Current and Future Computational Geoscience Directions: Successes & Failures

Seismology Working Group

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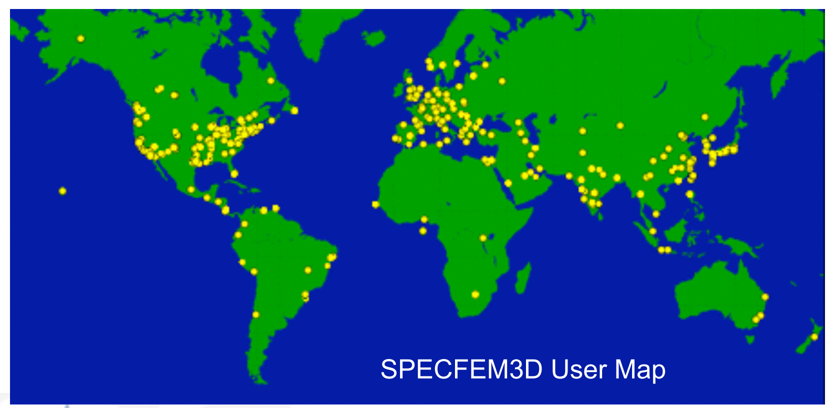
CIG Seismology Software

- MINEOS normal-mode synthetics
- SEISMIC_CMPL finite-difference package (Pau)
- SPECFEM3D Regional SEM synthetics
- SPECFEM3D_GLOBE Global SEM synthetics
- SPECFEM2D SEM package (CUBIT & Scotch-SEM)
- SPECFEM1D Introductory SEM package
- Princeton dynamic ray-tracing software
- SPICE Software Library link
- Soon:
  - LLNL finite-difference software
  - FLEXWIN data selection software
  - SPECFEM3D_SESAME (CUBIT-Scotch-SEM)

Seismology Download Statistics

	Sept.-Nov.	Dec.-Feb.
• Mineos 1.0.0	30	23
• SEISMIC_CMPL 1.0.1	72	67
• SPECFEM3D 1.4.3	92	68
• SPECFEM3D_GLOBE 4.0.3	111	57
• SPECFEM2D 5.2.2	54	42
• SPECFEM1D 1.0.0	51	37
• Total:	**704**	



CIG Seismology Workshops

- CIG-SPICE-IRIS Computational Seismology Workshop, October 9-11, 2007, Jackson, NH
  - ~60 International participants
  - Future joint meetings & collaborations
- Session at the 2008 IRIS Workshop
- Session at the 2009 Earthscope meeting

Current CIG Work

- Computational Seismology Science Gateway (Leif Strand)
  - Normal-mode synthetics (MINEOS)
  - Spectral-element synthetics (SPECFEM3D_GLOBE)
  - https://crust.geodynamics.org/portals/seismo/
- Integration of CITCOM and SPECFEM3D_GLOBE (Eh Tan & Leif Strand)

On-Demand Simulations

- SEM and mode synthetics via the CIG Seismology Web Portal:

https://crust.geodynamics.org/portals/seismo/

- SEM: 18 s to 27 s shortest period
- Modes: 5 s shortest period

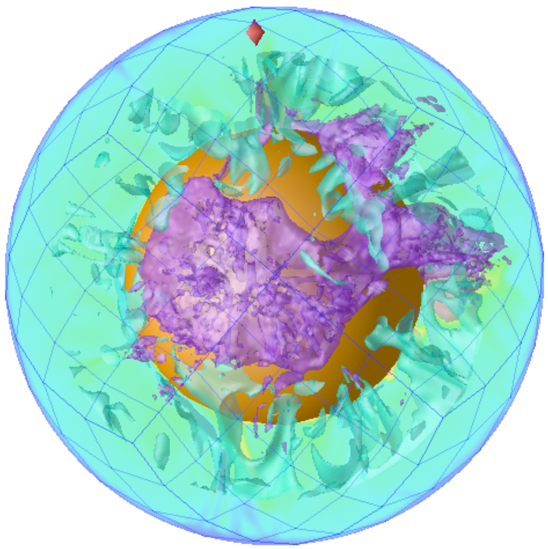
Soon: Near Real-Time Simulations

For every event reported by the Global Centroid-Moment Tensor (CMT) project:

- Spectral-Element Method (SEM) synthetics:
  - 3D model S362ANI (Kustowski et al. 2008)
  - Crust2.0 (Bassin et al.)
  - Topography & bathymetry
  - Rotation & ellipticity
  - Self-gravitation (Cowling)
  - Oceans
  - Accurate from 17 s to 800 s
- Mode synthetics:
  - PREM (Dziewonski & Anderson 1981)
  - Accurate at 8 s and longer
- Duration:
  - Mw < 7.5: 100 min (R1 & G1)
  - Mw >= 7.5: 200 min (R2 & G2)

Coupling CitcomS with SPECFEM3D

- CitcomS → *T, P, X* → mineral physics model → [illegible], *Vp, Vs* → SPECFEM3D → *seismograms*
    - Mineral physics model incorporated into CitcomS V3.1 (to be released)
    - SPECFEM3D interpolating [illegible], *Vp, Vs* from CitcomS grid
    - Deployed through CIG seismology portal



