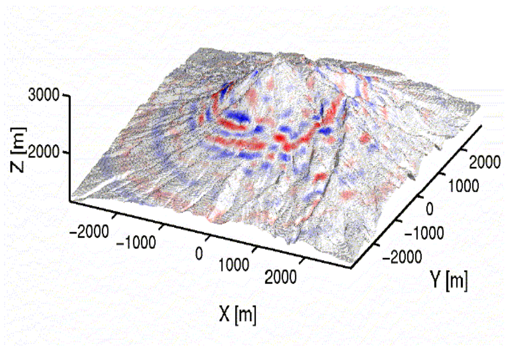
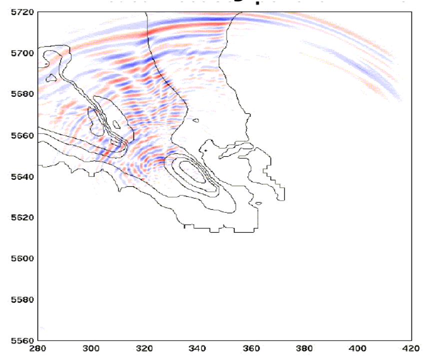
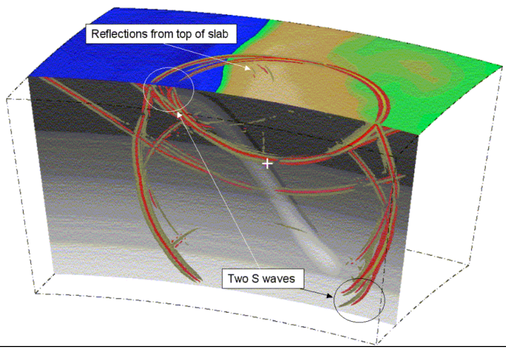
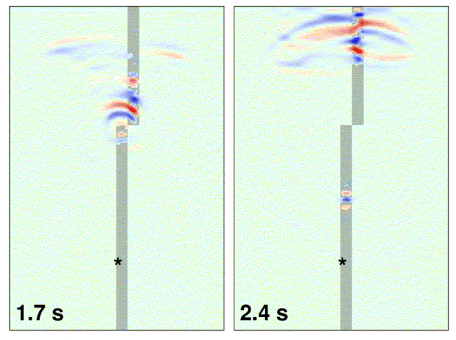
3-D Seismic Wave Propagation on a Global and Regional Scale: Earthquakes, Fault Zones, Volcanoes

Intermediate Report

Volcanoes[*]	Sedimentary Basins[*]
	
Subduction Zones[*]	**Fault Zones[*]**
	

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[*]Results from calculations on the Hitachi.

1. Summary of the goals

The accurate simulation of seismic wave propagation through realistic 3-D Earth models plays a fundamental role in several areas of geophysics: (1) in global seismology knowledge of the structure of the Earth's deep interior is crucial to understand the dynamic behaviour of our planet such as mantle convection, slab subduction or hot spot activity. Accurate synthetic 3-D seismograms which can be compared with globally recorded data require a numerical approach. The structural resolution of today's tomographic models can only be improved by exploiting the 3-D wave effects of the geodynamically important regions inside the Earth. (2) As deterministic earthquake fore-casting seems out of sight, the accurate prediction of likely ground motion following earthquakes in seismically active regions is a major goal which will allow measures (e.g. applying strict building codes) to be taken before major events. 3-D modelling will allow local (e.g. amplifying) effects such as low-velocity zone or topography to be studied. These so-called site effects will be investigated for several areas at risk (e.g. San Francisco Bay Area). (3) Active volcanic areas show very characteristic complex ground motion which is usually recorded on local networks monitoring the activity and risk of eruption. The origin of the seismically recorded signals are poorly understood. One of the reasons is the structural complexity of volcanic areas with strong 3-D heterogeneities, topography and sources in the summit region.
The first year of this project was dedicated to (1) Parallelization and implementation of algorithms for numerical wave propagation on the Hitachi SR8000-F1; (2) Verification of the codes and analysis of their efficiency; and (3) first applications to realistic problems. The results given below illustrate that the algorithms have been verified against analytical solutions and show excellent parallel performance. The computational speed for a typical run (including I/O etc.) reaches ca. 750Mflops per node.

