Computational Seismology: Narrowing the Gap Between Theory and Observations

Bernhard Schuberth, Michael Ewald, Heiner Igel, Markus Treml, Haijiang Wang, Gilbert Brietzke

Department für Geo- und Umweltwissenschaften, Bereich Geophysik,
Ludwig-Maximilians-Universität München, Theresienstrasse 41, 80333 München,
Germany, `bernhard@geophysik.uni-muenchen.de`

Summary. Numerical solutions to the problem of seismic wave propagation, that allow simulations of complete wave fields through 3D structures, are currently revolutionizing seismology and related fields. So far - in order to calculate theoretical seismograms in the observed frequency bands - one had to resort to solution methods with severe limitations (e.g., ray theoretical approximations, one-dimensional structures, perturbation theory, etc.). Only in the past few years, computational power has allowed us to simulate wave fields that can be directly compared to observations. Even though the computations still require substantial resources, the methodologies developed in the past decade are beginning to enter routine processing steps in all branches ranging from exploration seismics to global seismology. Here we present recent examples in global seismology (spectral element modeling of global wave propagation) and earthquake scenario simulations, their relation to shaking hazard estimation, and associated problems. The next decade will see fundamental changes in the way data fitting (inverse problem, parameter estimation) is done in seismology with the potential of advances in several fields of Earth Sciences.

1 Introduction

Many phenomena of (visco-)elastic (acoustic) wave propagation are the basis for diagnostic tools in fields such as medicine, meteorology, seismology, exploration geophysics, engineering, material sciences and others. Because of the increasing computational power, the methodologies used in these fields have dramatically converged in the past decade. Numerical solutions to wave propagation problems - using finite differences (FD), finite volumes (FV), finite and spectral element methods (FEM and SEM respectively) and others - are now common tools in most disciplines. While the algorithm development is now at a fairly advanced stage, the routine application of those tools with the associated potential large impact is just at the beginning. The KONWIHR project described here (numerical wave propagation) focused in the past years on the program development and verification. Below, we will link these developments to other ongoing projects and demonstrate that KONWIHR was fundamental in providing the more technical progress, thereby serving these related projects.

1.1 Current Issues in Computational Seismology

Several of the technical and scientific objectives and results were presented in the two previous project reports [?, ?]. These focused on the development of 3D wave propagation tools for media with strong topography [?, ?], the calculation of earthquake scenarios and the resulting ground motions [?, ?, ?, ?, ?, ?], the simulation of wave propagation in seismically active fault zones [?, ?, ?], the simulation of the actual rupture process during earthquakes [?, ?, ?] and finally the emerging field of numerical wave propagation on a global scale [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. It is beyond the scope of this paper to describe the results in detail. The main scientific advances are summarized here:

Earthquake Scenarios. 3D simulations of earthquake scenarios in seismically active regions (e.g., Cologne Basin) show that the 3D structure, source location, source mechanism, near-surface structure, etc. strongly influence the peak ground motion observed at a particular point in the region of interest (e.g., [?]). This has tremendous implications for seismic hazard studies, as many more aspects need to be taken into account for reliable estimations than was previously thought. The most important factor is the 3D seismic velocity structure, that is often not sufficiently well known. Studies are being undertaken (see Sect. 2.4) to incorporate uncertainties into the estimation of shaking hazard.

Dynamic Rupture. The physical processes that happen at the fault during rupture are still poorly understood. Recently it was discovered that - if across the fault the material properties change, a likely feature at many large deformation-rate strike slip faults such as the San Andreas in California - rupture at bi-material interfaces may dramatically influence the rupture behavior. A large number of simulations carried out as a parameter study illustrated the behavior of ruptures in such circumstances. It was shown that if rupture initializes in the vicinity of such material interfaces, the rupture is likely to migrate to this interface and continue to break that particular fault [?, ?, ?].

Global Seismology. Wave propagation on a planetary scale was so far predominantly carried out using quasi-analytical approaches (e.g., spherical harmonics) and perturbation theory. Only recently the impact of 3D structures on the observed wave field is being appreciated. A large part of the information contained in the recorded seismograms is still not used to understand the structure of the Earth's deep interior. With the tools developed in the Munich group (axi-symmetric approach [?] and spherical sections [?, ?, ?]) as well as a spectral element approach [?, ?, ?] that was developed elsewhere but was extended and installed on the Munich supercomputer facilities, a new era of global seismic data modeling is just beginning.