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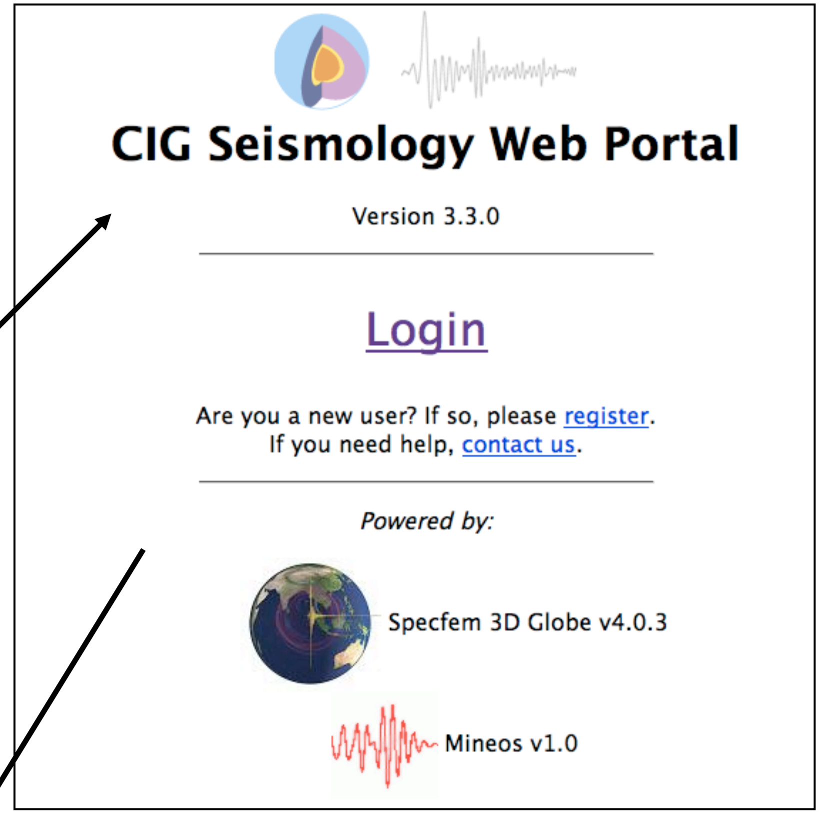


, Vp, Vs

download

seismograms

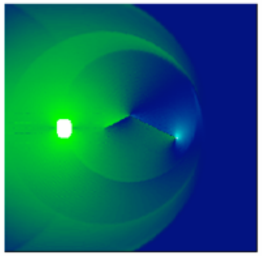
Details in Tan & Strand's poster

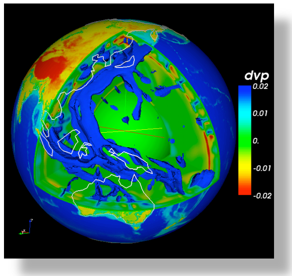
SPICE

- 2004 –2007, Marie Curie Research Training Network, funded by European Union
- 14 Partner institutions in 10 countries
- 14 PhD (3-yrs) and 14 postdoc (2-yrs) positions
- Annual research and training workshops
  - 2004 Numerical Methods, Venice, Italy
  - 2005 Large scale applications, Smolenice, Slovak Rep.
  - 2006 Inverse Problems, Kinsale
  - 2007 Wave propagation in other fields, Cargese
- 5 task groups
- Budget 5.5 Million Euro

SPICE Task Groups

- Reservoirs & Volcanoes
- Rupture and seismic hazard
- Global wave propagation
- Numerical Methods
- Software Library





1DFD_DS
The Fortran95 Computer Code for Finite-Difference Numerical Generation and Simulation of a 1D Seismic Wavefield in a 1D Heterogeneous Viscoelastic Medium Using the Displacement-Stress Staggered-Grid Finite-Difference Scheme

1DFD_DVS
The Fortran95 Computer Code for Finite-Difference Numerical Generation and Simulation of a 1D Seismic Wavefield in a 1D Heterogeneous Viscoelastic Medium Using the Displacement-Velocity-Stress Staggered-Grid Finite-Difference Scheme

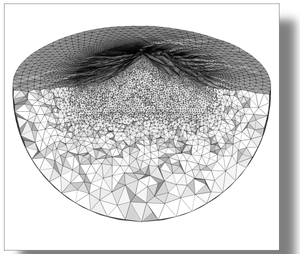
1DFD_VS
The Fortran95 Computer Code for Finite-Difference Numerical Generation and Simulation of a 1D Seismic Wavefield in a 1D Heterogeneous Viscoelastic Medium Using the Velocity-Stress Staggered-Grid Finite-Difference Scheme

3DFD_DVS
The program is designed for computation of seismic wavefields in 3D heterogeneous surface geological structures with planar free surface due to surface and near-surface point doublecouple sources

Direct Solution Method
DSM software for calculating full wave synthetics in a laterally homogeneous spherically symmetric earth model

FD3S
Finite-difference solver of the elastic wave equation in a spherical section. FD3S allows to model seismic wave attenuation as well as anisotropy with radial symmetry axis. The finite difference scheme is of fourth order in space and of second order in time. Arbitrarily complex Earth models can easily be included.

FD3S(AD)
FD3S(AD) is an extension of FD3S (see above) that allows to compute the derivative of an objective functional defined on a recorded seismic wavefield with respect to the model parameters. The computation of the derivative is based on the adjoint method.



QUEST

QUantitative estimation of Earth's sources and STructure

- **Improve the quality of structural and source images** derived from seismic data by incorporating 3-D simulation full waveform methods into the imaging process.
- **Develop novel approaches using passive imaging** that make use of virtual sources, investigate and broaden their domains of application on all scales.
- **Demonstrate the improved imaging power** through applications on a reservoir scale (CO_2-sequestration), volcanoes, active seismic faults, and planets.
- **Disseminate the developed methodologies to the user community** through an open source software repository and web-interfaced benchmark facilities.

Proposal submitted:	Sep 7, 2008
Expected project start:	Sep-Dec, 2009

Long Term Plans (2007)

