Seismic Wave Propagation in Media with Complex Geometries, Simulation of

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Glossary

Numerical methods Processes in nature are often described by partial differential equations. Finding solutions to those equations is at the heart of many studies aiming at the explanation of observed data. Simulations of realistic physical processes requires generally the use of numerical methods – a special branch of applied mathematics – that approximate the partial differential equations and allows solving them on computers. Examples are the finite-difference, finite-element, or finite-volume methods.

Spectral elements The spectral element method is an extension of the finite element method that makes use of specific basis functions describing the solutions inside each element. These basis functions (e. g., Chebyshev or Legendre polynomials) allow the interpolation of functions exactly at certain collocation points. This is often termed spectral accuracy.

Discontinuous Galerkin method The discontinuous Galerkin method is a flavor of the finite-element method that allows discontinuous behavior of the spatial or temporal fields at the element boundaries. The discontinuities – that might be small in the case of continuous physical fields such as seismic waves – then define so-called Riemann problems that can be handled using the concepts from finite-volume techniques. Therefore, the approximate solution is updated via numerical fluxes across the element boundaries.

Parallel algorithms All modern supercomputers make use of parallel architectures. This means that a large number of processors are performing (different) tasks on different data at the same time. Numerical algorithms need to be adapted to these hardware architectures by using specific programming paradigms (e. g., the message passing interface MPI). The computational efficiency of such algorithms strongly depends on the specific parallel nature of the problem to be solved, and the requirement for inter-processor communication.

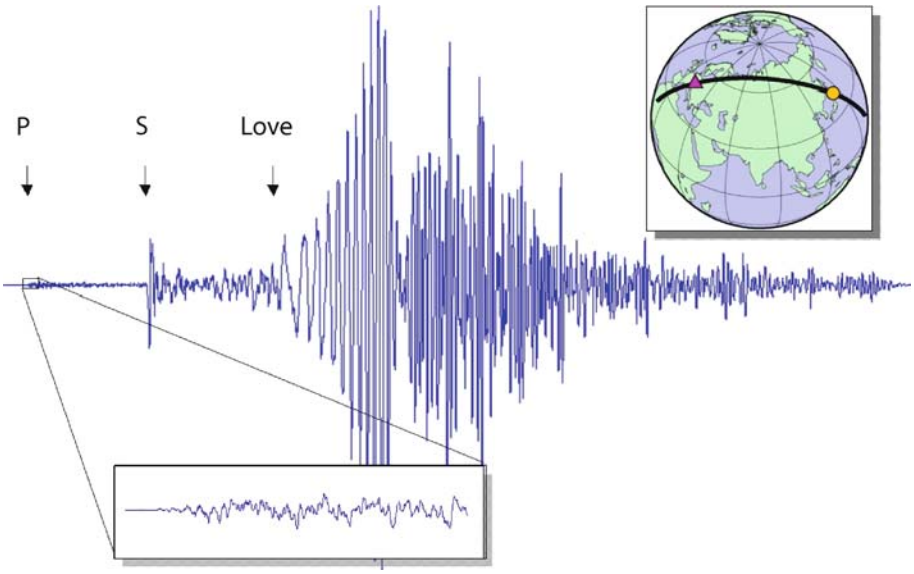
Grid generation Most numerical methods are based on the calculation of the solutions at a large set of points (grids) that are either static or depend on time (adaptive grids). These grids often need to be adapted to the specific geometrical properties of the objects to be modeled (volcano, reservoir, globe). Grids may be designed to follow domain boundaries and internal surfaces. Before specific numerical solvers are employed the grid points are usually connected to form triangles or rectangles in 2D or hexahedra or tetrahedra in 3D.

Definition of the Subject

Seismology is the science that aims at understanding the Earth's interior and its seismic sources from measurements of vibrations of the solid Earth. The resulting images of the physical properties of internal structures and the spatio-temporal behavior of earthquake rupture processes are prerequisites to understanding the dynamic evolution of our planet and the physics of earthquakes. One of the key ingredients to obtain these images is the calculation of synthetic (or theoretical) seismograms for given earthquake sources and internal structures. These synthetic seismograms can then be compared quantitatively with observations and acceptable models be searched for using the theory of inverse problems. The methodologies to calculate synthetic seismograms have evolved dramatically over the past decades in parallel with the evolution of computational resources and the ever increasing volumes of permanent seismic observations in global and regional seismic networks, volcano monitoring networks, and experimental campaigns. Today it is a tremendous challenge to extract an optimal amount of information from seismograms. The imaging process is still primarily carried out using ray theory or extensions thereof not fully taking into account the complex scattering processes that are occurring in nature.

To model seismic observations in their full complexity we need to be able to simulate wave propagation through 3D structures with constitutive relations that account for anisotropic elasticity, attenuation, porous media as well as complex internal interfaces such as layer boundaries or fault systems. This implies that numerical methods have to be employed that solve the underlying partial differential equations on computational grids. The high-frequency oscillatory nature of seismic wave fields makes this an expensive endeavor as far as computational resources are concerned. As seismic waves are propagating hundreds of wavelengths through scattering media, the required accuracy of the numerical approximations has to be of the highest possible order. Despite the fact that the physics of wave propagation is well understood, only recently computational algorithms are becoming available that allow us to accurately simulate wave propagation on many scales such as reservoirs, volcanoes, sedimentary basins, continents, and whole planets.

In addition to the imaging problem for subsurface structure and earthquake sources, the possibilities for 3D wave simulations have opened a new route to forecasting strong ground motions following large earthquakes in seismically active regions. In the absence of any hope to deterministically predict earthquakes, the calculation



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 1
Transverse velocity seismogram of the M8.3 Tokachi-Oki earthquake near Hokkaido observed at station WET in Germany with a broadband seismometer. The total seismogram length is one hour. Arrival times of body wave phases (P, S) and the onset of transversely polarized surface (Love) waves are indicated

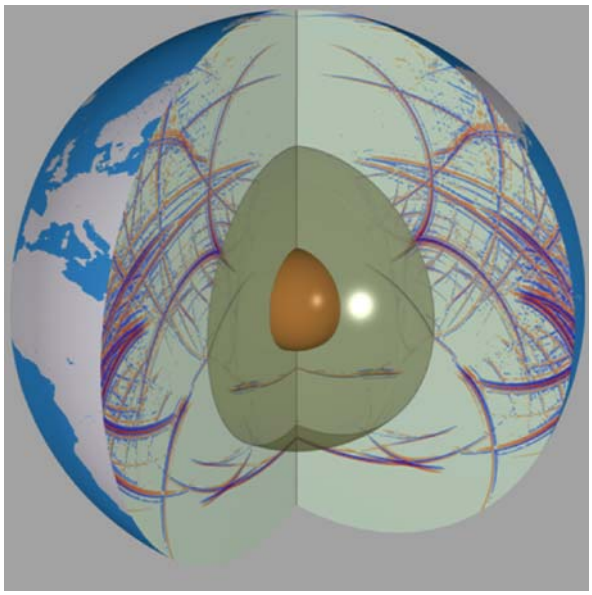
of earthquake scenarios in regions with sufficiently well known crustal structures and fault locations will play an important role in mitigating damage particularly due to potentially amplifying local velocity structures. However, to be able to employ the advanced 3D simulation technology in an efficient way, and to make use of the fast advance of supercomputing infrastructure, a paradigm shift in the concept of wave simulation software is necessary: The Earth science community has to build soft infrastructures that enable massive use of those simulation tools on the available high-performance computing infrastructure.

In this paper we want to present the state of the art of computational wave propagation and point to necessary developments in the coming years, particularly in connection with finding efficient ways to generate computational grids for models with complex topography, faults, and the combined simulation of soil and structures.

Introduction

We first illustrate the evolution of methodologies to calculate and model aspects of seismic observations for the case of global wave propagation. Seismology can look back at almost 50 years of systematic observations of earthquake induced teleseismic ground motions with the standardized global seismic and regional networks. The digital revolution in the past decades has altered the recording culture such that now seismometers are recording ground motions permanently rather than in trigger-mode, observations are becoming available in near-real time, and – because of the required sampling rates – the daily amount of observations automatically sent to the data centers is gigantic. If we take a qualitative look at a seismic observation (Fig. 1) we can illustrate what it takes to model either part or the whole information contained in such physical measurements.

In Fig. 1 a seismogram observed using a broadband seismometer (station WET in Germany) is shown. Globally observed seismograms following large earthquakes contain frequencies up to 1 Hz (P-wave motions) down to periods of around one hour (eigenmodes of the Earth) in which case modeling is carried out in the frequency domain. Seismograms of the kind shown in Fig. 1 contain many types of information. For large earthquakes the first part of the seismogram (inlet) contains valuable information on the spatio-temporal evolution of the earthquake rupture on a finite-size fault. A model of the fault slip history is a prerequisite to model the complete wave form of seismograms as the whole seismogram is affected by it unless severe low-pass filtering is applied. Information on the global seismic velocity structure is contained in the arrival times of numerous body-wave phases (here only P- and S-wave arrivals are indicated) and in the dispersive behavior of the surface waves (here the onset of the low-frequency Love waves is indicated). Further information is contained in the characteristics of the coda to body wave phases in-



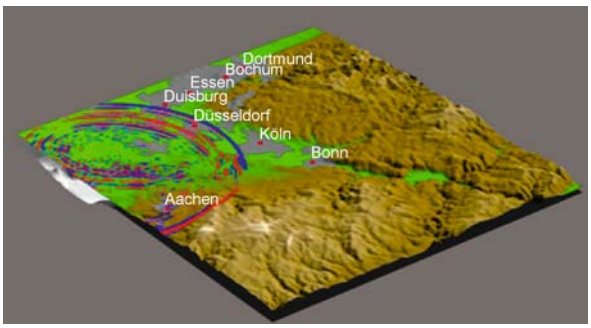
Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 2
Snapshot of wave propagation inside the Earth approx. 25 minutes after an earthquake occurs at the top part of the model. The radial component of motion is shown (blue and red denote positive and negative velocity, resp.). The simulation was carried out using an axi-symmetric approximation to the wave equation [55,58] and high-order finite-differences. Motion is allowed in the radial and horizontal directions. This corresponds to the P-SV case in 2D cartesian calculations. Therefore the wavefield contains both P- and S-waves and phase conversions

dicative of scattering in various parts of the Earth (see [62] for an account of modern observational seismology).

