Full-waveform inversion on heterogeneous HPC systems

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Abstract

We present a spectral-element implementation of full seismic waveform inversion for large heterogeneous HPC systems. In this we address the optimal parallelisation configurations of individual simulations, the large I/O requirements of adjoint simulations, and the scheduling of large numbers of forward and adjoint solves, typical for realistic inversions. Using GPU accelerators allows us to achieve a 3.5-4 times performance improvement over the best known homogeneous implementation. We achieve GPU memory throughput varying from 60-80% of the peak bandwidth, thus providing good utilisation of hardware resources. We demonstrate the practical applicability of our developments in a real-data application in the western Mediterranean. **With the help of GPU accelerators, we are able to model and invert seismic wave propagation in a frequency band that is broader than permitted by the use of CPUs alone, which helps bridging the traditional gap between crustal and mantle tomography.**

Keywords: Seismic tomography, heterogeneous HPC systems, wave propagation, full-waveform inversion, inverse theory, spectral-element method.

1. Introduction

Seismic tomography is in a transition period where methods based on simplified wave propagation physics are successively replaced by fully numerical

[☆]Fully documented code is available on the scientific software websites of the ETH Computational Seismology Group: www.cos.ethz.ch.

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4 approaches that allow seismologists to exploit the complete seismic recordings
5 for the benefit of improved tomographic resolution, provided that data quality
6 is sufficient. Conceptualised in the late 1970’s and early 1980’s [1, 2, 3, 4] such
7 *full-waveform inversions* have become applicable to today’s large seismic data
8 sets thanks to steadily increasing computational resources. Applications at local
9 scales in seismic exploration [5, 6, 7, 8], on regional scales [9, 10, 11, 12, 13, 14],
10 and for the entire Globe [15, 16] provide new insight into the structure, dynam-
11 ics and evolution of the Earth. While 3D inversion on standard CPU clusters
12 is still a major computational challenge taken up by few research groups, the
13 emergence of large heterogeneous high-performance computing (HPC) systems
14 has the potential to transform full-waveform inversion into a widely used routine
15 method.

16 Recognising the potential of heterogeneous HPC systems, several forward wave
17 propagation codes have been implemented on GPU graphic cards [17, 18, 19],
18 showing promising results. The next step, that is the transition from the forward
19 modelling of a single source (e.g. an earthquake or explosion) to the solution of a
20 seismic inverse problem, is complicated for two reasons: (i) Adjoint calculations
21 needed to compute gradients [20, 21, 22, 23, 24] require that very large amounts
22 of data are stored and read during the simulations. This is in conflict with
23 GPUs that require minimal I/O for optimal use. (ii) Acceptable tomographic
24 resolution can only be achieved when data from many sources, often hundreds
25 to thousands, are used. Therefore, individual simulations must be set up and
26 scheduled such that heterogeneous HPC systems are optimally harnessed. Run-
27 ning simulations sequentially on the largest possible number of nodes is mostly
28 inefficient.

29 In the following sections, we address these issues of I/O in adjoint simulations,
30 parallelisation setup and scheduling in the context of large heterogeneous HPC
31 systems. In addition to purely computational aspects, we present a real-data
32 full-waveform inversion of the Mediterranean region that underlines the appli-
33 cability of our developments.

34 This paper is organised as follows: In section 2 we provide a condensed review
 35 of seismic wave propagation modelling, including the governing equations of
 36 forward and adjoint simulations. A specific spectral-element implementation of
 37 these equations is presented in section 3. Following a brief description in section
 38 4 of the HPC system used for our developments, section 5 is dedicated to soft-
 39 ware engineering challenges, optimisation and parallelisation strategies, and the
 40 application architecture. A performance analysis and a real-data application
 41 are presented in sections 6 and 7, respectively.

42 2. Forward and inverse modelling of seismic wave propagation

43 To set the stage for our computational developments, we provide a condensed
 44 review of forward and adjoint seismic modelling, and the spectral-element dis-
 45 cretisation of the seismic wave equation. Additional details may be found in
 46 [20, 21, 25, 26, 22, 23, 27].

47 2.1. Forward modelling in visco-elastic anisotropic media

The propagation of seismic waves through the Earth is governed by the momentum-
 balance equation

$$\rho(\mathbf{x}) \ddot{u}_i(\mathbf{x}, t) - \sum_{j=1}^3 \partial_j \sigma_{ij}(\mathbf{x}, t) = f_i(\mathbf{x}, t), \quad \mathbf{x} \in V \subset \mathbb{R}^3, t \in [0, \infty), i = 1, 2, 3, \quad (1)$$

where $\rho > 0$ denotes mass density, σ_{ij} the symmetric stress tensor, f_i an external
 force density, and u_i the seismic wavefield [28, 29, 30]. Over-dots symbolise
 differentiation in time. The stress tensor and the wavefield are subject to the
 boundary and initial conditions

$$\sum_{j=1}^3 \sigma_{ij} n_j|_{\partial V} = 0, \quad u_i|_{t=0} = 0, \quad \dot{u}_i|_{t=0} = 0, \quad (2)$$

meaning that stresses in the direction of the surface normal n_j vanish along the
 boundary ∂V , and that the wavefield is at rest for time $t = 0$. The stress tensor

σ_{ij} is related to the gradients of the wavefield via the visco-elastic stress-strain relation

$$\dot{\sigma}_{ij}(\mathbf{x}, t) = \sum_{k,l=1}^3 \int_{t'=-\infty}^t \dot{C}_{ijkl}(\mathbf{x}, t-t') \partial_k \dot{u}_l(\mathbf{x}, t') dt', \quad (3)$$

where the elastic tensor C_{ijkl} satisfies the symmetry relations $C_{ijkl} = C_{jikl} = C_{klij}$. The time-dependence of C_{ijkl} controls the visco-elastic dissipation of the material, i.e. the conversion of elastic energy into heat as a function of frequency or time. To circumvent the numerically expensive solution of the convolution integral (3), the elastic tensor can be written as a superposition of N standard-linear solids:

$$C_{ijkl}(\mathbf{x}, t) = C_{ijkl}^r(\mathbf{x}) \left[1 + \tau_{ijkl}(\mathbf{x}) \sum_{p=1}^N D_p(\mathbf{x}) e^{-t/\tau_p(\mathbf{x})} \right]. \quad (4)$$

