Rupture, Waves, Imaging:
the role of high-performance computing (HPC)

Heiner Igel

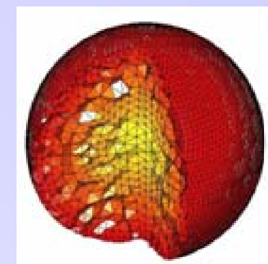
with R. Barsch, P. Bunge, G. Brietzke, A. Fichtner, F. Gallovic, M. Käser, J. de la Puente, B. Schuberth, M. Stupazzini, H. Wang
Department of Earth and Environmental Sciences, Munich, Germany

I The **beginning** of parallel computing in Europe

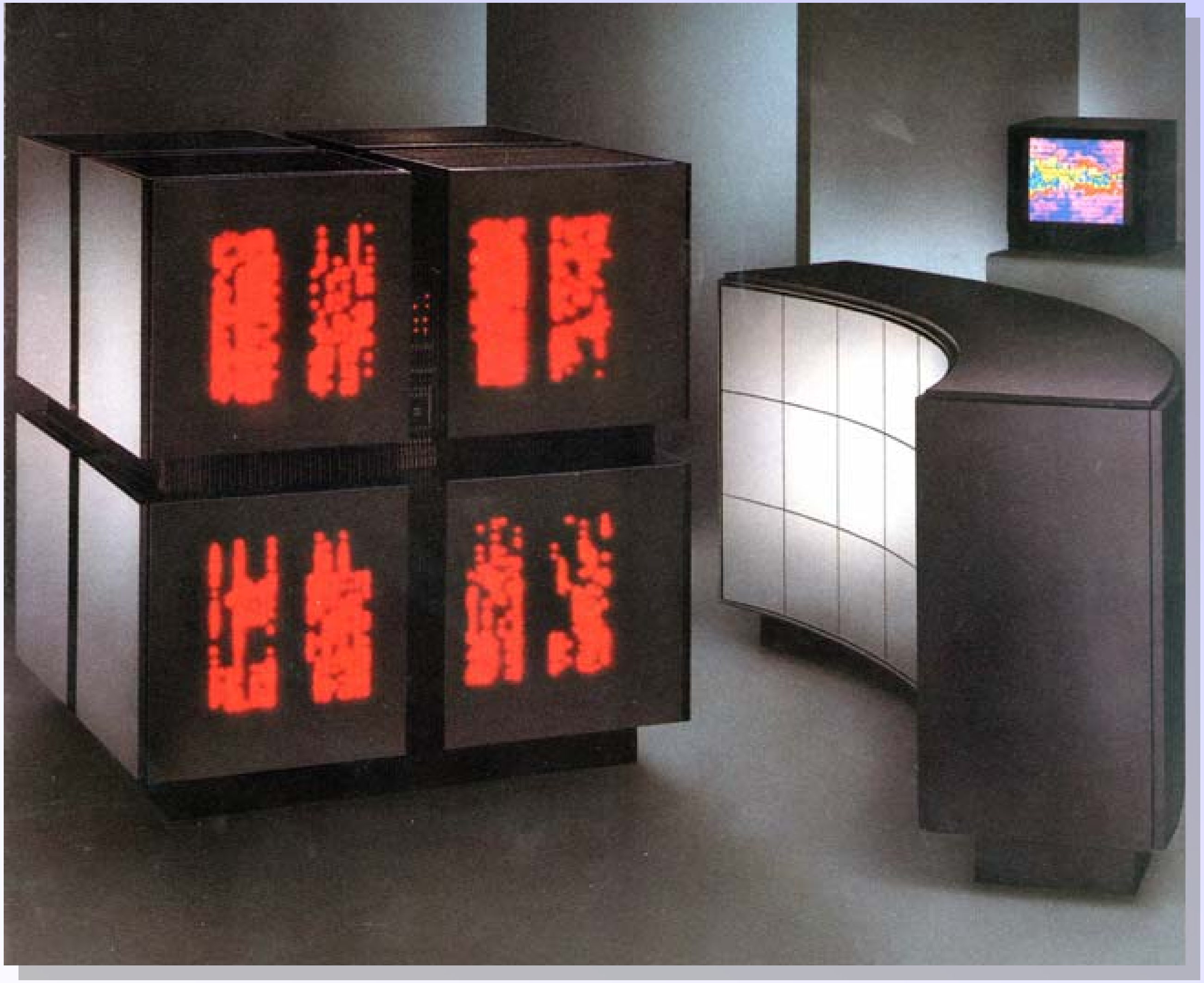
II Technical challenges for wave propagation
- The Grenoble valley **benchmark exercise**
- Waves on **unstructured grids**

III Science with HPC
- Understanding earthquake **rupture**
- Prediction of **strong ground motions**
- The **seismic signature of mantle convection**
- **Imaging** with 3-D methods – adjoint method

IV What is **missing**?

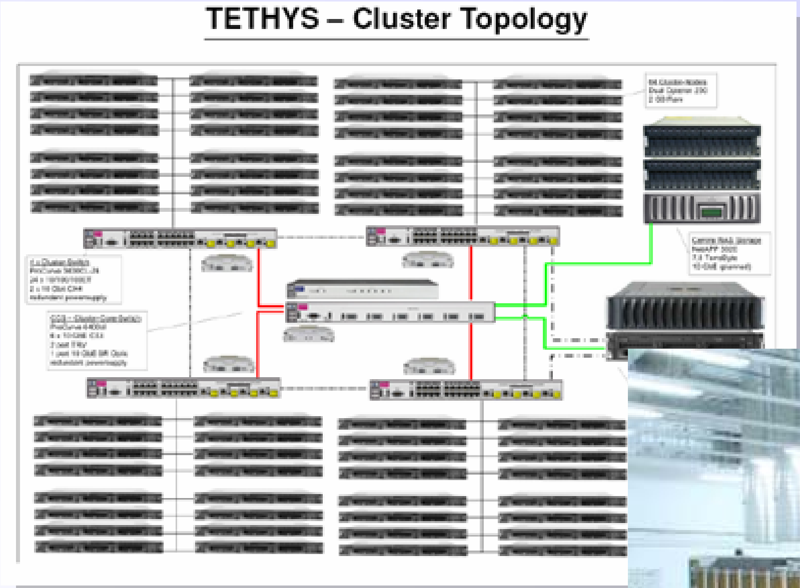


1990: Connection Machine CM-2



2007: Clusters and Supercomputers

Meso-scale

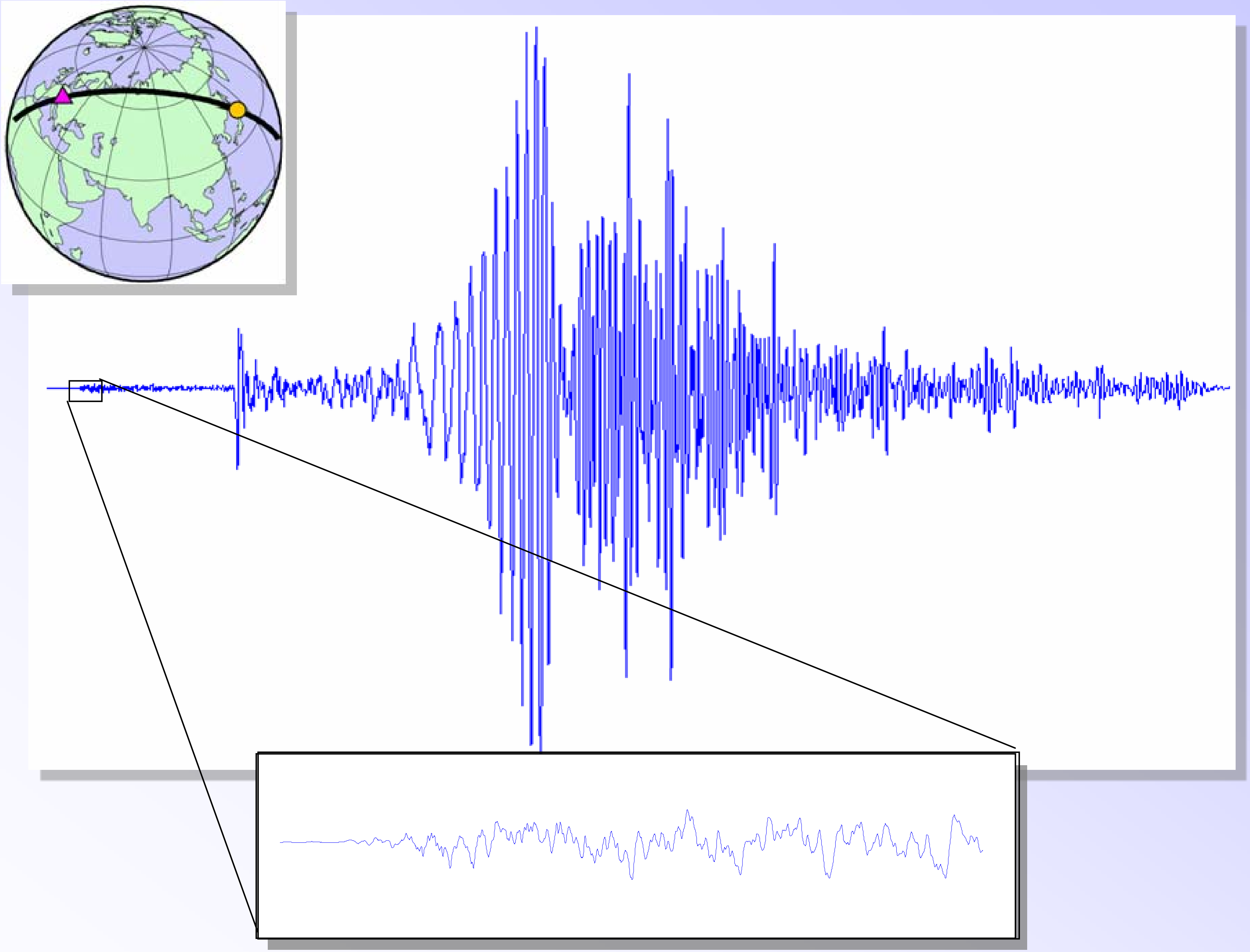


Source: Oeser et al., 2006

GCS
Gauss Centre for Supercomputing

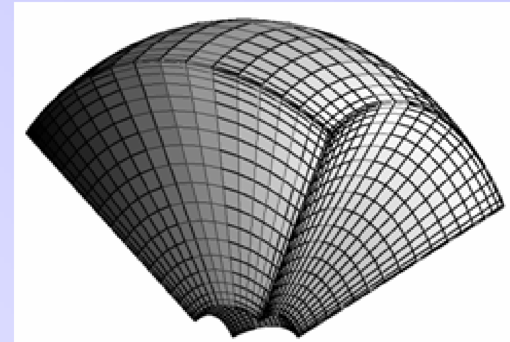
Super-scale

Source: LRZ Munich

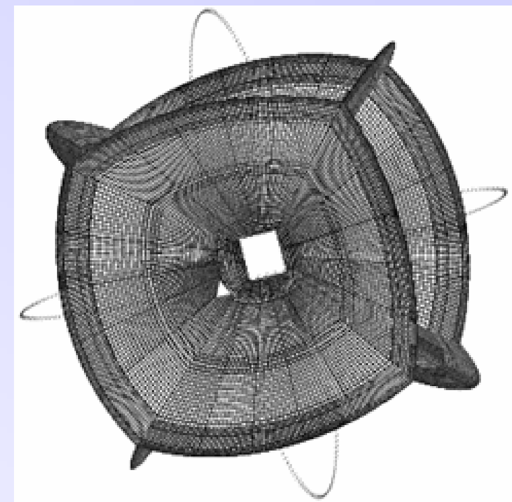


Spatial Scales and Memory

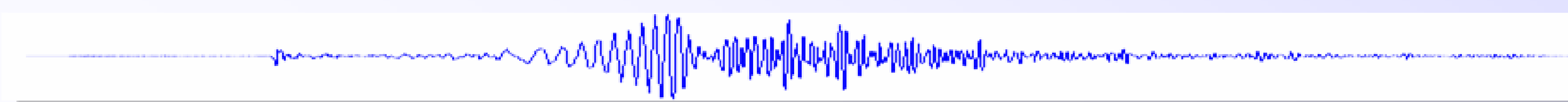
(back of the envelope)