After putting the KONWIHR project in the context of other activities, we will present recent results from three ongoing topics.

1.2 KONWIHR and Related Projects

There was strong beneficial interaction between the KONWIHR project and other studies. The technical lessons learned through the code development (debugging, profiling, parallelization) within KONWIHR lead to successful applications of the algorithms in projects like the **International Quality Network: Georisk** (www.iqn-georisk.de, funded by the German Academic Exchange Service); the **Geosensor Project** (BMBF, Geotechnologies program) that aims at understanding earthquake induced rotational motions [?]; a study that aims at understanding **the seismic signature of plumes** (German Research Foundation); and others. The experiences within the KONWIHR project were instrumental in the preparation for a large European network in computational seismology that was funded by the European Union in 2003. This project called **SPICE** (Seismic wave propagation and imaging in complex media: a European network, www.spice-rtn.org) is the first Research and Training Network in computational seismology connecting 14 European institutions and aims at developing a digital library with verified wave propagation codes for the Earth Science community. The project will also train young researchers in this field through workshops and online training material.

2 Recent Scientific Results

2.1 Spectral Element Modeling of Global Wave Propagation

In the last years the spectral element method became one of the most important tools in computational seismology. Being a modified finite element method, its name derives from the convergence behavior of the method with increasing order, which is the same as in the spectral methods.
First introduced for fluid dynamics [?], it was further developed in the 1990's for seismological applications ([?] and [?, ?]). Today the SEM can be used to simulate the wave propagation in global spherical Earth models including various features such as topography/bathymetry, laterally heterogenous velocity structures in the crust and the mantle, attenuation, anisotropy and also second order effects as for example Earth's rotation, gravity or the influence of ocean water on the wave field [?, ?]. The advantages of the method are not only the capability of dealing with the complex problems mentioned above, but also its high accuracy and the ease of implementing free boundary conditions. Especially for global Earth models, the latter is very appreciable.

The model for global wave propagation is built using the "cubed sphere" approach. This is illustrated in Fig. 1, where the initial cube is gradually distorted from left to right, until its six faces match the surface of the sphere. In the lower part of the picture the procedure is shown for one of the six "chunks" comprising the cubed sphere. The clue in this procedure is to keep a small cube in the interior of the mesh undistorted thus avoiding singularities in the center at $r = 0$.
In the current implementation of the SEM in a parallel MPI-FORTRAN code, the model space is decomposed for each chunk separately, but in the same manner. The number of divisions in both "horizontal" directions of the chunks has to be equal. In radial direction, the chunks are not split up. Thus, for given integer values n of possible divisions (1,2,3,...), the resulting number of processes for the whole sphere gets $6 \times n^2$ $(= 6, 24, 54, 96$ etc.).
As first tests on the SR8000 showed minor performance with auto-parallelization, we switched to intra-node MPI parallelization. The reasons for that are numerous indirect addressings in most of the loops, and therefore auto-parallelization of the loops fails. In addition, the communication between the processes is only at around 10% of the CPU time. Because of those reasons the number of nodes used on the HITACHI is very unusual compared to widely used 2^n values.
At the moment we use a standard setup for various calculations using 5×5 processors per chunk resulting in a total number of 150 processes. These are distributed on 19 nodes. The typical memory needed by our models, which are accurate for periods greater than 20 s, is between 60 to 90 GB, depending whether attenuation is incorporated or not. The typical runtime is 3.4 seconds per time step leading to a total runtime of 19 hours for the calculation of a 90 minute seismogram. This setup already allows us to enter a new realm of data modeling with dramatic improvement of misfit between observations and theory as shown in Sect. 2.2.

