



D6.5 Database of Earth Models

Version 1.0

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Change Log

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V0.2	First draft submitted for revision
V0.3	Second draft addressing the reviewer's comments and incorporating additional information and figures.
V0.4	Final version validated by reviewer.
V1.0	Document formatted for submission

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1. Executive Summary

The Pillar III earthquakes workflow, Urgent Computing Integrated Services for Earthquakes (UCIS4EQ), requires reliable Earth models for the forward modelling of ground motions. In this deliverable we present part of the work completed within Task 6.3 with focus on improving the underlying Earth models used for the UCIS4EQ simulations. The second generation Collaborative Seismic Earth Model (CSEM) – a multiscale global tomographic Earth model that incorporates a range of local-, regional- and global-scale updates – has been integrated into the UCIS4EQ workflow over the course of eFlows4HPC and serves as a starting point of the inversions, with the presented models developed as small-scale CSEM refinements. Those refinements aim to progressively adapt the CSEM model database to regional applications for seismic hazard studies in areas of interest. Such model improvements translate into the accuracy of the subsequent wave propagation simulations.

2. Introduction

The Pillar III earthquakes workflow, Urgent Computing Integrated Services for Earthquakes (UCIS4EQ), is a set of containerised micro-services that each tackle a different task, with interactions between those tasks orchestrated by PyCOMPSs, a workflow manager from the eFlows4HPC software stack. As new earthquakes with high-impact potential are recorded, their source characteristics are approximated and the corresponding wave propagation simulations are performed. The resulting synthetic shake maps for the affected areas are computed and uploaded automatically to B2DROP. UCIS4EQ has the potential to contribute to more accurate rapid-response predictions of the consequences of significant earthquakes and thus complement rapid analyses of the resulting ground motions and their impact. Simulations, however, are sensitive to model inputs – UCIS4EQ can only provide relevant information when the underlying physical models are sufficiently accurate.

In particular, as part of the work completed in Task 6.3 summarised in this deliverable, we have focused on working towards improving the Earth models used for the UCIS4EQ simulations. Constraining the 3D structure in the regions of interest is non-trivial, with the resulting model highly dependent on the quality and distribution of seismic data, as well as on the inversion method. As entire waveforms generated by UCIS4EQ are of interest to estimate the ground shaking parameters, we deem full-waveform inversion (FWI) – a method that inverts for the complete waveform – and the resulting models the most appropriate for our purpose. The methods and tools are briefly presented in Section 3.

The regional models are implemented as updates to the Collaborative Seismic Earth Model (CSEM), a state-of-the-art multiscale framework that supports evolutionary inversion of seismological data. As CSEM provides global coverage, an FWI model can be extracted for an arbitrary area and interpolated onto any mesh, lending itself perfectly to fully automated applications. The resolution, however, varies significantly across the globe, and thus affects the synthetic UCIS4EQ outputs. The multiscale approach also requires the treatment of all local sub-models on a global scale in order to ensure coherence and a good waveform fit globally, as described in Section 4.

CSEM model extraction was incorporated into the UCIS4EQ workflow in earlier stages of the eFlows4HPC project, with the subsequent regional refinements described in Section 5 offering greater resolution for selected test areas that serve as a UCIS4EQ testbed of FWI models for high-frequency simulations. In the long term, a full adaptation of the CSEM as a model database for area-independent synthetic seismic hazard studies would require further refinements, with an automation of some longer-wavelength updates envisaged in the DT-GEO project.

3. The FWI Methodology

Seismic full-waveform inversion is a PDE-constrained optimization problem, where the PDE (Partial Differential Equation) is a wave equation. As the process is iterative, multiple solutions of the wave equation ("forward problems") are required, with the cost of each solution growing with increasing domain size and decreasing model periods. In our case, the forward solutions are computed with Salvus, which is also the forward solver used for the solutions in UCIS4EQ. This ensures coherence required for best results, as the models are constrained for best waveform fit of synthetics of a given solver; they cannot be considered solver-agnostic unless very careful calibration of the modelling parameters between the solvers is performed.

In the following subsections we briefly describe the set of tools used for the presented global and local refinements of the CSEM, namely: *Inversionson* (Thrustarson et al., 2021; <https://github.com/solvithratar/Inversionson>), a tool that automates seismic FWI and minimises human and computational time, *Optson* (<https://swp.ethz.gitlab.io/optson/>), a tool that implements optimisation algorithms, and *Salvus* (Afanasiev et al., 2019; <https://mondaic.com/>), the wave equation solver.

3.1. Automation of FWI: *Inversionson*

Inversionson manages the seismic FWI process and automates all FWI steps, such as the computation of synthetics for all events, the windowing of the synthetics using the initial model, the computation of misfits, and the computation and smoothing of gradients. The package creates, submits, and monitors Salvus HPC jobs, and downloads results for updating the model on the local machine. Nonetheless, the automatic process needs to be monitored carefully to identify potential issues that require manual adjustments of inversion settings.

The package also incorporates the additional complexities of dynamic mini-batches (van Herwaarden et al., 2020), where the model gradient is approximated for each iteration with a carefully selected subset of events, as well as of wavefield-adapted event-specific meshes (Thrustarson et al., 2020). Both approaches significantly lower the computational cost of the FWI process without compromising the accuracy of the final model, with the mini-batches reducing the number of considered events per iteration, and the wavefield-adaptive meshes reducing the number of computational elements for a given simulation. Such reductions in computational costs allow reduction of the minimum period of the generated models relative to standard FWI provided that the data quality and the coverage are sufficient.

3.2. Optimisation algorithms: *Optson*

Originally, as described by Thrastarson et al. (2021), optimization routines were directly integrated in the Inversion workflow. They have recently been isolated into a separate python package, Optson, that manages the computation of misfits or gradients for a given model. Optson provides the flexibility of implementing new optimisation algorithms and is field agnostic, as it can be applied to any kind of optimization problem. With this abstraction from the specificities of seismic FWI, we increase software maintainability. Large monolithic codes are more difficult to manage, while with Optson it is easier to ensure the correctness of the optimization routines.

Optson supports the following optimisation algorithms: ADAM, limited memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS), stochastic L-BFGS, steepest descent, and stochastic gradient descent (SGD).

