnaire. The total number of attendees was 55 (including 9 DARE members) and less for the second technical part of the training. Almost a half of the non-DARE participants completed the evaluation questionnaire and some attendees agreed to participate in dedicated evaluation interviews. See other details in §3.2.2 and Deliverable D8.5.

Please indicate the option that closest indicates your role
55 responses



Figure 10: *Expertise of the webinar participants.* This includes all registered participants (9 of which are DARE members).

3.2.2 Evaluation Results

The training evaluation included short questionnaires to be filled in by the participants. Then, with respect to the volcanology school evaluation, also more detailed interviews to both training attendees and some DARE members were conducted by Aurora Constantin and Valentina Andries (WP2 – UEDIN) since we aimed for an additional, quantitative method to evaluate the utility and usability of the DARE platform and approach.

In the following sections the results of the questionnaires are analysed discussing the questions one by one (§3.2.2.1) and the general outcomes of the interviews are presented (§3.2.2.2).

3.2.2.1 Evaluation Questionnaires

The evaluation questionnaire, anonymously filled in by the attendees, is available at this link:

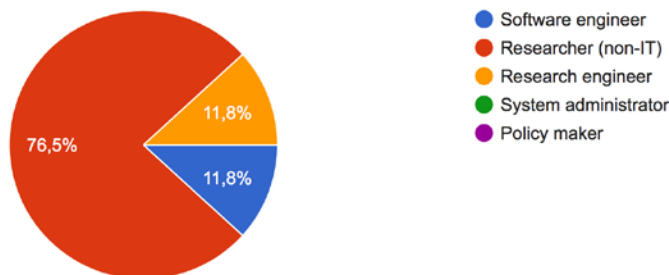
<https://forms.gle/AmUtJKrbckBmsrXz6>

The training webinar was organised in two separate parts (§3.2.1), thus the questionnaire is structured with a first set of questions related to the first part of the webinar and a second set for the more technical part of the webinar. Only the participants to the second part of the training were required to answer the second set of questions. Finally, additional open comments can be provided.

Question #1

Please indicate the option that closest indicates your role

17 risposte



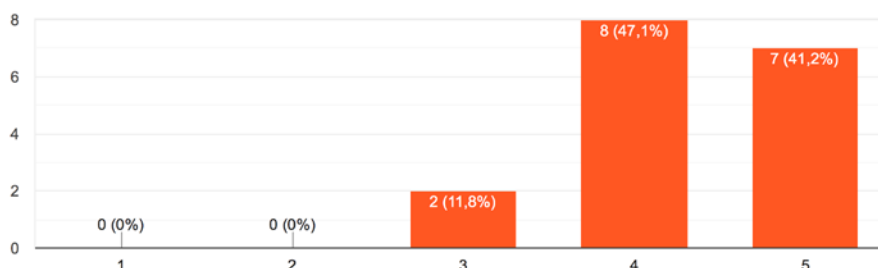
As anticipated, this question highlights the heterogeneity of the training participants which reflects the typical range of expertise in the seismological community. Most of them were researchers or research developers with domain specific competencies and also computing and development expertise. Research and software engineers were also interested in the DARE platform development and will address the more technical details for the deployment and maintenance of the platform.

Part I

Question #2

The webinar explained the main features of the DARE platform clearly

17 risposte



For these answers and all the following, '1'='Disagree', '5'='Agree'.