Adding a temporal and spatial scale to the above qualitative discussion reveals some important insight what it takes to simulate wave propagation on a planetary scale using grid-based numerical methods. Given the maximum frequency of around 1 Hz (P-waves) and 0.2 Hz (S-waves) the minimum wavelength in the Earth is expected to be O(km), requiring O(100 m) type grid spacing at least in the crustal part of the Earth leading to $O(10^{12})$ necessary grid points (or volume elements) for accurate numerical simulations. This would lead to memory requirements O(100 TByte) that are today possible on some of the world's largest supercomputers. The message here is that despite the rapid evolution of computational power, the complete modeling of teleseismic observations using approaches such as spectral elements (e. g., [63,64]) requiring tremendous numbers of calculations to constrain structure and sources will remain a grand challenge for some time to come. However, in many cases it is not necessary or not even desirable to simulate or model the whole seismogram, i. e. the complete observed frequency band. If we lower the cutoff frequency to 0.1 Hz (period 10 s), the required memory drops down to O(100 GByte). Such calculations can be done today on PC-clusters that can be inexpensively assembled and run on an institutional level (e. g., [8]). In addition, it means that the massive use of such forward simulations for imaging purposes and phenomenological investigations of wavefield effects is around the corner. This does not only apply to wave propagation or imaging on a planetary scale but in the same way to problems in volcanology, regional seismology, and exploration geophysics.

An illustration of global wave simulations using the finite difference method (e. g., [14,54,55,58,109,110,114]) is shown in Fig. 2 (more details on the methodologies are given in Sect. "The Evolution of Numerical Methods and Grids"). The snapshot of the radial component of motion at a time when the direct P-wave has almost crossed the Earth reveals the tremendous complexity the wave field exhibits even in the case of a spherically symmetric Earth model (PREM, [37]). The wavefield with a dominant period of ca. 15 seconds also highlights the short wavelengths that need to be propagated over very large distances. This is the special requirement for computational wave propagation that is quite different in other fields of computational Earth Sciences. While the theory of linear elastic wave propagation is well understood and most numerical methods have been applied to it in various forms, the accuracy requirements are so high that – particularly when models with complex geometrical features need to be modeled – there are still open questions as to what works best. One of the main goals of this paper is to highlight the need to focus on the grid generation process for various types of computational grid cells (e. g., rectangular, triangular in 2D, and hexahedral and tetrahedral in 3D) and the interface to appropriate highly accurate solvers for wave propagation problems.

As mentioned above computational modeling of strong ground motions following large earthquakes (see Fig. 3 for an illustration) is expected to play an increasingly important role in producing realistic estimates of shaking hazard. There are several problems that are currently unsolved: (1) to achieve frequencies that are interesting for earthquake engineers in connection with structural damage the near surface velocity structure needs to be known and frequencies beyond 5 Hz need to be calculated. In most cases this structure is not well known (on top of the uncertainties of the lower basin structures) and the required frequencies demand extremely large computational models. (2) In addition to structural uncertain-



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 3
Snapshot (horizontal component) for a simulation of the M5.9 Roermond earthquake in the Cologne Basin in 1992 [38]. The 3D sedimentary basin (maximum depth 2 km) leads to strong amplification and prolongation of the shaking duration that correlates well with basin depth. Systematic calculations may help mitigating earthquake induced damage

ties, there are strong dependencies on the particular earthquake rupture process that influence the observed ground motions. This suggests that many 3D calculations should be carried out for any characteristic earthquake of interest, to account for such variations (e. g., Wang et al. 2006). (3) The large velocity variations (e. g., 300 m/s up to 8 km/s) require locally varying grid densities which is difficult to achieve with some of the classical numerical methods in use (e. g. finite differences). Some of the potential routes are developed below.

In summary, computational simulation of 3D wave propagation will be more and more a central tool for seismology with application in imaging problems, earthquake rupture problems, questions of shaking hazard, volcano seismology and planetary seismology. In the following we briefly review the history of the application of numerical methods to wave propagation problems and the evolution of computational grids. The increasing complexity of models in terms of geometrical features and range of physical properties imposes the use of novel methodologies that go far beyond the initial approximations based on finite differences.

The Evolution of Numerical Methods and Grids

In this section we give a brief history of the application of numerical methods to the problem of seismic wave propagation. Such a review can not be complete, certainly gives a limited perspective, and only some key references are given. One of the points we would like to highlight is the evolution of the computational grids that are being employed for wave propagation problems and the consequences on the numerical methods of choice now and in the future.

Why do we need numerical approximations to elastic wave propagation problems at all? It is remarkable what we learned about the Earth without them! In the first decades in seismology, modeling of seismic observations was restricted to the calculation of ray-theoretical travel times in spherically symmetric Earth models (e. g., [13,16]). With the advent of computing machines these approaches could be extended to 2D and 3D media leading to ray-theoretical tomography and the images of the Earth's interior that we know today (e. g., [115]). The analytical solution of wave propagation in spherical coordinates naturally leads to spherical harmonics and the possible quasi-analytical solution of wave propagation problems in spherically symmetric media using normal modes. As this methodology leads to complete waveforms the term "waveform inversion" was coined for fitting the waveforms of surface waves by correcting the phase differences for surface waves at particular frequencies (e. g., [118]). This allowed the recovery of seismic velocity models particularly of crust and upper mantle (surface wave tomography). A similar approach in Cartesian layered geometry led to complete solutions of the wave equation in cylindrical coordinates through the summation of Bessel functions, the reflectivity method [46]. This method was later extended to spherical media through the Earth-flattening transformation [85]. Recently, ray-theory was extended allowing the incorporation of finite-frequency effects (e. g., [84]). The impact on the imaging process is still being debated.

Most of these methods are still today extremely valuable in providing first estimates of 2D or 3D effects and are important for the use in standard seismic processing due to their computational efficiency. Nevertheless, with the tremendous improvements of the quality of seismic observations we strive today to extract much more information on Earth's structure and sources from recorded waveforms. As waveforms are in most places strongly affected by 3D structural variations the application of numerical methods that solve "directly" the partial differential equations descriptive of wave propagation becomes mandatory. This necessity was recognized early on and the developments of numerical wave propagation began in the sixties of the 20th century.

Numerical Methods Applied to Wave Propagation Problems

The finite-difference technique was the first numerical method to be intensively applied to the wave propagation

problem (e. g., [1,6,61,77,82,83,88,89,116,117]). The partial differentials in the wave equation are replaced by finite differences leading to an extrapolation scheme in time that can either be implicit or explicit. The analysis of such simple numerical schemes led to concepts that are central to basically all numerical solutions of wave propagation problems. First, the discretization in space and time introduces a scale into the problem with the consequence that the numerical scheme becomes dispersive. This numerical dispersion – for the originally non-dispersive problem of purely elastic wave propagation – has the consequence that for long propagation distances wave pulses are no longer stable but disperse. The consequence is, that in any simulation one has to ascertain that enough grid points per wavelength are employed so that numerical dispersion is reduced sufficiently. Finding numerical schemes that minimize these effects has been at the heart of any new methodology ever since. Second, the so-called CFL criterion [24] that follows from the same theoretical analysis of the numerical scheme basically relates a "grid velocity" – the ratio between the space and time increments $\mathrm{d}x$ and $\mathrm{d}t$, respectively – to the largest physical velocity c in the model. In order to have a stable calculation, this ratio has to be smaller than a constant ε that depends on the specific scheme and the space dimension

$$c\frac{\mathrm{d}t}{\mathrm{d}x} \leq \varepsilon \,. \tag{1}$$

This simple relationship has important consequences: When the grid spacing $\mathrm{d}x$ must be small, because of model areas with low seismic velocities, then the time step $\mathrm{d}t$ has to be made smaller accordingly leading to an overall increase in the number of time steps and thus overall computational requirements. In addition, the early implementations where based on regular rectangular grids, implying that large parts of the model where carrying out unnecessary calculations. As shown below local time-stepping and local accuracy are important ingredients in efficient modern algorithms.

The fairly inaccurate low order spatial finite-difference schemes were later extended to high-order operators [26,48,49,50,51,56,76,103]. Nevertheless, the required number of grid points per wavelength was still large, particularly for long propagation distances. This has led to the introduction of pseudo-spectral schemes, "pseudo" because only the calculations of the derivatives where done in the spectral domain, but the wave equation was still solved in the space-time domain with a time-extrapolation scheme based on finite differences [10,45,47,67]). The advantage of the calculation of derivatives in the spectral domain is at hand: The Fourier theorem tells us that by multiplying the spectrum with ik, i being the imaginary unit and k the wavenumber, we obtain an *exact* derivative (exact to numerical precision) on a regular set of grid points. This sounds attractive. However, there are always two sides to the coin. The calculation requires FFTs to be carried out extensively and the original "local" scheme becomes a "global" scheme. This implies that the derivative at a particular point in the computational grid becomes dependent on any other point in the grid. This turns out to be computationally inefficient, in particular on parallel hardware. In addition, the Fourier approximations imply periodicity which makes the implementation of boundary conditions (like the free surface, or absorbing boundary conditions) difficult.

By replacing the basis functions (Fourier series) in the classical pseudo-spectral method with Chebyshev polynomials that are defined in a limited domain $(-1,1)$ the problem with the implementation of boundary problems found an elegant solution (e. g., [66,107,108]). However, through the irregular spacing of the Chebyshev collocation points (grid densification at the domain boundaries, see section below) new problems arose with the consequence that this approach was not much further pursued except in combination with a multi-domain approach in which the field variables exchange their values at the domain boundaries (e. g., [108]).