2. Description of computations run on the Hitachi

a. Technical Methods and Algorithms

The algorithms implemented by our group to date constitute numerical solutions to the elastic wave equations in Cartesian and spherical coordinates. The time-dependent partial differential equations are solved numerically using high-order finite-difference methods. This implies that – no matter the particular problem or coordinate system – the space-dependent fields are defined on a 3-D grid and the time extrapolation is carried out using a Taylor expansion. The space derivatives are calculated by explicit high-order finite-difference schemes which do not necessitate the use of matrix inversion techniques. This approach leads to naturally parallel problems where communication is only needed at the boundaries of the decomposed domains. A detailed description of the algorithms as well as the computer programs are given in a CD attached to this report.

Before complex 3D models were run on the Hitachi all algorithms were verified by comparing the numerical solutions to analytical solutions for simple (layered) model geometries. Thereby the parameter space for stable and accurate numerical solutions for the given problems could be identified. An example is given in Figure 1.

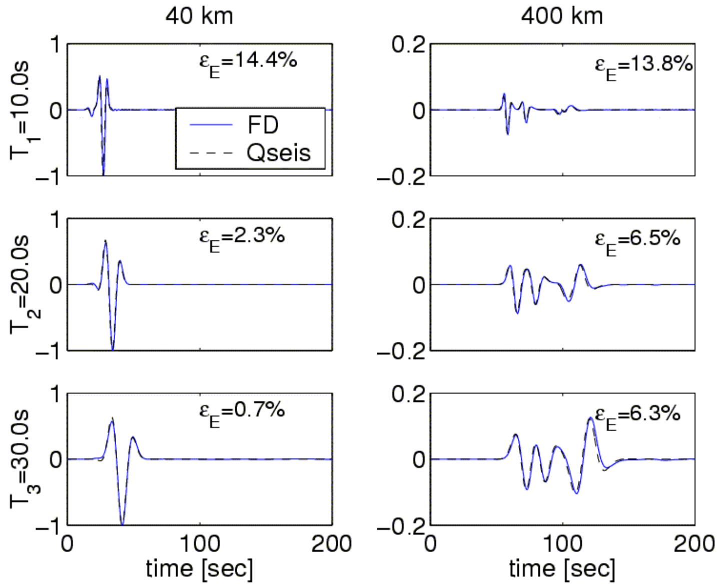

Figure 1: Comparison of numerical solution of elastic wave propagation (finite differences) for a layered model with analytical solutions. This verification is a prerequisite to move to more complex 3D models. All the algorithms mentioned in this report have been carefully verified (see attached Diplom theses). Numerical solution (FD in blue), analytical solution (Qseis, dashed in black).

b. Programming Techniques

Most of the programmes which were implemented on the Hitachi during the first year of the project were originally written in High-Performance Fortran (HPF). At the beginning we carried out extensive studies which programming model would be the best on the SR8000. Although – according to the Hitachi Manual – the HPF standard should be fully supported we encountered problems with I/O with very simple test programs. Furthermore, our HPF algorithms – developed on (then) DEC machines – were not portable (i.e. did not efficiently parallelize without modifications) and would have to be re-parallelized from scratch. Therefore we decided eventually to use the message-passing interface (MPI) for the *internode* parallelization. For the *intranode* parallelization it turned out – to our positive surprise – that for our finite-difference algorithms the automatic optimisation using the *-opt=ss -parallel* option gave excellent results. Therefore, the final programming model uses (1) the automatic parallelization for the shared-memory part and (2) the MPI model across the nodes. This seems to be the optimal approach for explicit FD algorithms.

In Figure 2 the domain decomposition used in the FD algorithms is illustrated. According to standard F90 rules we usually parallelize along the last axes of the 3D arrays. However, if this domain has only a small number of grid points, a decomposition with a 2D or 3D layout may further decrease the ratio between the region which needs to be communicated and the rest of the domain.

The parallel performance was tested with a code where all I/O was – as in production runs – carried out. An FD algorithm was run for 10 time steps on varying number of nodes. The memory in each node was kept constant, so the length of the array in the direction of parallelization was increased accordingly. The memory in each node was approximately 2Gbytes (which may be larger in future runs). The results of this test are shown in Figure 3. The run-time is plotted against the number of nodes used in the simulation. The overall simulation time remains almost constant independent of the number of nodes. This is the case for a 2-point or for a 4-point operator. The length of the spatial operators influences the size of the “shadows” as well as the number of floating-point operations. Figure 3 shows the excellent parallelization using the MPI approach.