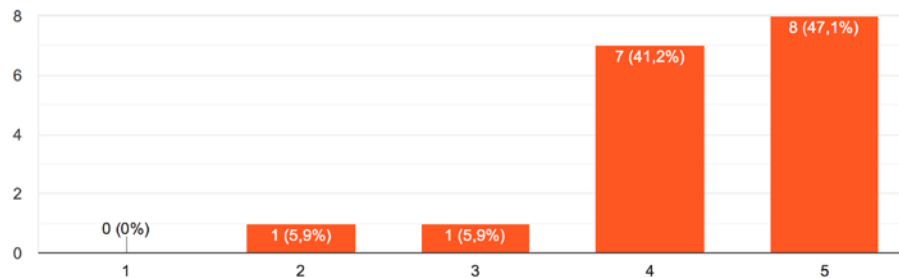
The answers reveal a very positive evaluation of the overall training webinar demonstrating that it was able to advertise the main features of the DARE platform and their usefulness for the EPOS seismological community. The short format chosen for the second training was suitable for capturing the interest of a broad audience through the introductory general presentations and the live demo,

concluding with the more detailed technical part which gives basic hints to start with platform deployment and use.

Question #3

The webinar provided enough pointers to additional information and documentation to get me started as a user

17 risposte

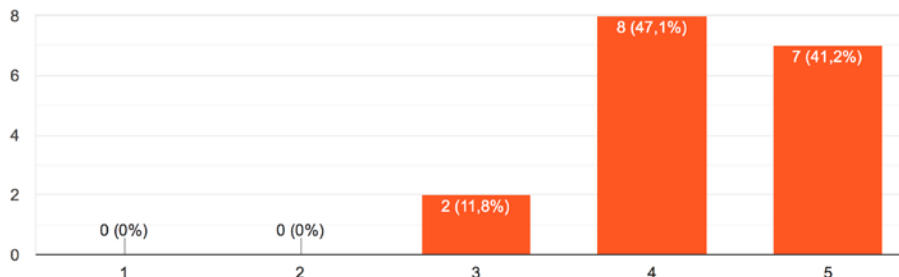


After the training, all the presentations were sent to the participants and they contained links to the online documentation on the DARE platform deployment and use, the DARE components and the tutorial Jupyter Notebook to execute the MT3D workflow. The majority of participants who answered the questionnaire found the material quite useful to start playing with the platform and use their temporary accounts for testing. By the end of the project all the documentations will be finalized including some videos recorded during the training events which can be useful for future users.

Question #4

The Earth-sciences use-case presented helped me to understand how the DARE platform can meet my requirements

17 risposte

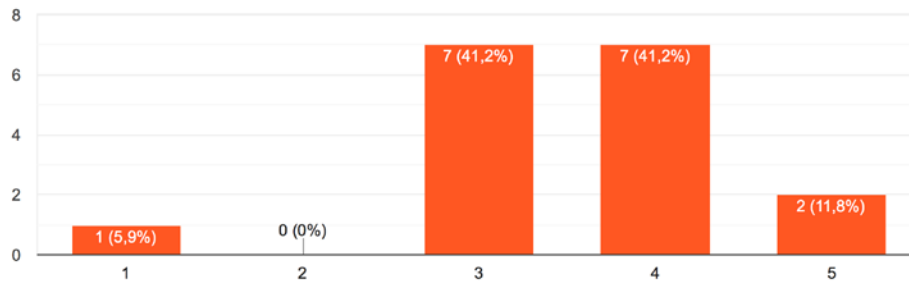


The answers are very satisfactory showing that the implementation of the MT3D workflow clearly exemplifies the utility of the DARE platform for seismological applications. The test case represents a typical issue faced by seismology researchers and developers. They recognised that the platform is a practical tool to approach this study, and also flexible enough to be adapted to other problems and analysis procedures.