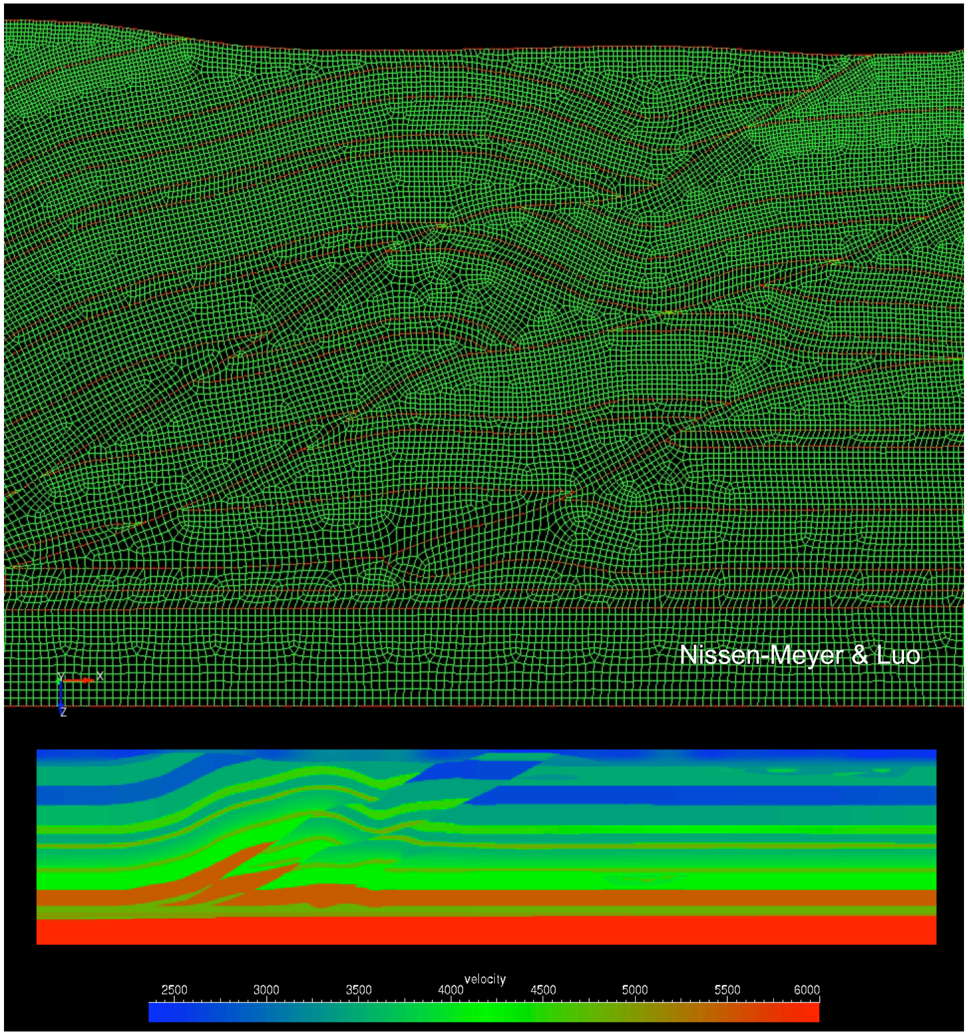
- **Automated/On-Demand Simulations**: CIG will work to further establish a Seismology Science Gateway, involving both automated and on-demand simulations. Automated simulations would provide near real-time 1D and/or 3D synthetics to accompany IRIS data for all events over a certain magnitude threshold using past and emerging events in the CMT catalog.
- **Seismic Model Database**: There is the need for a database of seismic models, including structural models of the crust and mantle together with databases of topography and bathymetry. Various resolutions are needed to match the capabilities of codes being developed under CIG. Mechanisms for the contribution of models must be established.
- **Data Processing Tools**: The SSC is considering whether CIG should investigate the feasibility of facilitating the development of data processing tools for field and laboratory use. These could include low-level routines for standard data manipulation (e.g., filtering, simple array analyses); higher level functionality such as earthquake location, traveltime picking, and moment tensor analysis; and high-level functionality such as tomography, receiver functions (perhaps with migration), and shear-wave splitting.
- **Visualization** of 2D and 3D seismic models is increasingly important in seismology and presents an area of great overlap with other CIG efforts that require coordination. Imaging/tomographic tools may be included productively within the CIG framework.

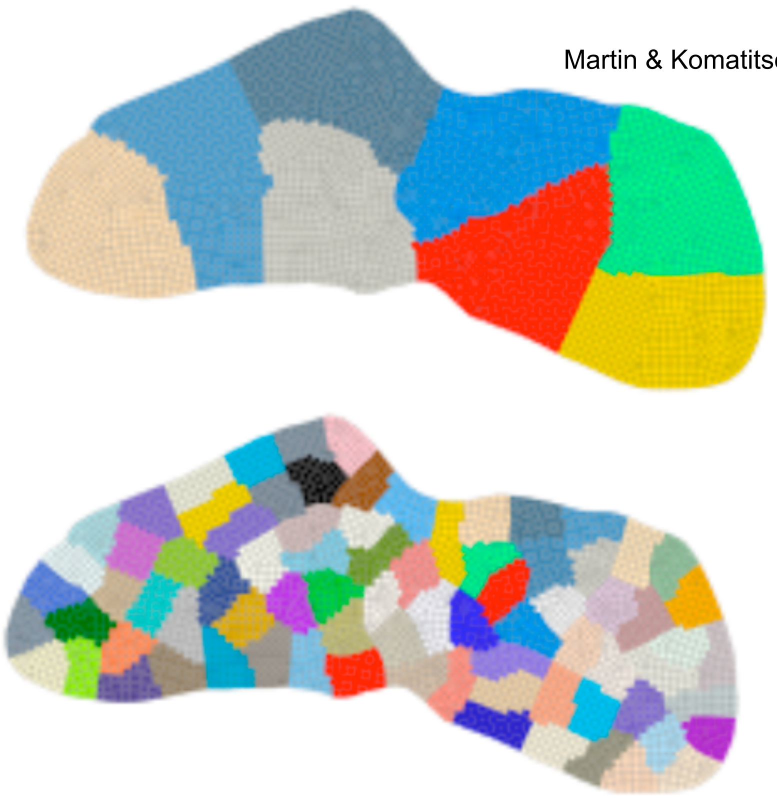
Successes & Failures

- Software Library
- IRIS-SPICE-CIG collaboration

- The Seismology Portal is currently not as widely used as anticipated
- Limited engagement of US seismologists