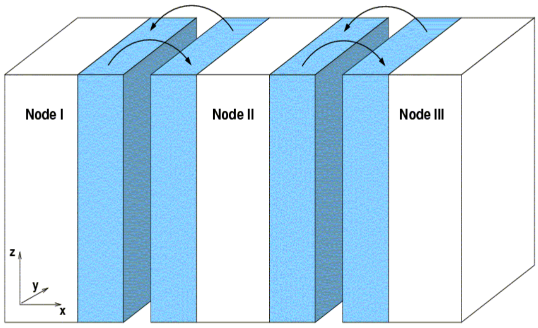

Figure 2: Domain decomposition across the nodes. The 3D spatial grids are decomposed along one (or two) axes. The blue regions denote the regions which have to be communicated to the neighbouring nodes.

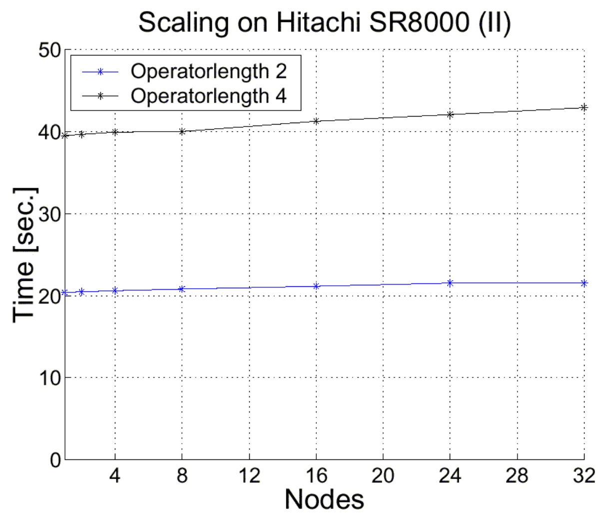

Figure 3: Scaling of the FD algorithms using the MPI language. The memory in each node and the number of time steps in the simulation is kept constant. The parallel performance is excellent.

Hardware Counters	1	2	3	4	5	6	7	8	Sum or Max
Inst TLB misses /sec	10.18D+00	9.09D+00	10.10D+00	9.09D+00	9.09D+00	10.10D+00	9.09D+00	8.58D+00	75.85D+00
Instruction Cache misses /sec	4.97D+03	1.32D+03	1.30D+03	1.29D+03	1.28D+03	1.36D+03	1.29D+03	1.37D+03	14.26D+03
Data Cache misses /sec	290.95D+03	286.83D+03	288.24D+03	286.95D+03	287.06D+03	287.05D+03	288.31D+03	254.28D+03	2.29D+06
Memory acc. instructions /sec	150.93D+06	149.63D+06	149.67D+06	149.63D+06	149.67D+06	149.66D+06	149.64D+06	145.14D+06	-983.82D+06
Total # of instructions /sec	300.00D+06	297.38D+06	297.47D+06	297.38D+06	297.46D+06	297.45D+06	297.41D+06	287.30D+06	202.63D+06
Floating point operations /sec	91.41D+06	90.65D+06	90.67D+06	90.65D+06	90.67D+06	90.67D+06	90.65D+06	90.65D+06	731.29D+06
Cycles	736.64D+06	742.86D+06	742.63D+06	742.86D+06	742.66D+06	742.69D+06	742.80D+06	742.80D+06	1.64D+09
Seconds	1.96D+00	1.98D+00	1.98D+00	1.98D+00	1.98D+00	1.98D+00	1.98D+00	1.98D+00	1.98D+00