3.3. Forward modelling: *Salvus*

Salvus (mondaic.com) is a high-performance software suite boosting the efficiency, scalability, and applicability of full-waveform modelling and inversion (FWI) through a modern and finely-tuned design based on spectral elements. Tailored to meet the challenges of modern FWI on both CPU and GPU architectures, Salvus solves multi-physics full-waveform forward and inverse problems in 2 and 3 dimensions, and fuses the flexibility of research codes with the performance of production-grade software. Custom unstructured mesh generation algorithms tailored for geophysical applications enable the simple and efficient incorporation of real-Earth topography, and fluid ocean layers with bathymetry can be included where appropriate.

In our work, mesh construction and wave propagation simulations are performed with Salvus while the inversion aspects are managed by the open-source packages described above in order to keep open the exploration of different research avenues.

4. The 2nd generation Collaborative Seismic Earth Model (CSEM)

The Collaborative Seismic Earth Model (CSEM) is a state-of-the-art multiscale global tomographic Earth model that evolves continuously via successive local-, regional- and global-scale updates. The second generation of the CSEM (Noe et al., in preparation) builds on its predecessor (Fichtner et al., 2018) as a starting model, incorporating recent regional and global refinements as well as providing a new set of tools for model processing and extraction. Across all regional updates, the second generation CSEM has been built using three-component waveform data from 1,845 events and 797,030 unique source-receiver pairs. The model resolution varies significantly across the globe, with scales ranging from hundreds of kilometres to entire continents.

To ensure coherence of the local and regional refinements, and to cover regions that have not been incorporated in the local- and regional-scale database of Earth models, a global long-period FWI is performed over multiple period bands to a minimum period of 50 seconds. Such global inversion consolidates the multiscale approach, bringing the regional and local models together by smoothing over regional boundaries.

As the CSEM is a composite of regional and global models, it can predict seismic waveforms globally for long-periods while it is possible to “zoom” into specific regions where the model explains wave propagation of shorter periods. Given that the global inversion ensures consistency, an FWI model can be extracted for an arbitrary area and interpolated onto any mesh, lending itself perfectly to a fully automated UCIS4EQ application. The CSEM, together with the corresponding software package CSEMlib that supports model treatment and extraction, has been integrated into UCIS4EQ over the course of the eFlows4HPC project and forms a basis for the database of Earth models for urgent simulations. A CSEM model can be extracted and interpolated over an arbitrary Salvus mesh in an automatic manner, either on the fly or for a static (existing) mesh, ensuring that UCIS4EQ can perform simulations on any desired region. It should be reiterated, however, that model resolution varies across the globe, rendering forward simulations of varying accuracy.

In this deliverable, we outline our preliminary work to adapt the CSEM to regional applications for seismic hazard studies. We are working towards regional refinements that extend the CSEM database, offering greater resolution for selected test areas. The models will both test the limits of FWI in terms of resolution in the context of possible automation of the generation of local models, and will serve as a UCIS4EQ testbed for high-frequency simulations. Further work towards the automation of regional FWI updates of the CSEM, both in the context of numerical wave propagation and beyond, will take place in the ongoing DT-GEO project.

In the two subsections below, we briefly discuss how both the global FWI step and the local model updates are performed.

4.1. Global inversion

As shown by Ajala & Persaud (2022), directly including densely sampled values within a coarser model does not always lead to an improved waveform fit for high frequencies over the entire domain. Thus, global FWI over all CSEM updates ensures the coherence of all models, injecting meaningful information on the edges of refinements and in-between them. This step is crucial, as erroneous regional tapering would lead to artefacts in simulated wavefields. The CSEM multiscale approach considers both regional and global results in a consistent final product that can reliably be used for numerical wave propagation for purposes such as UCIS4EQ.

The dataset for the global inversion comprises publicly available seismic data of 2,025 events between magnitudes 5.9 and 6.9 from Federation of Digital Seismograph Networks services, resulting in over 5.8 million unique source-receiver pairs. The considered period band has been progressively decreased over the course of the inversion, starting at 120-200s and ending at 50s-160s, resulting in a global model with a minimum period of 50s.

4.2. Local model integration

For the assimilation of the local models into a global one we follow the methodology presented in the first generation CSEM study (Fichtner et al., 2018). The desired pure Bayesian approach needed simplifications due to the infeasible prerequisite of high-dimensional densely sampled model spaces. The study demonstrated that the assumption of Gaussian model errors enables the maximum-likelihood model to be represented as the sum of successive regional refinements:

$$\mathbf{m}(\mathbf{x}) = \mathbf{m}_0(\mathbf{x}) + \text{sum}(\delta\hat{\mathbf{m}}_i(\mathbf{x}) \cdot \mathbf{T}_i(\mathbf{x})),$$

where \mathbf{m} is the final model in locations \mathbf{x} , \mathbf{m}_0 is the base model, $\hat{\delta\mathbf{m}}_i$ are the model updates from refinement i , the hat denotes an interpolation from the original parameterization onto \mathbf{x} , and the model-specific taper, \mathbf{T} , weighs the elements in the updates. Sufficiently wide cosine-tapers around the edges of the regional domains prevent abrupt artificial boundaries. Specific taper widths vary on a case-to-case basis.

When retrieving the CSEM for a specific area, the extraction searches the database of regional Earth models in a chronological order for models of geographical relevance. The extraction process onto any point cloud \mathbf{x} (representing the discretisation of the area) starts with the implementation of the base model onto the given points. Then the regional refinements from the database are sequentially interpolated. The entries in the list of regional CSEM refinements may have overlapping domains, as they are defined as updates with respect to the previous version of the CSEM. The final update stemming from the global inversions rounds off the model.

5. Regional updates

In this section we present the regional updates that will be integrated as CSEM refinements in the CSEM database of Earth models. These refinements are aimed specifically at regional applications for seismic hazard studies in the context of UCIS4EQ, offering higher resolution for selected test areas, but they will be integrated into the global CSEM for general use. It should be noted that we do not expect the local FWI models to reach the few-hertz-resolution of forward simulations of ground motions, but instead reach a highest resolution on the order of seconds or tens of seconds due to limitations on data availability and quality, among other considerations.

For each regional model, we invert for vertical P-wave velocity (V_{PV}), horizontal P-wave velocity (V_{PH}), vertical S-wave velocity (V_{SV}), horizontal S-wave velocity (V_{SH}), and density (ρ). The quality factor for bulk and shear modulus, and eta, are modelled but not inverted for. As data quality and availability, as well as coverage, vary between the areas, certain local models are easier to constrain than others and thus the choice of the period bands varies to ensure convergence.