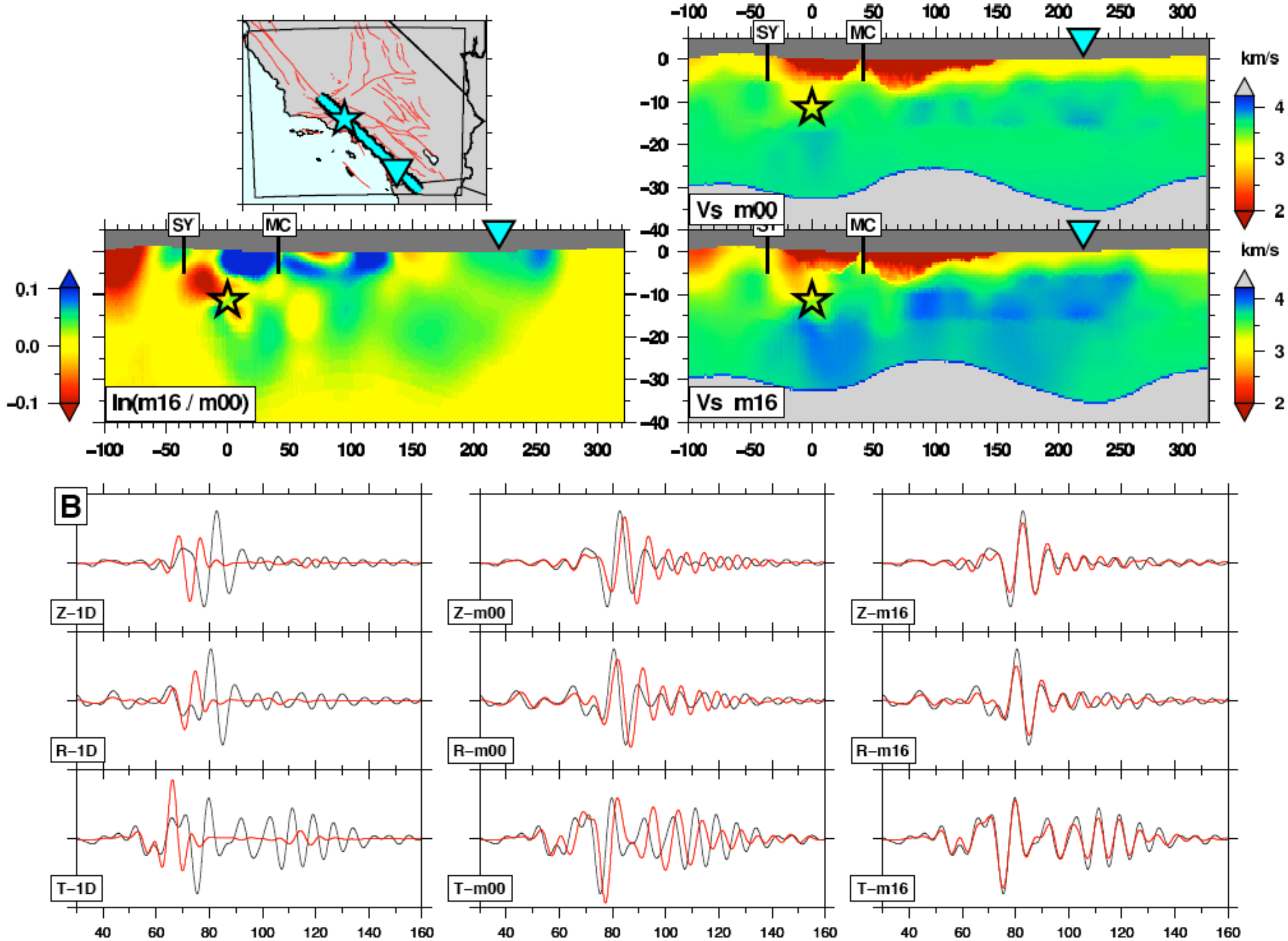
Future Efforts: Flexible Meshing & Load-Balancing





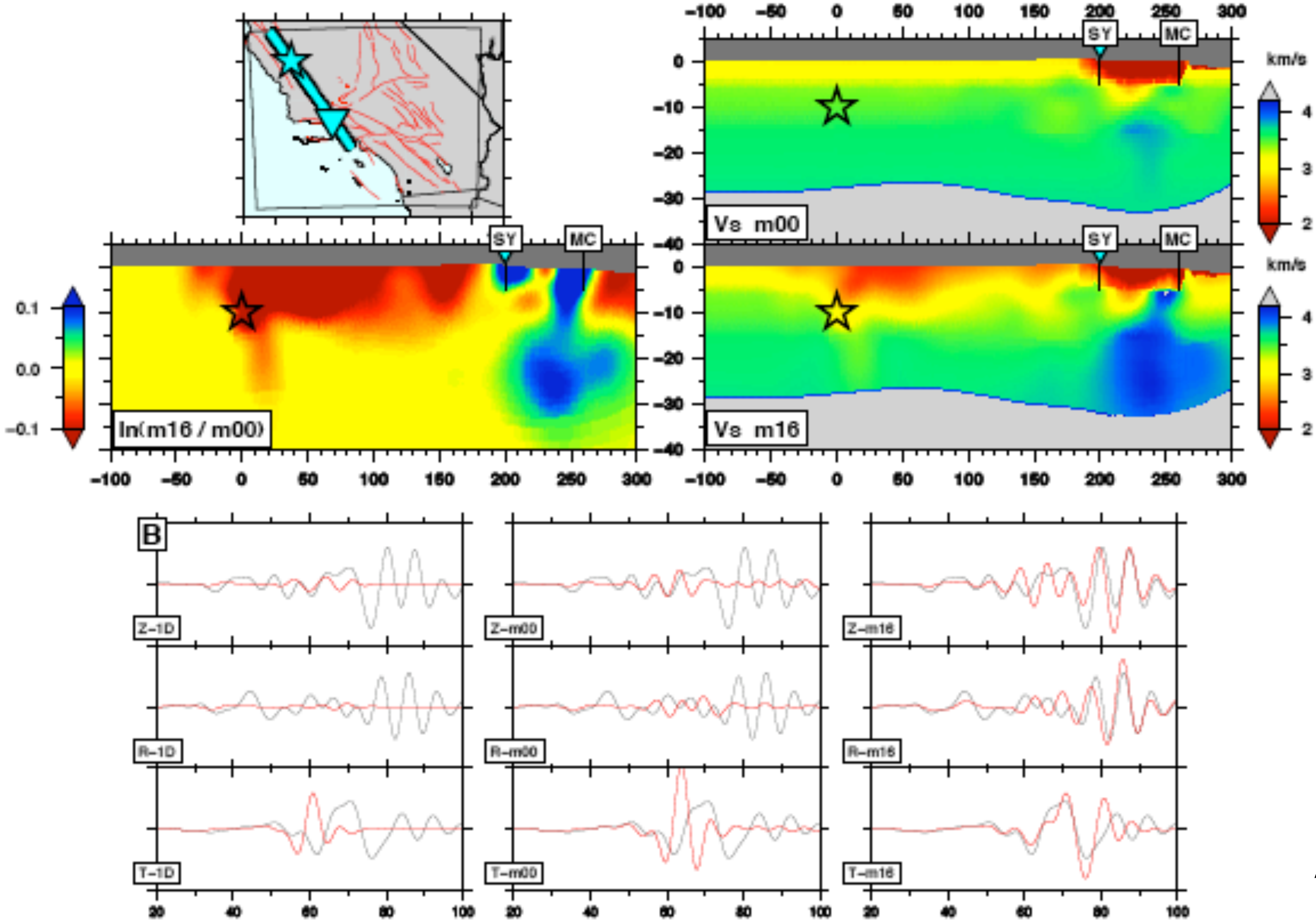
Meshing: CUBIT
Load-Balancing: Scotch
Solver: SEM