2.2 Convergence of Observations and Theory - Examples from Spectral Element Modeling

The SEM described above, was used in this study to show the decreasing misfit of theoretical simulations compared to real data with increasing complexity of the applied models. We simulated the M8.1 Tokachi-oki earthquake that happened on September 25, 2003. As a starting model we used a purely elastic (i.e., no attenuation), isotropic, spherically symmetric Earth model. The source itself was described as a point source double couple. In a second step we extended the simulation using a finite source model (Ji Chen, personal communication). The next step was using the same radially symmetric velocity structure but this time including attenuation for both source models. Finally, we included all effects, that are up to date incorporated in the SEM code, only excluding anisotropy. Thus, the final model consisted of a laterally heterogenous, attenuating 3D velocity structure for the Earth's crust and mantle together with a $2' \times 2'$ topography/bathymetry grid, as well as

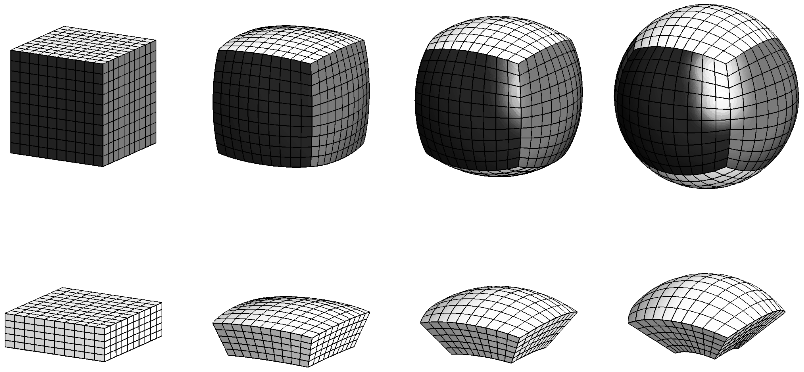

Fig. 1. Upper part: creation of a global Earth model by expanding an initial cube to the sphere (i.e., cubed sphere mesh). Keeping a small central cube undistorted avoids singularities at r=0. Lower part: same as above for only one of the six chunks of the cubed sphere mesh. (Picture courtesy of Peter Danecek).

rotation and gravity of the Earth and the effects of ocean water. Comparisons between respective simulations and observations are shown in Fig. 2. The bottom seismogram shows the transverse component (w.r.t. the great circle path from the source to the receiver) of the translational ground velocity recorded with a broad-band seismometer at the Geodetic Observatory Wettzell/Germany. The first two seismograms from top show the results for the radially symmetric Earth model without attenuation for point source (topmost trace) and finite source (second from top) simulations. The amplitudes were scaled to the S-wave amplitude of the real data which shows up at around 1350 s. The ratio of synthetic S-wave amplitude to the real amplitude (here called *amp*) is given in Fig. 2 for every seismogram. The third (point source) and fourth (finite source) traces from top show the results for the complex 3D Earth model described above. The simulations for the radially symmetric model with attenuation are not presented here, as they are very similar to the ones without attenuation. This illustrates that attenuation has much less effect on the amplitudes than the representation of the source by an extended fault plane (difference of *amp* of a factor of 10 for the two simulations using the radially symmetric model in Fig. 2). The azimuthal dependence of the amplitude is called the "directivity effect", which is a result of the anisotropic radiation from the large source area.

The results show a huge increase of fit to the real data with increasing incorporation of the various effects. The synthetic seismograms of the both source-type simulations for the 3D model are already quite close to reality, but show still too small amplitudes for the first part of the surface waves (between 2000 s and 2600 s). Nevertheless, the amplitudes of the finite source seismogram are closer to the observed ones. Thus, the complex 3D model with

a finite source representation is the best fitting one. To better illustrate this, Fig. 3 shows both seismograms plotted on top of each other. Only for displaying purposes, the synthetic seismograms (dark grey) have been offset by 5% of the maximum amplitude.
These comparisons show that with increasing effort and complexity of the models we are able to fit observations quite well. Thus, by studying even more complex aspects in future and continuously comparing the results to real data, the models of Earth's structure can be improved step by step with implications for other fields like geodynamics, tectonics and geodesy.