Question #5

I could see myself using this platform for my daily work

17 risposte

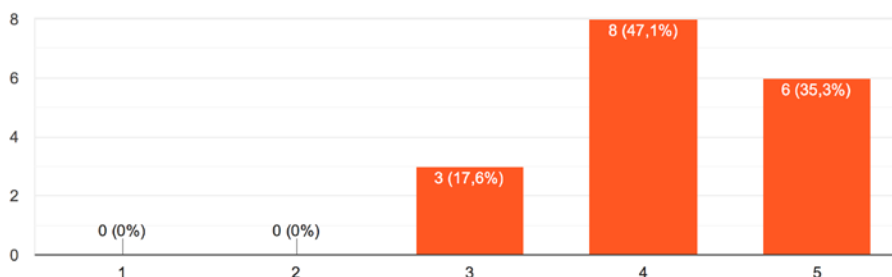


The answers confirm the promising results of the first training (§3.2 in Deliverable D6.3) during which the participants were very positive about using the DARE platform when it would become operational. In the second training we showed the latest updates of the platform and the implementation of a more complex and common seismological test case. This met the expectations of the Earth science community always looking for tools fostering the research outcomes and managing the increasing complexities of applets and huge dataset analysis.

Question #6

I think the various components of the platform (WaaS, provenance, registries, jupyter environment, etc.) are well integrated

17 risposte

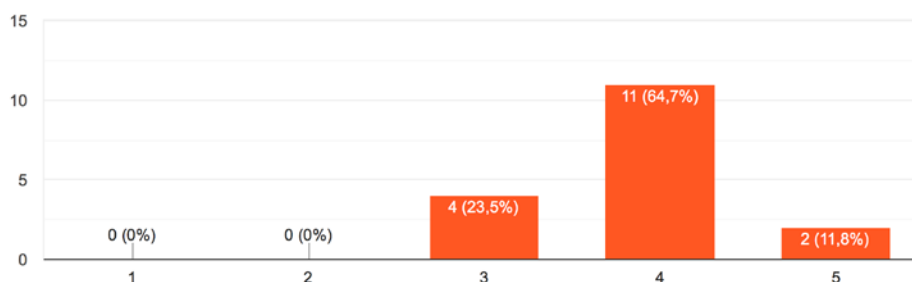


The integration of different and heterogeneous components in a single powerful tool is also very much appreciated by the attendees, an achieved goal of the DARE project. The users can focus on their work and exploit the advantages of the different components without the need of manually activating them and taking care of their specificities.

Question #7

I would imagine that research developers and engineers would learn how to use this platform quickly

17 risposte



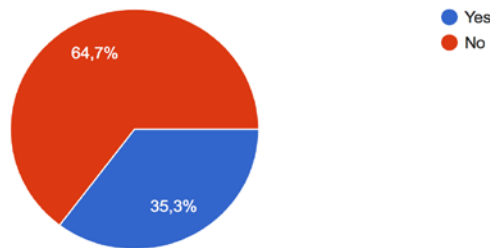
The attendees recognised that a learning stage is necessary for the research developers and engineers in order to explore all the DARE platform functionalities and understand how they can be used to benefit the researchers' work. This phase could be initially a bit slow since developers may not be

familiar with all the components but in general the use of largely common tools as Kubernetes, Dockers and Jupyter Notebooks will facilitate the process.

Question #8

Did you participate in Part 2, on deployment and the hands-on session?

17 risposte



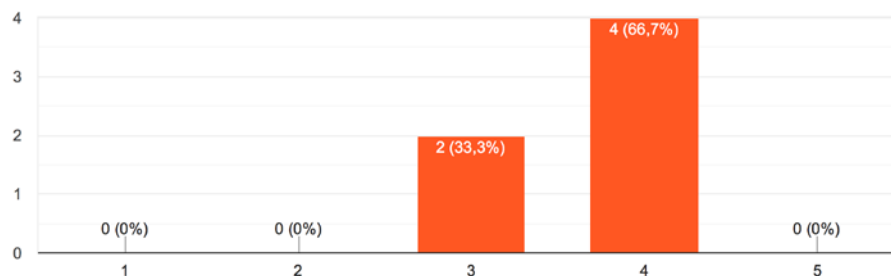
The second part of the webinar was dedicated to the presentation of technical guidelines to deploy the DARE platform in local or institutional resources and to use the DARE components to implement and execute workflows. Not all the attendees participated in part II and only some of them answered the questions pertaining to that part.