Highest frequency:	**1 Hz**
Shortest wavelength:	2 km (crust)
Shortest wavelength:	5 km (mantle)
Grid points per wavelength:	5
Grid spacing:	200 m (crust)
Grid spacing:	500 m (mantle)



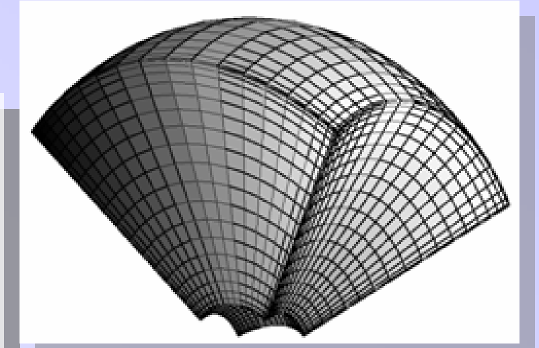
Required grid points: $O(10^{12})$
Required memory: O(100 TBytes)

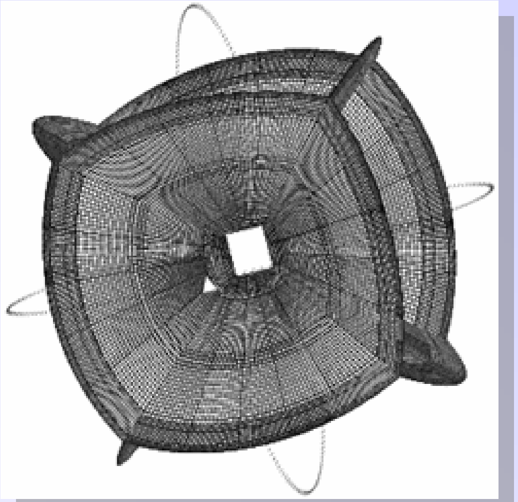


Spatial Scales and Memory

(back of the envelope)

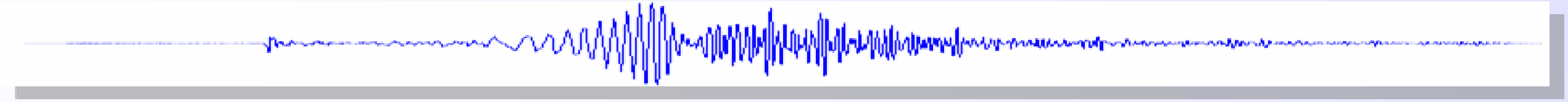
Highest frequency:	**0.1 Hz**
Shortest wavelength:	20 km (crust)
Shortest wavelength:	50 km (mantle)
Grid points per wavelength:	5
Grid spacing:	2000 m (crust)
Grid spacing:	5000 m (mantle)

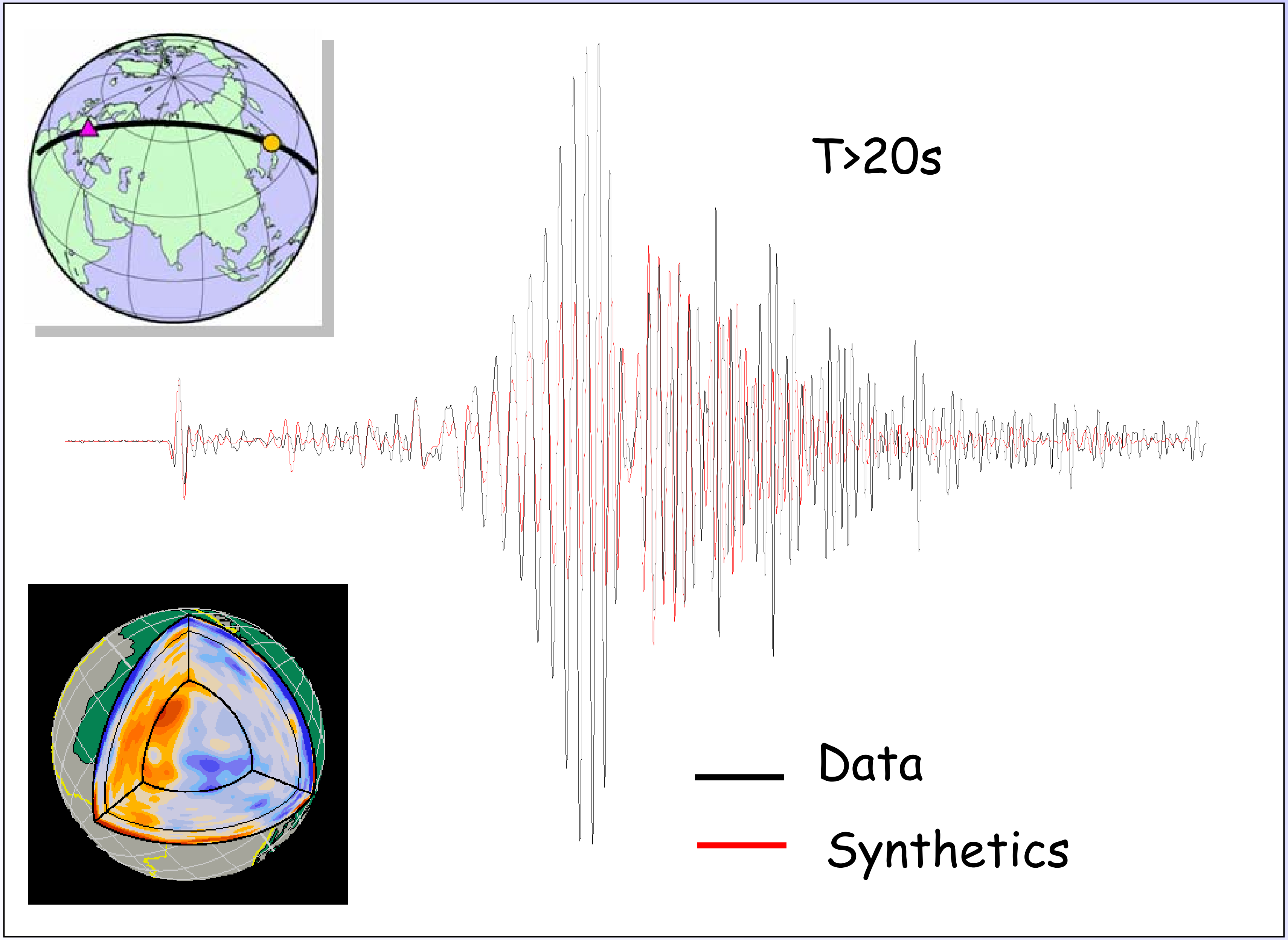




Required grid points: $O(10^9)$

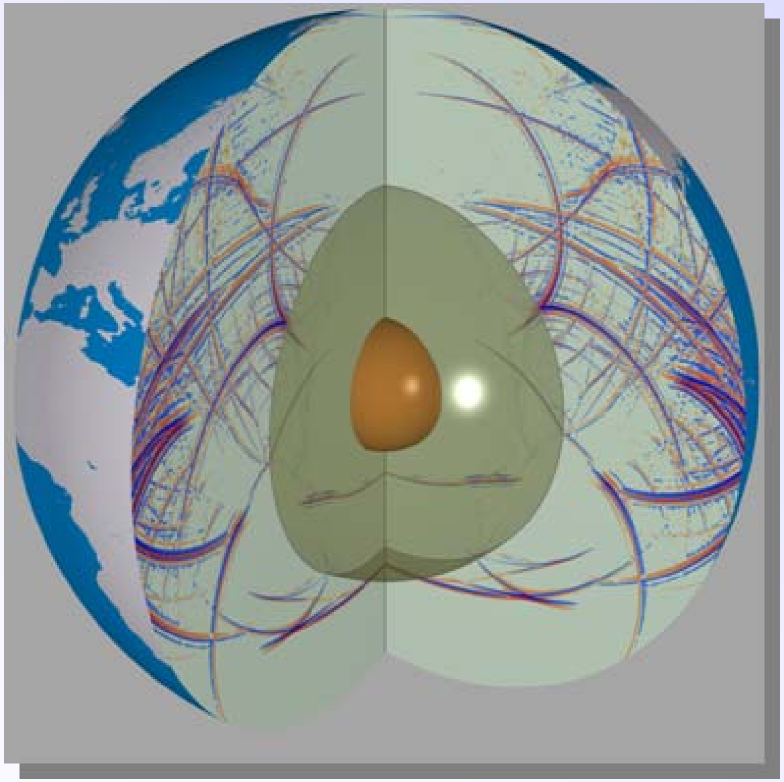
Required memory: O(100 GBytes)