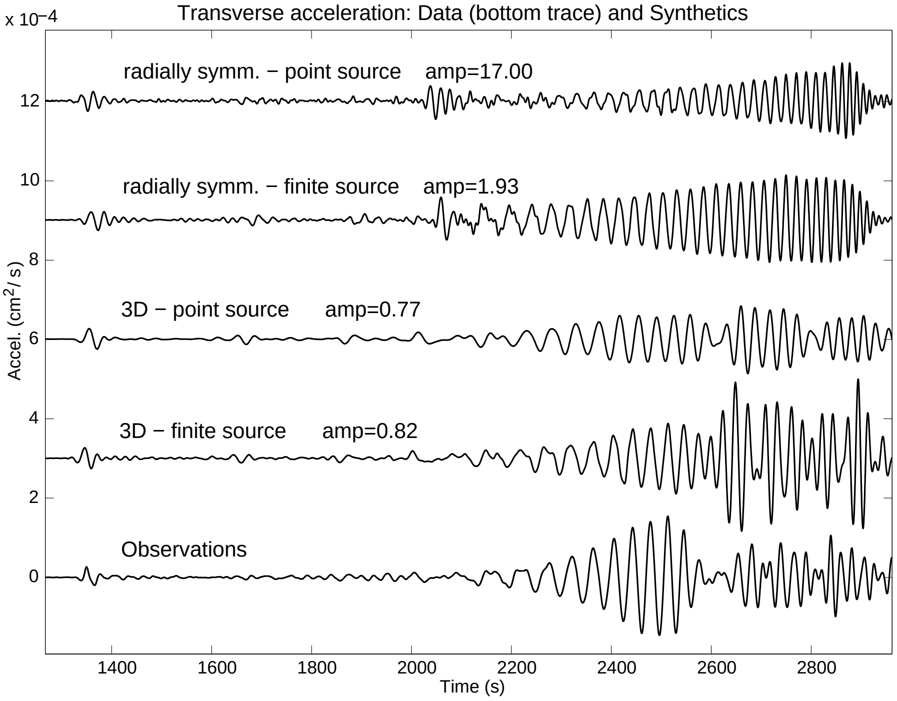

Fig. 2. Simulations using different Earth and source models compared to real data of the M8.1 Tokachi-oki earthquake, September 25 2003: The bottom trace shows the broad-band seismogram recorded at Wettzell/Germany. The two top traces show seismograms for a radially symmetric Earth model using a point source (uppermost trace) and a finite source model. The two middle traces show simulations using a 3D velocity model incorporating attenuation (anelasticity), topography/bathymetry, Earth's rotation and gravity and ocean water together with finite and point source representations (second and third trace from below respectively). All synthetic seismograms have been scaled to the S-wave amplitude of the observations. The given factor (amp) is the ratio of the synthetic S-wave amplitude and the S-wave amplitude of the real data.