So far, the numerical solutions described are all based on the *strong* form of the wave equation. The finite-element method is another main scheme that found immediate applications to wave propagation problems (e. g., [79]). Finite element schemes are based on solving the *weak* form of the wave equation. This implies that the space- and time-dependent fields are replaced by weighted sums of basis (also called trial) functions defined inside elements. The main advantage of finite element schemes is that elements can have arbitrary shape (e. g., triangular, trapezoidal, hexahedral, tetrahedral, etc.). Depending on the polynomial order chosen inside the elements the spatial accuracy can be as desired. The time-extrapolation schemes are usually based on standard finite differences. There are several reasons why finite-element schemes were less widely used in the field of wave propagation. First, in the process a large system matrix needs to be assembled and must be inverted. Matrix inversion in principle requires global communication and is therefore not optimal on parallel hardware. Second, in comparison with the finite-element method, finite- difference schemes are more easily coded and implemented due to their algorithmic simplicity.

A tremendous step forward was the introduction of basis functions inside the elements that have spectral accuracy, e. g., Chebyshev or Legendre polynomials [11,15,39,40,65,86,90,98]. The so-called spectral element scheme became particularly attractive with the discovery that – by using Legendre polynomials – the matrices that required inversion became diagonal [65]. This implies that the scheme does no longer need global communication, it is a local scheme in which extrapolation to the next time step can be naturally parallelized. With the extension of this scheme to spherical grids using the cubed-sphere discretization [63,64] this scheme is today the method of choice on many scales unless highly complex models need to be initiated.

Most numerical schemes for wave propagation problems were based on regular, regular stretched, or hexahedral grids. The numerical solution to unstructured grids had much less attention, despite the fact that highly complex models with large structural heterogeneities seem to be more readily described with unstructured point clouds. Attempts were made to apply finite volume schemes to this problem [31], and other concepts (like natural neighbor coordinates [7] to find numerical operators that are applicable on unstructured grids [72,73,78]). These approaches were unfortunately not accurate enough to be relevant for 3D problems. Recently, a new flavor of numerical method found application to wave propagation on triangular or tetrahedral grids. This combination of a discontinuous Galerkin method with ideas from finite volume schemes [33,70] allows for the first time arbitrary accuracy in space and time on unstructured grids. While the numerical solution on tetrahedral grids remains computationally slower, there is a tremendous advantage in generating computational grids for complex Earth models. Details on this novel scheme are given below.

Before presenting two schemes (spectral elements and the discontinuous Galerkin method) and some applications in more detail we want to review the evolution of grids used in wave propagation problems.

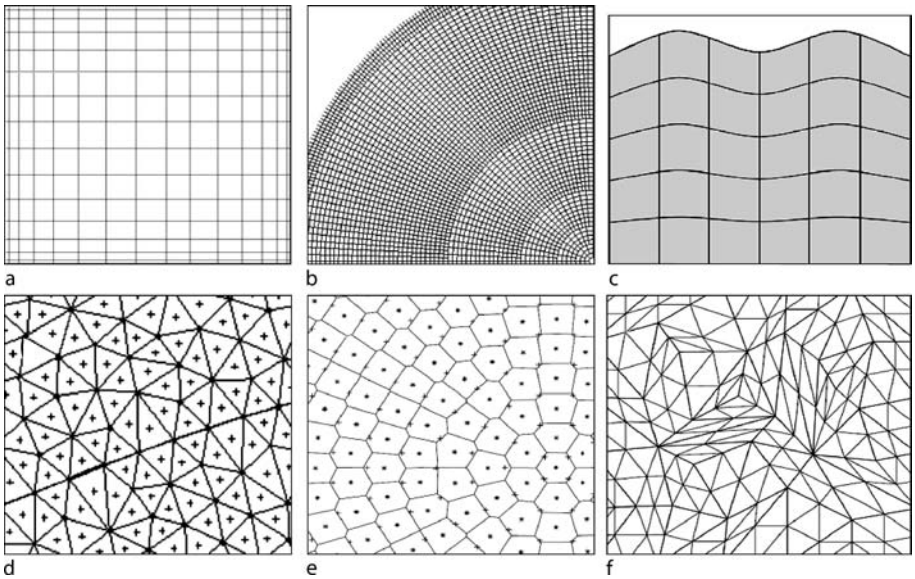
Grids for Wave Propagation Problems

The history of grid types used for problems in computational wave propagation is tightly linked to the evolution of numerical algorithms and available computational resources. The latter in the sense that – as motivated in the introduction – even today realistic simulations of wave propagation are still computationally expensive. This implies that it is not sufficient to apply stable and simple numerical schemes and just use enough grid points per wavelength and/or extremely fine grids for geometrically complex models. Optimal mathematical algorithms that minimize the computational effort are still sought for as the recent developments show that are outlined in the following sections.

In Fig. 4 a number of different computational grids in two space dimensions is illustrated. The simple-most equally-spaced regular finite-difference grid is only of practical use in situations without strong material discontinuities. With the introduction of the pseudospectral method based on Chebyshev polynomials grids as shown in Fig. 4a grids appeared that are denser near the domain boundaries and coarse in the interior. While this enabled a much more efficient implementation of boundary conditions the ratio between the size of the largest to the smallest cell depends on the overall number of grid points per dimension and can be very large. This leads to very small time steps, that can in some way be compensated by grid stretching [9] but overall the problem remains. An elegant way of allowing grids to be of more practical shape is by stretching the grids using analytical functions (Fig. 4c, this basically corresponds to a coordinate transformation, e. g., [50,107]). By doing this either smooth surface topography or smoothly varying internal interfaces can be followed by the grid allowing a more efficient simulation of geometrical features compared to a blocky representation on standard finite difference grids.

The problem of global wave propagation using spherical coordinates (here in the two-dimensional, axi-symmetric approximation) nicely illustrates the necessity to have spatially varying grid density (e. g., [42,43,53,59,89,109]). The grid shown in Fig. 4b demonstrates that in spherical coordinates a regular discretization leads to grid distances that get smaller and smaller towards the center of the Earth. This is in contrast to what is required to efficiently model the Earth's velocity structure: Velocities are small near the surface (requiring high grid density) and increase towards the center of the Earth (requiring low grid density). One way of adjusting is by re-gridding the mesh every now and then, in this case doubling the grid spacing appropriately. This is possible, yet it requires interpolation at the domain boundaries that slightly degrades the accuracy of the scheme.

The problems with grid density and complex surfaces cry for the use of so-called unstructured grids. Let us define an unstructured grid as an initial set of points (a point cloud), each point characterized by its spatial coordinates. We wish to solve our partial differential equations on this point set. It is clear that – with appropriate grid generation software – it is fairly easy to generate such grids that obey exactly any given geometrical constraints be it in connection with surfaces or velocity mod-

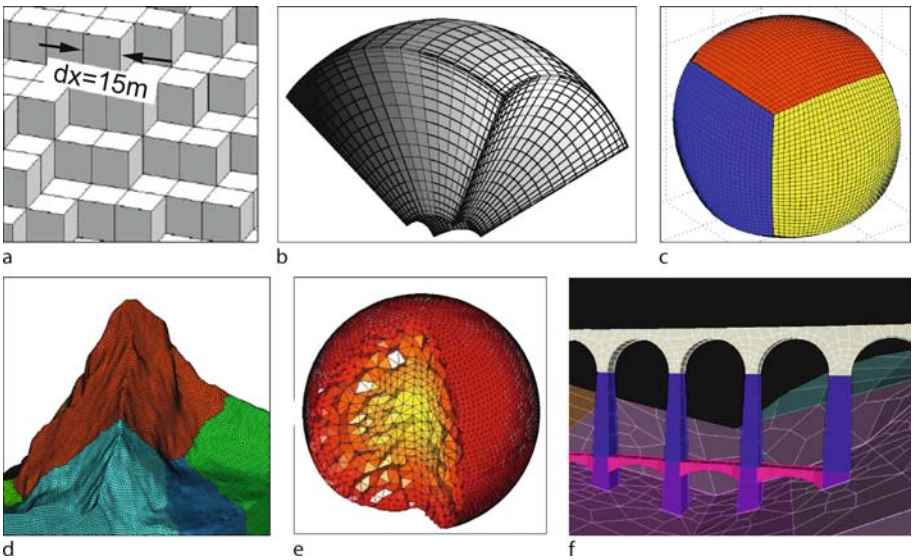


Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 4
Examples of 2D grids used for wave propagation simulations. a Chebyshev grid with grid densification near the domain boundaries. b Multidomain finite-difference grid in regular spherical coordinates. c Stretched regular finite-difference grid that allows following smoothly varying interface or surface boundaries. d Triangular staggered grid following an interface that allows finite-difference type operators. e Unstructured grid with associated Voronoi cells for calculations using the finite-volume method. f Triangular cells for finite-element type calculations. See text for details and references

els (i. e., varying grid density). It is important to note that such point clouds cannot be represented by 2D or 3D matrices as is the case for regular or regular stretched grid types. This has important consequences for the parallelization of numerical schemes. The first step after defining a point set is to use concepts from computational geometry to handle the previously unconnected points. This is done through the idea of Voronoi cells, that uniquely define triangles and their neighbors (Delauney triangulation). In Fig. 4d an example is shown for a triangular grid that follows an internal interface [72]. For finite-difference type operators on triangular grids a grid-staggering makes sense. Therefore, velocities would be defined in the center of triangles and stresses at the triangle vertices. Voronoi cells (Fig. 4e) can be used as volumetric elements for finite volume schemes [31,73]. For finite-element schemes triangular elements (Fig. 4f, e. g., [70]) with appropriate triangular shape functions are quite standard but have not found wide applications in seismology.