Future Efforts: Imaging



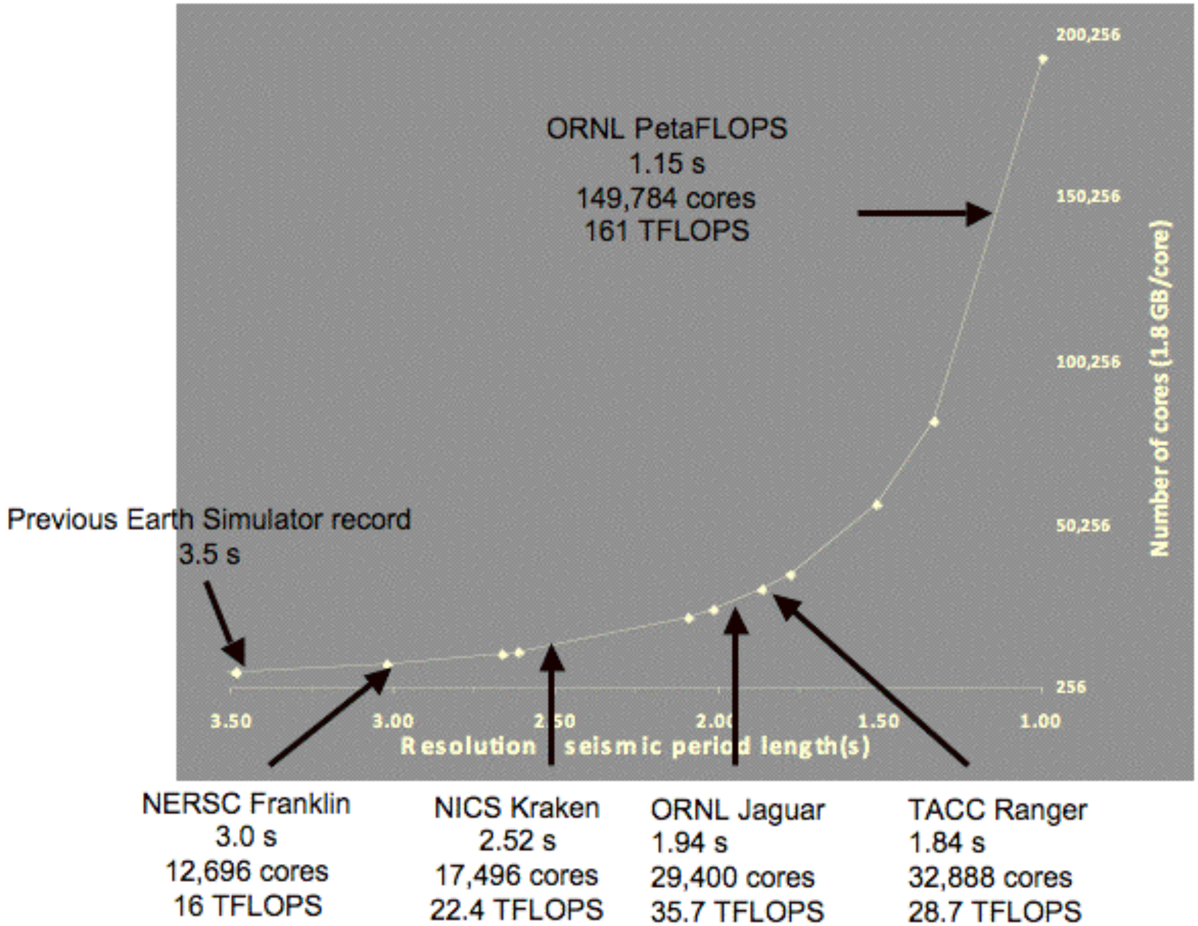
Adjoint Tomograpgy:
Carl Tape

Future Efforts: Imaging



Adjoint Tomograpgy:
Carl Tape

Future Efforts: Peta-Scale Computing



Carrington et al. (SC'08)

Testing seismic tomography models using numerical simulation of wave propagation

Ebru Bozdağ & Jeannot Trampert
Department of Earth Sciences, Utrecht University, Utrecht, the Netherlands

It is very well known that Earth's crust has a very strong influence on surface waves. Therefore, crustal corrections are a crucial step in surface wave tomography to enhance mantle structures. In Bozdağ & Trampert [2008], we investigated crustal effects on tomographic mantle images. We estimated crustal corrections using first order ray theoretical and finite frequency approximations and compared them to those obtained from full 3-D wave simulations with the spectral element method. We observed that crustal effects cannot be completely removed from seismograms and produce errors larger than those in phase velocity measurements at periods shorter than 60 and 80 s for Rayleigh and Love waves, respectively. In addition, Rayleigh and Love waves are affected by the crust in a different way. As a consequence, our observations indicate that imperfect crustal corrections could have a large impact on inferences of radial mantle anisotropy. Part of mantle anisotropy could be uncorrected crustal signal. Possible solutions are to use 3-D reference models or to invert crust and mantle together instead of applying crustal corrections.

In Bozdağ & Trampert [2009], we investigated to what extent current tomographic mantle images represent the real Earth's mantle. For this purpose, we compared real seismograms to those computed by the spectral element method in some 3-D mantle models. In particular, we examined the effect of damping on our interpretation of the mantle by choosing differently damped mantle models. Surprisingly, synthetic seismograms are statistically insensitive to differently damped models. These observations point to a crustal signal which could not be properly removed from the data by corrections. In addition, we observed a large amplitude signal which is usually ignored in classical mantle tomography. The amplitude mismatches are most likely due to our ignorance in attenuation. Body wave amplitudes however are more sensitive to focusing/defocusing effects than surface waves.