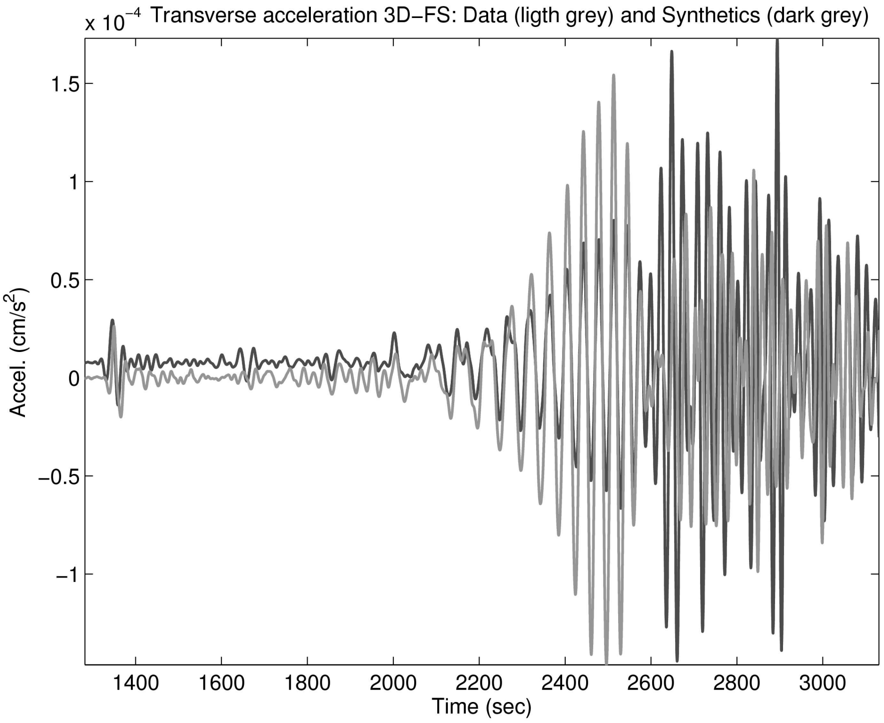

Fig. 3. Comparison of the best fitting simulation (3D – finite source; plotted in dark grey) to the real observations (light grey). The seismograms are offset in vertical direction by 5% of the maximum amplitude for better distinction. Especially the first part of the surface waves between 2000 s and 2600 s fit very well in waveform and phase.

2.3 Effects of Plume Structures on the Wave Field

Apart from studying the effects of Earth's structure at a global scale, it is useful to examine the effects of prominent regional features in the Earth isolated in order to improve understanding of their specific influence. A prominent structure on a regional scale would be for example subduction zones. However, in recent years the hot topic of the scientific community has been mantle plumes. From earlier studies using a regional, Cartesian 3D code [**?**], the development headed for examination of the influence of plumes on incoming teleseismic wavefields. For this purpose a hybrid 2D axi-symmetric/regional spherical 3D code was developed, allowing for an effective computation of the wavefield by concentrating computational power on the area around the structure of interest [**?**]. Meanwhile, the focus is on a full 3D spectral element approach because it allows for a wider range of studies. Its drawback are the enormous requirements in computational power.

Using the same code as described in Sect. 2.1, we additionally implemented plume models and are now beginning to systematically study effects of plume geometry and the nature of the spatial perturbation pattern of plumes. In this first plume parameter study to date we aim at finding a typical ”signature” of a plume in the wavefield. A further goal is to be able in future to suggest optimal experiment configuration in order to detect this signature with the least effort possible. This has become necessary since experiments carried out to image plume structures became more and more expensive, especially when employing ocean bottom seismometers, which are furthermore very difficult to install and maintain. Nevertheless, they turn out to be mandatory for studying important ocean island plumes such as Hawaii.

2.4 Earthquake Scenarios: Uncertainties in Ground Motion Estimation

In this study 3D FD techniques are applied to simulate wave propagation of earthquake scenarios in seismically active regions and thus assess the seismic hazard of such areas. Amplifications of ground motion due to low velocity structures such as sedimentary basins is of special interest in these investigations. Our studies of earthquake scenario simulations concentrate on basins near the city of Cologne and the Beijing metropolitan area [**?**, **?**].

In FD ground motion simulations the velocity model is discretized onto a spatial grid on which the wave equations are solved. This solution provides the complete 3D wave field over the model space. Information on the ground motion in terms of velocity, acceleration or displacement according to the purposes of the simulation can be determined at any point (typically on the surface). Quantities relevant for engineering purposes (e.g., intensity or shaking duration) are then derived from these values.

Results from FD simulations are afflicted with errors caused by two major sources: 1) approximation errors, due to uncertainties of the input data (e.g., velocities, q-values, densities, source location especially source depth etc.) and 2) modeling errors, due to natural imperfections of mathematical abstractions of real physical events depending on the algorithms used in the simulations.

Whereas modeling errors can be minimized by properly chosen operator accuracy and simulation parameters, the influence of uncertainties in the input data are hard to quantify. To investigate such effects multiple simulations were performed using varying models within realistic error margins on the input data sets. We chose basin depth and hypocenter depth as parameter axes along which the model is modified.

Figure 4 shows five synthetic seismograms for the same earthquake scenario at the same receiver location using velocity models varying in terms of basin depth by -10, -5, 0, 5 and 10% respectively relative to the original model. Notable effects on waveforms can be observed in the later arrivals which are caused by surface waves multiply scattered within the sedimentary basin.

