D-NA2.3.2: Training applications: updated selection and documentation with best practice guides

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1	E. Casarotti (INGV)	30/03/2014	Initial draft for comments
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3	E. Casarotti (INGV)	07/04/2014	2nd version with Igel's comments taken into account

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Executive Summary

The main objectives of WP2/NA2 are: (1) select existing pilot data-intensive applications and design sound use case scenarios; (2) analyze and define a use case implementation strategy during the project with WP8, WP7 and WP9; (3) support and evaluate the "productising" transition of the methods and their implementation performed by WP8; (4) support and evaluate the deployment and the efficiency of the pilot applications and their use case scenarios on the VERCE platform; (5) define in collaboration with NA3 documentation and tailored training session material; (6) provide requirements and support to WP7 and WP9 for tailored interfaces of the scientific gateways targeted to the developers and the users. VERCE's primary objective consists of "enabling" existing data- and HPC-intensive software applications through the development of processing elements (PEs) within dedicated workflows. It follows that the applications to be enabled or under enablement are all well developed and already have their own line of development. This also implies that they have already chosen their dissemination strategies through tutorials, web portals, etc.

During this RP and according to the activities and deliverables provided in the DoW, NA2 continued the validation and evaluation of the enabled applications deployment and use cases reported in the D-NA2.1. The activities involved interactions with WP7/SA3 in the realisation of the VERCE gateway front-end, in particular seismolgists provided guidelines, suggestions, beta testing efforts and models/meshes to implement the current stage of the forward simulation portal. Technical details of the portal are in SA3 reporting deliverable.

1 Introduction

During the review and the Steering Committee, SC, meetings both held in Paris in April and July, respectively, it was decided to give precedence to the HPC compute-intensive use case to the goal of providing by March 2014 a working and ready-to-be-tested beta-version. This use case entails the development of waveform simulation of earthquake events and, as describe in deliverable D-SA3.3.1, the VERCE Science Gateway reached its *beta* release. In the reporting period object of this document, NA2 has interacted closely with WP7/SA3 in the realisation of the VERCE gateway front-end. In the following sections, we present the summary of these activities where NA2 provided seismological feedback from the user community perspective. In this document, we provide a detail description of velocity model/mesh requirements.

2 Forward Modeling VERCE Gateway

During this reporting term, NA2 continued to provided feedback to SA3 shaping the user experience of the Forward Modelling GUI. We expect that the main end-users of VERCE gateway will be geoscientists and we suggest a beta release that exposes the waveform computation as a service for the needs of the seismological community.

Briefly, the VERCE Forward Modelling GUI is composed of two sections: an interactive map integrating geological overlayers and a tabbed windows for the definition of the workflow parameters and the submission of the simulation. As initially defined in the previous reporting period, users can (i) select the solver (from a list of available codes already deployed within the VERCE computational resources), (ii) specify the input parameters, (iii) include the mesh that they wish to adopt for the simulations, (iv) identify seismic stations and earthquakes for simulation.

Feedbacks from computational seismologists show that the GUI represents a critical improvement of the current process of preparing the forward simulation and, even if in a beta stage, it has been implemented effectively.

In order to achieve a ready-to-be-tested beta-version of the portal, during the previous reporting period, NA2 suggested (i) to focus on SPECFEM3D, (ii) to expand the library of tomographic models and meshes, (iii) to allow the submission of models and meshes by users, (iv) to design a more flexible workflow submission control.

All the requested features have been implement. We refers to SA3.3.1 deliverable for technical details and figures. In the following section, we provide guidelines for the models and meshes requirement.

3 Tomographic Models and Meshes

The portal provides access to the full features of SPECFEM3D including the possibility to simulate point- or finite-source on unlimited number of receivers recording the full 3D wavefield in terms of displacement, velocity and acceleration. Movie,snapshot, shakemaps and kernel could be also recovered. The beta-version of Forward Simulation VERCE portal provides a small library of tomographic models/meshes and the possibility for the user to collaborate to expand this library submitting his case, so virtually it is possible to simulate seismic signals in any model described as unstructured hexahedral mesh in SPECFEM3D format (see the manual https://github.com/geodynamics/specfem3d/tree/master/doc/USER_MANUAL for more information).)