Hardware Counters (% of all)	1	2	3	4	5	6	7	8	Sum or Max
Instruction TLB misses [%]	14.84	12.17	12.17	12.17	12.17	12.17	12.17	12.17	100.00
Data TLB misses [%]	13.42	12.08	13.42	12.08	12.08	13.42	12.08	11.41	100.00
Instruction Cache misses [%]	34.87	9.32	9.20	9.12	9.06	9.59	9.13	9.71	100.00
Data Cache misses [%]	12.73	12.65	12.71	12.66	12.66	12.66	12.72	11.22	100.00
Memory acc. instructions [%]	12.73	12.65	12.71	12.66	12.66	12.66	12.72	11.22	100.00
Total # of instructions [%]	12.56	12.55	12.55	12.55	12.55	12.55	12.55	12.13	100.00
Floating point operations [%]	12.50	12.50	12.50	12.50	12.50	12.50	12.50	12.50	100.00
Cycles [%]	12.41	12.51	12.51	12.51	12.51	12.51	12.51	12.51	100.00
Seconds [%]	12.41	12.51	12.51	12.51	12.51	12.51	12.51	12.51	100.00

Figure 4: Log file for one node of a typical run. Note the excellent *intranode* parallelization which is obtained using *the –opt=ss –parallel* compiler options.

A Hitachi Log file for one of the test runs (slightly different grid size) is shown in Figure 4. The overall computational speed per node amounts to ca. 730Mflops. It is important to note that this result is representative for a production run with all I/O.

c. Resources Needed for Next Period

The requirements for a *standard* simulation has been outlined in the original proposal. The requirements mentioned still hold. A high-resolution 3-D seismic simulation of an earthquake will be simulated on a O(1000x1000x500) grid (x,y,z-direction, respectively). The number of variables to be permanently stored in parallel

for elastic wave propagation problems is approx. (stresses and displacements at two different time steps, elastic parameters) 24. Thus the memory requirement for such a run would be on the order of 100 GBytes (double precision). The duration of a simulation – depending on the desired length of seismogram and the number of processors used – is estimated to be of 100-500 processor hours (which would have to be divided by the number of processors used). We initially asked for 160.000hours of which 40.000 were allocated in the first year.
Because of the various projects which were funded during last year (see below) and the many exciting scientific problems which are now possible with the implemented and verified codes we ask for an additional **150.000hours** for the second year.

3. **Scientific and technical results**

In the following results from the various projects which made use of the Hitachi in Year 1 of the project will be presented. Note that all publications and papers cited are stored on the accompanying CD-Rom.

a. **Volcano topography in 3-D seismic wave propagation** (Diplom thesis, paper in preparation): How does the (usually strong) topography affect the seismic wavefield observed on volcanoes? How can we model the topographic effects and the scattering effects inside the medium? In this thesis two methods (grid-stretching and a staircase method) which allow the modelling of topographic effects were implemented and tested for a realistic topography (digital elevation map of the Merapi volcano, Indonesia). An important result is that one of the method (grid-stretching) fails for real topography and has to be discarded. This project led to the first 3D simulation of wave propagation through a real volcano model. There are numerous applications for this technique. We intend to use this code to investigate (1) the seismic signature of pyroclastic flows; (2) seismic sources inside magma chambers and volcanic dykes; (3) scattering vs. topographic effects as observed on Merapi. This project will continue as a Ph.D. project (DFG).

b. **Site effects of the Cologne Basin** (Diplom thesis, paper in preparation): As reliable deterministic earthquake prediction is not in sight, the simulation of realistic earthquake scenarios is one of the most important tools to assess the seismic risk of active regions. In this project the first 3D calculation for the area in Germany with the highest seismic risk – the Cologne Basin – were carried out. The simulations show remarkably good agreement with observed data as far as the amplitudes for the ground motion is concerned which tells us that we are on the right way to be able to predict the possible ground motion amplification due to 3D structure for this (and other) areas. This project will continue as a Ph.D. project funded by the MunichRe which has obvious interest in such calculations. Within the KONWIHR project (NBW) this area of research will focus on the effects of topography in seismically active regions.

c. **The seismic signature of plumes** (Diplom thesis, paper in preparation): Hot spots like Hawaii, the Galapagos Islands or Iceland are characterized by large scale hot plumes underneath them, which are though to consist of rising material from inside the mantle. However, it is not clear, how deep the roots of the plumes are. Answering this question has strong implications for the dynamics of the Earth's interior (mantle convection). In this project 3D simulation for plume models were investigated. These simulations will be important to design future large scale experiments around hot spots which are planned within the OPP (Ocean Plume Project) in the near future. This project will be continued as a Ph.D. project (DFG).