These phases are most sensitive to slight variations on the basin shape as resonant amplification occurs to different extents and at different points in time. A variation of ±30% in peak ground velocity like in this example would result in a difference in predicted seismic intensity of one unit on the Mercalli scale. The expected shaking level would change for example from so-called "severe" to "violent" which has distinct implications on local building codes. Source depth is another input parameter in earthquake scenario modeling afflicted with noticeable error. Besides the expected effects of earlier arrival times and higher amplitudes with declining source depth our investigations show a strong impact on resonant wave trains that can account for quite the opposite behavior. Such effects are due to the interaction of source location, velocity model and receiver location and can be quantified only by 3D simulations. Our goal is to pin down the most critical model parameters and quantify their influence on the simulation results.

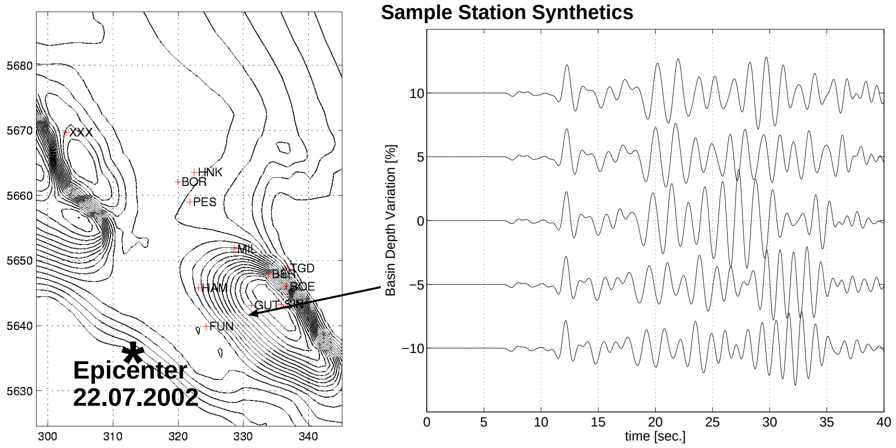

Fig. 4. Left part: contour map of the sedimentary basin depth in the Cologne area. Right part: synthetic seismograms for the same earthquake scenario (the Alsdorf, July 22 2002 earthquake) and receiver location using velocity models with varying basin depth by -10, -5, 0, +5 and +10% respectively. Note the strong influence of the model variation on the later phases of the individual traces.

3 General Conclusions and Outlook

In the field of seismology the calculation of synthetic (theoretical) seismograms for generally heterogeneous 3D media by numerical means is now beginning to complement (maybe soon in large part to replace) the previous tools (ray theory, 1D-, 2D-approximations) used to process, analyse and explain observations. For realistic problems, these calculations will remain large-scale computing problems with the necessity of parallel programming for some time. However, with the more and more common cluster facilities and the exciting prospects of GRID computing, the developed codes are likely to become routine tools for the seismological community. Providing these new facilities to the non-specialist Earth scientist (i.e., non program-developer) is one of the most important tasks for the coming years and will require substantial software engineering particularly in the domain of www-interfaces and data bases.

The results that are beginning to appear (e.g., [**?**]), demonstrate that the scientific value of synthetic seismograms (i.e., the results of large scale simulations) is approaching that of observations. This has tremendous consequences as it suggests that not only the observations (seismograms measured around the world) should be archived and made publicly available but also the synthetic seismograms. This problem is taken up within the European SPICE project (see Sect. 1.2) and has led to an international working group of Earth scientists and seismic network managers with the aim of defining common data formats to store synthetic data in the same way as observations, also using the same infrastructure (e.g., international seismic data centers like www.iris.org). As an example, this will imply that in the not so distant future, scientists will be able to download not only observed seismograms for specific sites, but also theoretical seismograms computed using the latest 3D reference Earth model. It is likely that this will allow new ways of rapidly interpreting seismograms and progress in the associated fields such as (1) the determination of earth structure, (2) the recovery of earthquake rupture properties, and (3) the reliable estimation of shaking hazards.

Acknowledgement. We like to acknowledge funding through the KONWIHR Project, and the Leibniz-Rechenzentrum and its steering committees for providing access to the Hitachi SR8000. We also want to thank the LRZ supporting staff for their help. These projects where partly supported through the DAAD (IQN-Georisk) and the German Research Foundation.