The relaxed moduli $C_{ijkl}^r = \lim_{t \rightarrow \infty} C_{ijkl}$ and the relaxation parameters τ_{ijkl} , D_p and τ_p are chosen to match a prescribed dissipation of the material [31, 32, 33, 34, 35]. Introducing (4) in (3) transforms the stress-strain relation into

$$\begin{aligned} \dot{\sigma}_{ij}(\mathbf{x}, t) = & \sum_{k,l=1}^3 C_{ijkl}^r(\mathbf{x}) [1 + \tau_{ijkl}(\mathbf{x}) s(\mathbf{x})] \partial_k \dot{u}_l(\mathbf{x}, t) \\ & + \sum_{k,l=1}^3 C_{ijkl}^r(\mathbf{x}) \tau_{ijkl}(\mathbf{x}) \sum_{p=1}^N M_{p,kl}(\mathbf{x}, t), \end{aligned} \quad (5)$$

with $s = \sum_{p=1}^N D_p$. The memory variables $M_{p,kl}$ satisfy the ordinary differential equation

$$\dot{M}_{p,kl} = -\frac{1}{\tau_p} M_{p,kl} - \frac{D_p}{\tau_p} \partial_k \dot{u}_l. \quad (6)$$

48 Together, equations (1), (5) and (6) constitute the set of differential equations
 49 that must be solved numerically for the seismic wavefield $u_i(\mathbf{x}, t)$, subject to the
 50 boundary and initial conditions (2).

51 2.2. Adjoint modelling and full waveform inversion

The solution of a seismic inverse problem rests on the quantification of a misfit J between waveforms $u_i^{\text{obs}}(\mathbf{x}_r, t)$ observed in a time interval $[0, T]$ at receiver

positions $\mathbf{x}_{r=1,2,\dots,R}$, and the corresponding synthetic waveforms $u_i(\mathbf{x}_r, t, \mathbf{m})$ computed for an Earth model $\mathbf{m} = (\rho, C_{ijkl})$. The specific form of the misfit functional $J(\mathbf{m})$ depends on the concrete application and on the nature of the data [36, 37, 38, 39, 40, 41, 42]. To minimise J with respect to $\mathbf{m}$ using gradient-based methods, we require the variation of J , which can be written in terms of a Fréchet or sensitivity kernel $\mathbf{K}$:

$$\delta J = \int_V \mathbf{K}(\mathbf{x}) \cdot \delta \mathbf{m}(\mathbf{x}) d\mathbf{x}. \quad (7)$$

For the parameters ρ and C_{ijkl}^r , the Fréchet kernels take the specific forms

$$K_\rho(\mathbf{x}) = - \sum_{i=1}^3 \int_0^T \dot{u}_i(\mathbf{x}, t) \dot{u}_i^\dagger(\mathbf{x}, t) dt, \quad K_{C_{ijkl}^r}(\mathbf{x}) = \int_{t=0}^T \partial_i u_j(\mathbf{x}, t) \partial_j u_k^\dagger(\mathbf{x}, t) dt, \quad (8)$$

respectively [20, 21, 22, 23, 24]. The adjoint wavefield $u_i^\dagger(\mathbf{x}, t)$ is governed by the following set of equations: (i) the adjoint momentum-balance equation

$$\rho(\mathbf{x}) \ddot{u}_i^\dagger(\mathbf{x}, t) - \sum_{j=1}^3 \partial_j \sigma_{ij}^\dagger(\mathbf{x}, t) = f_i^\dagger(\mathbf{x}, t), \quad \mathbf{x} \in V \subset \mathbb{R}^3, t \in [0, \infty), i = 1, 2, 3, \quad (9)$$

(ii) the adjoint stress-strain relation that couples the adjoint stress tensor $\sigma_{ij}^\dagger$ to the adjoint field $u_i^\dagger$,

$$\dot{\sigma}_{ij}^\dagger(\mathbf{x}, t) = \sum_{k,l=1}^3 \int_{t'=-\infty}^t \dot{C}_{ijkl}(\mathbf{x}, t' - t) \partial_k \dot{u}_l^\dagger(\mathbf{x}, t') dt', \quad (10)$$

and (iii) the adjoint subsidiary conditions

$$\sum_{j=1}^3 \sigma_{ij}^\dagger n_j|_{\partial V} = 0, \quad u_i^\dagger|_{t=T} = 0, \quad \dot{u}_i^\dagger|_{t=T} = 0. \quad (11)$$

52 The adjoint source $f_i^\dagger$ is uniquely determined by the misfit functional J , and so
53 are the adjoint wavefield and the Fréchet kernels.

54 The terminal conditions on the adjoint field (11) impose that the adjoint equa-
 55 tions must be solved in reverse time. Consequently, the forward field u_i must be
 56 made available during the adjoint equation solve in order to compute the time
 57 integrals in (8) on the fly. To achieve this task in the hypothetical absence of
 58 visco-elastic dissipation, the wavefield from the end of the forward simulation
 59 can be propagated backwards in time, therefore not requiring significant storage
 60 capacities. In realistic dissipative media, backward propagation is numerically
 61 unstable, and the forward field must be stored at sufficiently many time steps
 62 to enable efficient checkpointing [43]. The massive I/O related to reading and
 63 writing snapshots of the forward field is a major challenge on modern HPC
 64 systems that we address in this paper.

65 *2.3. Numerical solution*

Depending on the particular application, various techniques have been devel-
 oped to solve the seismic wave equation numerically. These include finite-
 difference [44, 45, 46, 47, 48], spectral-element [49, 50, 25, 26, 51], and dis-
 continuous Galerkin [52, 53, 54] methods. Regardless of the specific method,
 the space-discretised equations can generally be cast into the generic form

$$\sum_j M_{ij} \ddot{\bar{u}}_j + \sum_j K_{ij} \bar{u}_j = \bar{f}_i, \tag{12}$$

66 with the discretised wavefield $\bar{u}_j$, the mass matrix M_{ij} , the stiffness matrix
 67 K_{ij} , and the discretised external force $\bar{f}_i$. In our application we obtain (12)
 68 through a spectral-element discretisation of the elastic wave equation. For this,
 69 the computational domain is subdivided into non-overlapping elements G_e that
 70 are mapped to the unit cube Λ (figure 1). In Λ , material parameters and the
 71 wavefield are approximated by Lagrange polynomials, where the GLL points
 72 serve as interpolation points. GLL quadrature then leads to a discrete system
 73 with diagonal mass matrix that allows for efficient explicit time stepping.
 74 Despite the specific choice of a forward problem solver, the following computa-
 75 tional developments are equally applicable to time-domain forward and adjoint
 76 wave equation solvers where the discrete system is the same as in equation (12).