In the following subsections, we present general information on the inversion settings, objective function plots for the validation dataset, as well as a representative section of the original CSEM V_{SH} model and a resulting V_{SH} model for each period band. The objective function is a measure of the difference between measured data and simulations on the FWI Earth model; during the inversion we use the training dataset, where the objective function should always decrease with iterations. Here the objective function is plotted for the validation dataset (that is, for events not seen by the inversion) which is used to confirm that the model is not overfitting the data used. Unlike for the training dataset, the objective function for the validation dataset does not necessarily always decrease with each iteration, but it should follow a decreasing trend.

The presented models are work in progress, with the aim of carefully lowering the shortest period considered in order to increase the resolution progressively and reliably, without introducing artefacts in the models. Therefore, the models have not yet been integrated back into CSEM, as only the final period band will contribute to the global model.

5.1. The Mediterranean

The Mediterranean region is one of the best-resolved regions in the CSEM, with the lowest period down to 8 seconds in the small subregion comprising Western Turkey and the Marmara sea (Çubuk-Sabuncu et al., 2017). The region therefore serves as the main testing area for UCIS4EQ. Given good data coverage, high data quality, and a significant seismic risk, we choose to focus on refining the model for this region further. Our methodologies have significantly improved since the 2017 study, reducing computational costs, allowing us to use the available data more effectively and thus to spatially extend the region of high resolution coverage.

Table 1 provides a summary of the inversion. Figure 1 shows the current CSEM model for the region. Figures 2, 4, and 6 show the misfit reduction for the independent validation dataset in each iteration for the period bands of 50-100s, 35-100s, and 25-50s, respectively. Figures 3, 5 and 7 show the updated model at 50 km for 50s, 35s and 25s minimum period.

Table 1. Summary of The Mediterranean inversion.

The Mediterranean: general information	
Latitude range (min-max)	20°N - 60°N
Longitude range (min-max)	0°E - 60°E
Maximum depth	2000km
Performed period bands	50s - 100s, 35s -100s, 25s - 50s
Planned period bands	20s - 50s, 15s - 45s, 12s - 40s, 10s - 30s, 8s - 30s, 5s - 30s
The Mediterranean: 50s inversion	
Number of iterations	27
Misfit reduction: inversion	28%
Misfit reduction: validation	47%
Model size	414.5 MB
Event magnitude range (min-max)	5.6 - 6.8
Number of events	66
Number of validation events	15
Size of dataset	32 GB
The Mediterranean: 35s inversion	

Number of iterations	19
Misfit reduction: inversion	7%
Misfit reduction: validation	8%
Model size	414.5 MB
Event magnitude range (min-max)	5.5 - 6.8
Number of events	87
Number of validation events	15
Size of dataset	44 GB
The Mediterranean: 25s inversion	
Number of iterations	25
Misfit reduction: inversion	+8%
Misfit reduction: validation	25%
Model size	2.6 GB
Event magnitude range (min-max)	5.4 - 6.8
Number of events	107
Number of validation events	15
Size of dataset	53 GB

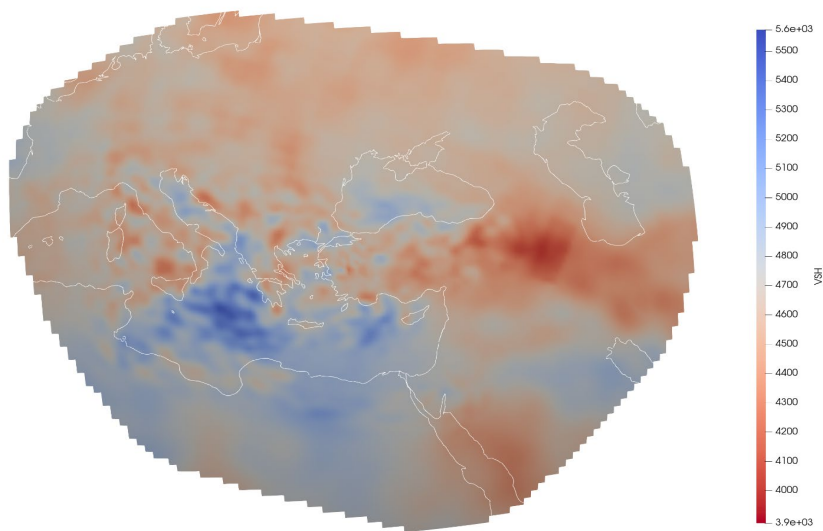


Figure 1. VSH slice of the Mediterranean region in the CSEM at 50 km depth. Inversion results from this deliverable will be used to improve this model region.

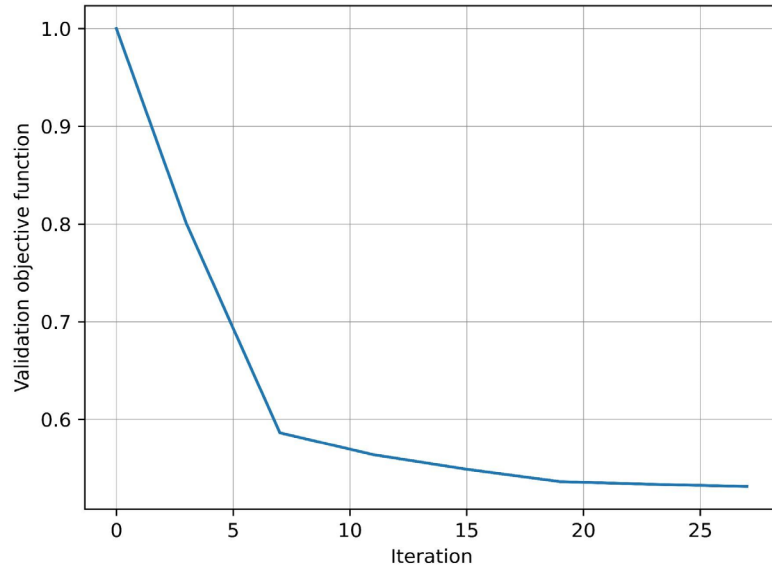


Figure 2. Objective function for the Mediterranean for the validation dataset at 50 seconds minimum period.