d. **The seismic signature of subduction zones** (Diplom thesis (about to be finished), 1 paper in print, one paper in preparation): Subduction zones contain the largest earthquakes on Earth. Knowledge of there structural details not only is important for hazard assessment but also to understand the dynamics of subduction and mantle convection. In this project a 3D algorithm in spherical coordinates was implemented and earthquakes in subduction zones simulated. We were able to simulate particular wave effects observed in nature which – in the future – can be used to further constrain the structure of subduction zones.

e. **Fault zone wave propagation** (Ph.D. thesis and Diplom thesis, both in preparation ; one paper in print, one paper submitted, one paper in preparation). Fault zones (FZ) are though to consist of a highly localized damage zone with low seismic velocity and high attenuation. The structure of FZs at depth has important implications for the size of (future) earthquakes and the dynamic behaviour of the rupture. Only recently it was observed that right above FZs a particular wave type (guided waves) can be observed which may allow imaging FZs at depth. Numerical simulations play an important role in developing imaging schemes and assess their reliability. Several papers are presently being written on the phenomenology of waves in FZs by our group.

4. Reasons to Extend this Project

As demonstrated above in the first year of this project we implemented and verified several algorithms for various specific problems in computational seismology. The algorithms, as well as their implementation on one of the largest machines in the world available to Earth Scientists has given the projects considerable international attention. This is expressed in the numerous presentations at Meetings and the papers in print, submitted or in preparation. Yet, it is only now that our algorithms are really in production mode and that we can attack the scientific problems. Based on some of the initial results in Year 1 several research projects were funded (see below). For the outcome of these projects large-scale computations are crucial.

Example: The 3D structure of sedimentary basins strongly influence the ground motion after earthquakes. However, to properly assess the seismic hazard to a region like the Cologne basin, the Los Angeles basin, or the San Francisco Area a large number of likely earthquake scenarios (O(100)) are necessary. The Hitachi would offer the opportunity to carry out such a detailed study for the first time. This project would benefit from collaboration with the University of Southern California. A travel grant for exchange of staff and students has been granted by the Bavarian Californian Technology Institution (BaCaTec) in 2001.

5. Current and Future Projects with Relevance to High-Performance Computing at the Institute of Geophysics (Project leader Prof. Dr. Heiner Igel)

a. Wave Propagation in a heterogeneous spherical Earth (DFG, 2000-2002)
b. The seismic signature of plumes (DFG, 2001-2003)
c. The simulation and interpretation of rotational motions after earthquakes (BMBF, 2002-2005)
d. Numerical wave propagation in seismically active regions (KONWIHR, initially until 2002, may be further extended).
e. International Quality Network: Georisk (www.iqn-georisk.de) funded by the DAAD, 2001-2003. Will allow students, post-docs, professors from other countries to visit our Institute and take part in research projects. In combination with our simulation algorithms this may allow us to combine the numerical aspects with data from regions at risk. Involved countries: USA, Indonesia, China, New Zealand, Japan. The core of this network is a research group (1 post-doc, 3 PhD students) residing in Munich working of risk and hazard related problems in seismology and volcanology.

6. Publications (with results from simulations on Hitachi SR-8000)

Igel, H., Nissen-Meyer, T., Jahnke, G., 2001. Wave propagation in 3-D spherical sections: effects of subduction zones, Phys. Earth Planet. Int., in print.
Igel, H., Jahnke, G., Ben-Zion, Y., 2001. Numerical simulation of fault zone guided waves: accuracy and 3-D effects, Pure and Applied Geophysics, in print.
Jahnke, G., Igel, H., Ben-Zion, Y., 2001. Fault zone guided waves: the effects of 3D structure, submitted to Geophys. J. Int.

Ewald, M. 2001. Numerical simulation of site effects with applications to the Cologne basin, Diplom thesis, Institute of Geophysics, LMU, paper in preparation.
Ripperger, J., 2001. Volcano topography in 3-D seismic wave simulation, Diplom thesis, Institute of Geophysics, LMU, paper in preparation.
Nissen-Meyer, T., 2001 (to be finished beginning of september). Wave propagation through 3D subduction zones. Diplom thesis, Institute of Geophysics, LMU, further paper in preparation.
Strasser, M., 2001. Seismic signature of subduction zones, Diplom thesis, Institute of Geophysics, LMU, paper in preparation.

All these publications plus some movies are on the attached CD-Rom.