3.1 Library of Tomographics Model and Meshes

The meshing process is a crucial step for any simulation and any solver. Meshing a geological volume based upon hexadral elements is often difficult, tedious and art-crafting task. Nevertheless, the accuracy of this process is critical for a accurate result in the seismigrams.

The aim of the Model and Mesh Library is to keep all of the complexity of model creation away from the users responsibilities, in order to decrease the initial steep learning process of meshing.

NA2 provided 3 real case examples: (i) central Italy (small, 200K+ elements), (ii) sourthern Italy (medium, 1M+ elements), (iii) northern Italy (large, 3M+ elements). The tomographic model has been published by Di Stefano et al. 2009[1].

The mesh have been selected to provide a variety of performance, ranging from a small example, that can be executed on 64 cores, to a larger one, that we suggest to run on more than 400 cores.

Each case is distributed with information about the geographical limits of the mesh and the adopted coordinate system. Furthermore, NA2 has tested each mesh and selected an optimal set of parameter, in particular the simulation time step has been carefully chosen to avoid numerical instabilities and possible errors in the job submission.

Using the library, the user can quickly focus on seismograms, play with the tools of the VERCE portal and provide useful feedback in the occuring beta-testing period. The obtained seismogram could have numerical and geophysical significance for seismic wave periods down to 2 seconds (i.e., $T \geq 2$ s).

3.2 User Submission of Tomographics Model and Meshes

As shown in SA3.3.1 deliverable, from the *Solver* tab of the Forward Modeling GUI, users can now submit new meshes and velocity models which will be evaluated and "sanity checked" by the *Verce-application-manager*. NA2 acts as *Verce-application-manager* in this project, waiting for automatic tools to validate the meshes. User should provide an optimal set of parameters and geographical information as the system coordinate.

After NA2's approval the new mesh and model metadata will be included into the mesh database, and the actual files deployed within the target infrastructure. The contribution of the users is crucial in the expansion of the library. A large collection of models/meshes is a valuable features of the VERCE portal both for beginners and for experienced users.

The evalution of the first submitted model is ongoing. It is a large example from Chile. Furthermore, an interesting opportunity is currently scrutinized as first industrial example. Specifically, an induced seismicity young scientist asked to be part of the beta-testing with a model that requires exclusive usage by the user. The potential interest in this kind of problem leads NA2 and SA3 to explore the possibility to provide him exclusivity and support in the creation of the model/mesh, even if this kind of usage was not initially planned neither encouraged.

4 Authentication and security

The process of authentication has been enormously simplified during the reporting period. Nevertheless, the possibiliy to access at EGI and PRACE resources via the VERCE Virtual Organisations requires special care at security level. We are offering through the VERCE Science Gateway the possibility to

[1] Di Stefano, R., E. Kissling, C. Chiarabba, A. Amato, and D. Giardini (2009), Shallow subduction beneath Italy: Three-dimensional images of the Adriatic-European-Tyrrhenian lithosphere system based on high-quality P wave arrival times, J. Geophys. Res., 114, B05305, doi:10.1029/2008JB005641.

produce and upload users proxy certificates interactively. NA2 hightlights the complexity of the system that could lead to early abandon of users. Now, VERCE is providing user documentation, which will be available via the portal pages. Moreover, Videos and Demos of the tools are available on the home page, for immediate access. Nevertheless, last tests on the portal demonstrated that this process is still a difficult step for beginners, even due to minor annoyances like incompatibilities of the process to early version of JAVA and modern internet browsers.

5 Conclusions and Future Work

During the last year of developments of the VERCE Science Gateway NA2 and SA3 matured a deep collaboration, implementing in the Foward Simulations Portal the requested features during last period. If technical aspects have been address by SA3, NA2 provided fundamental seismological points of view and tests.

The upcoming period will be definitely focused on improving the current services on the basis of the collected feedbacks. NA2 can consider two phases: 1) automatizing the meshing check in order to provide the user with a simpler and quicker automatic submission, 2) improving the visualizisation of synthetics, 3) collecting the feedbacks from seismological community in order to improve the forward modeling portal, 4) adding multiple features likes Shakemovies creation and visualization, 5) creating the workflow for comparison of data and synthetics, leading the path to the inverse problem use case. Last point will benefit from the developments for the data-intensive use case, that will be included in the upcoming period.