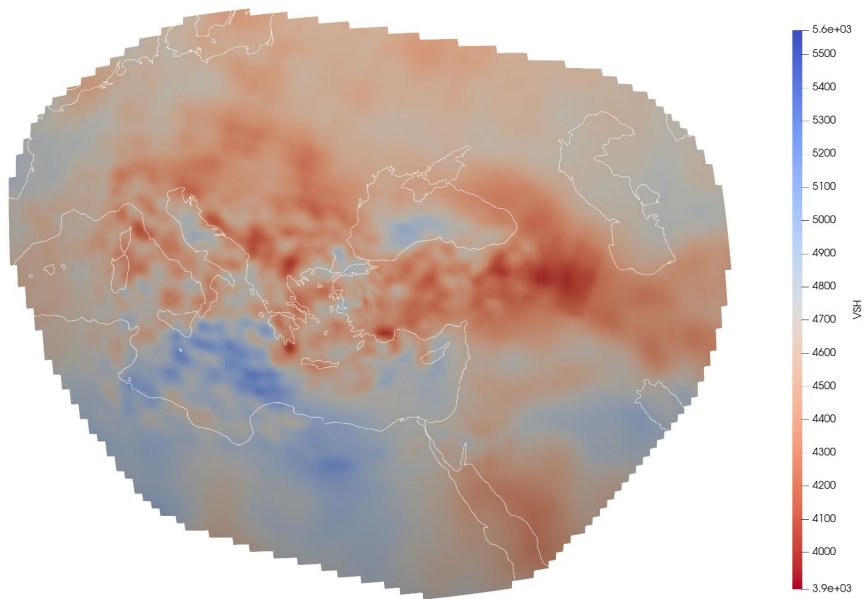


Figure 3. VSH slice of the Mediterranean model at 50 km depth at 50 seconds minimum period.

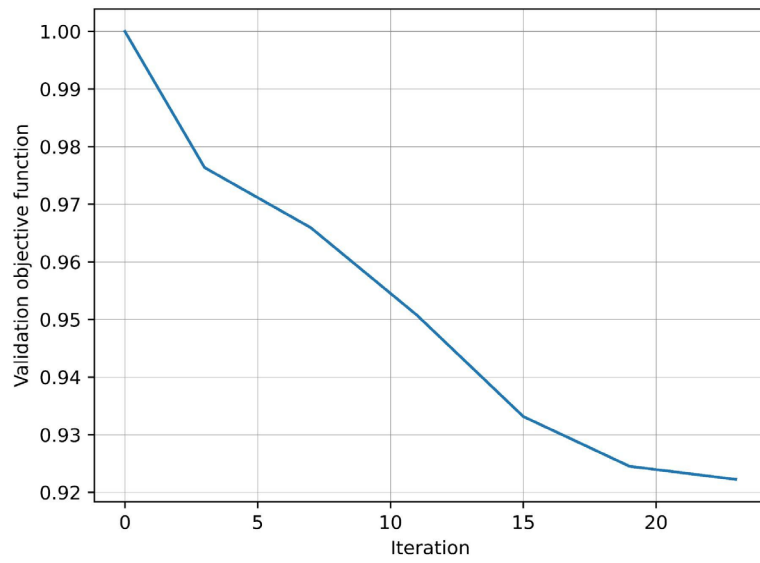


Figure 4. Objective function for the Mediterranean for the validation dataset at 35 seconds minimum period.

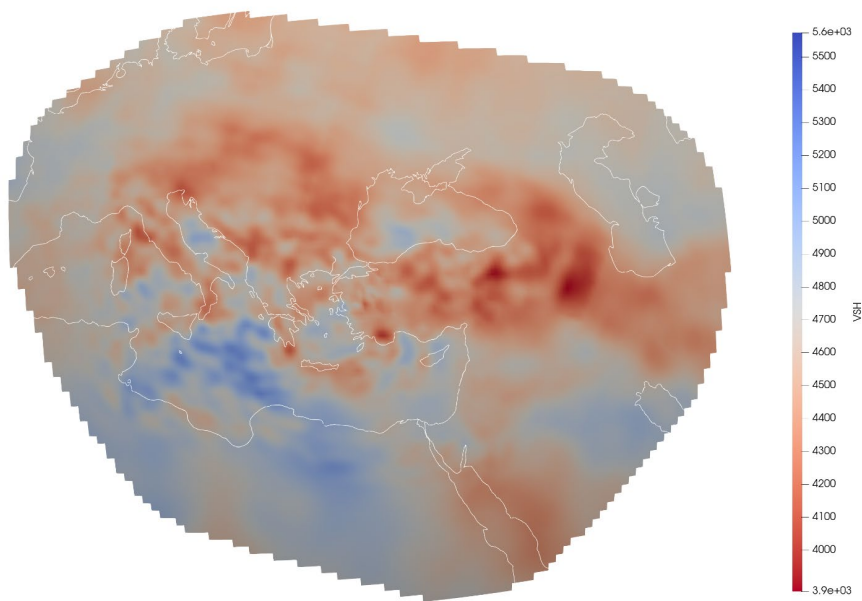


Figure 5. VSH slice of the Mediterranean model at 50 km depth at 35 seconds minimum period.

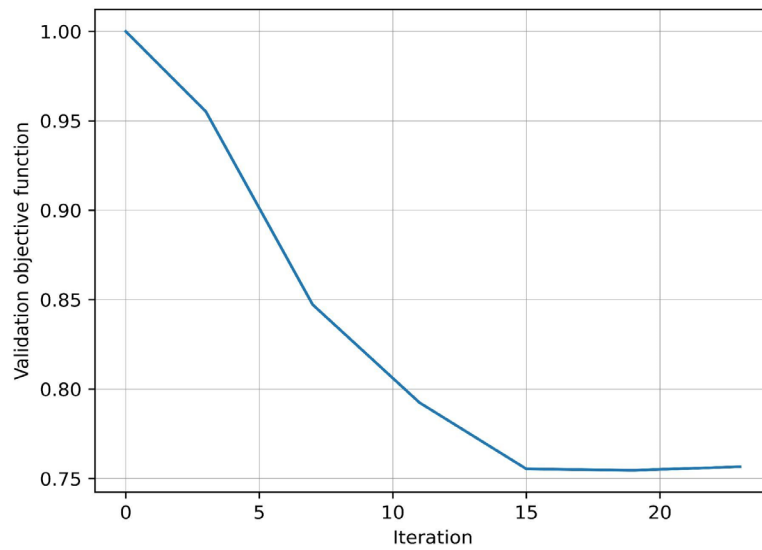


Figure 6. Objective function for the Mediterranean for the validation dataset at 25 seconds minimum period.