Part II

Question #9

The webinar provided enough information to acquire and deploy the DARE platform

6 risposte

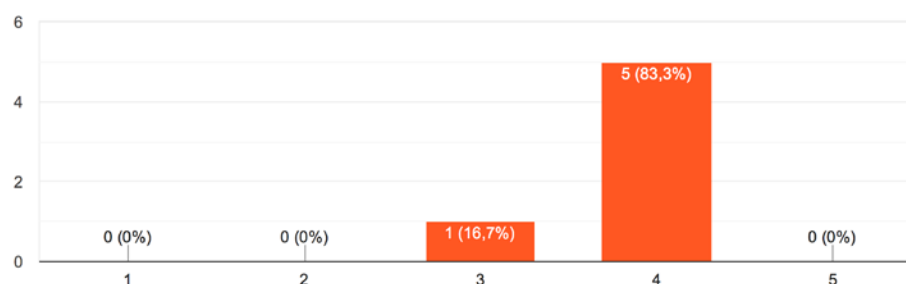


As for the questions in Part I about general information for starting users, the answers to question #9 show that the training provided quite complete information to approach the technical deployment of the platform. Availability of the video tutorial describing guidelines on the platform deploy will complement the training event for future users.

Question #10

The hands-on experience was informative of the platform's capabilities

6 risposte

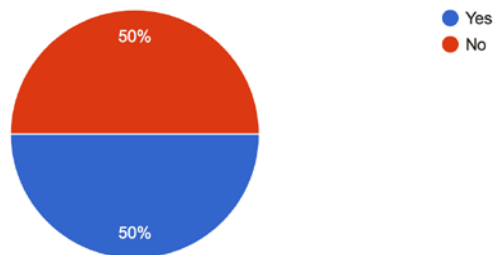


A quick demo of the MT3D workflow execution using the Jupyter Notebook was shown in the first part of the training. At the end of the second part, the participants were guided through the practical instructions to implement and execute scientific workflows in the platform and, based on the answers, they considered these presentations useful to learn the platform usage and get started with it.

Question #11

Would you like to participate in a follow-up interview, to help us assess the usability of the DARE platform?

6 risposte



Three of the training participants gave the availability to be interviewed by the evaluation team. The results are reported in §3.2.2.2.

Additional feedback

Question #12

Which features did you like the most about the DARE platform?

6 risposte

-
easy way to deploy workflows - jupyter notebooks
Scalability, open source usage
the integration of many subsystems with less need to manage detail than normal
Abstraction
the fact that DARE platform hides complexity

The answers to this open question highlight that the training not only presented the main features of the DARE platform clearly (question #1), but correctly enhanced the main advantages of its usage for scientific applications. Participants caught the benefits for their work and the expectations evidenced in the first training (Deliverable D6.3) about the initial prototype of the platform were satisfied. Use of Jupyter Notebooks as interface with the platform resulted to be a good choice since it's a common tool for the research developers and meets their need of easily interacting with the operational components. At the same time, abstraction and detail handling, some of the main goals of DARE, are very appreciated.

Question #13

Which features did you like the least about the DARE platform?

4 risposte

-

need some time to understand the overall functioning of the platform

complexity of the installation

n/a

These answers confirm, as in question #7, that in order to fully exploit the richness of the platform functionalities, an initial training phase is necessary both for domain scientists and research engineers. The interested communities should spend some time to learn how to deploy and use a DARE instance but this will finally be beneficial for their daily work offering a powerful, ready-to-use tool to implement and execute their applications. The answers also suggest that the seismological community could be interested in further training events that allow it to overcome the initial complexities of the platform installation.

Question #14

What do you suggest we improve about the platform?

6 risposte

n/a

A seminar close to geophysical community background

I have not enough knowledge to suggest improvements

Using Singularity instead of docker as a container should be better for HPC computations

reduce the amount of information required by increasing integration and automation

The answers suggest that future, more focused trainings would be very appreciated also by the scientific Earth science community. Moreover, it is clear that the DARE platform has many potentialities that can be further exploited and the communities interested in its adoption can enrich it with improved/additional functionalities also more suitable for specific applications.