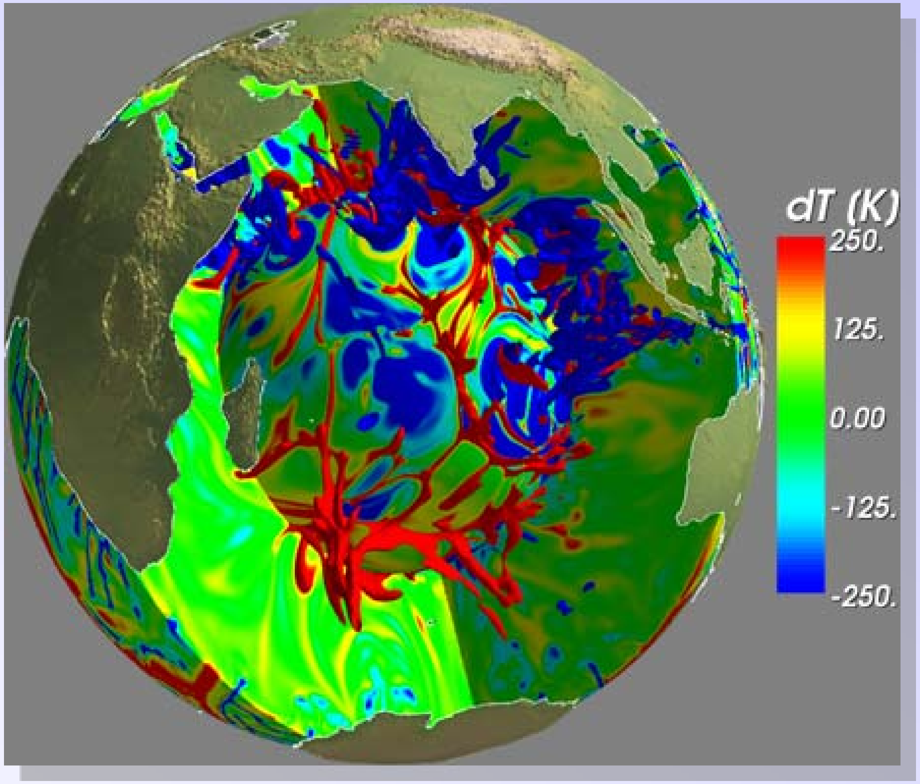


T>20s
Data
Synthetics

Seismology and Geodynamics



Courtesy: G. Jahnke



Courtesy: H.P. Bunge, B. Schuberth

Numerical simulation of seismic wave propagation

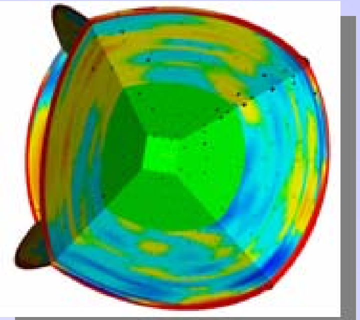
Elastic wave equations

$$\rho \partial_t^2 u_i = \partial_j (\sigma_{ij} + M_{ij}) + f_i$$

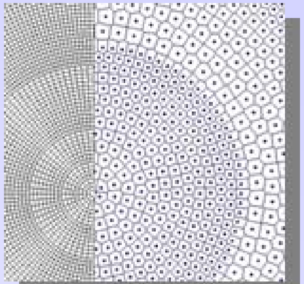
$$\sigma_{ij} = c_{ijkl} \varepsilon_{kl}$$

$$\varepsilon_{kl} = 1/2 (\partial_k u_l + \partial_l u_k)$$

3D Model

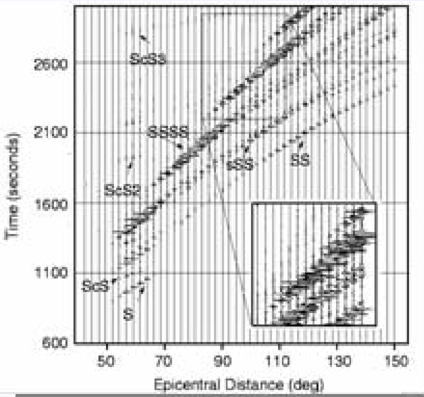


Grid

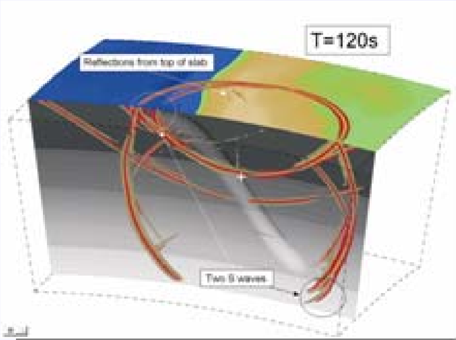


Parallelisation

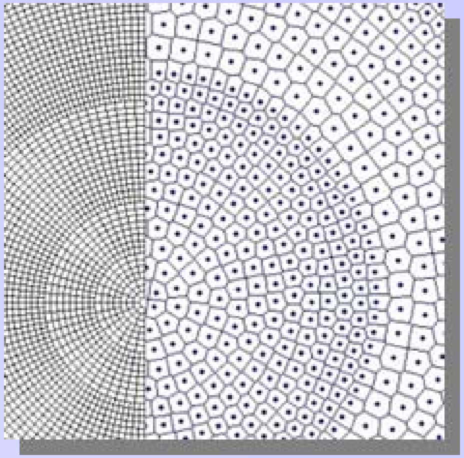
Synthetic seismograms



Simulation



Numerical methods



- **Finite Differences** (**high order**, optimal operators)
- Pseudospectral methods (Chebyshev, Fourier)
- **Finite/spectral elements** on hexahedral grids
- **Unstructured grids** (**finite volumes/elements**, natural neighbours) or combinations
- Parallelization using MPI (message passing interface)

-> for rupture problems special internal boundary conditions apply

3D numerical simulation of seismic wave propagation in the Grenoble valley (M6 earthquake)

Forward modeling benchmark (Chaljub et al., 2006)

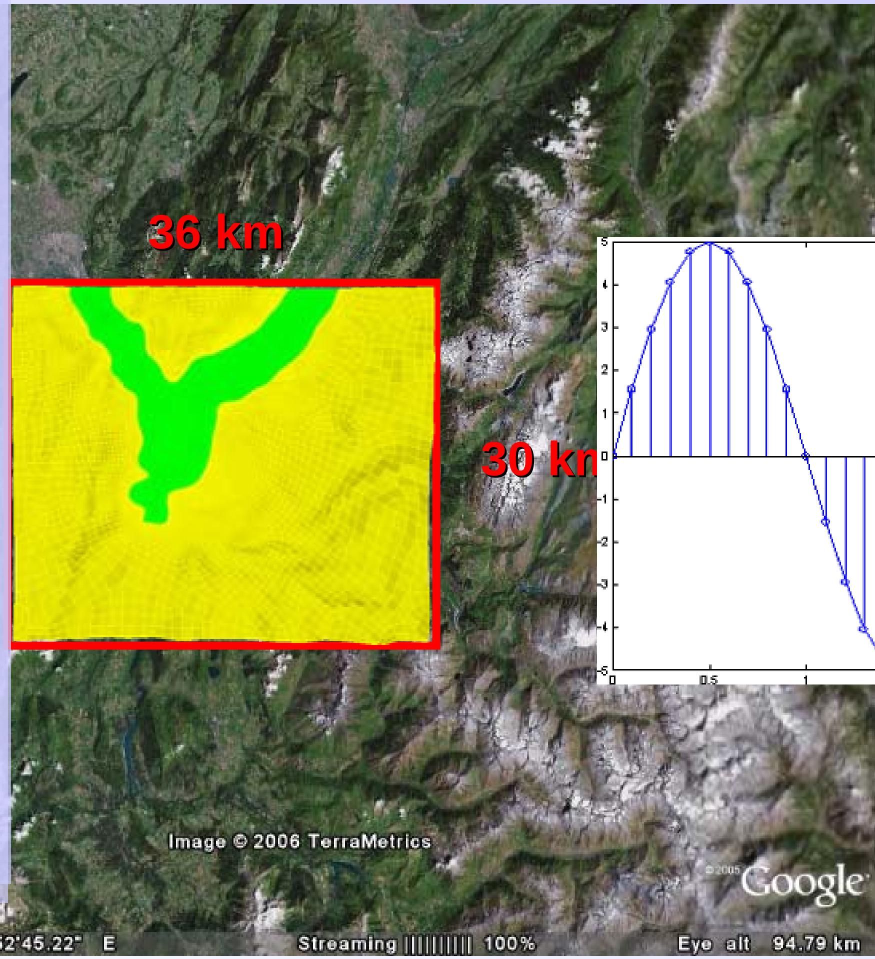
3D numerical simulation of seismic wave propagation in the Grenoble valley (M6 earthquake)