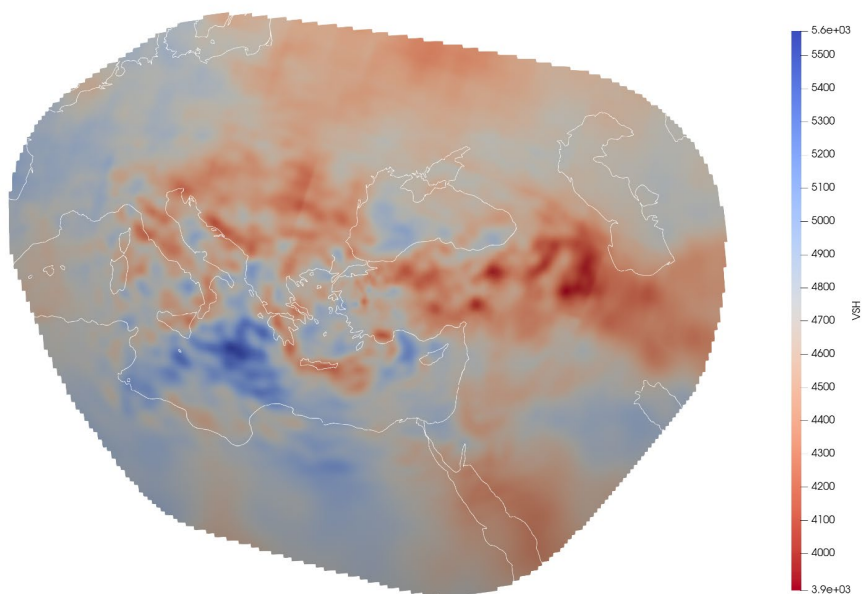


Figure 7. VSH slice of the Mediterranean model at 50 km depth at 25 seconds minimum period.

5.2. Iceland

Unlike other European areas, Iceland has no regional refinements in the CSEM and thus no pronounced heterogeneities. We choose it as a study area to test the new methodologies on the small scale, as the source-receiver distribution in the region makes the inversion particularly challenging.

Table 2 provides a summary of the inversion. Figure 8 shows the current CSEM model for the region. Figures 9 and 11 show the misfit reduction for the independent validation dataset in each iteration for the period bands of 30-70s and 25-70s, respectively. Figure 15 shows the model at 50 km for 30s minimum period, while Figure 17 for the 25s.

Table 2. Summary of the Iceland inversion.

Iceland: general information	
Latitude range (min-max)	52°N - 78°N
Longitude range (min-max)	6°W - 30°W
Maximum depth	570 km
Performed period bands	30 - 70s, 25 - 70s
Planned period bands	22 - 70s, 15 - 50s
Iceland: 30s inversion	
Number of iterations	14
Misfit reduction: inversion	37%
Misfit reduction: validation	6%
Model size	163 MB
Event magnitude range (min-max)	4.6 - 6.2
Number of events	153
Number of validation events	30
Size of dataset	7.3 GB
Iceland: 25s inversion	
Number of iterations	25
Misfit reduction: inversion	35%
Misfit reduction: validation	4%
Model size	281 MB
Number of events	153
Number of validation events	30
Size of dataset	7.3 GB

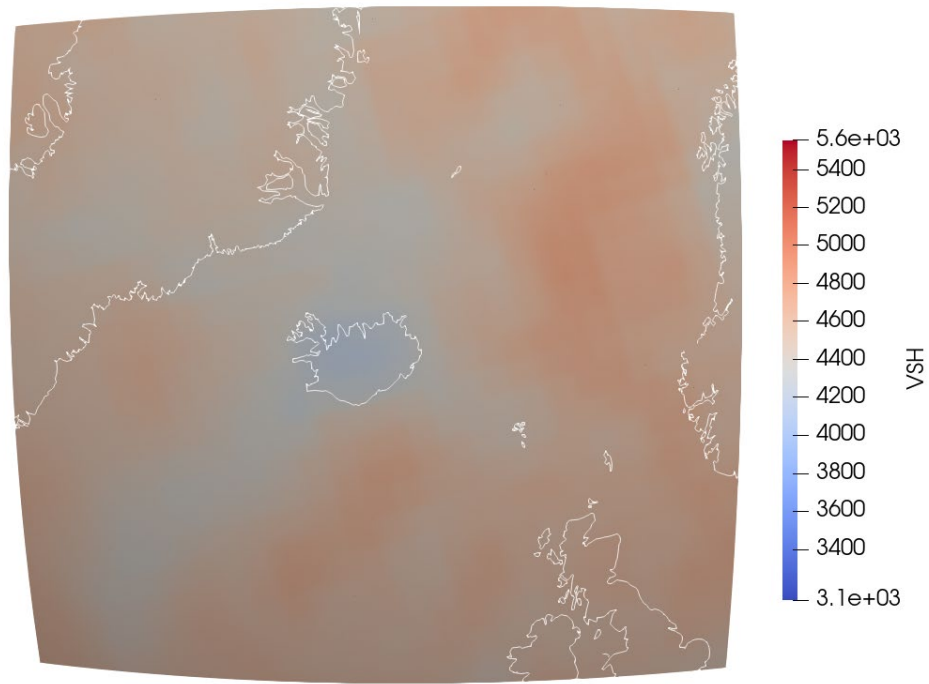


Figure 8. VSH slice of the Iceland region in the CSEM at 50 km depth. Inversion results from this deliverable will be used to improve this model region.

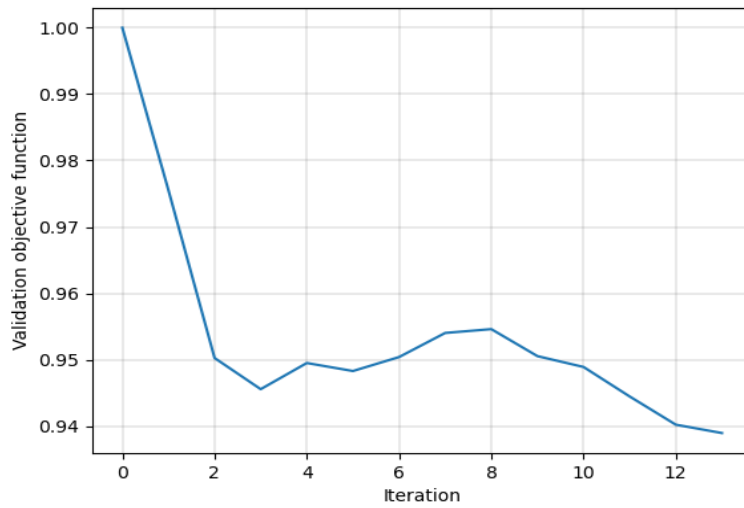


Figure 9. Objective function for Iceland for the validation dataset at 30 seconds minimum period.