Figure 1: Schematic illustration of the mapping between the unit cube Λ and the physical-domain element G_e , which is a small spherical-subsection of the Earth.

3. SES3D: Spectral-element visco-elastic wave propagation in a 3D spherical section

We have implemented the computational approach described above in a software package named SES3D. SES3D operates in the natural spherical coordinates, which is untypical for spectral-element approaches. The advantages are a compact programme code, fast computations for spherical sections that are sufficiently far from the poles and the core, and the easy implementation of 3D models. A single run of SES3D performs either a forward simulation with or without storage of the wavefield, or an adjoint simulation where a previously stored forward field is read and combined with the adjoint field to produce sensitivity kernels. Each run, forward or adjoint, corresponds to an earthquake or other seismic event that is processed independently.

SES3D data are represented as 3D arrays mostly falling into the following categories: (i) physical model parameters including elastic tensor components C_{ijkl}^r , density ρ , and relaxation parameters τ_{ijkl} , (ii) source fields for moment tensor and vector forces, including adjoint sources, (iii) snapshots of the forward field required for adjoint calculations, (iv) static fields such as the mass matrix, and (v) dynamics fields that are recomputed in every iteration, including velocities $\dot{u}_i$, velocity gradients $\partial_j \dot{u}_i$, stresses σ_{ij} , and stress rates $\dot{\sigma}_{ij}$. Among these fields the displacements and stress rates are accumulated (integrated) during the entire iterative process.

198 The time step algorithm exposes a large amount of data-level parallelism that
199 can be harnessed by computing systems with multiple independent processing
200 elements. For this, the computational domain is partitioned into a fixed number
201 of sub-domains, each being assigned to one processing element. Information be-
202 tween elements is exchanged when stress rates at element boundaries are shared
203 between neighbouring sub-domains. If processing elements themselves provide
204 hardware facilities for parallel computations, they can exploit the algorithm
205 data parallelism by performing parallel computations of field values for differ-
206 ent grid points within a sub-domain. This is exactly the case for heterogeneous
207 massively parallel computing systems, which we use in the present work.

208 **4. Instrument: heterogeneous massively parallel computing systems**

209 In recent years, the combination of GPU-accelerated computing with more tra-
210 ditional ideas of massively parallel systems, consisting of multiple nodes with
211 distributed memory, led to the introduction of heterogeneous high-performance
212 systems. Such systems consist of large numbers of nodes interconnected via high
213 throughput networks, where each node provides a mix of processing elements
214 with different architectures, like a small number of sequential CPU cores and
215 one or a few GPU accelerators. These emerging systems provide an opportu-
216 nity for manifold application performance increase and are more energy-efficient.
217 However, since they have higher hardware complexity and are more difficult to
218 program, the transition to heterogeneous computing is highly disruptive from
219 the software engineering perspective. Efficient use of GPU resources requires a
220 programming methodology that is completely different from those used for mul-
221 tiple sequential processors running in parallel, typical for the recent decades.
222 Thus, to exploit potential benefits of heterogeneous computing, novel program-
223 ming methodologies must be created.

224 A typical example for massively parallel heterogeneous high-performance com-
225 puting systems is "Piz Daint", a supercomputer of the Cray XC 30 family op-
226 erated by the Swiss National Supercomputing Center (CSCS). It features 5,272

127 computing nodes, each being equipped with an 8-core 64-bit Intel Sandy Bridge
 128 CPU (Intel Xeon E5-2670), an NVIDIA Tesla K20x GPU accelerator with 6
 129 GB GDDR5 memory, and 32 GB of host memory. The nodes are connected by
 130 the proprietary "Aries" interconnect from Cray. In this study, we aimed at the
 131 implementation of SES3D on "Piz Daint".

132 **5. Methodology: Software engineering challenges**

133 *5.1. Need for a new software engineering methodology*

134 The proposed implementation presented us with various engineering challenges
 135 arising from a need to split the code into two distinct parts running on the CPU
 136 and GPU devices that require different techniques for programming and per-
 137 formance optimisation. Furthermore, special attention had to be paid to work
 138 distribution and interaction between CPU and GPU, especially during I/O in-
 139 tensive adjoint runs.

140 We based the implementation process on the assumption that the transition to
 141 a heterogeneous computing model will have impact on all aspects of the appli-
 142 cation architecture. This means, in particular, that it would not be sufficient to
 143 extract the most critical parts of the code and re-implement them as optimised
 144 kernels running on GPUs. Instead, the entire application architecture has to
 145 be re-engineered because any inefficiency in the serial part of the application
 146 can easily offset the benefits of using GPUs. Therefore, we decided to employ a
 147 hybrid programming model based on a combination of several well-established
 148 software development technologies, including C as a host programming lan-
 149 guage, MPI 3.0 as a library for the inter-node communication, and CUDA as
 150 a toolkit for programming NVIDIA GPU accelerators. We are using compil-
 151 ers and libraries of Cray Programming Environments 5.1 in combination with
 152 NVIDIA CUDA Toolkit 5.5.

153 *5.2. Optimisation methodology*

154 SES3D manages large volumes of data arranged in ~ 100 arrays. Interchange
 155 of these data volumes between GPU memory and CPU memory at every it-

eration would incur a large performance overhead. Due to the nature of the algorithm, this interchange cannot be done asynchronously. To use GPU capabilities efficiently, it is necessary to host all data arrays on GPU permanently and implement all computations on GPU. The role of the corresponding host CPU should be limited to I/O operations, inter-node communication, and management of the workflow. We thus try to keep data interchange between the GPU and the surrounding environment at the absolutely necessary minimum.

Data interchange between the computing nodes may cause overhead that can offset benefits provided by the GPU. It was therefore essential to tune inter-node communication carefully to keep data interchange between GPU devices of different nodes reasonably fast. Our implementation relies on MPI as a principal communication platform. However, we decided to replace the classic MPI point-to-point communication by one-sided communication based on the MPI Remote Memory Access (RMA) that, according to the results of our empirical study, provide better performance for all parallelisation configurations.

For the optimisation of CUDA kernels, we tuned the layout of data arrays to enable coalesced access to device memory, and we used GPU shared memory to reduce the number of redundant device memory accesses. Whenever feasible, we implemented highly optimised re-usable kernels for commonly used functions like array reductions. We extensively used the NVIDIA profiler *nvprof* to measure performance of individual CUDA kernels and data transfers between CPU hosts and GPU devices.