Question #15

Any other comments?

3 risposte

I heard from the DARE platform first, when I received the invitation to this webinar from my institute / professor (I currently changed from Master to PhD). So, this platform and its concept is still quite new for me and it was difficult for me to answer the question in this questionnaire in a helpful way. However, this webinar was a good overview. And with the provided slides (thanks!) and the links inside, it is more or less easy to get more information and a better understanding of the whole thing.

My answers are not typical as I am involved as a system architect in the project

no

Although there is only one useful answer, it reflects the general positive impression from previous answers, showing that the training aroused the interest of new users and provided the basics to get started with the platform.

As a general comment, the training webinar offered a thorough overview of the platform functionalities and advantages, and the promising expectations about the usefulness of the initial DARE prototype (Deliverable D6.3) have been finally met by the latest, more mature release of the platform.

3.2.2.2 Evaluation Interviews

The evaluation interviews aimed to assess the usability of the DARE platform in general terms without focusing on a particular use case. The data analysis thereby provided an overall feedback which applies to both seismological and climate (Deliverable D7.4) scientific applications due to the level of participation and the characteristics of the participants. Thus, this section is also reported in Deliverables D7.4 (§3.3) and D2.2 (§5.3.2) for completeness. Readers who have read it in one of those deliverables are advised to skip to §4.

Study Design

Aims

The interview-study aims were to evaluate:

1. ease of use
2. user satisfaction
3. utility of the DARE platform
4. DARE impact on the speed of the engineers' responses to research requirements
5. impact of the platform on researchers' productivity
6. impact of the platform on the innovation in research community

In addition, the study aimed to collect:

1. usability and functionality issues
2. suggestions to improve the platform.

Participants

We have recruited 6 participants, from various backgrounds. Two of them helped us to pilot the interview questions. All of them have been involved in the development of the platform to varying extents, and they all have programming skills.

Procedure

We conducted semi-structured interviews to obtain insights arising from participants' perspectives and experiences. The interview questions were developed to probe several areas of exploration, such as the ease of use of the DARE platform, its learnability, its potential for integration with other services, and for automation of research methods. They asked about data-use policies.

Initially, we piloted the interviews with two DARE team members. This tested our interview questions and interview data-collection procedure.

Data Collection and Analysis

The data has been collected online, using the Zoom platform for video-conferencing. The sessions were recorded for analysis purposes. Similar to the previous evaluation (§3.1.2), a thematic analysis top-down approach was employed. Codes were given to the participants (from P1 to P6) to maintain anonymity in reports and publications.

Results and Discussion

Here is a summary of main findings of the interviews, clustered thematically. Readers are referred to [Constantin & Andries 2020] for a complete report.

Successful experience

Overall, all the participants found that the experience of using DARE led to success. Discussing what contributed to their success, they mentioned that developing targets for use cases was accomplished (N=2)⁹, and the structure of the platform in itself was deemed to be versatile and functional, because it “hides some of the complexity of the execution” (P3). Its components have also been mentioned as contributing to a successful experience with the platform, primarily the workflows that are already set up (N=4), or the fact that DARE sets up the environment with all the libraries that users may need (P6).

Ease of use

The participants generally found the platform easy to use (N=5). We employ caution when presenting this result as all interviewees were in some way involved in its development. They were able to identify potential areas for improvement, and suggestions for additional features and training to improve the use of the platform.

Less successful platform features

The participants discussed these in terms of features that might be missing and could be added, referring to the lack of maturity of the platform, rather than unsuccessful features. Examples included the lack of a user interface, for finding files and logs (P4). Instead they had to use the DARE API for that purpose (P4). The difficulty of installation (P5), the potential assumption that the users should have some cloud computing knowledge to use the platform (P6), as well as computational and programming skills (P3). There was confusion around the provenance and the API documentation regarding types of data (P2).