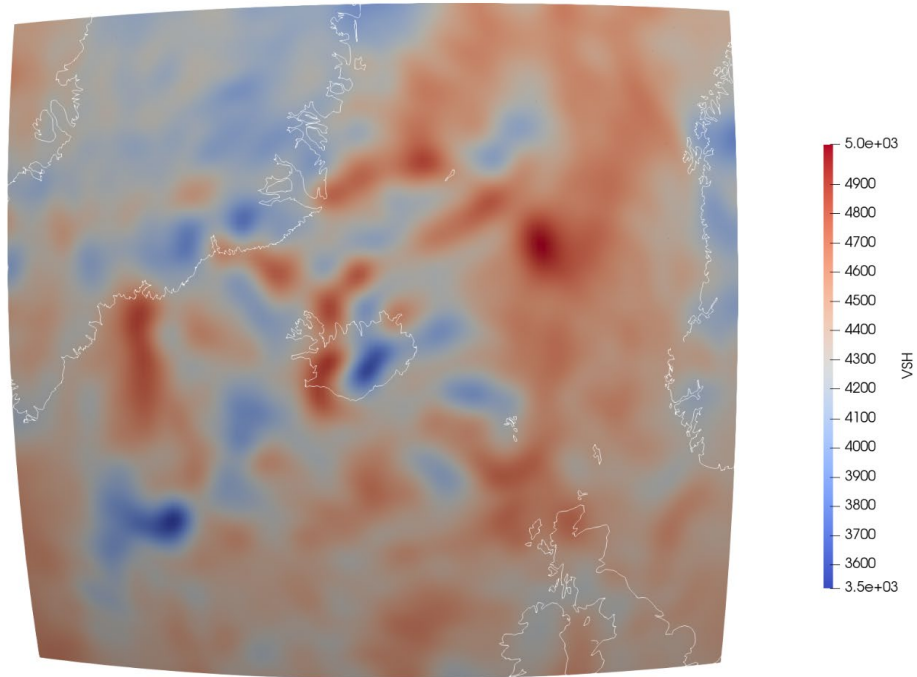


Figure 10. VSH slice of the Iceland model at 50 km depth at 30 seconds minimum period.

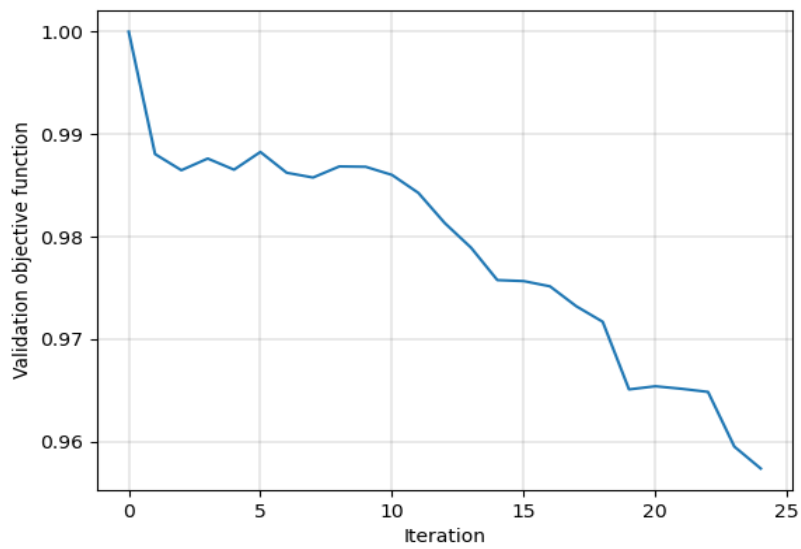


Figure 11. Objective function for Iceland for the validation dataset at 25 seconds minimum period.

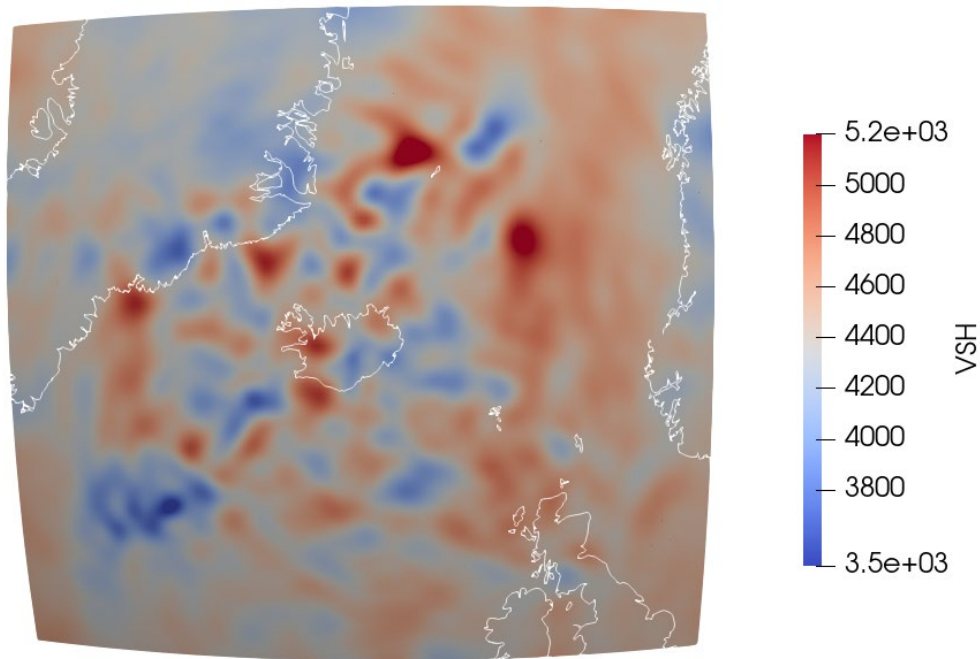


Figure 12. VSH slice of the Iceland model at 50 km depth at 25 seconds minimum period.

5.3. Chile

The high seismic risk in the area makes Chile a region of interest for UCIS4EQ studies. The Northern part of the continent is well-resolved in the CSEM, while the Southern part requires further work. Incorporating a new study into the CSEM will preserve the high resolution in the north and add structural heterogeneities in the south.