The algorithm for the forward and adjoint simulations where wavefield snapshots are written and read, respectively, requires a substantial amount of data interchange between the application and external storage. This interchange takes place once per a pre-defined number of iterations, typically 10-30 [55]. As explained in section 2.2, snapshots of the forward wavefield are written to large external files during the forward simulations; in the adjoint mode they are read from these files in reverse order. The storage requirements for typical applications, such as the one presented in section 7, are on the order of 1-10 TB.

186 Adjoint mode I/O operations add penalty to the overall performance. This is
 187 tolerable in homogeneous configurations but increases dramatically in hetero-
 188 geneous cases. This increase occurs because in heterogeneous configurations
 189 each GPU device takes over the work that otherwise would be performed by
 190 a big number of CPU cores and therefore much larger volumes of data have
 191 to be interchanged between each computing node and external storage. Our
 192 empirical performance study of interchange with the external storage suggests
 193 that the related I/O penalty is tolerable if data are read or written sequentially.
 194 Unfortunately, this is not a case in the adjoint mode when data are read in the
 195 reverse order. To solve this problem we introduced buffering of read operations
 196 in the adjoint mode. For each array to be read the application allocates a buffer
 197 large enough to hold approximately 30 consecutive array instances which are
 198 pre-fetched via a single read request. This approach allowed us to reduce the
 199 run time and make it comparable to that of forward simulations with wavefield
 200 storage.

201 *5.3. Choice of parallelisation scheme*

202 Our implementation on massively parallel computing architectures is facilitated
 203 by parallelisation configurations that specify 3D processor grids consisting of
 204 CPU cores in the homogeneous case or GPU devices (and respective computing
 205 nodes) in the heterogeneous case. The whole computational domain is parti-
 206 tioned into sub-domains, each sub-domain being mapped to a single element
 207 of the respective processor grid. We make the distinction between "wide" and
 208 "compact" parallelisation configurations. Wide configurations are characterised
 209 by a relatively large processor grid size and rather small amount of data as-
 210 signed to each processor grid element. Compact configurations have a substan-
 211 tially smaller grid size and respectively larger size of data sets assigned to each
 212 processing element.

213 The initial implementation of SES3D processed all events sequentially, that is,
 214 at each moment all computing nodes were involved in processing of the same
 215 event. This sequential scenario appears impractical for the compact paralleli-

216 sation configurations. These configurations provide superior performance in
 217 heterogeneous cases, however, the absolute wall clock time required to process
 218 the large number of events in a realistic full-waveform inversion sequentially
 219 is too large. On the other hand, the number of computing resources involved
 220 in computations for the compact parallelisation configurations is substantially
 221 (usually in order of magnitude of more) smaller than in case of wide config-
 222 urations. (This subject is discussed further in the section 6 dedicated to the
 223 application performance.) Therefore, if a comparable number of computing re-
 224 sources is available for both compact and wide configurations, then the compact
 225 configuration may utilise these resources in full by splitting them into smaller
 226 groups, then distributing all events to be processed evenly among these groups
 227 and allowing them to process events in parallel.

228 We implemented support for parallel event processing in SES3D. If a number
 229 of processing elements allocated at application start is a multiple of a num-
 230 ber specified by a parallelisation configuration, the application automatically
 231 splits available processing elements in groups and partitions a list of events into
 232 chunks, assigning each chunk to its own group for parallel processing.

233 *5.4. Application architecture*

234 Each program instance consists of a sequential part running on the CPU core
 235 and a massively parallel part running on the GPU device (see figure 2). The
 236 sequential part includes modules for application initialisation, inter-node com-
 237 munication, mass storage I/O, and management of control and data flow for
 238 operations offload to the GPU. The massively parallel part is represented as a
 239 set of CUDA kernels that reside and run on GPU, each kernel implementing a
 240 certain computational function applied to a large stream of parallel processing
 241 threads. The sequential part orchestrates activation of CUDA kernels. CUDA
 242 kernels perform all computations of the SES3D time step algorithm, including
 243 the computation of external forces, velocity gradients and stress rates and the
 244 time extrapolation of stresses and velocities. Furthermore, there are kernels
 245 implementing functionality specific for various computation modes, such as the

246 computation of synthetic seismograms, intermediate wavefield snapshots and
247 Fréchet kernels.

248 All major data sets are replicated between the CPU and GPU memories. The
249 CPU is responsible for initialisation of all data sets at the processing start for
250 each event. These data sets are then copied once to the GPU memory, where
251 they reside until completion of the event processing. Further data interchange
252 between CPU and GPU is kept at minimum and takes place only when inter-
253 node communication or mass storage I/O operation is required. Copying of data
254 between the CPU and GPU is performed using synchronous memory manage-
255 ment primitives of CUDA. We keep a separate set of data files per processing
256 element and use plain binary format and standard C I/O libraries. The overall
257 number of files is not performance-critical. We have made experiments keeping
258 values of each parameter for the entire simulation domain in a single file and
259 using the MPI parallel I/O for the shared access, however, this did not provide
260 any performance gain.

261 Programming instances arranged this way form a *gang* that performs parallel
262 wave modelling on all sub-domains for a single event. Since usually a single sim-
263 ulation involves tens of events that can be processed independently, a typical
264 application configuration contains multiple gangs, every gang being responsible
265 for processing a distinct part of the entire event set (see figure 3). Distribution
266 of work among gangs is done statically at the application initialisation phase
267 based on a simple algorithm aiming at uniform load balancing.

268 6. Performance

269 We use a simple yet practical method for performance assessment. The wall
270 clock time for each configuration and test run is measured. Based on this
271 figure, the number of iterations processed per minute per computing node is
272 calculated. While we have chosen several SES3D use cases in the development
273 stage, we limit the following description to a representative scenario featuring

Figure 2: Schematic illustration of the application architecture.

Figure 3: Schematic illustration of 10 gangs of 11 computing nodes each processing 60 events in parallel.

274 a $77 \times 68 \times 77$ grid of blocks, and 10 events of 14,000 iterations each. For this
 275 case we used the following parallelisation configurations:

Configuration	Processor grid	Nodes	CPU	GPU
Homogeneous, compact	$11 \times 1 \times 7$	10	77	
Heterogeneous, compact	$11 \times 1 \times 1$	11	11	11
Homogeneous, wide	$11 \times 17 \times 7$	164	1309	
Heterogeneous, wide	$11 \times 1 \times 11$	121	121	121

277 We measured performance for both CPU and GPU versions, and for both com-
 278 pact and wide parallelisation configurations. At each run, 10 events were pro-
 279 cessed in a sequence with 14,000 iterations for each event. We conducted sep-
 280 arate tests for each of three supported computation modes: (i) forward sim-
 281 ulations without storage of wavefield snapshots, (ii) forward simulations with
 282 storage of wavefield snapshots, and (iii) adjoint simulations. The following wall
 283 clock times have been recorded in one of the representative test series (results
 284 expressed as hours:mins:secs).