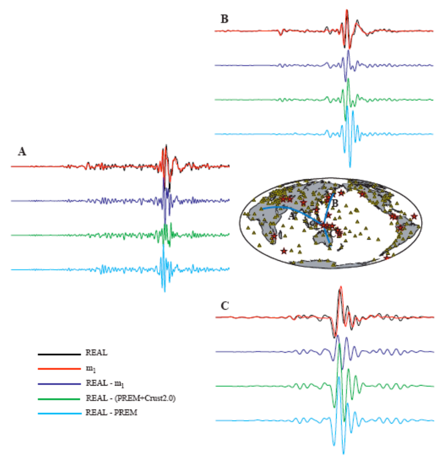


***Figure** An example for comparison of real seismograms with the synthetic ones computed in 1D (PREM) and 3D crust (Crust2.0) and mantle (m_1) models by SPECFEM3D. Blue, green and cyan seismograms show the waveform differences.*

The computation of synthetic seismograms in these studies was performed by SPECFEM3D-GLOBE package that we obtained from CIG.

References
Bozdağ, E. & Trampert, J., 2008. On crustal corrections in surface wave tomography, **Geophysical Journal International**, 172, 1066-1082.
Bozdağ, E. & Trampert, J., 2009. Assessment of tomographic mantle models using spectral element seismograms, **Geophysical Journal International**, under revision.

Evaluating the effectiveness of current 3-D earth models for use in rapid earthquake source characterisation

Alison Kirkby and Phil Cummins, Geoscience Australia

Tsunami warning systems typically use only magnitude and location to identify potentially tsunamigenic earthquakes, but slip distribution may also have an influence if the fault rupture length is comparable to the tsunami propagation distance. For example, the M_W 9.3 Sumatra-Andaman earthquake in 2004 had a rupture length of >1200km, so that even coastlines 1000s of km distant from the source could experience tsunami heights sensitive to details of the fault slip.

Slip model inversions typically use waveform calculations that only approximately account for 3D structure, and these often involve a minimum distance for their application, delaying the time in which data can be used to produce a slip model. The purpose of this project is to explore whether this distance threshold can be reduced by using seismograms accurately calculated for 3D earth structure. We compared synthetic surface wave seismograms calculated for a point source representation of the 12 September, 2007 Mw=8.5 earthquake off Sumatra using (a) an asymptotic method accounting for 3D structure via a global phase velocity map, and (b) calculations using SPECFEM3D via the CIG portal. The calculated waveforms were compared with each other via cross-correlation (Figure 1.).

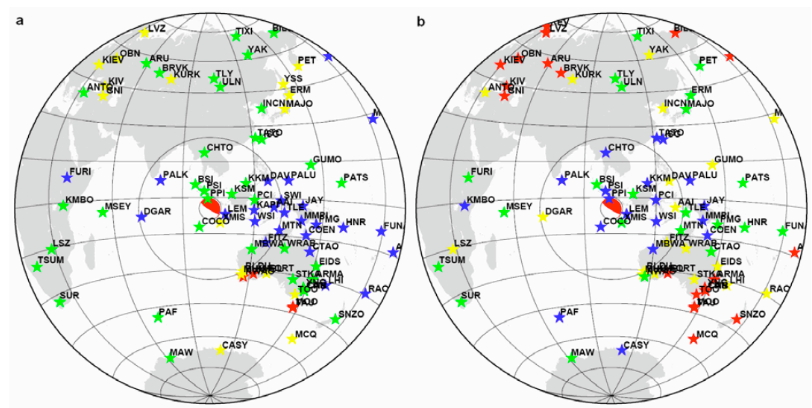


Figure 1. Results of cross correlating point source synthetics from 1D and 3D earth models for the Sumatra event, plotted according to: (a) correlation coefficients (vertical component) of <0.85 (red), 0.85 – 0.90 (yellow), 0.90 – 0.95 (green), 0.95 – 1.00 (blue), (b) correlation coefficients (transverse component).

The results, and similar ones for the 2007 Solomon Islands earthquake, show geographically coherent patterns of low and high correlation. Most of the correlations within the 30º distance threshold, where we expected our use of a phase velocity map might break down, are high. The regions of poorly correlated synthetics are generally at large distance form the source and exhibit some similarity for the two events studied – in particular, some correlations were poor in southern Australia, particularly for the transverse component synthetics.

The results suggest that the effects of 3D structure on the seismic waveform data used for finite fault rupture modelling should be further investigated, especially if its use is to be considered for the Australian stations important for the Australian Tsunami Warning System. Future work will focus on comparing synthetics computed for finite fault models with actual data.

Adjoint tomography for the Middle East

Daniel Peter[1], Arthur Rodgers[2], Brian Savage[3], Jeroen Tromp[1]
[1] Princeton University, [2]Lawrence Livermore National Laboratory, [3]University of Rhode Island

Using [SPECFEM3D_GLOBE], we evaluate 3D models of the Middle East by computing full waveforms for several regional earthquakes. We measure traveltime shifts between observed broadband data and synthetic seismograms for distinct seismic phases within selected time windows using a recently developed automated measurement algorithm [FLEXWIN]. We take advantage of [SPECFEM3D_GLOBE] together with the package [ADJOINT_TOMO] in order to calculate the sensitivity to seismic structure of the traveltime measurements for all available seismic network recordings for a fully numerical 3D seismic tomography approach.

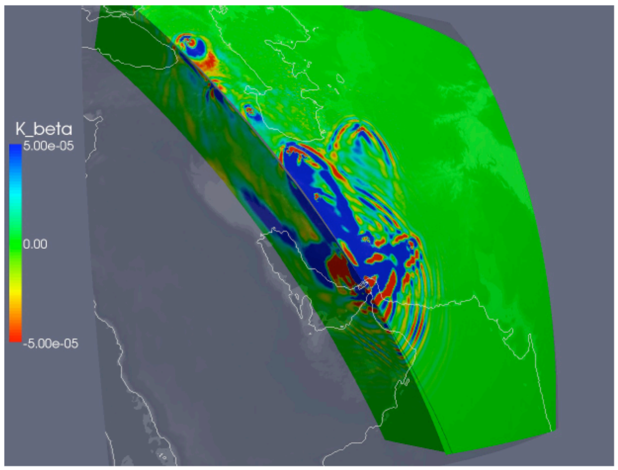


Figure 1: Shear-velocity event kernel for an earthquake in the strait of Hormuz recorded 2005 by several regional stations. Sensitivities are shown on a horizontal cross-section at 5 km depth and a vertical cross-section through the source and a station location down to a depth of 670 km.