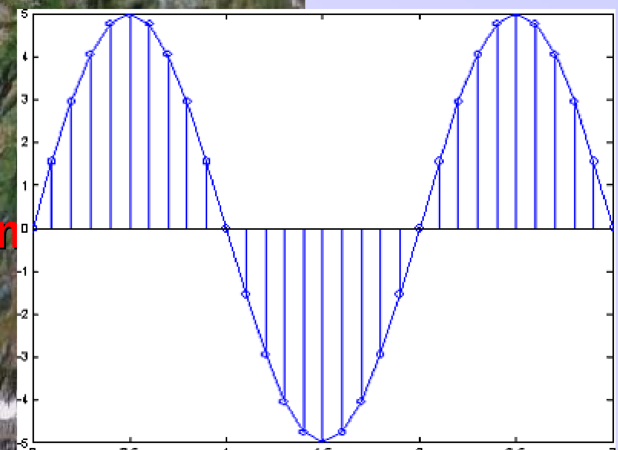
Bedrock

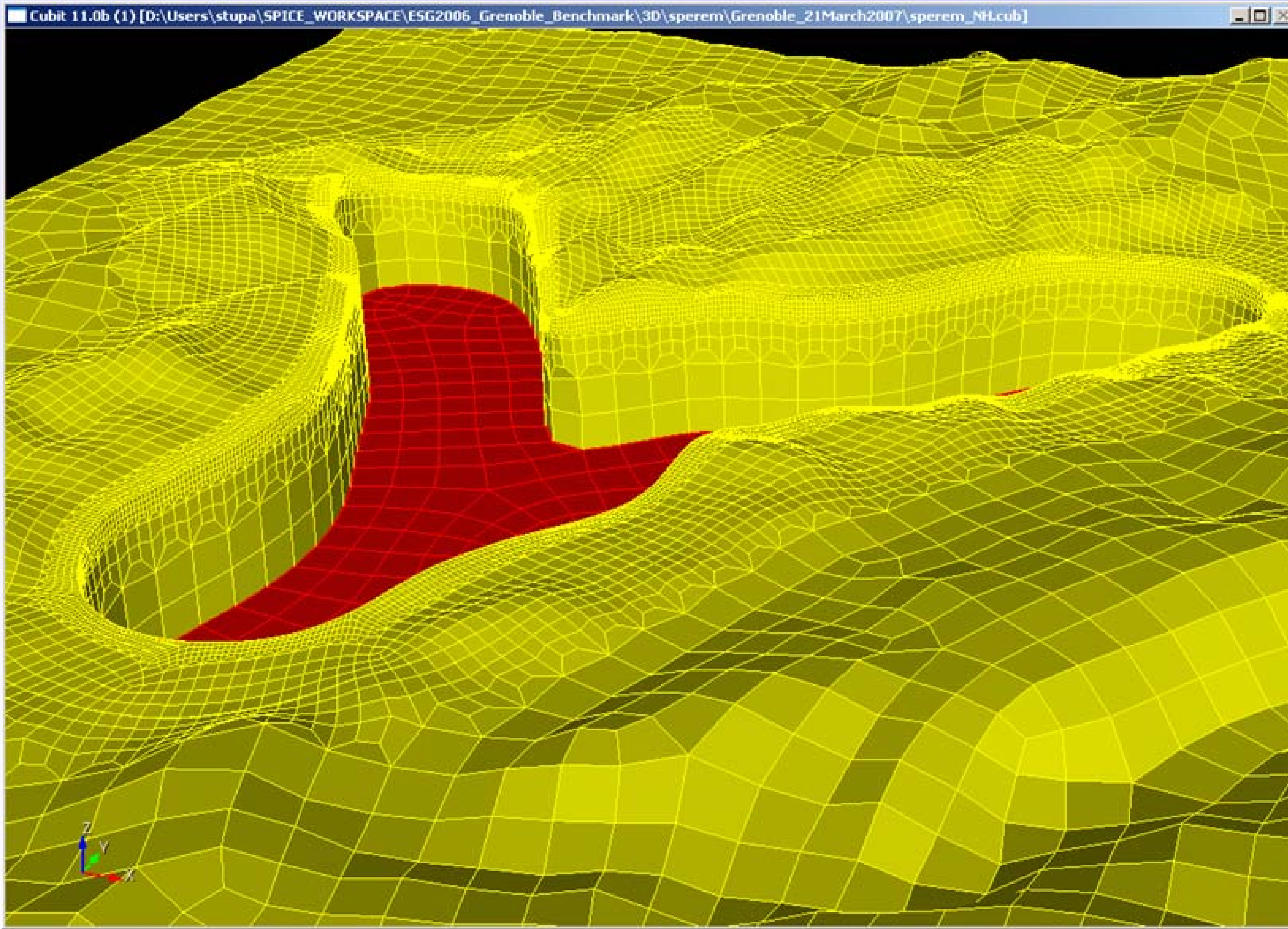
$V_S = 3200m/s$

$f_{max} = 3Hz$

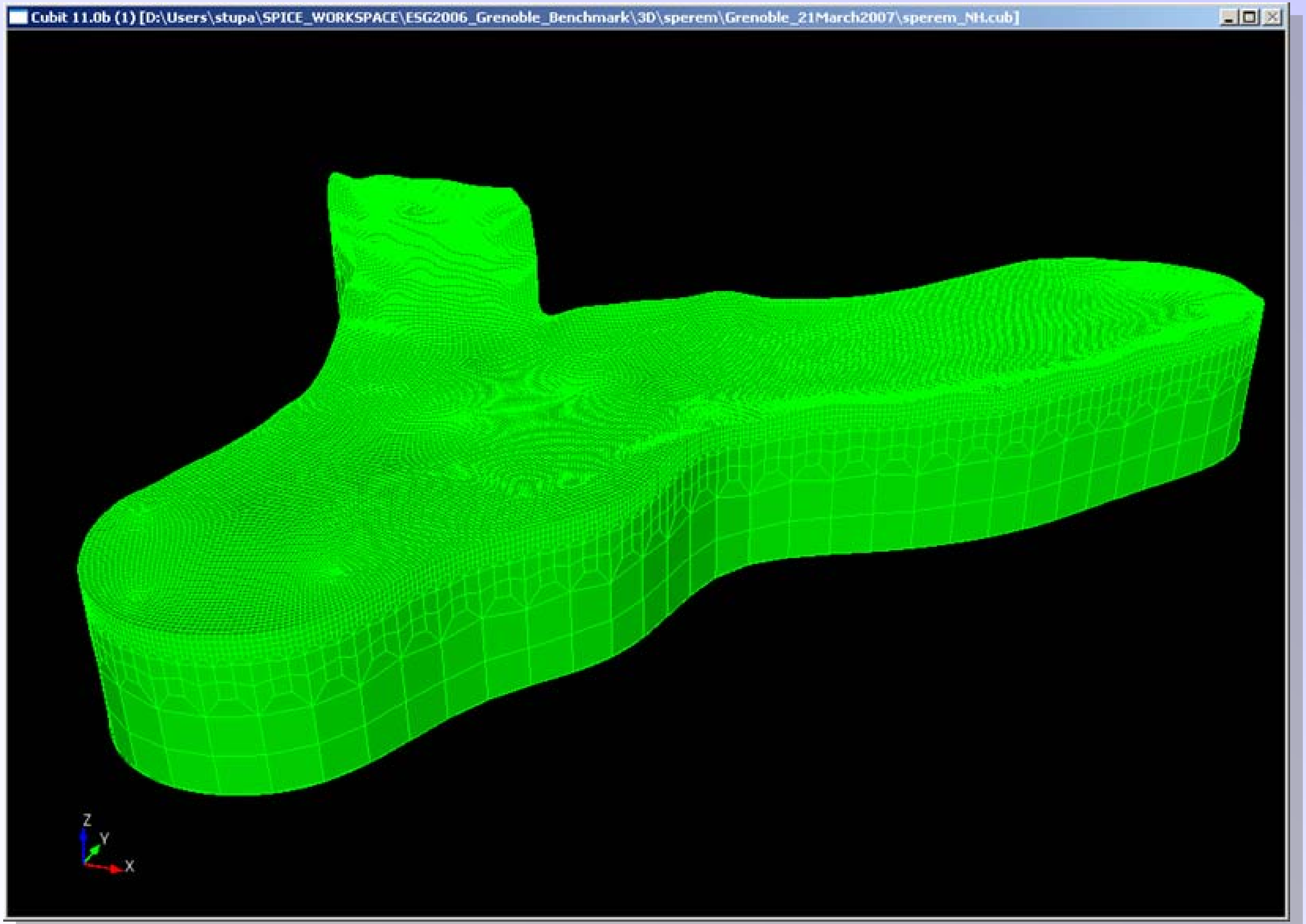
$\lambda_{min} = V_S/f_{max} = 1066.7m$





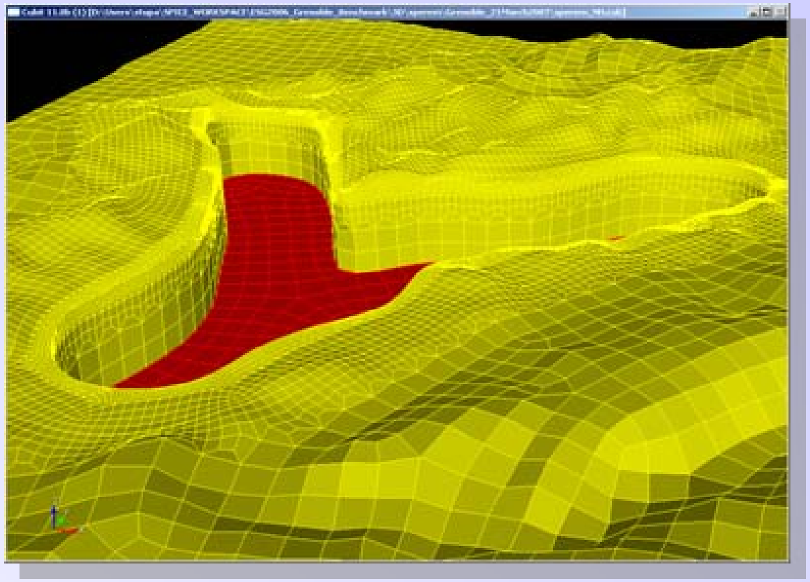


Stupazzini et al. (2006)


Cubit 11.0b (1) [D:\Users\stupa\SPICE_WORKSPACE\ESG2006_Grenoble_Benchmark\3D\sperem\Grenoble_21March2007\sperem_NH.cub]
Z
Y
X

The Courant Criterion

$$v_P\left(\frac{dt}{dx}\right)\leq \varepsilon$$



Smallest grid size

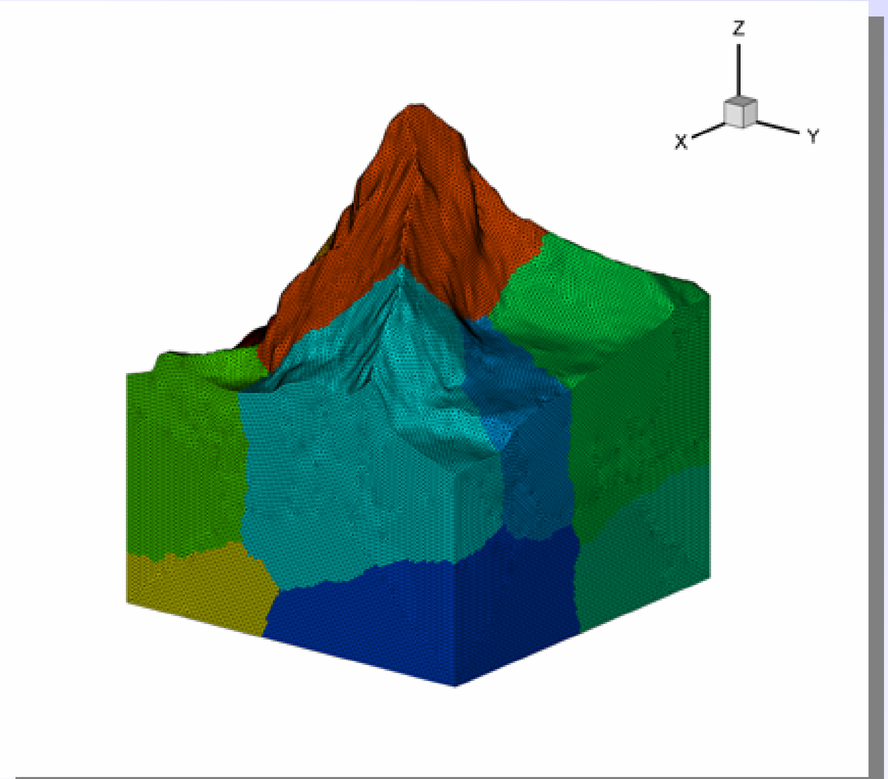
Largest velocity

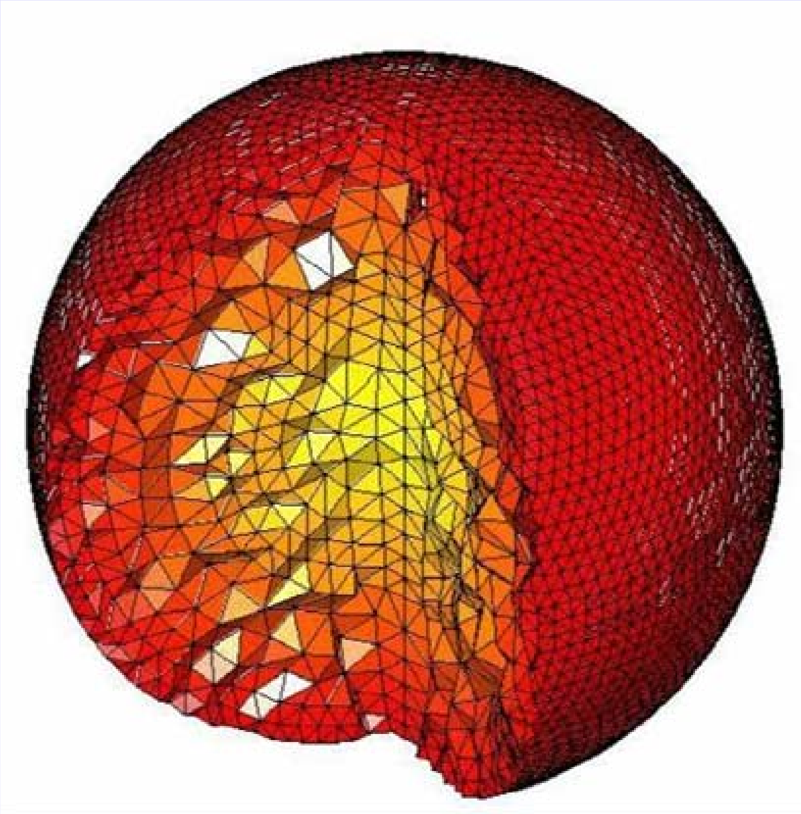
Problems …

- … **grid generation** is cumbersome with hexahedra, trying to honor complex geometries and material heterogeneities …