Table 3 provides a summary of the inversion. Figure 13 shows the current CSEM model for the region. Figures 14 and 16 show the misfit reduction for the independent validation dataset in each iteration for the period bands of 35-70s and 25-70s, respectively. Figure 15 shows the model at 50 km for 35s minimum period, with Figure 17 for the 25s.

Table 3. Summary of the Chile inversion.

Chile: general information	
Latitude range (min-max)	18°S - 54°S
Longitude range (min-max)	60°W - 80°W
Maximum depth	770 km
Performed period bands	35 - 70s, 25 - 70s

Planned period bands	20 - 50s
Chile: 35s inversion	
Number of iterations	26
Misfit reduction: inversion	17%
Misfit reduction: validation	12%
Model size	149 MB
Event magnitude range (min-max)	5.0 - 6.3
Number of events	111
Number of validation events	30
Size of dataset	2.5 GB
Chile: 25s inversion	
Number of iterations	28
Misfit reduction: inversion	30%
Misfit reduction: validation	13%
Model size	438 MB
Event magnitude range (min-max)	5.0 - 6.3
Number of events	111
Number of validation events	30
Size of dataset	2.5 GB

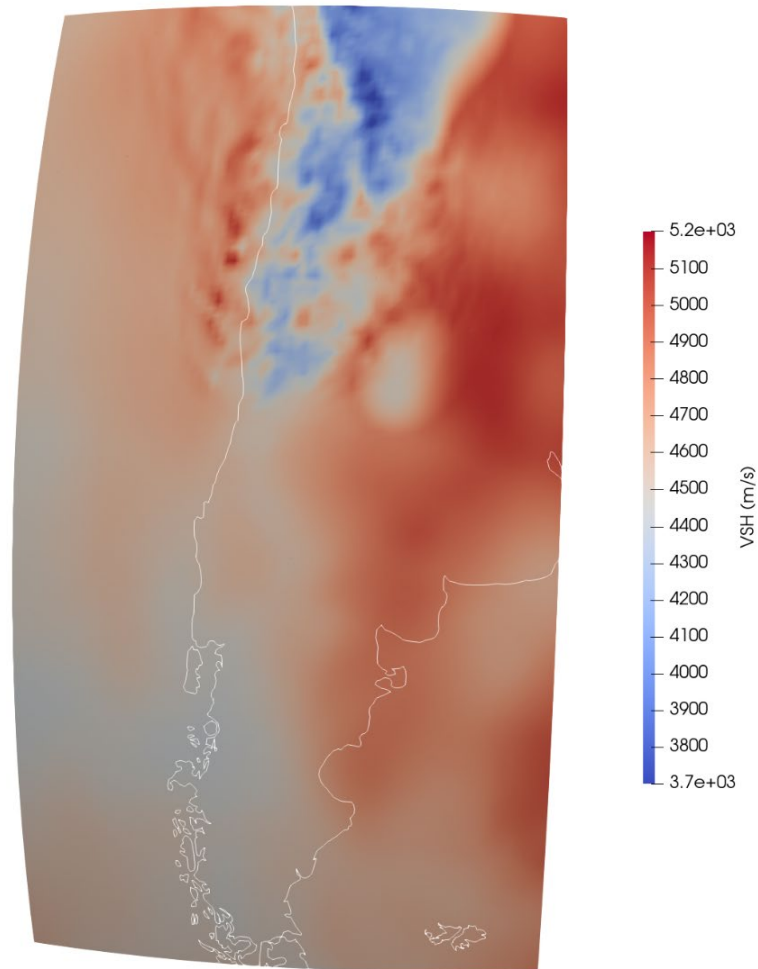


Figure 13. VSH slice of the Chile region in the CSEM at 50 km depth. Inversion results from this deliverable will be used to improve this model in the Southern part of the continent, while preserving the existing high-resolution information in the North.

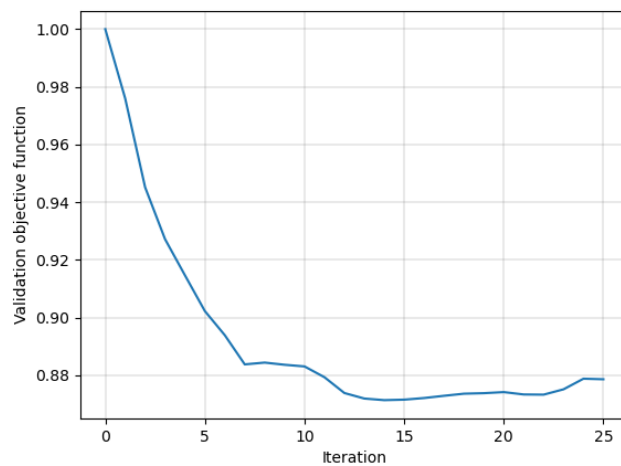


Figure 14. Objective function for Chile for the validation dataset at 35 seconds minimum period.

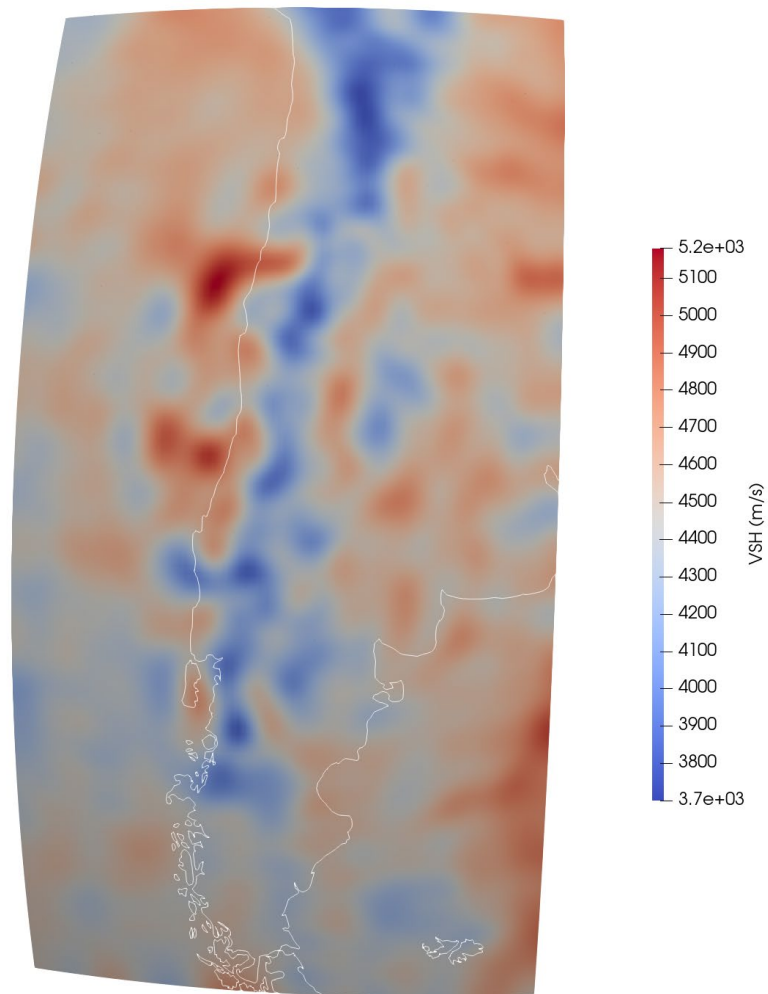


Figure 15. VSH slice of the Chile model at 50 km depth at 35 seconds minimum period.