Configuration	simulation mode	Time
CPU, compact, $11 \times 1 \times 7$ (10 nodes)	forward without storage	7:00:16
	forward with storage	7:12:10
	adjoint	7:18:39
GPU, compact, $11 \times 1 \times 1$ (11 nodes)	forward without storage	1:18:24
	forward with storage	1:49:22
	adjoint	1:52:49
CPU, wide, $11 \times 17 \times 7$ (164 nodes)	forward without storage	0:21:32
	forward with storage	0:22:40
	adjoint	0:26:46
GPU, wide, $11 \times 1 \times 11$ (121 nodes)	forward with storage	0:16:24
	forward without storage	0:20:42
	adjoint	0:31:10

286 The following performance figures (iterations / node / minute) have been cal-
 287 culated for forward simulations without wavefield storage:

Configuration	Performance
GPU, 11 x 1 x 1	140000/11/78.5 = 162.1
GPU, 11 x 1 x 11	140000/121/16.5 = 70.1
CPU, 11 x 1 x 7	140000/10/420.5 = 33.3
CPU, 11 x 17 x 7	140000/164/21.5 = 39.7

These figures fully support our original assumption stating that wide configurations favour homogeneous (CPU-based) versions since smaller data sets fit CPU caches better. On the other hand, compact configurations provide more benefits for heterogeneous (GPU-based) versions because GPU devices achieve better performance processing reasonably large data sets that suit better for amortisation of latencies in the GPU streaming processors. Furthermore, by comparison of the best performances for CPU and GPU cases, the speedup achieved on the heterogeneous architecture for the given use case can be calculated as $162.1/39.7 = 4.1$ times.

There exist certain technical limits for the further performance improvement on the heterogeneous architecture. SES3D is a typical memory-bound application, therefore performance of its CUDA kernels is constrained by the peak memory bandwidth of the GPU device. For NVIDIA K20x this bandwidth equals 250 GB/s. Profiling of our kernels reports the GPU device memory throughput varying between 160 and 200 GB/s, that is, between 60% and 80% of the peak bandwidth.

Performance comparison done for problems with different overall size but the same problem size per processing element has demonstrated the weak scaling efficiency of SES3D does not depend significantly on the number of processing elements for configurations consisting of up to a few hundred of computing nodes on "Piz Daint". The strong scaling efficiency behaves differently for homogeneous and heterogeneous configurations. For homogeneous configurations the strong scaling efficiency is higher for big numbers of processing elements (CPUs), while for heterogeneous configurations it is higher for the smaller number of processing elements (GPUs). Furthermore, simulations with higher frequency

314 resolution will require the proportionally larger number of time steps and grid
 315 size in each dimension. Therefore, the computational complexity grows by the
 316 factor of N^4 with the increase of the simulation frequency by the factor of N .

317 7. Application: Full-waveform inversion for the western Mediter- 318 ranean region

319 We tested the GPU implementation of SES3D in a full-waveform inversion in
 320 the western Mediterranean region. For this, we used 13,089 three-component
 321 recordings from 52 regional earthquakes. For broadband stations belonging to
 322 permanent national/regional networks we obtained seismic waveform data from
 323 global (IRIS, www.iris.edu) and European (ORFEUS, www.orfeus-eu.org) data
 324 centres. This was complemented by data from the temporary IberArray [56].
 325 The source-receiver distribution is shown in figure 4.

326 We partitioned the computational domain into 1,603,584 elements, within which
 327 all fields are represented by tensorised polynomials of degree 4. The total number
 328 of grid points was 200,448,000. Taking at least two elements per minimum
 329 wavelength to ensure sufficiently accurate solutions, this setup allowed us to
 330 model wave propagation at periods as low as 12 s. To optimise GPU usage,
 331 each event was processed on only 48 nodes. However, since the 52 earthquakes
 332 were subdivided into 26 gangs with 2 earthquakes each, a total of 1,248 nodes
 333 was used simultaneously. The forward simulation of all earthquakes was typi-
 334 cally accomplished within slightly more than 1 hour.

335 For the processing of seismic waveform data and the selection of measurement
 336 time windows, we used the Large Scale Seismic Inversion Framework of Krischer
 337 et al. [57]. A previous full-waveform inversion for all Eurasia at longer periods
 338 [58] served as initial model. After 20 conjugate-gradient iterations, the initial
 339 misfit was reduced by nearly 80 %. Figure 5 shows the final distribution of the
 340 isotropic S velocity v_s , defined as a weighted average of the velocities of vertically
 341 polarised (v_{sv}) and horizontally polarised (v_{sh}) shear waves: $v_s^2 = \frac{2}{3}v_{sv}^2 + \frac{1}{3}v_{sh}^2$
 342 [59, 60].

Figure 4: Source-receiver distribution in the western Mediterranean. Beachballs indicate the source mechanisms and locations of the 52 earthquakes used in our inversion. Great circles connecting sources and receivers are plotted in lighter colour when coverage is high. The black and gray boxes mark the boundary of the computational domain and the inner boundary of the absorbing layer.

Figure 5: Horizontal slices through the 3D distribution of isotropic S velocity v_s at various depths.

343 The final model, discussed in terms of the regional geology in [61], is remark-
 344 able in that 3D structure within both the thin crust at mostly less than 40 km
 345 depth and the underlying mantle can be resolved. This is in contrast to tradi-
 346 tional seismic tomography, where either crust or mantle were fixed, depending
 347 on the specific region of interest. The ability to model and invert seismic wave
 348 propagation at shorter periods with the help of heterogeneous HPC systems,
 349 bridges the resolution gap between crustal and seismic tomography; and it will
 350 eventually lead to the unification of these two seismic imaging branches. The
 351 work presented here constitutes a step in this direction.