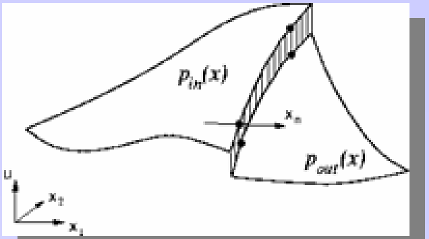
- … large variations in seismic velocities (i.e. required grid size) lead to **very small time steps** – overkill in a large part of the model …

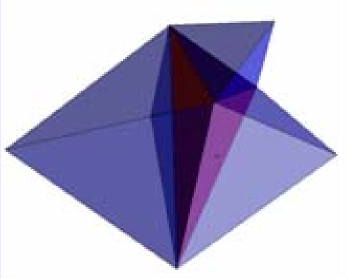
Waves on unstructured grids?
tetrahedral

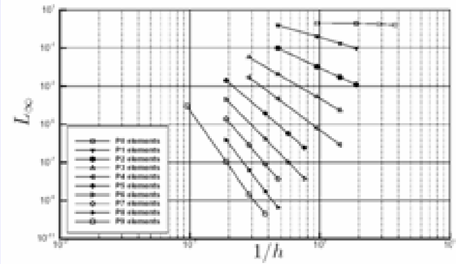


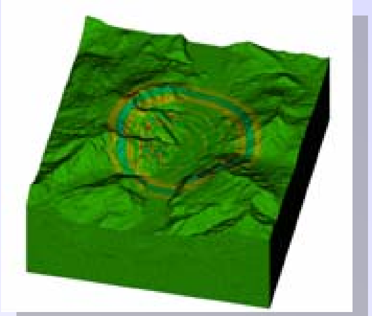


Arbirtrarily high-orDER - Discontinuous Galerkin









- Combination of a **discontinous Galerkin method** with ADER time integration
- Piecewise polynomial approximation combined with the fluxes across elements (**finite volumes**)
- **Time integration as accurate as space derivatives**, applicable also to strongly irregular meshes (not so usually for FD, FE, SE)
- Method developed in **aero-acoustics** and **computational fluid dynamics**
- The scheme is entirely local, not large matrix inversion -> **efficient parallelization**
- Algorithms on tetrahedral grids **slower** than spectral element schemes on hexahedra

ADER-DG in *Geophysical Journal International* a.o.

Käser, M., and M. Dumbser (2006), An Arbitrary High Order Discontinuous Galerkin Method for Elastic Waves on Unstructured Meshes I: **The Two-Dimensional Isotropic Case** with External Source Terms, *Geophysical Journal International*, *166*(2), 855-877.

Dumbser, M., and M. Käser (2006), An Arbitrary High Order Discontinuous Galerkin Method for Elastic Waves on Unstructured Meshes II: **The Three-Dimensional Isotropic Case**, *Geophysical Journal International*, *167*(1), 319-336.

Käser, M., M. Dumbser, J. de la Puente, and H. Igel (2007), An Arbitrary High Order Discontinuous Galerkin Method for Elastic Waves on Unstructured Meshes III: **Viscoelastic Attenuation**, *Geophysical Journal International*, *168*, 224-242.

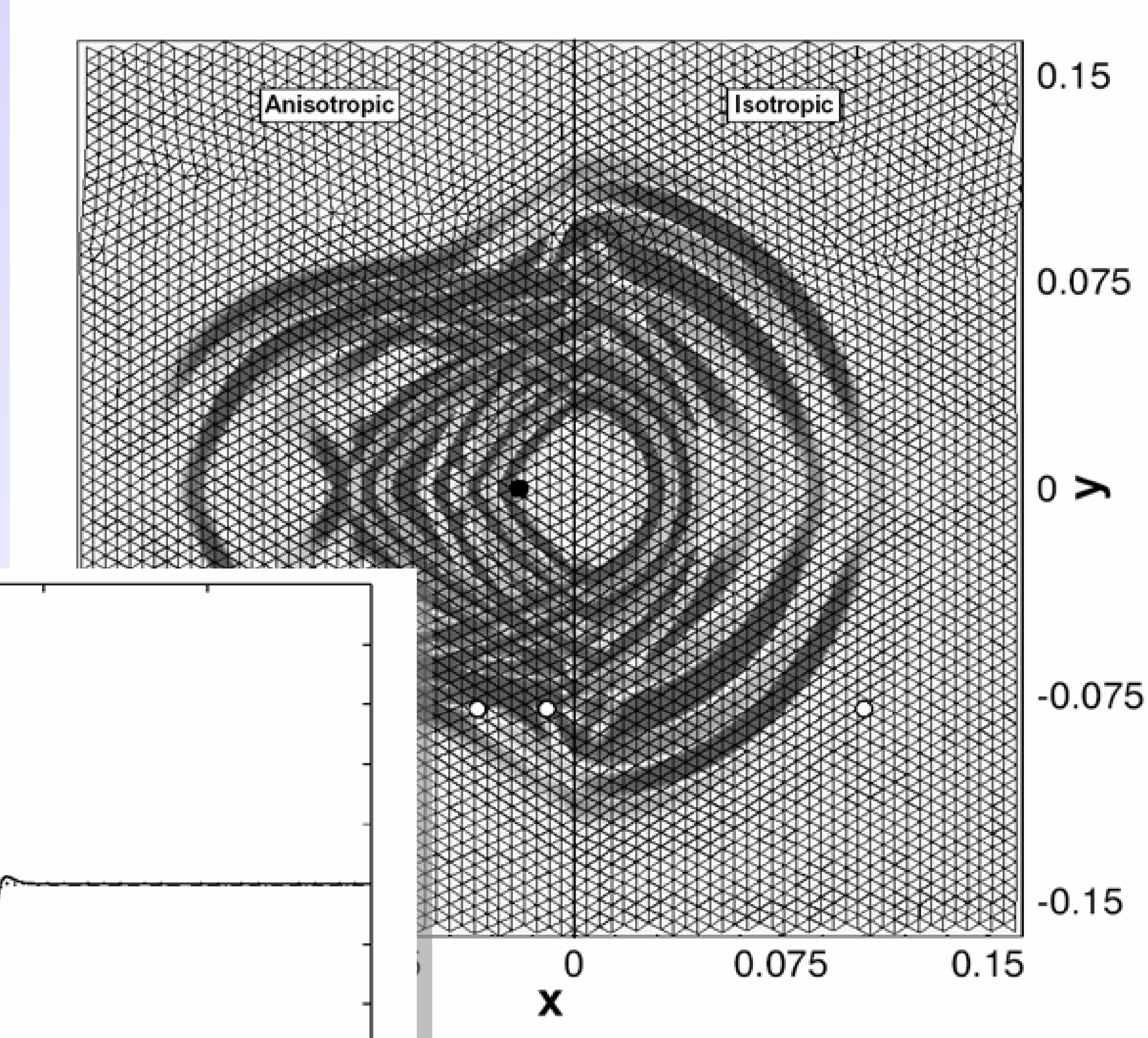
De la Puente, J., M. Käser, M. Dumbser, and H. Igel (2007), An Arbitrary High Order Discontinuous Galerkin Method for Elastic Waves on Unstructured Meshes IV: **Anisotropy**, *Geophysical Journal International*, in press.

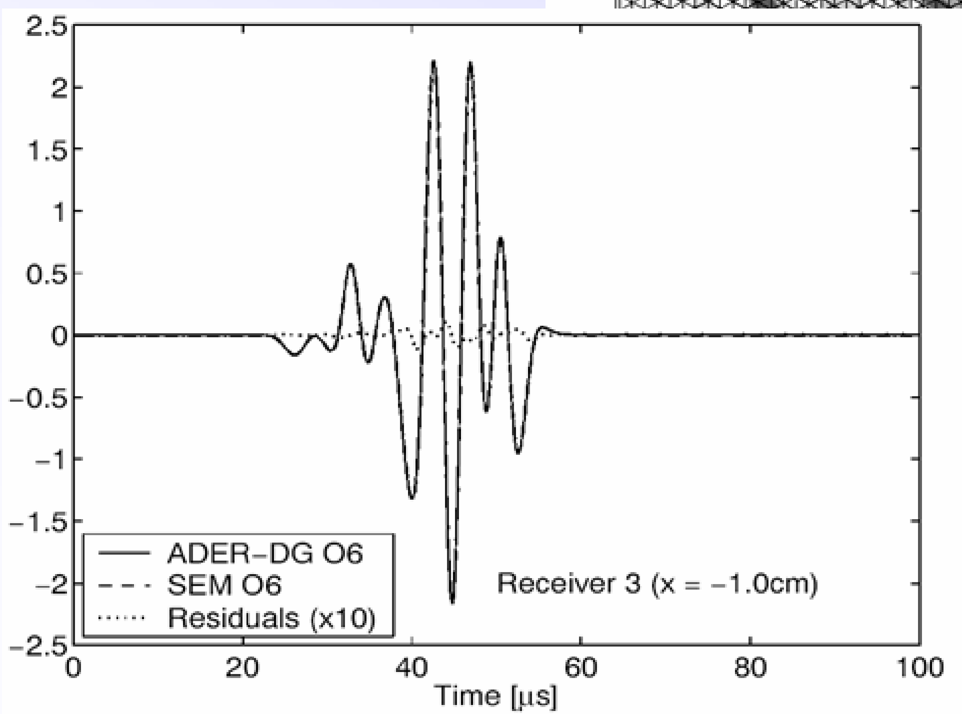
Dumbser, M, M. Käser, and E Toro (2007), An Arbitrary High Order Discontinuous Galerkin Method for Elastic Waves on Unstructured Meshes V: **Local Time Stepping and p-Adaptivity**, *Geophys. J. Int.*, in press

Käser, M., P. M. Mai, and M. Dumbser (2007), On the Accurate Treatment of **Finite Source Rupture Models** Using ADER-DG on Tetrahedral Meshes, *Bull. Seis. Soc. Am.*, in press.