Training needed for using the platform

All the participants agreed that training would be beneficial for the users and developers. More specifically, an initial training stage was described as essential as the platform has plenty of functionality to offer, and the opportunity and support to explore that in depth should be provided (N=2). Perhaps some training, more specifically aimed at individuals who may not have a background in computer science (N=2), to provide support with the development of workflows and helper functions would be useful. Providing examples which can be sorted by functions, objectives, etc. was also mentioned (P5). Videos to explain how to register an application, and videos to introduce each aspect of the platform’s functionality (P6).

Responsibility for knowledge transfer

All the participants agree that the developers have the initial responsibility for providing support (e.g. to organise webinars). A collaboration between research engineers and domain-specific engineers was also mentioned (N=2). Lastly, one of the participants suggested a community forum could be developed over time, similar to Stack Overflow, provided that enough members would actively engage.

Productivity and innovation in communities

All the participants agreed that by using the platform, the productivity of the users would increase. This was motivated by explaining that the platform is aimed at reducing the engineering time by hiding the technical details (N=3), allowing the users to spend more time developing their specific applications and, consequently, on research. More specifically, the platform can be used via an API call, not needing to worry about the workflows or the infrastructure (N=2). Most of the participants thus considered that, by reducing the time previously spent on infrastructure complexities, the platform can accelerate innovation in the users’ communities, by enabling them to focus more on research.

Integration with external and local services

All the participants considered that the platform integrated very well with both external and local services, given the services that were tested so far. Examples of good integration included the European

⁹ Indicates number of interviewees that gave this response, 2 in this case.

seismic archives which could be downloaded for use (P3). DARE was described as modular and independent thanks to Kubernetes (P4) and well connected to the climate computational resources infrastructure (P5). DARE was also described as one of the first platforms to allow the communities to transfer into a cloud, which should be the future of operations (P6).

Automation of research methods and development practices

The participants knew that automation was one of the goals of DARE (to hide some technical details) and they all believe that this was achieved to some extent. More specifically, all resources are shareable between users, by enabling the use and sharing of workflow systems, and large-scale parallelisation without the users' input.

Additional automation and functionality

These can be added to the platform, depending on community's needs (N=2), e.g., graphical interfaces could help beginners (P2), the addition of a desktop version with the same libraries, for local deployment (P6), as well as a visual representation of the user's repository (P6) may be helpful.

Conclusions and caveat

We would have recruited more responders and conducted more interviews had face-to-face events been possible. The participants supported the view that the platform is usable, and that it would be easy to use (depending on the users' background and skills). The platform supports automation of some common practices, and it allows additional functionality to be added. Training should be provided by developers in the early stages and extended by the communities themselves, to facilitate understanding of the different opportunities enabled by the platform. Some of the replies indicate limitations in the training, e.g., regarding difficulty in finding files and logs when the data catalogue and provenance (P4) have these facilities. However, readers are warned that all the interviewees were or had been members of the DARE project, so the results should be considered with caution.

4 General Conclusions

The seismological MT3D test case was successfully implemented and executed in the latest release of the DARE platform accomplishing the requirements delineated in the initial plan (Deliverable D6.1) and the targeted updates emerged during the second phase of the project (Deliverables D6.3 and D6.2). Based on this, also the RA test case was improved in order to make its execution more general and consistent with the other test cases.

A new test case in the volcanology field (VC) was proposed and effectively implemented following the same strategy in order to broaden the interest to another community in the EPOS framework, as suggested during the mid-term review.

These advances will be beneficial for future implementations of more complex test case scenarios as it could be the Ensemble Simulation (ES) test case, a statistical analysis of ground motion parameters which would combine multiple executions of RA and MT3D test cases, or other multidisciplinary applications in Earth science. In particular, ES was cited in Deliverable D6.1 as a possible EPOS test case but during the second phase of the project the priority was given to the MT3D test case and, based on the mid-term review, to the unanticipated VC test case to engage the volcanology community. Given the advanced status of the project now entering the final compilation and evaluation stage, work allocation with focus on the ES test case is set as a desirable but subordinated goal of WP6 within the remaining funding period.