If the grid spacing of a regular finite-difference grid scheme in 3D would have to be halved this would result in an overall increase of computation time by a factor of 8 (a factor 2 per space dimension and another factor 2 because of the necessary halving of the time step). This simply means that the accuracy of a specific numerical scheme and the saving in memory or computation time is much more relevant in three dimensions. The evolution of grids in three dimensions is illustrated with examples in Fig. 5. A geometrical feature that needs to be modeled correctly particularly in volcanic environments is the free surface. With standard regular-spaced finite-difference schemes only a stair-step representation of the surface is possible (Fig. 5a, e. g., [87,92]). While the specific numerical implementation is stable and converges to the correct solution a tremendous number of grid points is necessary to achieve high accuracy.

Chebyshev grids and regular grids were applied to the problem of wave propagation in spherical sections (Fig. 5b, e. g., [52,57]). The advantage of solving the problem in spherical coordinates is the natural orthogonal coordinate system that facilitates the implementation of boundary conditions. However, due to the nature of spherical coordinates the physical domain should be close to the equator and geographical models have to be rotated accordingly. A highly successful concept for wave propagation in spherical media was possible through the adoption of the cubed-sphere approach in combination with spectral-elements (Fig. 5c, [63,64]). The cubed-sphere discretization is based on hexahedral grids. Towards the center of the Earth the grid spacing is altered to keep the number of elements per wavelength approximately constant.



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 5
Examples of 3D grids. a Stair-step representation of a complex free surface with finite-difference cells. b Chebyshev grid in spherical coordinates for a spherical section. c Cubed sphere grid used for spectral-element and multi-domain Chebyshev calculations. d Tetrahedral grid of the Matterhorn. e Tetrahedral grid of the Earth's interior with the grid density tied to the velocity model. f Hexahedral grid of bridge structure and subsurface structure for spectral-element calculations. See text for details and references

Computational grids for wave propagation based on tetrahedra (Fig. 5d,e) are only recently being used for seismic wave propagation in combination with appropriate numerical algorithms such as finite volumes [34] or discontinuous Galerkin (e. g., [70]). The main advantage is that the grid generation process is greatly facilitated when using tetrahedra compared to hexahedra. Generating point clouds that follow internal velocity structures and connecting them to tetrahedra are straight forward and efficient mathematical computations. However, as described in more detail below, tetrahedral grids require more involved computations and are thus less efficient than hexahedral grids. Complex hexahedral grids – even for combined modeling of structure and soil (Fig. 5f) are possible but – at least at present – require a large amount of manual interaction during the grid generation process. It is likely that the combination of both grid types (tetrahedral in complex regions, hexahedral in less complex regions) will play an important role in future developments.

In the following we would like to present two of the most competitive schemes presently under development, (1) the spectral element method and (2) the discontinuous Galerkin approach combined with finite-volume flux schemes. The aim is to particularly illustrate the role of the grid generation process and the pros and cons of the specific methodologies.

3D Wave Propagation on Hexahedral Grids: Soil-Structure Interactions

We briefly present the spectral element method (SEM) based on Lagrange polynomials, focusing only on its main features and on its implementation for the solution of the elasto-dynamic equations. The SEM can be regarded as a generalization of the finite element method (FEM) based on the use of high order piecewise polynomial functions. The crucial aspect of the method is the capability of providing an arbitrary increase in spatial accuracy simply enhancing the algebraic degree of these functions (the spectral degree SD). On practical ground, this operation is completely transparent to the users, who limit themselves to choosing the spectral degree at runtime, leaving to the computational code the task of building up suitable quadrature points for integration and new degrees of freedom. Obviously, the increasing spectral degree implies raising the required computational effort.

On the other hand, one can also play on the grid refinement to improve the accuracy of the numerical solution, thus following the standard finite element approach. Spectral elements are therefore a so-called "$h-p$" method, where "h" refers to the grid size and "p" to the degree of polynomials. Referring to Faccioli et al. [40], Komatitsch and Vilotte [65], Chaljub et al. [15] for further details, we briefly remind in the sequel the key features of the spectral

element method adopted. We start from the wave equation for the displacement $\boldsymbol{u}$:

$$\rho \frac{\partial \boldsymbol{u}^2}{\partial t^2} = \operatorname{div} \sigma_{ij}(\boldsymbol{u}) + f \,, \quad i, j = 1 \ldots \mathrm{d}(\mathrm{d} = 2, 3) \quad (2)$$

where t is the time, $\rho = \rho(x)$ the material density, $f = f(x, t)$ a known body force distribution and σ_{ij} the stress tensor. Introducing Hooke's law:

$$\sigma_{ij}(\boldsymbol{u}) = \lambda \operatorname{div} \boldsymbol{u} \delta_{ij} + 2\mu \varepsilon_{ij}(\boldsymbol{u}) \,, \quad (3)$$

where

$$\varepsilon_{ij}(\boldsymbol{u}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (4)$$

is the strain tensor, λ and μ are the Lamé coefficients, and δ_{ij} is the Kronecker symbol, i. e. $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$, otherwise.

As in the FEM approach, the dynamic equilibrium problem for the medium can be stated in the weak, or variational form, through the principle of virtual work [121] and through a suitable discretization procedure that depends on the numerical approach adopted, can be written as an ordinary differential equations system with respect to time:

$$[M]\, \ddot{\boldsymbol{U}}(t) + [K]\, \boldsymbol{U}(t) = \boldsymbol{F}(t) + \boldsymbol{T}(t) \quad (5)$$

with matrices $[M]$ and $[K]$, respectively the mass and stiffness matrices, and vectors $\boldsymbol{F}$ and $\boldsymbol{T}$ representing the contributions of external forces and traction conditions, respectively. In our SE approach, $\boldsymbol{U}$ denotes the displacement vector at the Gauss–Lobatto–Legendre (GLL) nodes, that correspond to the zeroes of the first derivatives of Legendre polynomial of degree N. The advancement of the numerical solution in time is provided by the explicit 2nd order leap-frog scheme. This scheme is conditionally stable and must satisfy the well known and already mentioned Courant–Friedrichs–Levy (CFL) condition. The key features of the SE discretization are described in the following.

Like in the FEM standard technique, the computational domain may be split into quadrilaterals in 2D or hexahedra in 3D, both the local distribution of grid points within the single element and the global mesh of all the grid points in the domain must be assigned. Many of these grid points are shared amongst several spectral elements. Each spectral element is obtained by a mapping of a master element through a suitable transformation and all computations are performed on the master element. Research is in progress regarding the introduction of triangular spectral elements [80]. The nodes within the element where displacements and spatial derivatives are computed, on which volume integrals are evaluated, are not necessarily equally spaced (similar to the Chebyshev approach in pseudospectral methods mentioned above). The interpolation of the solution within the element is done by Lagrange polynomials of suitable degree. The integration in space is done through Gauss–Lobatto–Legendre quadrature formula.

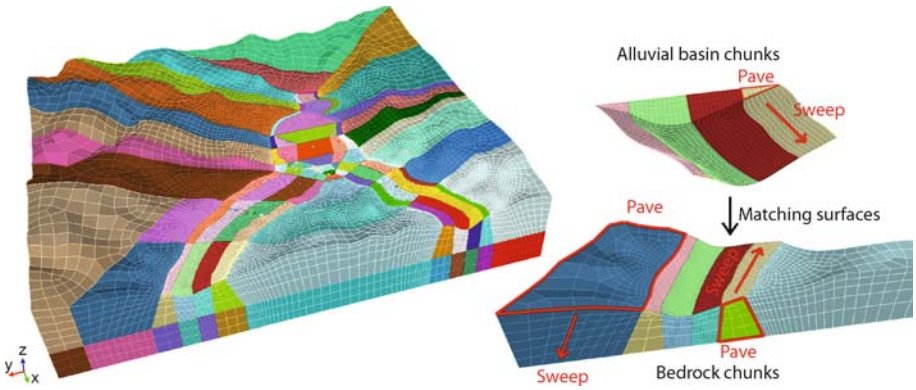
Thanks to this numerical strategy, the exponential accuracy of the method is ensured and the computational effort minimized, since the mass matrix results to be diagonal. The spectral element (SE) approach developed by Faccioli et al. [40] has been recently implemented in the computational code GeoELSE (GeoELasticity by Spectral Elements) [93,102,120] for 2D/3D wave propagation analysis. The most recent version of the code includes: (i) the capability of dealing with fully unstructured computational domains, (ii) the parallel architecture, and (iii) visco-plastic constitutive behavior [30]. The mesh can be created through an external software (e. g., CUBIT [25]) and the mesh partitioning is handled by METIS [81].

Hexahedral Grids

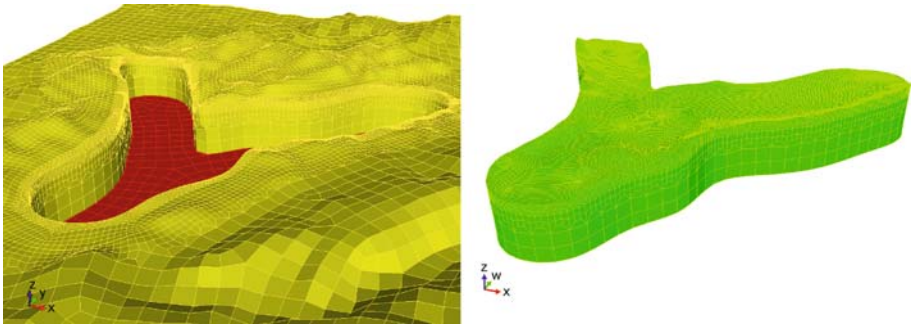
As already mentioned in the SEM here presented the computational domain is decomposed into a family of non overlapping quadrilaterals in 2D or hexahedra in 3D. The grid discretization should be suitable to accurately propagate up to certain frequencies. Obviously, owing to the strong difference of the mechanical properties between soft-soil and stiff-soil (or building construction material) and to the different geometrical details as well, the grid refinement needed in the various parts of the model varies substantially. Therefore, a highly unstructured mesh is needed to minimize the number of elements. While 3D unstructured tetrahedral meshes can be achieved quite easily with commercial or non commercial software, the creation of a 3D non structured hexahedra mesh is still recognized as a challenging problem. In the following paragraph we provide state of the art results concerning the mesh creation.