Coming soon: poroelasticity, combined hexahedral and tetrahedral grids, dynamic rupture

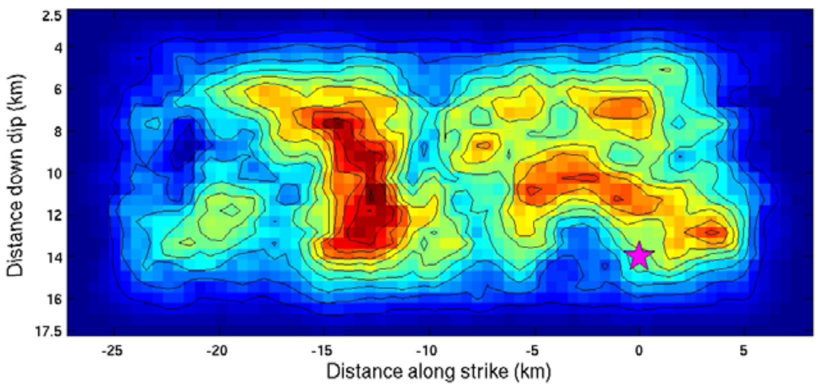
Anisotropic Material



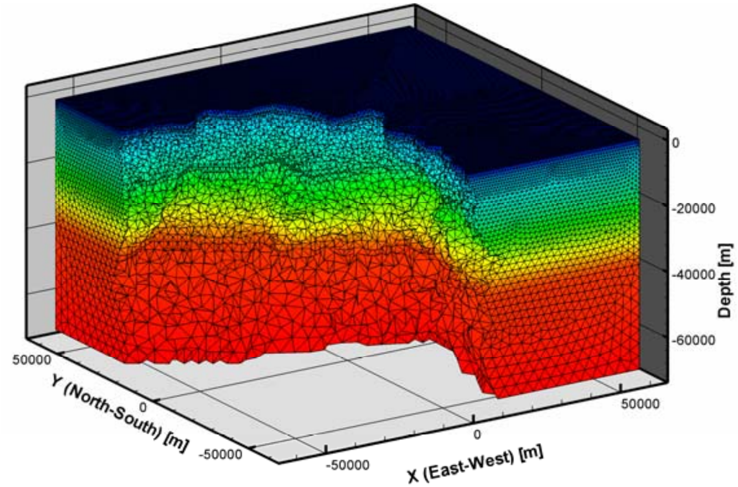


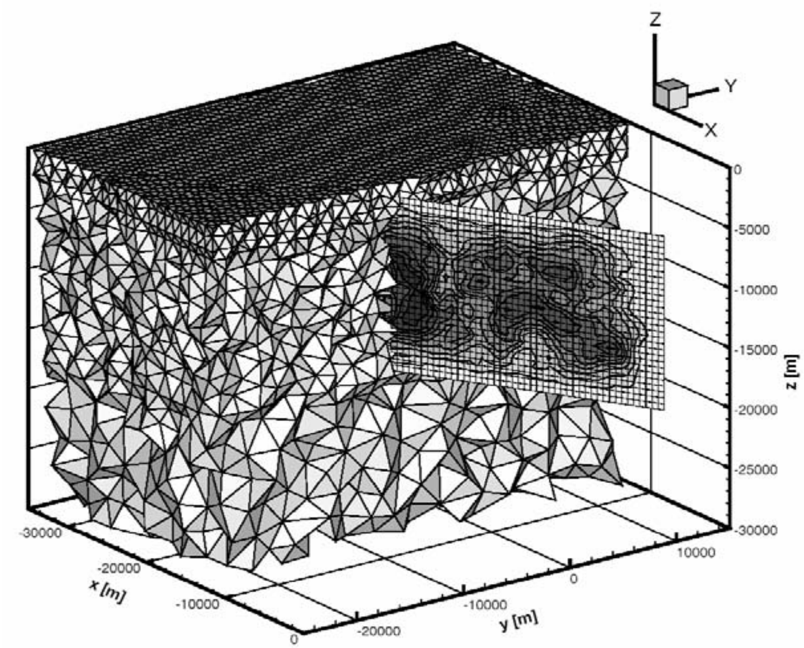
Arbitrarily shaped finite sources

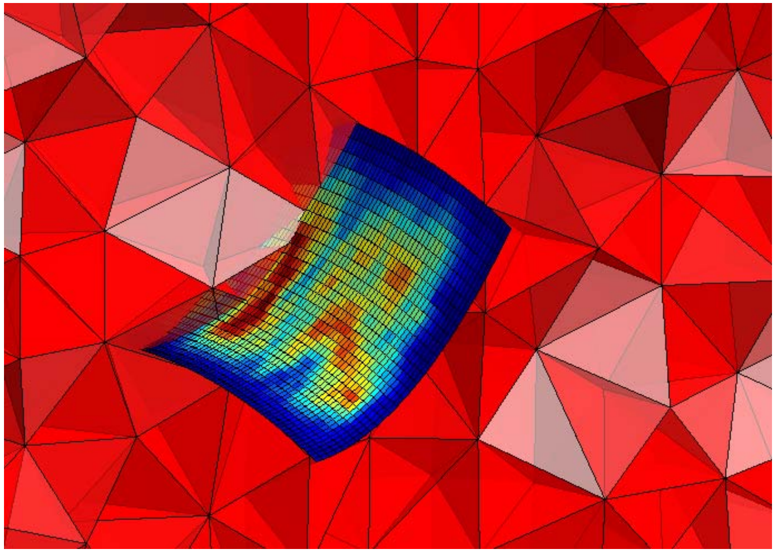
Slip map of an earthquake fault



Mesh spacing is proportional to P-wave velocity



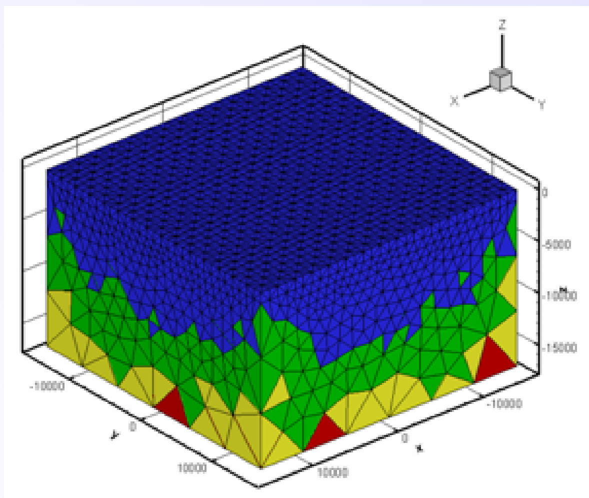


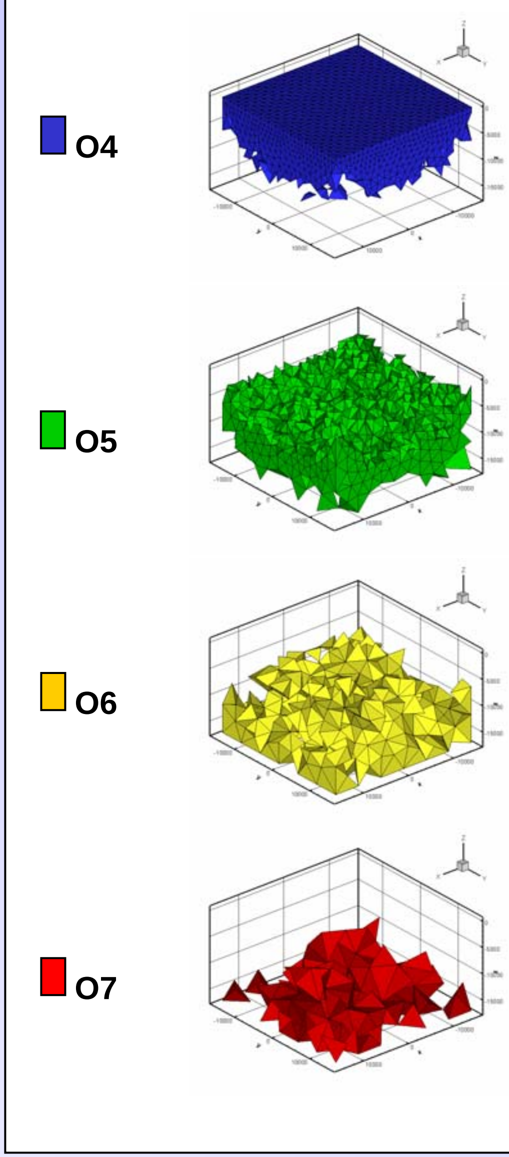


Käser, Mai, Dumbser, 2007

Local precision

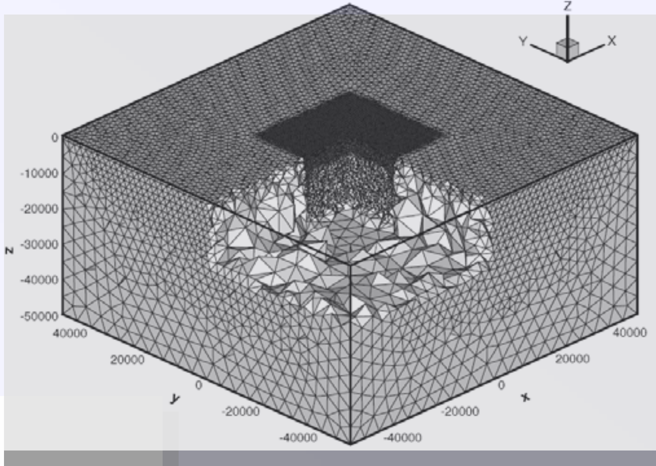
- Use high precision (i.e., high-order polynomials) only where necessary
- High precision where cells are large (high velocities)
- Low precision where cells are small (because of structural heterogeneities)