References

[1] Peter, D., A. Rodgers, B. Savage and J. Tromp, 2008. Adjoint tomography for the Middle East, AGU fall meeting 2008, paper presented.

An unsplit convolutional Perfectly Matched Layer improved at grazing incidence for the seismic wave equation

R. Martin, *University of Pau, France*
D. Komatitsch, *University of Pau, France; Institut universitaire de France, Paris, France*

The Perfectly Matched Layer absorbing boundary condition has proven to be very efficient from a numerical point of view for the elastic wave equation to absorb both body waves with non-grazing incidence and surface waves. However, at grazing incidence the classical discrete Perfectly Matched Layer method suffers from large spurious reflections that make it less efficient for instance in the case of very thin mesh slices, in the case of sources located close to the edge of the mesh, and/or in the case of receivers located at very large offset. We demonstrate how to improve the Perfectly Matched Layer at grazing incidence for the differential seismic wave equation based on an unsplit convolution technique. The improved PML has a cost that is similar in terms of memory storage to that of the classical PML. We illustrate the efficiency of this improved Convolutional Perfectly Matched Layer based on numerical benchmarks using a finite-difference method on a thin mesh slice for an isotropic material and show that results are significantly improved compared with the classical Perfectly Matched Layer technique. We also show that, as the classical model, the technique is intrinsically unstable in the case of some anisotropic materials.

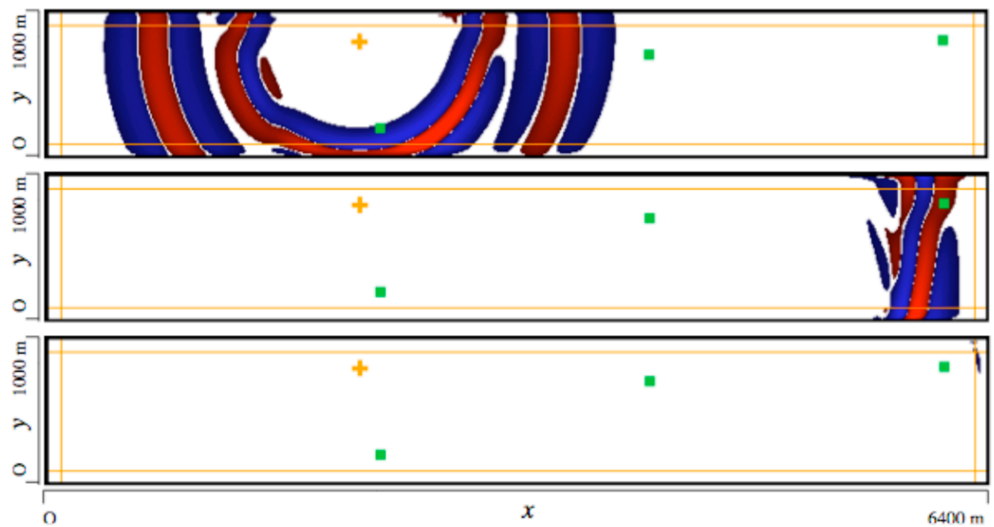


Figure 1: *Snapshots in a (x,y) plane of the v_y component of the three-dimensional velocity vector for a model corresponding to a thin slice with C-PML conditions implemented on the six sides. We represent the component in red (positive) or blue (negative) at each grid point. The orange cross indicates the position of the source. The four vertical or horizontal orange lines represent the edge of each layer PML. No spurious wave of significant amplitude is visible, even at grazing incidence.*

Simulation of seismic wave propagation in a 3D asteroid model using an unstructured MPI spectral-element method and non-blocking communications

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J. Labarta, *Barcelona Supercomputing Center, Spain*

We implement spectral-element calculations in parallel in an asteroid based upon MPI. Homogeneous an fractured models are meshed using the CUBIT mesh generator developed at Sandia National Laboratorie (USA) and the unstructured meshes are partitioned using the SCOTCH graph partitioning library, whicl focuses on balancing the size of the different domains and minimizing the edge cut to optimize loa balancing in our parallel non-blocking MPI implementations. Balancing the size of the domains ensure that no processor core remains idle for a significant amount of time while others are still running at eacl iteration of the time loop, while a small edge cut reduces the number and the size of the communications Contributions between neighboring elements that are located on different processor cores are added usin non-blocking MPI sends and receives. Internal force contributions from the outer elements of a give mesh partition are computed first and sent to the neighbors of that mesh slice using a non-blocking MP send. Similarly, each processor core issues non-blocking MPI receives. Communications are the overlapped by the calculations.

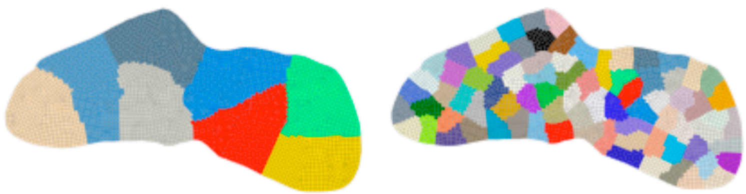

Figure 1: *Partitioning of a homogeneous model mesh obtained in the case of 8 (left) and 80 (right) domains. The number of elements along the interface of the partitions is small compared to the number o elements inside each partition in the case of 8 domains and overlapping of communications with calculations works fine. But for 80 domains, this number becomes comparable or even higher than the number of inner elements and overlapping tends to fail with poor performances.*

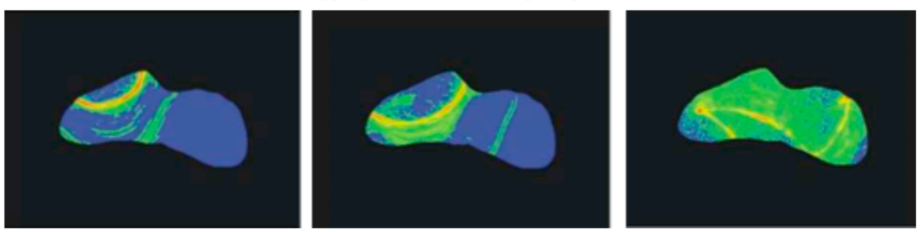

Figure 2: *Snapshots of the propagation of simulated 3D seismic waves in the geological model for a tota duration of 20 seconds in the case of a 3D asteroid model with a regolith layer. Snapshots are shown at 4~s, 6~s and 15~s on the 3D surface. We represent the vertical component of the displacement vector.*