Grid Generation

Hexahedral grids have more severe restrictions in meshing efficiently. This is basically related to the intrinsic difficulty that arises from the mapping of the computational domain with this particular element. As a consequence automatic procedures have difficulty capturing specific boundaries, create poor quality elements, the assigned size is difficult to be preserved and the generation process is usually much slower compared to the tetrahedral mesh generation algo-



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 6
3D numerical model used for the simulations of ESG06 "Grenoble Benchmark". "Honoring" technique: The computational domain is subdivided into small chunks and each one is meshed starting from the alluvial basin down to the bedrock. For simplicity only the spectral elements are shown without GLL nodes



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 7
3D numerical model used for the simulations of ESG06 "Grenoble Benchmark". "Not Honoring" technique: The computational domain is meshed with a coarse mesh and then refined twice approximately in the area where the alluvial basin is located

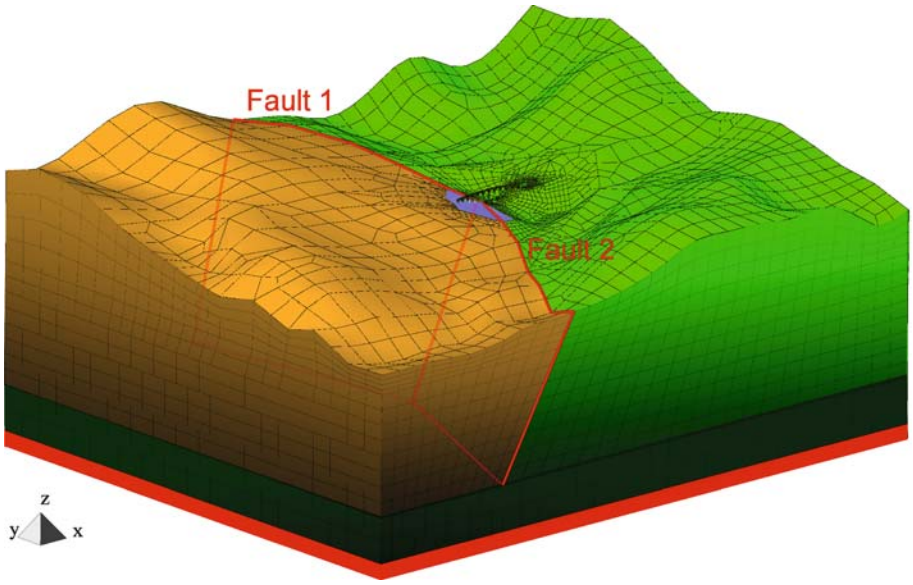
rithms. On the other hand the advantages of hexahedral meshes are usually related to the lower computational cost of the wave propagation solutions with respect to the one based on triangular meshes or hexahedral structured grids (like in the finite difference method).

Nevertheless certain problems can be addressed reasonably well with specific solutions. A quite typical case in earthquake seismology is the study of the alluvial basin response under seismic excitation. In handling this problem, a first strategy is to try to "honor" the interface between the sediment (soft soil) and the bedrock (stiff soil). The two materials are divided by a physical interface and the jump in the mechanical properties is strictly preserved. The major drawback of this approach is that usually it requires strong skills from the user to build-up the mesh and a significant amount of working time (Fig. 6). Given that the "honoring approach" is not always feasible in a reasonable time (or with a reasonable effort) a second strategy is worth to be mentioned: The so called "not honoring" procedure. In this second case the mesh is refined in proximity of the area where the soft deposit are localized but the elements do not respect the interface. On a practical ground the mechanical properties are assigned node by node and the sharp jump is smoothed through the Lagrange interpolation polynomial and substituted with smeared interfaces (Fig. 7). At the present time it is still strongly under debate if it is worth to honor or not the physical interfaces.

Finally, we highlight the fact that meshing software (e. g., CUBIT [25]) is available that seems to be extremely promising and potentially very powerful for the creation of geophysical and seismic engineering unstructured hexahedral meshes. Further very interesting mesh generation procedures based on hexahedral are under investigation [99].

Scale Problem with Structure and Soil

In engineering practice one of the most common approaches to design buildings under seismic load is the im-

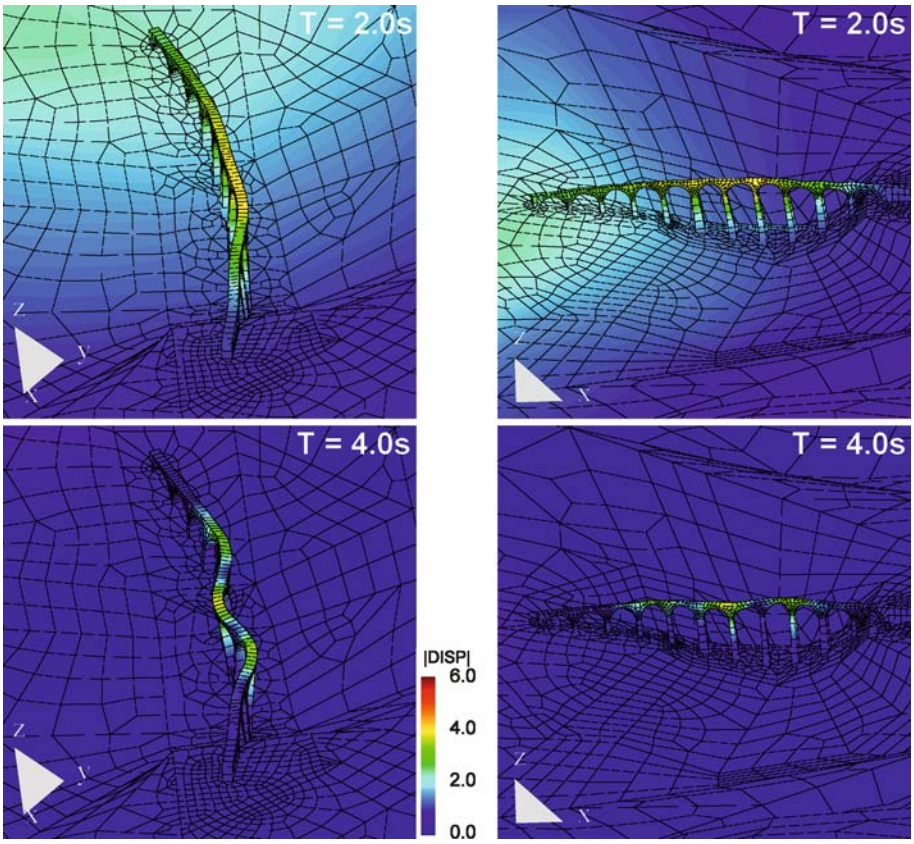


Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 8
3D model of Acquasanta bridge and the surrounding geological configuration. The investigated area is 2 km in length, 1.75 km in width and 0.86 km in depth. The model was designed to propagate waves up to 5 Hz with a SD = 3 (Order 4) and has 38,569 hexahedral elements and 1,075,276 grid points. The contact between calcareous schists (*brown color*) and serpentine rocks (*green color*) is modeled with two sub-vertical faults (*red-line*). *Cyan color* represents the alluvial and weathered deposits

position of an acceleration time history to the structure, basically acting like an external load. An excellent example of this technique can be found in recent publications (e. g., [68,69]) and in the study of the so-called "urban-seismology", recently presented by Fernandez-Ares et al., [44]. In this case the goal is to understand how the presence of an entire city can modify the incident wave-field. Due to the size of the simulation and the number of buildings, the latter are modeled as single degrees of freedom oscillators. The interaction between soil and structure is preserved but the buildings are simplified. For important structure (e. g.: Historical buildings, world heritage buildings, hospitals, schools, theaters, railway and highways) it is worth to provide an ad-hoc analysis capable to take into account the full complexity of the phenomena.

Here we present an example of a fully coupled modeling (Fig. 8): A railway bridge and its geotechnical-topographical surroundings. The Acquasanta bridge on the Genoa-Ovada railway, North Italy, is located in the Genoa district and represents a typical structure the ancestor of which can be traced back to the Roman "Pont du Gard". This structural type did not change significantly along the centuries, thanks to the excellent design achieved no less than 1900 years ago. The Acquasanta bridge structure is remarkable both for the site features and the local geological and geomorphological conditions. The foundations of several of the piers rest on weak rock; moreover, some instability problems have been detected in the past on the valley slope towards Ovada.

Several simulations have been performed with GeoELSE, in order to evaluate the influence of seismic site effects on the dynamic response of the Acquasanta bridge. A fully coupled 3D soil-structure model was designed: The grid is characterized by a "subvertical fault" between calcareous schists and serpentine rocks. This is in accordance with available data, even if further investigations in future should identify more in detail the tectonic structure of the area. The geometry of weathered materials overlaying the calcareous schists on the Ovada side has been assumed according to available information. The dimension of hexahedral elements ranges some tens of centimeters to about 1000 m. With such a model, the problem can be handled in its 3D complexity and we can examine the following aspects that are usually analyzed under restrictive and simplified assumptions: (i) soil-structure interaction, (ii) topographic amplification, (iii) soft soil amplification (caused by the superficial alluvium deposit shown in cyan), (iv) subvertical fault (red line) between the schists, on the Ovada side, and serpentine rock, on the Genoa side. For excitation a shear plane wave (x-direction) was used (Ricker wavelet, fmax = 3 Hz, $t0 = 1.0\,s$. and amplitude = 1 mm) propagating vertically from the bottom (red elements in Fig. 8).



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 9
Snapshots of the modulus of the displacement vector and the magnified deformed shape of the bridge (in mm)

In Fig. 9 we present some snapshots of the modulus of the displacement vector and the magnified deformed shape of the bridge. It is worth to note that at $T = 2$ s the motion of the bridge is almost in-plane (direction x), while at $T = 4$ s is clearly evident how the coupling between the in-plane and out-plane (y-direction) motion starts to be important.