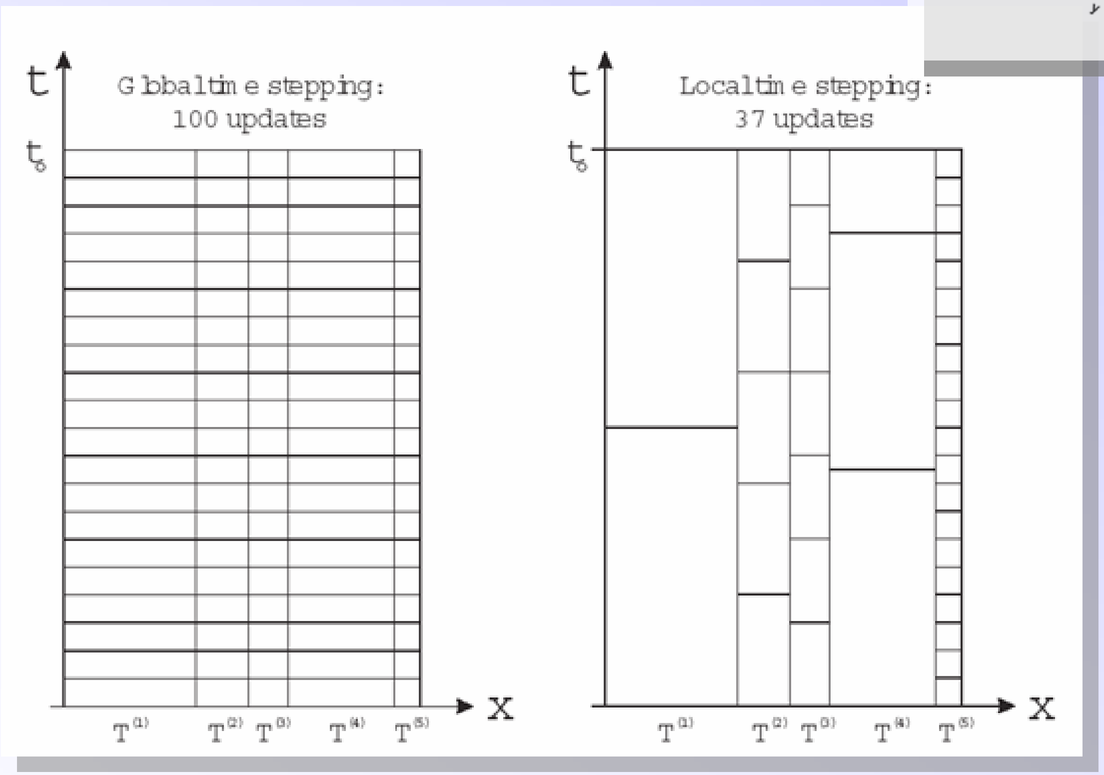




Käser et al. (2006)

Local time-stepping





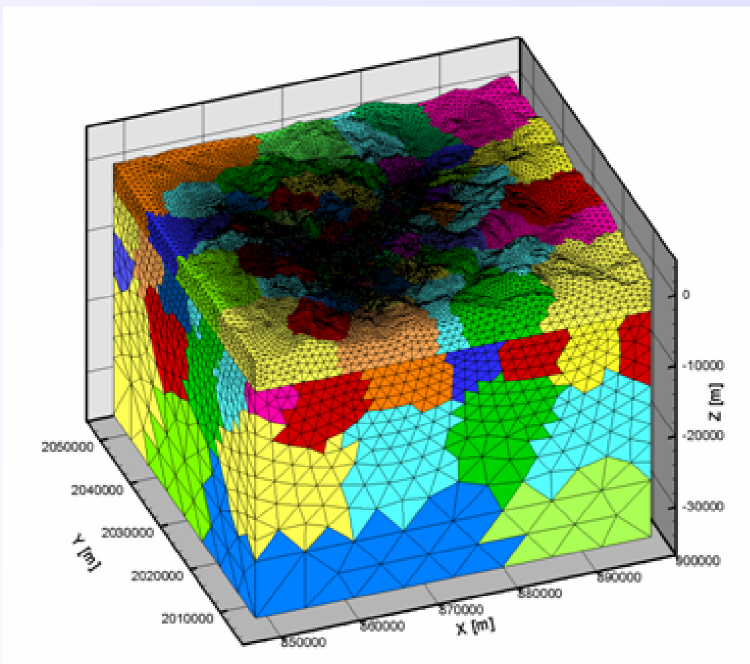
global ***local***

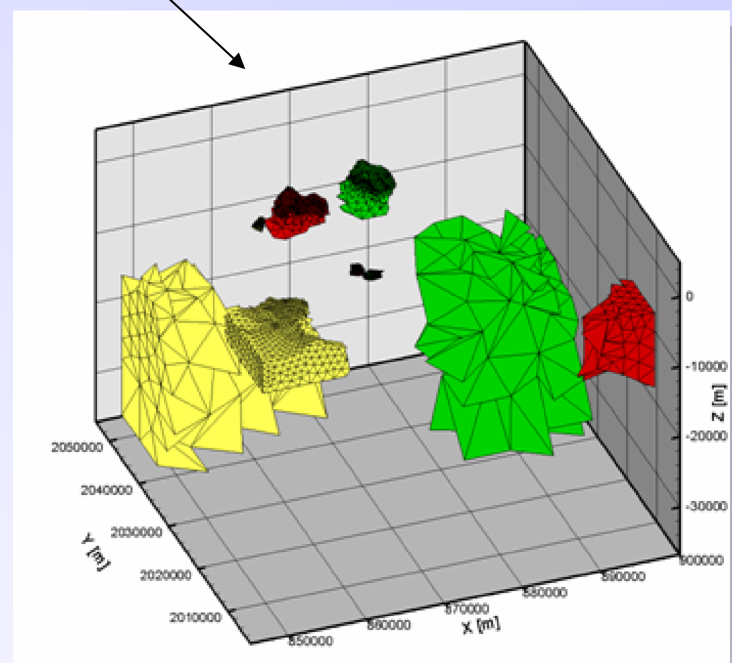
Local time-stepping is possible without loosing the accuracy of the scheme

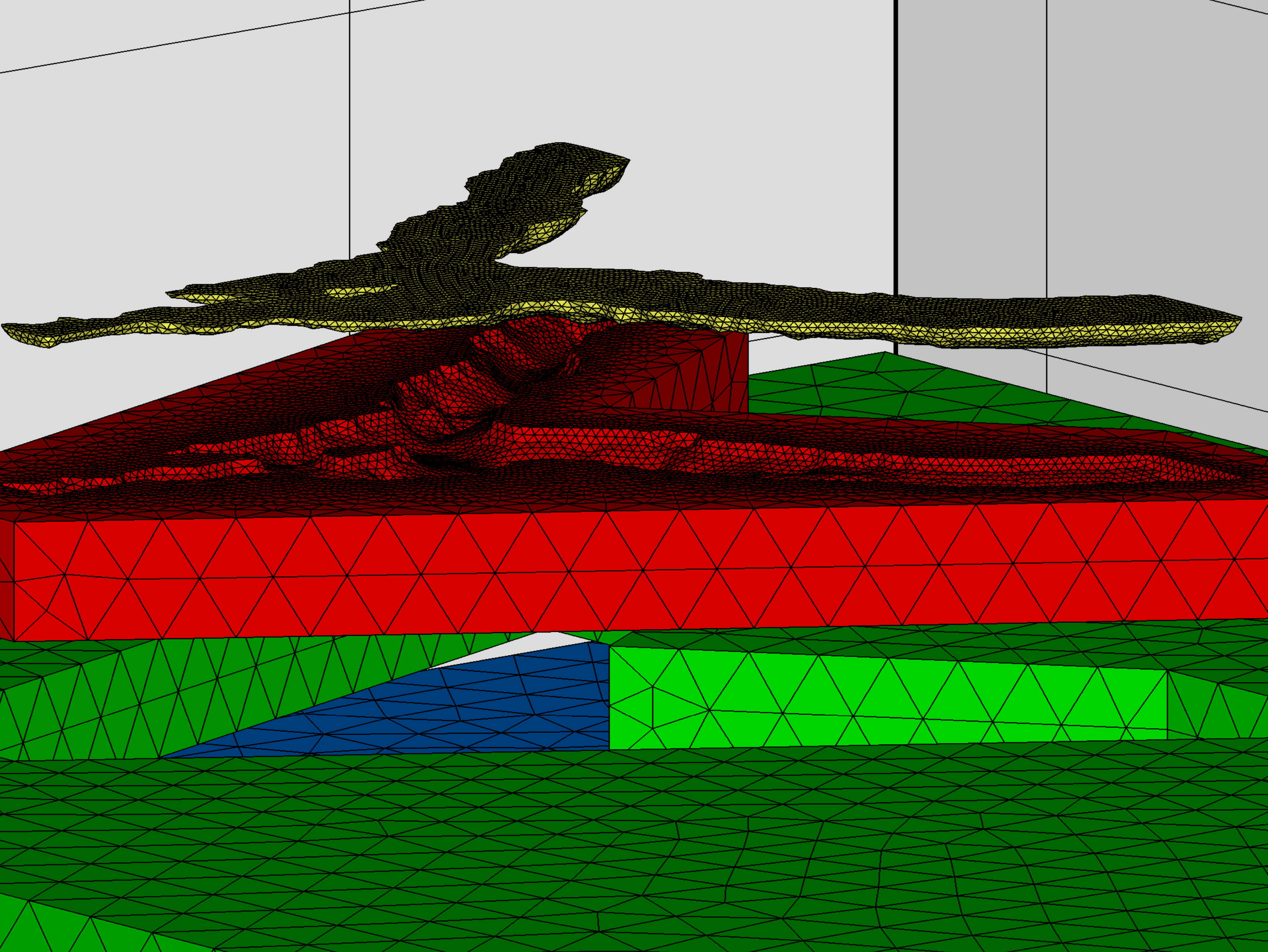
Mesh Partitioning and Parallel Computing