High-Frequency Simulations of Global Seismic Wave Propagation Using SPECFEM3D_GLOBE

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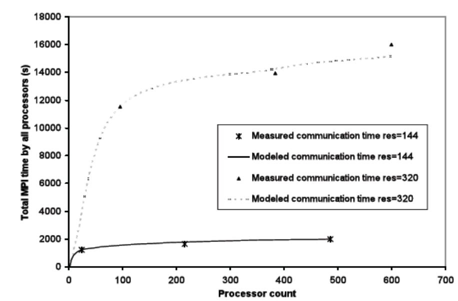
SPECFEM3D_GLOBE is a spectral-element application enabling the simulation of global seismic wave propagation in 3D anelastic, anisotropic, rotating and self-gravitating Earth models at unprecedented resolution. A fundamental challenge in global seismology is to model the propagation of waves with periods between 1 and 2 seconds, the highest frequency signals that can propagate clear across the Earth. These waves help reveal the 3D structure of the Earth's deep interior and can be compared to seismographic recordings. We broke the 2 second barrier using the 62K processor Ranger system at TACC. Indeed we broke the barrier using just half of Ranger, by reaching a period of 1.84 seconds with sustained 28.7 Tflops on 32K processors. We obtained similar results on the XT4 Franklin system at NERSC and the XT4 Kraken system at University of Tennessee Knoxville, while a similar run on the 28K processor Jaguar system at ORNL, which has more memory per processor, sustained 35.7 Tflops (a higher flops rate) with a 1.94 shortest period. For the final run we obtained access to the ORNL Petaflop System, a new very large XT5 just coming online, and achieved 1.72 shortest period and 161 Tflops using 149,784 cores.

With this landmark calculation we have enabled a powerful new tool for seismic wave simulation, one that operates in the same frequency regimes as nature; in seismology there is no need to pursue periods much smaller because higher frequency signals do not propagate across the entire globe.

We employed performance modeling methods to identify performance bottlenecks and worked through issues of parallel I/O and scalability. Improved mesh design and numbering results in excellent load balancing and few cache misses. The primary achievements are not just the scalability and high teraflops number, but a historic step towards understanding the physics and chemistry of the Earth's interior at unprecedented resolution.



Fitted curves for total communication time (in seconds) for all cores for different resolutions.

Three-Dimensional Simulations of Seismic-Wave Propagation in the Taipei Basin with Realistic Topography Based upon the Spectral-Element Method

Shiann-Jong Lee[1], How-Wei Chen[2], Qinya Liu[3], Dimitri Komatitsch[4,5], Bor-Shouh Huang[1] and Jeroen Tromp[6]

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[2] Institute of Geophysics, National Central University, Jung-Li, Taiwan, ROC
[3] Seismological Laboratory, California Institute of Technology, Pasadena, California, USA
[4] Institut universitaire de France, 103 boulevard Saint-Michel, 75005 Paris, France
[5] Department of Modeling and Imaging in Geosciences, CNRS UMR 5212 and INRIA Magique3D, University of Pau, France
[6] Department of Geosciences, Princeton University, Princeton, USA

We use the spectral-element method to simulate strong ground motion throughout the Taipei metropolitan area. Mesh generation for the Taipei basin poses two main challenges: 1) the basin is surrounded by steep mountains, and 2) the city is located on top of a shallow, low wave-speed sedimentary basin. To accommodate the steep and rapidly varying topography, we introduce a thin high-resolution mesh layer near the surface. The mesh for the shallow sedimentary basin is adjusted to honor its complex geometry and sharp lateral wave-speed contrasts. Variations in Moho thickness beneath Northern Taiwan are also incorporated in the mesh. Spectral-element simulations show that ground motion in the Taipei metropolitan region is strongly affected by the geometry of the basin and the surrounding mountains. The amplification of ground motion is mainly controlled by basin depth and shallow shear-wave speeds, although surface topography also serves to amplify and prolong seismic shaking.

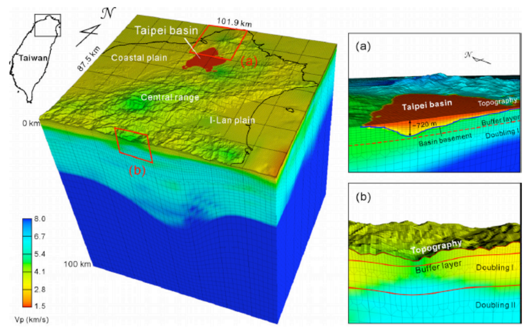

Fig.1 Spectral-element mesh for northern Taiwan. (a) Mesh implementation for the Taipei basin. (b) Mesh that incorporates realistic topography.

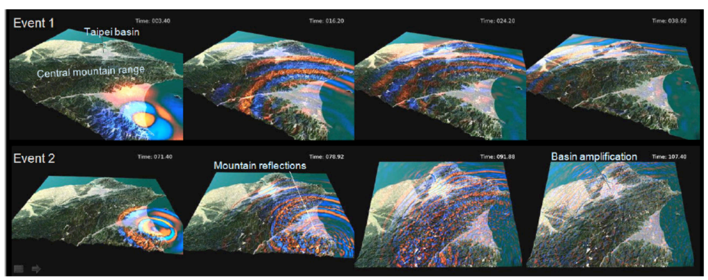

Fig.2 3-D SEM simulation and visualization of March 6, 2005 Ilan earthquake doublet. The amplification due to soft materials in the Taipei basin as well as the reflected and refracted waves generated by scattering from the mountains are clearly observed in these visual images.

Reference

Lee, S. J., H. W. Chen, Q. Liu, D. Komatitsch, B. S. Huang and J. Tromp, 2008. Three-dimensional simulations of seismic wave propagation in the Taipei basin with realistic topography based upon the spectral-element method, *Bull. Seism. Soc. Am.*, 98, 253-264, doi: 10.1785/0120070033.