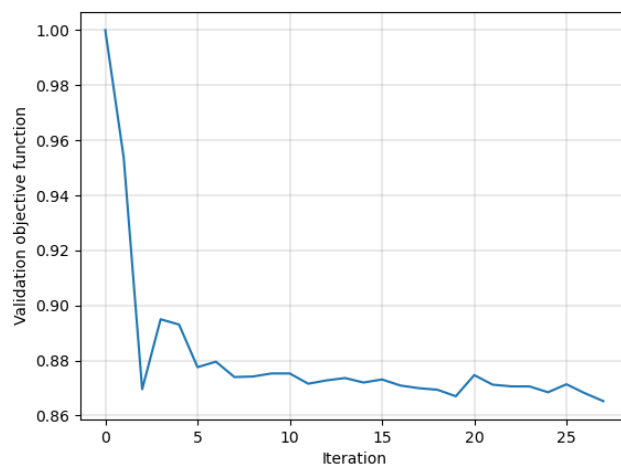


Figure 16. Objective function for Chile for the validation dataset at 25 seconds minimum period.

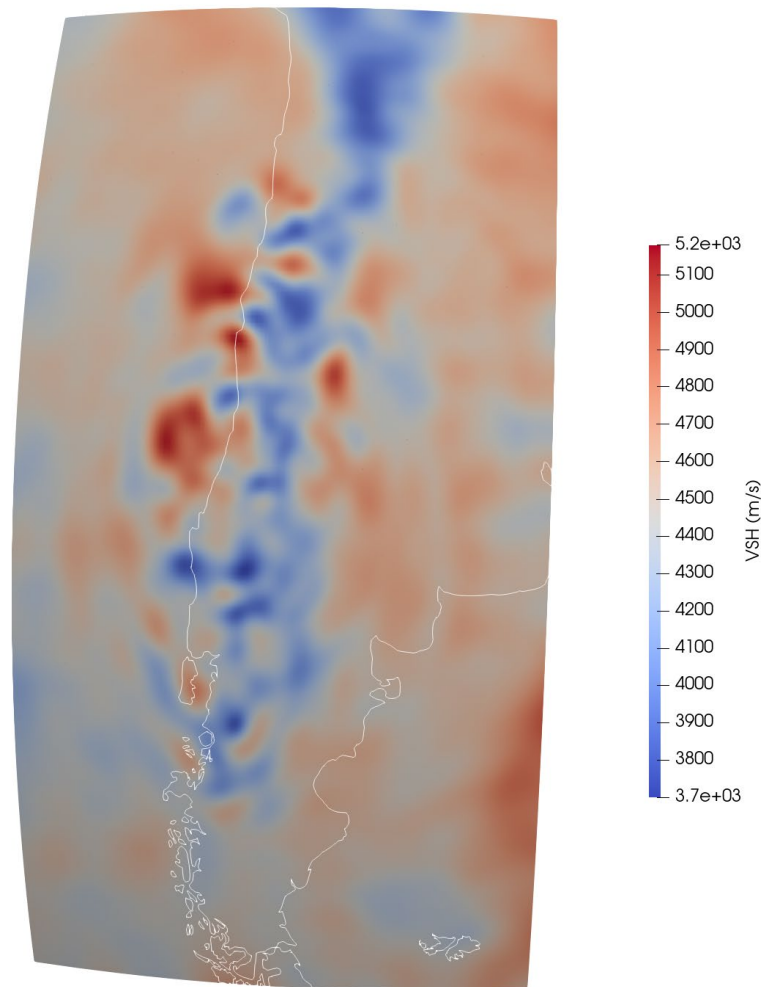


Figure 17. VSH slice of the Chile model at 50 km depth at 25 seconds minimum period.

6. Conclusion

This deliverable reports progress on part of the work completed within Task 6.3 with focus on improving the Earth models for the UCIS4EQ forward modelling of ground motions. The FWI tools, as well as the underlying model database – the second generation Collaborative Seismic Earth Model (CSEM) that incorporates a range of local-, regional- and global-scale updates – have been presented. The CSEM has been integrated into the UCIS4EQ workflow over the course of eFlows4HPC and is currently used for the simulations in an automated fashion. The CSEM also serves as a starting point of the regional inversions that have been performed during the eFlows4HPC project, with the presented models developed as small-scale CSEM refinements that adapt the CSEM model database to regional applications for seismic hazard studies. The inversions require careful treatment of data, with progressive introduction of short-period information to reliably increase model resolution without introducing artefacts. Certain areas are easier to constrain for short periods than others and the progress of the inversion (that is, the chosen period bands and the convergence) is region dependent, as data quality and availability, as well as coverage, varies. The presented models are therefore works in progress, with further period bands

planned for each area. It should be noted that we do not expect the local FWI models to reach the few-hertz-resolution of forward simulations of ground motions. Nonetheless, the improved model resolution translates into the accuracy of the subsequent wave propagation simulations and thus is an important step in improving the reliability of UCIS4EQ runs.

7. Acronyms and Abbreviations

<i>Term or abbreviation</i>	<i>Description</i>
HPC	High Performance Computing
UCIS4EQ	Urgent Computing Integrated Services for EarthQuakes
CSEM	Collaborative Seismic Earth Model
FWI	Full Waveform Inversion
PDE	partial differential equation
L-BFGS	limited memory Broyden-Fletcher-Goldfarb-Shanno
SGD	Stochastic gradient descent
V_{PV}	Vertical P-wave velocity
V_{PH}	Horizontal P-wave velocity
V_{SV}	Vertical S-wave velocity
V_{SH}	Horizontal S-wave velocity

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