352 8. Discussion

353 A major challenges in the GPU implementation of full-waveform inversion is
 354 the large I/O caused by the reading and writing of wavefield snapshots during
 355 the simulations. It arises from the need to have synchronous access to the for-
 356 ward and adjoint fields in the computation of Fréchet kernels. In media without
 357 attenuation, this synchronous access can be achieved by the time reversed prop-
 358 agation of the forward wavefield from the final state of the forward simulation
 359 to time $t = 0$ [62]. Since seismic wavefields in the Earth can be strongly atten-
 360 uated, reverse-time propagation is inherently unstable. The instability can be
 361 avoided by ignoring attenuation in the time reversed simulation, though at the
 362 cost of inaccurate kernels that may slow down or even prevent convergence. To
 363 ensure convergence in the presence of a realistic attenuating Earth, the forward
 364 wavefield should be stored whenever possible.

365 Using the GPU-based version of SES3D package is not more difficult than that
 366 of the conventional CPU-only version since no GPU-specific detail is exposed
 367 to the end-user and no computer science background is required for running the
 368 application. However, using the GPU-related technologies for building similar
 369 HPC applications in seismology in general represents a significant challenge.
 370 Transition to heterogeneous architectures has a clear disruptive effect since it
 371 requires a substantial revision of programming paradigms and demands higher

372 programming skills from developers. In particular, we note that substantial code
 373 duplication took place during the development of SES3D. The same computa-
 374 tion algorithms have been implemented twice, as serial C code and as code of
 375 GPU CUDA kernels. This code duplication is regarded as a significant disadvan-
 376 tage that cannot be efficiently addressed within the chosen programming model,
 377 which, in our opinion, leaves substantial room for improvement of programmer
 378 productivity. In the future this improvement might be achieved by introduction
 379 of more advanced programming models that would replace the present het-
 380 erogeneous mix of relatively low-level technologies thus reducing complexity of
 381 application code, improving its portability, increasing programmer productivity
 382 and being accessible for developers who are not experts in software engineer-
 383 ing. Acceptability of GPU accelerators for development of new applications
 384 by the wider seismologist community depends on the availability of such high
 385 level programming models and respective tools. Their creation must involve the
 386 multi-disciplinary collaboration of seismologists and computer scientists.

387 It must be noted, that the waveform simulations in SES3D implement just one
 388 of various performance-critical steps of the seismic inversion process. Once the
 389 substantial performance improvement is achieved for the simulation modules,
 390 we have to shift focus to the optimisation of other steps, in particular, compu-
 391 tation of misfits and updating the model. We intend to address these issue at
 392 the next stages of our research.

393 At the high level, our engineering approach is similar to the one used for
 394 the seismic wave propagation package SPECFEM3D [62]. Like our solution,
 395 SPECFEM3D supports large-scale homogeneous and GPU-enabled heteroge-
 396 neous computers and is implemented using MPI / CUDA. Furthermore, the
 397 entire package and not just individual kernels had been ported to CUDA and
 398 special attention had been paid to the optimization of data motions at all lev-
 399 els. Although the authors of SPECFEM3D and SES3D have faced the similar
 400 development challenges, in some cases they addressed them in different ways.
 401 In particular, in our work we target the issue of updating the shared grid nodes

402 with the purpose built race-free algorithm, thus avoiding the need for using
 403 more sophisticated methods like mesh colouring. We have decided not to imple-
 404 ment overlapping of data motion for inter-node and host-accelerator transfers
 405 because in case of SES3D the volumes of data to be transferred at each iter-
 406 ation are relatively modest and potential performance gains do not justify the
 407 respective increase in the code complexity. We employ the various techniques for
 408 CUDA optimizations, focusing mainly on mediating the limited global memory
 409 throughput by the extensive use of the GPU shared memory; in this respect the
 410 SES3D approach apparently differs in detail from that used in SPECFEM3D
 411 given the different code structure of two packages. Finally, we note that the
 412 parallelisation strategy of SES3D is specifically tailored towards the solution of
 413 large inverse problems that involve a large number of events.

414 9. Conclusions

415 We present a spectral-element implementation of full seismic waveform inver-
 416 sion for large heterogeneous HPC systems. In our development, we addressed
 417 the optimal parallelisation configurations of individual simulations, the large
 418 I/O requirements of adjoint simulations, and the scheduling of large numbers of
 419 forward and adjoint solves, typical for realistic inversions.

420 We have demonstrated that wide parallelisation configurations are more bene-
 421 ficial for the homogeneous (CPU-only) application version while compact con-
 422 figurations yield better performance in the heterogeneous (GPU-enabled) case.

423 Adjoint mode I/O operations add a significant penalty to the overall performance
 424 of the heterogeneous application version running in compact configurations. We
 425 solve this problem by prefetching a reasonably big number of consecutive data
 426 records into a large memory buffer via a single I/O request. This approach
 427 successfully reduces the run time of adjoint simulations to that of forward sim-
 428 ulations.

429 The multi-event processing in the inverse problem solution is most efficient when

430 events are grouped into gangs. While all gangs operate in parallel, events are
431 processed sequentially within each of them.

432 Using GPU accelerators allowed us to achieve 3.5-4 times performance improve-
433 ment over the best known homogeneous implementation on "Piz Daint". The
434 new implementation achieves the GPU memory throughput varying from 60%
435 to 80% of the peak bandwidth, thus providing good utilisation of hardware re-
436 sources.

437 We demonstrated the practical applicability of our developments in a real-data
438 application in the western Mediterranean. With the help of GPU accelerators,
439 we were able to model and invert seismic wave propagation at periods as short
440 as 12 s over ~ 2000 km distance, thereby bridging the resolution gap between
441 crustal and seismic tomography.

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454 **References**

- 455 [1] A. Bamberger, G. Chavent, P. Lailly, Une application de la théorie du
456 contrôle à un problème inverse sismique., Ann. Geophys. 33 (1977) 183–
457 200.