The developed workflows were presented in the WP6 training events organised during the second phase of the project. The volcanology school of July 2020 showcased the self-sufficiency of the users,

specifically MSc students, in interacting and using the platform also adding customised solutions. The seismology training webinar of November 2020 demonstrated the last updates of the platform and pilot implementation advertising them to a broad audience and gathering potential future users. This heterogeneity in the training attendees allowed us to collect the platform utility and usability evaluations from different levels of users, finally composed to obtain an overall assessment of the DARE project outcomes.

The promising impressions from the first training event were confirmed by these latest dissemination events. The trainings were judged to be very informative to guide first users through the exploitation of the DARE platform functionalities. A large interest has been evidenced among research scientists, developers and engineers of the reference seismological and volcanological communities letting us envisage future applications of the platform also after the end of the project.

5 References

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[Braun & Clarke] Braun V., Clarke V., 2006. *Using thematic analysis in psychology*. *Qualitative research in psychology*, 3(2): 77-101.

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[Sauro 2011] Sauro J., 2011. *A practical guide to the system usability scale*. Denver: Create Space.

[Scognamiglio *et al.* 2009] Scognamiglio L., Tinti E., Michelini A., 2009. *Real-time determination of seismic moment tensor for the Italian region*. *Bull. Seism. Soc. Am.* 99, 2223–2242.

6 Annex: Documentation

- DARE platform
 - API documentation <https://project-dare.gitlab.io/dare-platform/api/>
 - Platform installation/deployment <https://project-dare.gitlab.io/dare-platform/installation/>
 - Jupyter Lab <https://jupyter.dare.scai.fraunhofer.de>
 - Provenance viewer <https://platform.dare.scai.fraunhofer.de/sprovflow-viewer/html/view.jsp>
- RA test case

- Jupyter Notebook for RA test case
https://gitlab.com/project-dare/dare-examples/-/blob/master/wp6/WP6_RA.ipynb
- dispel4py sub-workflows composing the test case
https://gitlab.com/project-dare/WP6_EPOS/-/tree/RA_total_script/processing_elements/Download_Specfem3d_Misfit_RA
- SPECFEM3D docker and CWL workflow
<https://gitlab.com/project-dare/dare-platform/-/tree/master/containers/exec-context-specfem3d>
<https://gitlab.com/project-dare/dare-platform/-/tree/master/containers/specfem3d>
https://gitlab.com/project-dare/WP6_EPOS/-/tree/RA_total_script/specfem3d/specfem3d_test_input_cwl
- MT3D test case
- Jupyter Notebook for MT3D test case
https://gitlab.com/project-dare/dare-examples/-/blob/master/wp6/WP6_MT3D.ipynb
- dispel4py sub-workflows composing the test case
https://gitlab.com/project-dare/WP6_EPOS/-/tree/RA_total_script/processing_elements/MT-3D/workflow
(SPECFEM3D docker and CWL workflow are the same as the RA test case above).
- VC test case
- Jupyter Notebook for VC test case
https://gitlab.com/project-dare/dare-examples/-/blob/master/volcanology/admin/dare_volcanology.ipynb
- dispel4py sub-workflows composing the test case
https://gitlab.com/project-dare/wp6_volcanology/
- FALL3Dpy docker and CWL workflow
<https://gitlab.com/project-dare/dare-platform/-/tree/master/containers/exec-context-FALL3DPy>
- Tutorial documentation
- <https://gitlab.com/project-dare/dare-examples/-/tree/master/tutorial>
- <https://gitlab.com/project-dare/dare-examples/-/tree/master/volcanology>
- video <http://project-dare.eu/2020/12/11/dare-participated-eosc-expo2020/>