The study of the soil-structure interaction problem could be easily enhanced (i) improving the input excitation of the model here presented and (ii) taking into account complex constitutive behavior both from the soil and the structure side. The former is already available in GeoELSE thanks to the recent implementation [41,93] of the domain reduction method (DRM), a methodology that divides the original problem into two simpler ones [4,119], to overcome the problem of multiple physical scales that is created by a seismic source located some kilometers away from the structure with typical element size of the order of meters and located over a relatively small area (less than 1 km^2) on soft deposit. The latter still needs to be improved because of the lack of a complete tool capable to handle in 3D non linear soil behavior, non-linear structural behavior and the presence of the water, that play a crucial role in the failure of buildings. Partial response to this problem can be found in the recent work of Bonilla et al. [5] and in the visco-plastic rheology recently introduced in GeoELSE [30].

3D Wave Propagation on Tetrahedral Grids: Application to Volcanology

As indicated above, the simulation of a complete, highly accurate wave field in realistic media with complex geometry is still a great challenge. Therefore, in the last years a new, highly flexible and powerful simulation method has been developed that combines the Discontinuous Galerkin (DG) Method with a time integration method using Arbitrary high order DERivatives (ADER) of the approximation polynomials. The unique property of this numerical scheme is, that it achieves arbitrarily high approximation order for the solution of the governing seismic

wave equation in space and time on structured and unstructured meshes in two and three space dimensions.

Originally, this new ADER-DG approach [32,35] was introduced for general linear hyperbolic equation systems with constant coefficients or for linear systems with variable coefficients in conservative form. Then, the extension to non-conservative systems with variable coefficients and source terms and its particular application to the simulation of seismic waves on unstructured triangular meshes in two space dimensions was presented [70]. And finally, the further extension of this approach to three-dimensional tetrahedral meshes has been achieved [33]. Furthermore, the accurate treatment of viscoelastic attenuation, anisotropy and poroelasticity has been included to handle more complex rheologies [28,29,71]. The governing system of the three-dimensional seismic wave equations is hereby formulated in velocity-stress and leads to the hyperbolic system of the form

$$\frac{\partial \boldsymbol{Q}_p}{\partial t} + A_{pq}\frac{\partial \boldsymbol{Q}_q}{\partial \xi} + B_{pq}\frac{\partial \boldsymbol{Q}_q}{\partial \eta} + C_{pq}\frac{\partial \boldsymbol{Q}_q}{\partial \zeta} = S_p \,, \quad (6)$$

where the vector $\boldsymbol{Q}$ of unknowns contains the six stress and the three velocity components and S is the source term. The Jacobian matrices A, B and C include the material values as explained in detail in [33,70].

The ADER-DG Method: Basic Concepts

The ADER-DG method is based on the combination of the ADER time integration approach [113], originally developed in the finite volume (FV) framework [96,97,111] and the Discontinuous Galerkin finite element method [18,19,20,21,22,23,91]. As described in detail in [33] in the ADER-DG approach the solution is approximated inside each tetrahedron by a linear combination of space-dependent polynomial basis functions and time-dependent degrees of freedom as expressed through

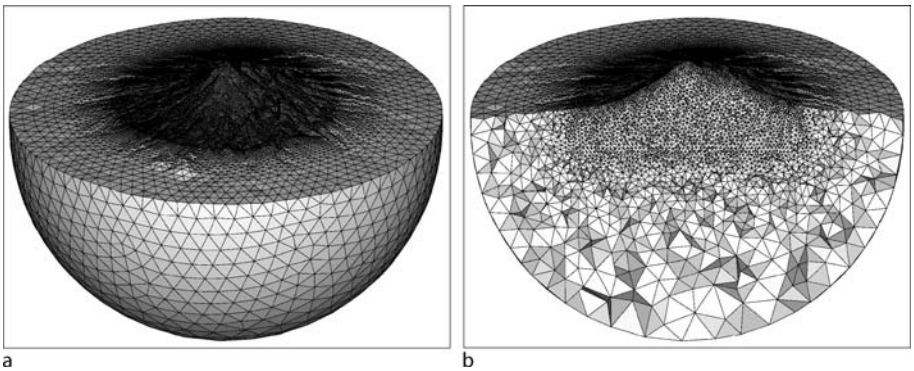
$$(\boldsymbol{Q}_h)_p(\xi,\eta,\zeta,t) = \hat{\boldsymbol{Q}}_{pl}(t)\boldsymbol{\Phi}_l(\xi,\eta,\zeta) \,, \quad (7)$$

where the basis functions Φ_l form an orthogonal basis and are defined on the canonical reference tetrahedron. The unknown solution inside each element is then approximated by a polynomial, whose coefficients – the degrees of freedom $\hat{\boldsymbol{Q}}_{pl}$ – are advanced in time. Hereby, the solution can be discontinuous across the element interfaces, which allows the incorporation of the well-established ideas of numerical flux functions from the finite volume framework [75,112]. To define a suitable flux over the element surfaces, so-called Generalized Riemann Problems (GRP) are solved at the element interfaces. The GRP solution provides simultaneously a numerical flux function as well as a time-integration method. The main idea is a Taylor expansion in time in which all time derivatives are replaced by space derivatives using the so-called Cauchy–Kovalewski procedure which makes recursive use of the governing differential Eq. (6). The numerical solution of Eq. (6) can thus be advanced by one time step without intermediate stages as typical e. g. for classical Runge–Kutta time stepping schemes. Due to the ADER time integration technique the same approximation order in space and time is achieved automatically. Furthermore, the projection of the elements in physical space onto a canonical reference element allows for an efficient implementation, as many computations of three-dimensional integrals can be carried out analytically beforehand. Based on a numerical convergence analysis this new scheme provides arbitrary high order accuracy on unstructured meshes. Moreover, due to the choice of the basis functions in Eq. (7) for the piecewise polynomial approximation [23], the ADER-DG method shows even spectral convergence.

Grid Generation: Unstructured Triangulations and Tetrahedralization

Both tetrahedral and hexahedral elements are effectively used to discretize three-dimensional computational domains and model wave propagation with finite element type methods. Tetrahedra can be the right choice because of the robustness when meshing any general shape. Hexahedra can be the element of choice due to their ability to provide more efficiency and accuracy in the computational process. Furthermore, techniques for automatic mesh generation, gradual mesh refinement and coarsening are generally much more robust for tetrahedral meshes in comparison to hexahedral meshes. Straightforward tetrahedral refinement schemes, based on longest-edge division, as well as the extension to adaptive refinement or coarsening procedures of a refined mesh exist [3,12]. In addition, parallel strategies for refinement and coarsening of tetrahedral meshes have been developed [27].

Less attention has been given to the modification of hexahedral meshes. Methods using iterative octrees have been proposed [74,95], but these methods often result in nonconformal elements that cannot be accommodated by some solvers. Lately also conformal refinement and coarsening strategies for hexahedral meshes have been proposed [2]. Other techniques insert non-hexahedral elements that result in hybrid meshes that need special solvers that can handle different mesh topologies. Commonly, the geometrical problems in geosciences arise through rough surface topography, as shown for the Mer-



a b

Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 10
Tetrahedral mesh for the model of the volcano Merapi. The zone of interest, such as the free surface topography and the volcano's interior are discretized by a fine mesh, whereas the spatial mesh is gradually coarsened towards the model boundaries

api volcano in Fig. 10, and internal material boundaries of complex shape that lead to wedges and overturned or discontinuous surfaces due to folding and faulting. However, once the geometry of the problem is defined by the help of modern computer aided design (CAD) software, the meshing process using tetrahedral elements is automatic and stable. After the mesh generation process, the mesh vertices, the connectivity matrix and particular information about boundary surfaces are typically imported to a solver.

The computational possibilities and algorithmic flexibility of a particular solver using the ADER-DG approach for tetrahedral meshes are presented in the following.

Local Accuracy: *p*-Adaptation

In many large scale applications the computational domain is much larger than the particular zone of interest. Often such an enlarged domain is chosen to avoid effects from the boundaries that can pollute the seismic wave field with possible, spurious reflections. Therefore, a greater number of elements has to be used to discretize the domain describing the entire model. However, in most cases the high order accuracy is only required in a restricted area of the computational domain and it is desirable to choose the accuracy that locally varies in space. This means, that it must be possible to vary the degree p of the approximation polynomials locally from one element to the other [36]. As the ADER-DG method uses a hierarchical order of the basis functions to construct the approximation polynomials, the corresponding polynomial coefficients, i. e. the degrees of freedom, for a lower order polynomial are always a subset of those of a higher-order one. Therefore, the computation of fluxes between elements of different approximation orders can be carried out by using only the necessary part of the flux matrices.

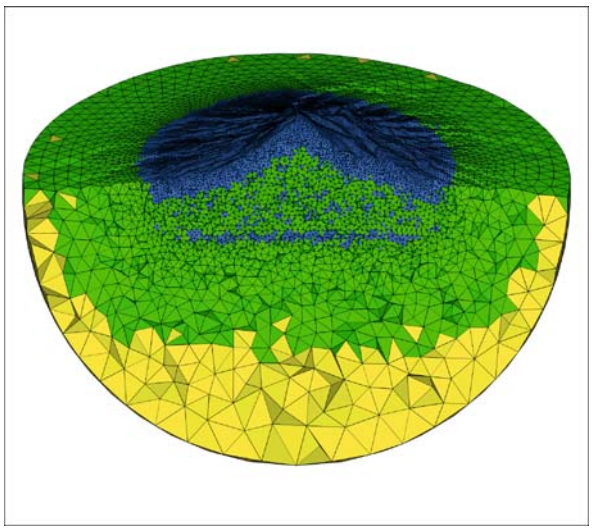
Furthermore, the direct coupling of the time and space accuracy via the ADER approach automatically leads to a local adaptation also in time accuracy, which often is referred to as p_t-adaptivity. In general, the distribution of the degree p might be connected to the mesh size h, i. e. the radius of the inscribed sphere of a tetrahedral element. In particular, the local degree p can be coupled to the mesh size h via the relations

$$p = p_{\min} + (p_{\max} - p_{\min}) \left(\frac{h - h_{\min}}{h_{\max} - h_{\min}} \right)^r , \qquad (8)$$

$$p = p_{\max} - (p_{\max} - p_{\min}) \left(\frac{h - h_{\min}}{h_{\max} - h_{\min}} \right)^r , \qquad (9)$$

where the choice of the power r determines the shape of the p-distribution. Note, that depending on the choice of the first term and the sign the degree p can increase as in Eq. (8) or decrease as in Eq. (9) with increasing h, starting from a minimum degree $p_{\min}$ up to a maximum degree $p_{\max}$. This provides additional flexibility for the distribution of p inside the computational domain. An example of a p-distribution for the volcano Merapi is given in Fig. 11.