- 458 [2] A. Bamberger, G. Chavent, C. Hemons, P. Lailly, Inversion of normal inci-
459 dence seismograms., *Geophysics* 47 (1982) 757–770.
- 460 [3] P. Lailly, The seismic inverse problem as a sequence of before stack migra-
461 tions, in: J. Bednar, R. Redner, E. Robinson, A. Weglein (Eds.), *Conference*
462 *on Inverse Scattering: Theory and Application*, Soc. Industr. appl. Math.,
463 Philadelphia, PA., 1983.
- 464 [4] O. Gauthier, J. Virieux, A. Tarantola, Two-dimensional nonlinear inversion
465 of seismic waveforms: numerical results., *Geophysics* 51 (1986) 1387–1403.
- 466 [5] R. Pratt, C. Shin, G. Hicks, Gauss-Newton and full Newton methods in
467 frequency domain seismic waveform inversion, *Geophys. J. Int.* 133 (1998)
468 341–362.
- 469 [6] A. J. Brenders, R. G. Pratt, Full waveform tomography for lithospheric
470 imaging: results from a blind test in a realistic crustal model, *Geophys. J.*
471 *Int.* 168 (2007) 133–151.
- 472 [7] B. Smithyman, R. G. Pratt, J. Hayles, R. Wittebolle, Detecting near-
473 surface objects with seismic waveform tomography, *Geophysics* 74 (2009)
474 WCC119–WCC127.
- 475 [8] M. V. Afanasiev, R. G. Pratt, R. Kamei, G. McDowell, Waveform-based
476 simulated annealing of crosshole transmission data: A semi-global method
477 for estimating seismic anisotropy, *Geophys. J. Int.* (2014) in press.
- 478 [9] P. Chen, L. Zhao, T. H. Jordan, Full 3D tomography for the crustal struc-
479 ture of the Los Angeles region., *Bull. Seismol. Soc. Am.* 97 (2007) 1094–
480 1120.
- 481 [10] C. Tape, Q. Liu, A. Maggi, J. Tromp, Seismic tomography of the southern
482 California crust based upon spectral-element and adjoint methods., *Geo-*
483 *phys. J. Int.* 180 (2010) 433–462.

- 484 [11] L. Colli, A. Fichtner, H.-P. Bunge, Full waveform tomography of the upper
485 mantle in the South Atlantic region: Imaging westward fluxing shallow
486 asthenosphere?, *Tectonophysics* 604 (2013) 26–40.
- 487 [12] F. Rickers, A. Fichtner, J. Trampert, The Iceland - Jan Mayen plume
488 system and its impact on mantle dynamics in the North Atlantic region:
489 Evidence from full-waveform inversion, *Earth Planet. Sci. Lett.* 367 (2013)
490 39–51.
- 491 [13] A. Fichtner, E. Saygin, T. Taymaz, P. Cupillard, Y. Capdeville, J. Tram-
492 pert, The deep structure of the North Anatolian Fault Zone, *Earth Planet.*
493 *Sci. Lett.* 373 (2013) 109–117.
- 494 [14] H. Zhu, E. Bozdağ, J. Tromp, Seismic structure of the European upper
495 mantle based on adjoint tomography, *Geophys. J. Int.* 201 (2015) 18–52.
- 496 [15] E. Bozdag, M. Lefebvre, W. Lei, D. Peter, J. Smith, D. Komatitsch,
497 J. Tromp, Global adjoint tomography: Combining Big Data with HPC
498 Simulations, in: *AGU Fall Meeting*, 2014, pp. S11G–04.
- 499 [16] M. V. Afanasiev, D. Peter, K. Sager, S. Simute, L. Ermert, L. Krischer,
500 A. Fichtner, Foundations for a multiscale collaborative Earth model, *Geo-*
501 *phys. J. Int.* 204 (2016) 39–58.
- 502 [17] D. Michea, D. Komatitsch, Accelerating a three-dimensional finite-
503 difference wave propagation code using gpu graphics cards, *Geophys. J.*
504 *Int.* 182 (2010) 389–402.
- 505 [18] D. Komatitsch, G. Erlebacher, D. Göddeke, D. Michea, High-order finite-
506 element seismic wave propagation modeling with MPI on a large GPU
507 cluster, *J. Comp. Phys.* 229 (2010) 7692–7714.
- 508 [19] D. Komatitsch, Fluid-solid coupling on a cluster of GPU graphics cards for
509 seismic wave propagation, *C. R. Mechanique* 339 (2011) 125–135.

- 510 [20] A. Tarantola, Inversion of seismic reflection data in the acoustic approxi-
511 mation, *Geophysics* 49 (1984) 1259–1266.
- 512 [21] A. Tarantola, Theoretical background for the inversion of seismic wave-
513 forms, including elasticity and attenuation, *Pure Appl. Geophys.* 128 (1988)
514 365–399.
- 515 [22] J. Tromp, C. Tape, Q. Liu, Seismic tomography, adjoint methods, time
516 reversal and banana-doughnut kernels, *Geophys. J. Int.* 160 (2005) 195–
517 216.
- 518 [23] A. Fichtner, H.-P. Bunge, H. Igel, The adjoint method in seismology - I.
519 Theory, *Phys. Earth Planet. Inter.* 157 (2006) 86–104.
- 520 [24] P. Chen, Full-wave seismic data assimilation: Theoretical background and
521 recent advances, *Pure Appl. Geophys.* 168 (2011) 1527–1552.
- 522 [25] D. Komatitsch, J. P. Vilotte, The spectral element method: an effective
523 tool to simulate the seismic response of 2d and 3d geological structures,
524 *Bull. Seism. Soc. Am.* 88 (1998) 368–392.
- 525 [26] D. Komatitsch, J. Tromp, Spectral-element simulations of global seismic
526 wave propagation, part I: validation, *Geophys. J. Int.* 149 (2002) 390–412.
- 527 [27] A. Fichtner, *Full Seismic Waveform Modelling and Inversion.*, Springer,
528 Heidelberg., 2010.
- 529 [28] F. A. Dahlen, J. Tromp, *Theoretical Global Seismology*, Princeton Univer-
530 sity Press. NJ, 1998.
- 531 [29] B. L. N. Kennett, *The seismic wavefield I. - Introduction and theoretical*
532 *development.*, Cambridge University Press., 2001.
- 533 [30] K. Aki, P. Richards, *Quantitative Seismology.*, University Science Books.,
534 2002.

- 535 [31] H. Emmerich, M. Korn, Incorporation of attenuation into time-domain
536 computations of seismic wave fields, *Geophysics* 52 (1987) 1252–1264.
- 537 [32] J. O. A. Robertsson, J. O. Blanch, W. W. Symes, Viscoelastic finite-
538 difference modelling, *Geophysics* 59 (1994) 1444–1456.
- 539 [33] J. O. Blanch, J. O. A. Robertsson, W. W. Symes, Modelling of a constant
540 Q : Methodology and algorithm for an efficient and optimally inexpensive
541 viscoelastic technique, *Geophysics* 60 (1995) 176–184.
- 542 [34] A. Fichtner, M. van Driel, Models and Fréchet kernels for frequency-
543 (in)dependent Q , *Geophys. J. Int.* 198 (2014) 1878–1889.
- 544 [35] M. van Driel, T. Nissen-Meyer, Optimized visco-elastic wave propagation
545 for weakly dissipative media, *Geophys. J. Int.* 199 (2014) 1078–1093.
- 546 [36] E. Crase, A. Pica, M. Noble, J. McDonald, A. Tarantola, Robust elastic
547 nonlinear waveform inversion - Application to real data, *Geophysics* 55
548 (1990) 527–538.
- 549 [37] Y. Luo, G. T. Schuster, Wave-equation travelttime inversion., *Geophysics*
550 56 (1991) 645–653.
- 551 [38] L. S. Gee, T. H. Jordan, Generalized seismological data functionals, *Geo-*
552 *phys. J. Int.* 111 (1992) 363–390.
- 553 [39] A. Fichtner, B. L. N. Kennett, H. Igel, H.-P. Bunge, Theoretical back-
554 ground for continental- and global-scale full-waveform inversion in the time-
555 frequency domain., *Geophys. J. Int.* 175 (2008) 665–685.
- 556 [40] T. van Leeuwen, W. A. Mulder, A correlation-based misfit criterion for
557 wave-equation travelttime tomography, *Geophys. J. Int.* 182 (2010) 1383–
558 1394.
- 559 [41] R. Brossier, S. Operto, J. Virieux, Robust elastic frequency-domain full
560 waveform inversion using the l_1 norm, *Geophys. Res. Lett.* 36 (2009)
561 L20310.

- [42] R. Brossier, S. Operto, J. Virieux, Which data residual norm for robust elastic frequency-domain full waveform inversion?, *Geophysics* 75 (2010) R37–R46.
- [43] A. Griewank, A. Walther, An implementation of checkpointing for the reverse or adjoint mode of computational differentiation, *Trans. Math. Software* 26 (2000) 19–45.
- [44] Z. Alterman, F. C. Karal, Propagation of elastic waves in layered media by finite-difference methods, *Bull. Seis. Soc. Am.* 58 (1968) 367–398.
- [45] D. M. Boore, Love waves in nonuniform waveguides: finite difference calculations, *J. Geophys. Res.* 1970 (1970) 1512–1527.
- [46] P. Moczo, J. Kristek, V. Vavrycuk, R. Archuleta, L. Halada, 3D heterogeneous staggered-grid finite-difference modeling of seismic motion with volume harmonic and arithmetic averaging of elastic moduli, *Bull. Seis. Soc. Am.* 92 (2002) 3042–3066.
- [47] T. Bohlen, Parallel 3-D viscoelastic finite difference modelling, *Comput. Geosci.* 28 (2002) 887–899.
- [48] P. Moczo, J. Kristek, M. Galis, *The finite-difference modelling of earthquake motions: waves and ruptures*, Cambridge University Press, 2014.
- [49] G. Seriani, E. Priolo, Spectral element method for acoustic wave simulation in heterogeneous media, *Finite Elements in Analysis and Design* 16 (1994) 337–348.
- [50] E. Faccioli, F. Maggio, R. Paolucci, A. Quarteroni, 2D and 3D elastic wave propagation by a pseudospectral domain decomposition method, *J. Seismology* 1 (1997) 237–251.
- [51] T. Nissen-Meyer, M. van Driel, S. Stähler, K. Hosseini, S. Hempel, L. Auer, A. Fournier, AxiSEM: broadband 3-D seismic wavefields in axisymmetric media, *Solid Earth* 5 (2014) 425–445.

- 589 [52] J. de la Puente, M. Dumbser, M. Käser, H. Igel, An arbitrary high-order
590 discontinuous galerkin method for elastic waves on unstructured methods
591 - iv. anisotropy, *Geophys. J. Int.* 169 (2007) 1210–1228.
- 592 [53] M. Dumbser, M. Käser, J. de la Puente, Arbitrary high order finite volume
593 schemes for seismic wave propagation on unstructured meshes in 2D and
594 3D, *Geophys. J. Int.* 171 (2007) 665–694.
- 595 [54] M. Dumbser, M. Käser, E. Toro, An arbitrary high-order discontinuous
596 Galerkin method for elastic waves on unstructures meshes, Part V: Local
597 time stepping and p -adaptivity, *Geophys. J. Int.* 171 (2007) 695–717.
- 598 [55] A. Fichtner, B. L. N. Kennett, H. Igel, H.-P. Bunge, Full seismic waveform
599 tomography for upper-mantle structure in the Australasian region using
600 adjoint methods., *Geophys. J. Int.* 179 (2009) 1703–1725.
- 601 [56] J. Díaz, A. Villaseñor, J. Gallart, J. Morales, A. Pazos, D. Córdoba, J. Pul-
602 gar, J. L. García-Lobón, M. Harnafi, TopoIberia Seismic Working Group,
603 The IBERARRAY broadband seismic network: A new tool to investigate
604 the deep structure beneath Iberia, *ORFEUS Newsletter* 8 (2009) 1–6.
- 605 [57] L. Krischer, A. Fichtner, S. Zukauskaitė, H. Igel, Large-scale seismic inver-
606 sion framework, *Seis. Res. Lett.* (2015) in revision.
- 607 [58] A. Fichtner, J. Trampert, P. Cupillard, E. Saygin, T. Taymaz, Y. Capdev-
608 ille, A. Villasenor, Multi-scale full waveform inversion, *Geophys. J. Int.* 194
609 (2013) 534–556.
- 610 [59] V. Babuška, M. Cara, *Seismic anisotropy in the Earth.*, Kluwer Academic
611 Publishers, Dordrecht, Boston, London., 1991.
- 612 [60] M. Panning, B. Romanowicz, A three-dimensional radially anisotropic
613 model of shear velocity in the whole mantle, *Geophys. J. Int.* 167 (2006)
614 361–379.

- 615 [61] A. Fichtner, A. Villasenor, Crust and upper mantle of the western Mediter-
616 ranean - Constraints from full-waveform inversion, *Earth Planet. Sci. Lett.*
617 428 (2015) 52–62.
- 618 [62] M. Rietmann, P. Messmer, T. Nissen-Meyer, D. Peter, P. Basini, D. Ko-
619 matitsch, O. Schenk, J. Tromp, L. Boschi, D. Giardini, Forward and adjoint
620 simulations of seismic wave propagation on emerging large-scale GPU ar-
621 chitectures, in: *International Conference for High Performance Computing,*
622 *Networking, Storage and Analysis, SC, IEEE, 2012*, p. 10.1109/SC.2012.59.