Here the idea is to resolve the slowly propagating surface waves with high accuracy, whereas the waves propagating towards the absorbing model boundaries pass through a zone of low spatial resolution. This approach leads to numerical damping due to an amplitude decay that reduces possible boundary reflections. Furthermore, the computational cost is reduced significantly due to the strongly reduced number of total degrees of freedom in the model.



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 11
The local degree *p* of the approximation polynomial depends on the insphere radius of each tetrahedral element and is given in color code. Close to the surface topography an approximation polynomial of degree $p = 5$ (*blue*) is used, whereas in depth the degree is reduced to $p = 4$ (*green*) and $p = 3$ (*yellow*)

Local Time Stepping: Δt-Adaptation

Geometrically complex computational domains or spatial resolution requirements often lead to meshes with small or even degenerate elements. Therefore, the time step for explicit numerical schemes is restricted by the ratio of the size h of the smallest element and the corresponding maximum wave speed in this element. For global time stepping schemes all elements are updated with this extremely restrictive time step length leading to a large amount of iterations. With the ADER-DG approach, time accurate local time stepping can be used, such that each element is updated by its own, optimal time step [36]. Local time-stepping was used in combination with the finite-difference method [42,106].

An element can be updated to the next time level if its actual time level and its local time step Δt fulfill the following condition with respect to all neighboring tetrahedra n:

$$t + \Delta t \leq \min(t_n + \Delta t_n) \,. \tag{10}$$

Figure 12 is visualizing the evolution of four elements (I, II, III and IV) in time using the suggested local time stepping scheme. A loop cycles over all elements and checks for each element, if condition (10) is fulfilled. At the initial state all elements are at the same time level, however, element II and IV fulfill condition (10) and therefore can be updated. In the next cycle, these elements are already advanced in time (grey shaded) in cycle 1. Now elements I and IV fulfill condition (10) and can be updated to their next local time level in cycle 2. This procedure continues and it is obvious, that the small element IV has to be updated more frequently than the others. A synchronization to a common global time level is only necessary, when data output at a particular time level is required as shown in Fig. 12.

Information exchange between elements across interfaces appears when numerical fluxes are calculated. These fluxes depend on the length of the local time interval over which a flux is integrated and the corresponding element is evolved in time. Therefore, when the update criterion (10) is fulfilled for an element, the flux between the element itself and its neighbor n has to be computed over the local time interval:

$$\tau n = [\max(t, tn) \,, \;\; \min(t + \Delta t, tn + \Delta tn)] \,. \tag{11}$$

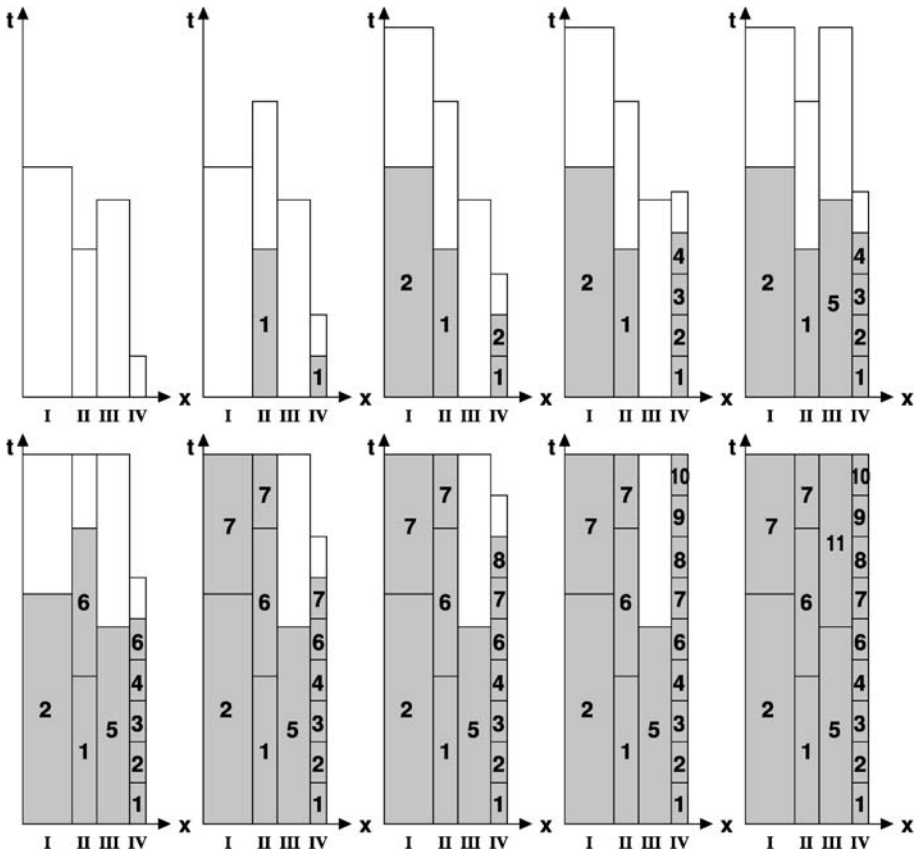
As example, the element III fulfills the update criterion (10) in cycle 5 (see Fig. 12). Therefore, when computing the fluxes only the remaining part of the flux given by the intervals in Eq. (11) has to be calculated. The other flux contribution was already computed by the neighbors II and IV during their previous local updates. These flux contributions have been accumulated and were stored into a memory variable and therefore just have to be added.

Note that e. g. element IV reaches the output time after 10 cycles and 9 local updates, which for a global time stepping scheme would require $9 \times 4 = 36$ updates for the all four elements. With the proposed local time stepping scheme only 16 updates are necessary to reach the same output time with all elements as indicated by the final number of grey shaded space time elements in Fig. 12.

Comparing these numbers leads to a speedup factor of 2.25. For strongly heterogeneous models and local time step lengths this factor can become even more pronounced. However, due to the asynchronous update of elements that might be spatially very close to each other the mesh partitioning for parallel computations becomes an important and difficult issue. Achieving a satisfying load balancing is a non-trivial task and still poses some unresolved problems as explained in the following.

Mesh Partitioning and Load Balancing

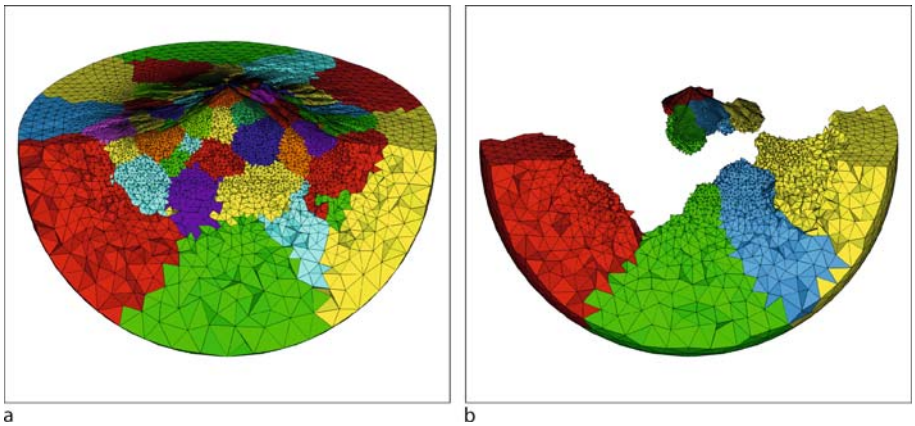
For large scale applications it is essential to design a parallel code that can be run on massively parallel supercomputing facilities. Therefore, the load balancing is an important issue to use the available computational resources efficiently. For global time stepping schemes with-



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 12
Visualization of the local time stepping scheme. The actual local time level *t* is at the top of the *gray shaded* area with numbers indicating the cycle, in which the update was done. *Dotted lines* indicate the local time step length Δt with which an element is updated

out *p*-adaptation standard mesh partitioning as done e. g. by METIS [60] is sufficient to get satisfying load balancing. The unstructured tetrahedral mesh is partitioned into subdomains that contain an equal or at least very similar number of elements as shown in Fig. 13. Therefore, each processor has to carry out a similar amount of calculations. However, if *p*-adaptation is applied, the partitioning is more sophisticated as one subdomain might have many elements of high order polynomials whereas another might have the same number of elements but with lower order polynomials. Therefore, the parallel efficiency is restricted by the processor with the highest work load. However, this problem can usually be solved by weighted partitioning algorithms, e. g. METIS.

In the case of local time stepping, mesh partitioning is becoming a much more difficult task. One solution is to divide the computational domain into a number of zones, that usually contain a geometrical body or a geological zone that typically is meshed individually with a particular mesh spacing *h* and contains a dominant polynomial order. Then each of these zones is partitioned separately into subdomains of approximately equal numbers of elements. Then each processor receives a subdomain of each zone, which requires a similar amount of computational work as shown in Fig. 13. In particular, the equal distribution of tetraheda with different sizes is essential in combination with the local time stepping technique. Only if each processor receives subdomains with a similar amount of small and large elements, the work load is balanced. The large elements have to be updated less frequently than the smaller elements and therefore are computationally cheaper. Note, that the separately partitioned and afterwards merged zones lead to non-connected subdomains for each processor (see Fig. 13). This increases the number of element surfaces between subdomains of different processors and therefore increases the communication required. However, communication is typically low as the degrees of freedom have to be exchanged only once per



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 13
Standard partitioning of the computational domain (*left*) and an example of 4 subdomains grouped together for more efficient local time stepping

time step and only for tetrahedra that have an interface at the boundary between subdomains. Therefore, the improvements due to the new load balancing approach are dominant and outweigh the increase in communication.

However, care has to be taken as the distribution of the polynomial degree p or the seismic velocity structure might influence the efficiency of this grouped partitioning technique. A profound and thorough mesh partitioning method is still a pending task as the combination of local time stepping and p-adaptivity requires a new weighting strategy of the computational cost for each tetrahedral element considering also the asynchronous element update. The automatic partitioning of unstructured meshes with such heterogeneous properties together with the constraint of keeping the subdomains as compact as possible to avoid further increase of communication is still subject to future work.

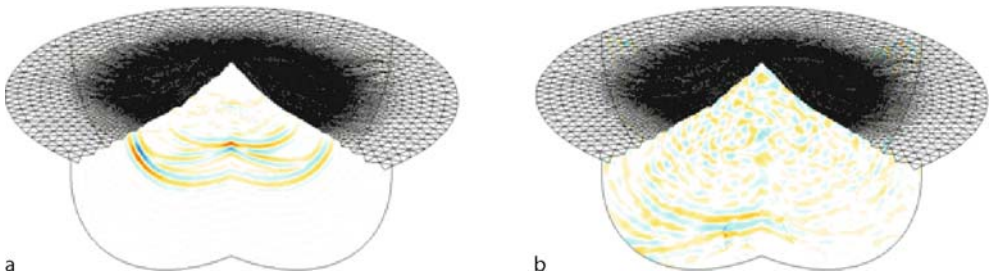
In Fig. 13 an example of a grouped partition of the tetrahedral mesh is shown for 4 processors. Two non-connected subdomains indicated by the same color are assigned to each processor including small – and therefore computationally expensive – tetrahedra that are updated frequently due to their small time step, and much larger elements that typically are cheap due to their large time step. This way, the work load often is balanced sufficiently well over the different processors.

Relevance of High Performance Computing: Application to Merapi Volcano

In recent years the development of the ADER-DG algorithm including the high order numerical approximation in space and time, the mesh generation, mesh adaptation, parameterization, and data visualization created the basis of an efficient and highly accurate seismic simulation tool. Realistic large scale applications and their specific requirements will further guide these developments. On the other hand, the study and incorporation of geophysical processes that govern seismic wave propagation insures, that the simulation technology matches the needs and addresses latest challenges in modern computational seismology. Hereby, the accurate modeling of different source mechanisms as well as the correct treatment of realistic material properties like anelasticity, viscoplasticity, porosity and highly heterogeneous, scattering media will play an important role.

However, only the combination of this state-of-the-art simulation technology with the most powerful supercomputing facilities actually available can provide excellent conditions to achieve scientific progress for realistic, large scale applications. This combination of modern technologies will substantially contribute to resolve current problems, not only in numerical seismology, but will also influence other disciplines. The phenomenon of acoustic, elastic or seismic wave propagation is encountered in many different fields. Beginning with the classical geophysical sciences seismology, oceanography, and volcanology such waves also appear in environmental geophysics, atmospheric physics, fluid dynamics, exploration geophysics, aerospace engineering or even medicine.

With the rapid development of modern computer technology and the development of new highly accurate simulation algorithms computer modeling just started to herald a new era in many applied sciences. The 3D wave propagation simulations in realistic media require a substantial amount of computation time even on large par-



Seismic Wave Propagation in Media with Complex Geometries, Simulation of, Figure 14
Snapshots of the seismic wave field after an explosive event close to the summit of Merapi volcano. The free surface topography introduces strong scattering of the waves making it extremely difficult to invert for the seismic source mechanism or the exact source location

allel computers. Extremely powerful national supercomputers already allow us to run simulations with unrivaled accuracy and resolution. However, using the extremely high accuracy and flexibility of new simulation methods on such massively parallel machines the professional support of experts in supercomputing is absolutely essential. Only professional porting, specific CPU-time and storage optimizations of current software with respect to continuously changing compilers, operating systems, hardware architectures or simply personnel, will ensure the lifetime of new simulation technologies accompanied by ongoing improvements and further developments. Additionally, the expertise and support in the visualization of scientific results using technologies of Virtual Reality for full 3D models not only enhances the value of simulation results but will support data interpretation and awake great interest in the new technology within a wide research community.

As an example, volcano monitoring plays an increasingly important role in hazard estimation in many densely populated areas in the world. Highly accurate computer modeling today is a key issue to understand the processes and driving forces that can lead to dome building, eruptions or pyroclastic flows. However, data of seismic observations at volcanoes are often very difficult to interpret. Inverting for the source mechanism, i. e. seismic moment tensor inversion, or just locating an exact source position is often impossible due to the strongly scattered wave field caused by an extremely heterogeneous material distribution inside the volcano. Furthermore, the rough topography alone can affect the wave field by its strongly scattering properties as shown in Fig. 14.

Therefore, it is fundamental to understand the effects of topography and scattering media and there influence on the seismic wave field. A systematic study of a large number of scenarios computed by highly accurate simulation methods to provide reliable synthetic data sets is necessary to test the capabilities of currently used inversion tools. Slight changes in parameters like the source position, the source mechanism or the elastic and geometric properties of the medium can then reveal the limits of such tools and provide more precise bounds of their applicability in volcano seismology.

Finally, the implementation of the ADER-DG method is still much more expensive than other state-of-the-art implementations of existing methods. However, a fair comparison between accuracy and computational cost is still a pending task. The main reason for the CPU-time difference is the much larger number of tetrahedral elements than hexahedra that have to be used to cover the same volume. Furthermore, due to the choice of the basis functions, the flux computations are expensive, as the matrix-matrix multiplications involved are not sparse.

However, the ADER-DG method is currently implemented on hexahedral meshes to make fair comparisons possible. Preliminary tests show, that the change of mesh topology from tetrahera to hexahedra significantly reduces the computational cost. However, final results are subject to future investigations.

Discussion and Future Directions

As indicated in the introduction and highlighted in the previous sections, computational tools for wave propagation problems are getting increasingly sophisticated to meet the needs of current scientific problems. We are far away from simple finite-difference time schemes that are solving problems on regular grids on serial computers in which case the particular programming approach did not affect dramatically the overall performance. Today, competitive algorithms are results of years of partly highly professional coding. Implementations on high-performance computing hardware requires in-depth knowledge of parallel algorithms, profiling, and many technical aspects of modern computations. To make complex scientific soft-

ware available to other researchers requires implementation and testing on many different (parallel) platforms. This may involve parallelization using different programming paradigms (e. g., the combination of OpenMP and MPI on nodes of shared memory machines), and interoperability on heterogeneous computational GRIDs.

This has dramatic consequences particularly for young researchers in the Earth Sciences who want to use advanced computational tools to model observations. While in the early days a finite-difference type algorithm could be understood, coded, implemented and tested in a few weeks, this is no longer possible. In addition, standard curricula do not offer training in computational methods allowing them to efficiently write and test codes. This suggests that at least for some, well-defined computational problems verified and professionally engineered scientific software solutions should be provided to the community and also professionally extended and maintained in close collaboration with scientists. In seismology we are in a quite fortunate situation. In contrast to many other fields of physical sciences, our constitutive relations (e. g., stress-strain) are fairly well understood, and – as indicated in this paper – numerical solutions for 3D problems and their implementation on parallel hardware are well advanced. Another argument for stable tested "community"-codes for wave propagation is the fact that advancement in many scientific problems (e. g., imaging the Earth's interior, quantifying earthquake-induced shaking hazard) relies on zillions of forward modeling runs with only slight variations of the internal velocity models.

As far as technical developments are concerned, the efficient initialization of complex 3D models on computational grids is still a great challenge. Realistic models may be composed of complex topography, families of overlapping fault surfaces, discontinuous interfaces, and varying rheologies (e. g., elastic, anisotropic, viscoelastic, viscoplastic, porous). This may require the combination of tetrahedral and hexahedral grid in models with strongly varying degree of complexity. Ideally, standards for Earth models (and synthetic data) formats should be established by the communities that allow easy exchange and multiple use of models with different simulation tools (e. g., wave propagation, deformation, earthquake rupture). In addition, the rapid developments towards PetaFlop computing opens new questions about the scalability and efficient parallelization of current and future algorithms.

As the forward problem of wave propagation is at the core of the seismic imaging problem for both source and Earth's structure, in the near future we will see the incorporation of 3D simulation technology into the imaging process. Provided that the background seismic velocity models are fairly well known (e. g., reservoirs, global Earth, sedimentary basins), adjoint methods provide a powerful analytical tool to (1) relate model deficiencies to misfit in observations and (2) quantify the sensitivities to specific aspects of the observations (e. g., [100,104,105]). As the core of the adjoint calculations is the seismic forward problem, the challenge is the actual application to real data and the appropriate parametrizations of the model and the data that optimize the data fitting process.

In summary, while we look back at (and forward to) exciting developments in computational seismology, a paradigm shift in the conception of one of the central tools of seismology – the calculation of 3D synthetic seismograms – is necessary. To extract a maximum amount of information from our high-quality observations scientists should have access to high-quality simulation tools. It is time to accept that "*software is infrastructure*" and provide the means to professionally develop and maintain community codes and model libraries at least for basic Earth science problems and specific focus regions. Developments are one the way along those lines in the SPICE project (Seismic Wave Propagation and Imaging in Complex Media, a European Network [101]), the Southern California Earthquake Center (SCEC [94]) and the CIG Project (Computational infrastructure in geodynamics [17]).

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