the problem of load blancing

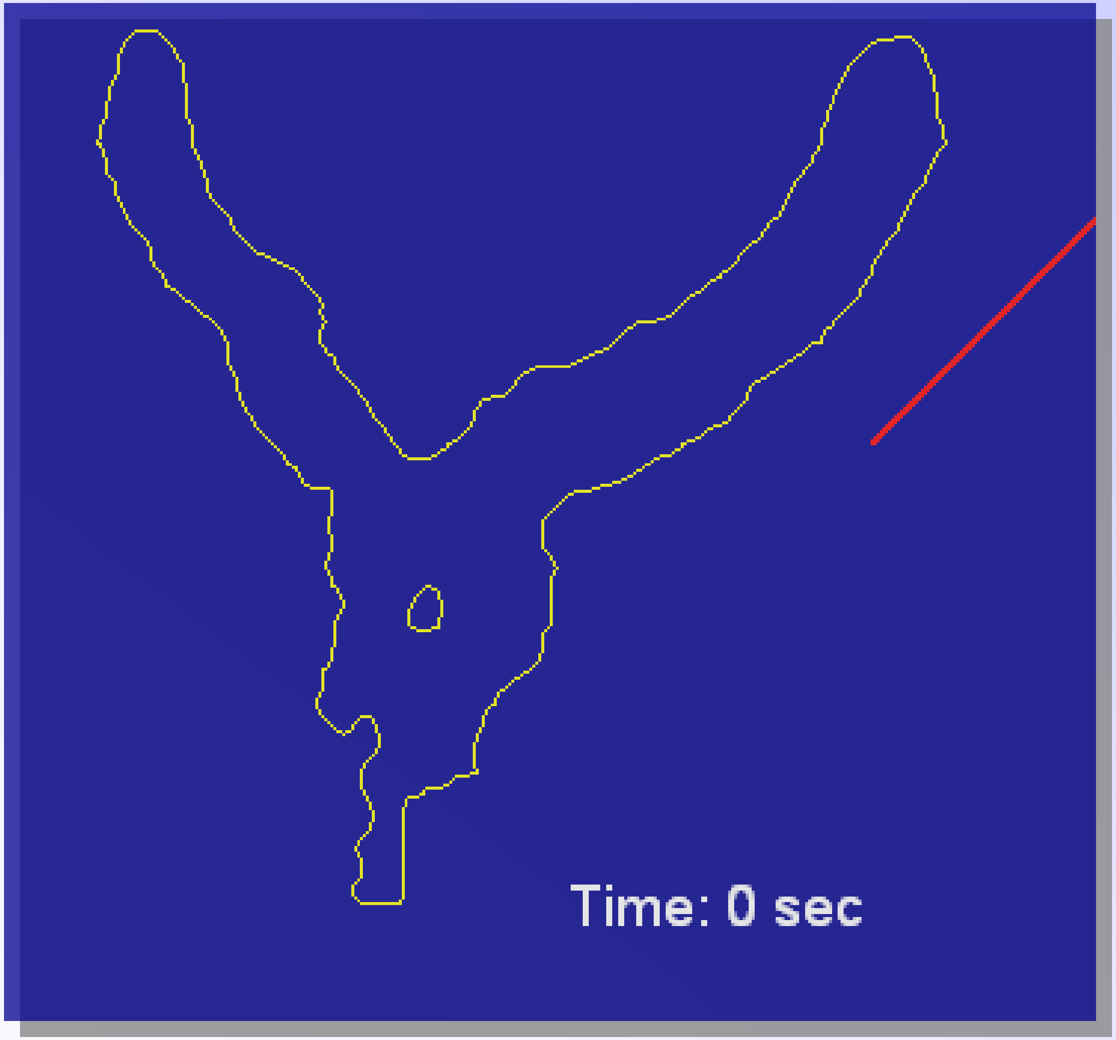
Same color means same processor

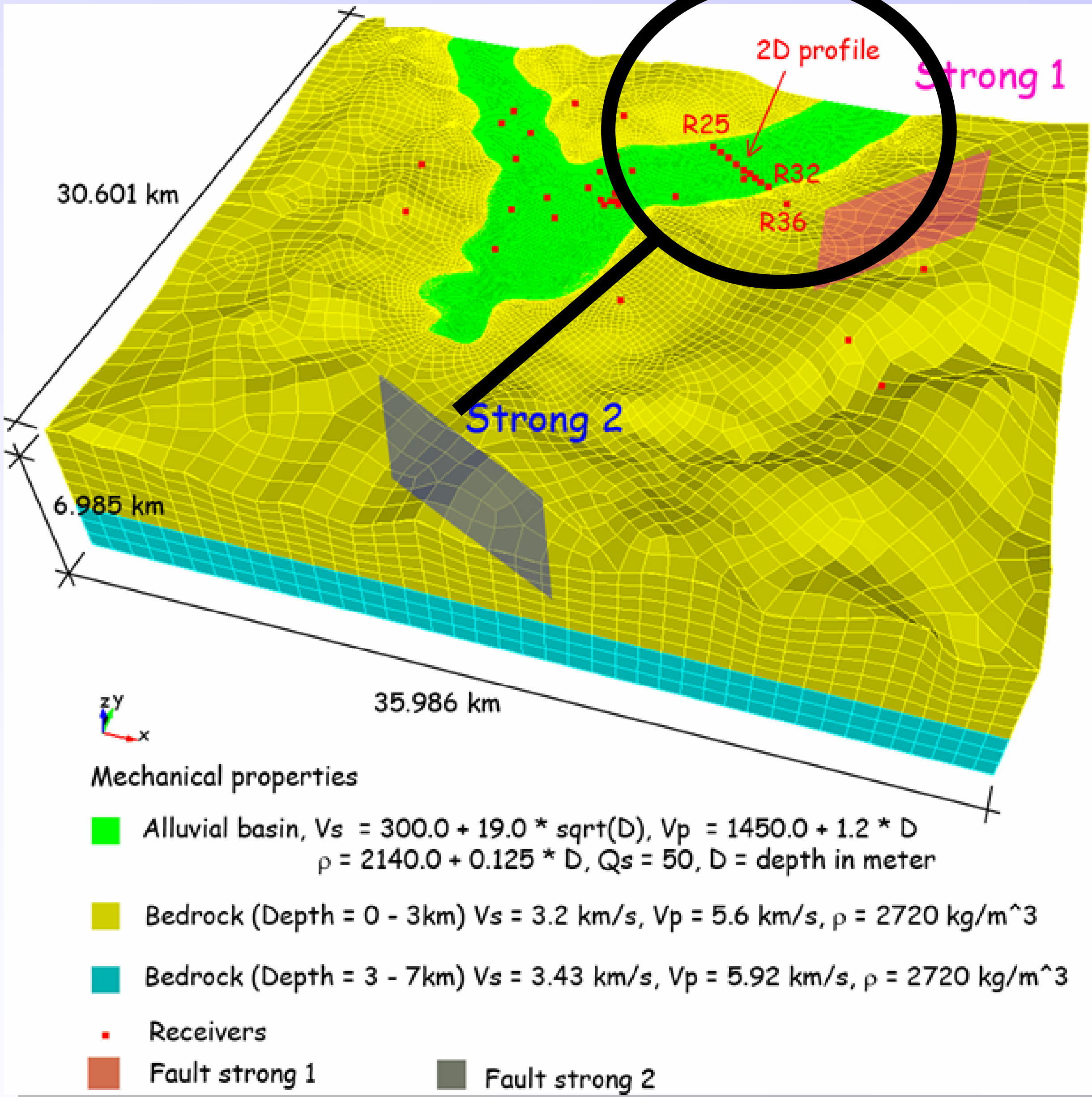




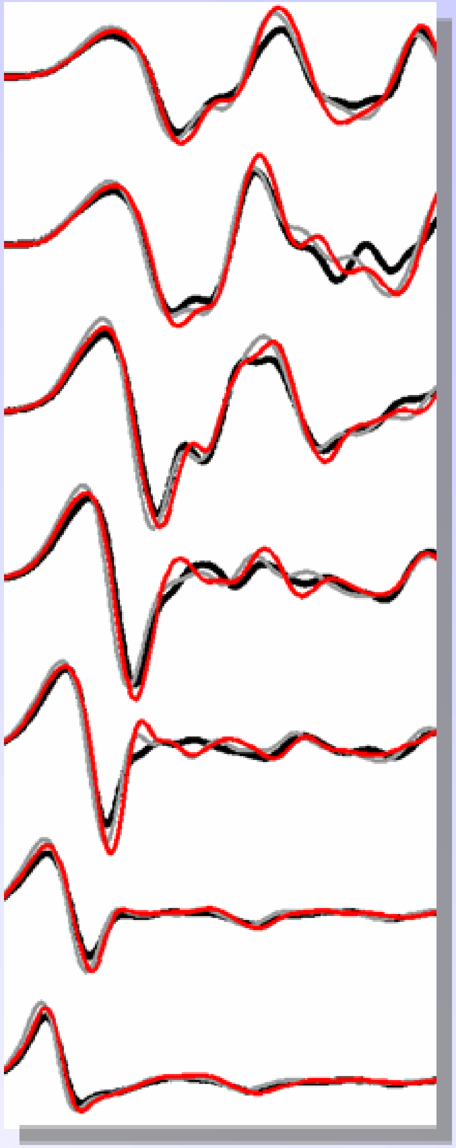


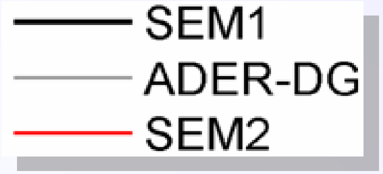
Grenoble Basin Simulation



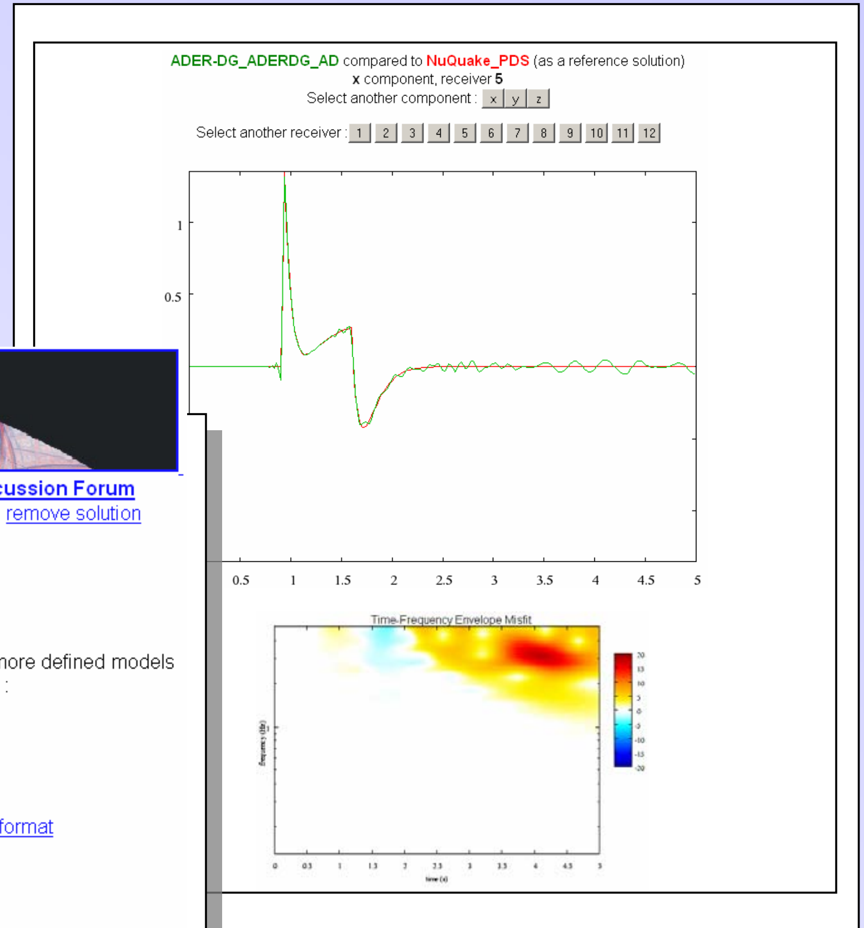

2D profile
Strong 1
R25
R32
R36
30.601 km
Strong 2
6.985 km
35.986 km
z y
x
Mechanical properties
Alluvial basin, Vs = 300.0 + 19.0 * sqrt(D), Vp = 1450.0 + 1.2 * D
ρ = 2140.0 + 0.125 * D, Qs = 50, D = depth in meter
Bedrock (Depth = 0 - 3km) Vs = 3.2 km/s, Vp = 5.6 km/s, ρ = 2720 kg/m^3
Bedrock (Depth = 3 - 7km) Vs = 3.43 km/s, Vp = 5.92 km/s, ρ = 2720 kg/m^3
Receivers
Fault strong 1
Fault strong 2

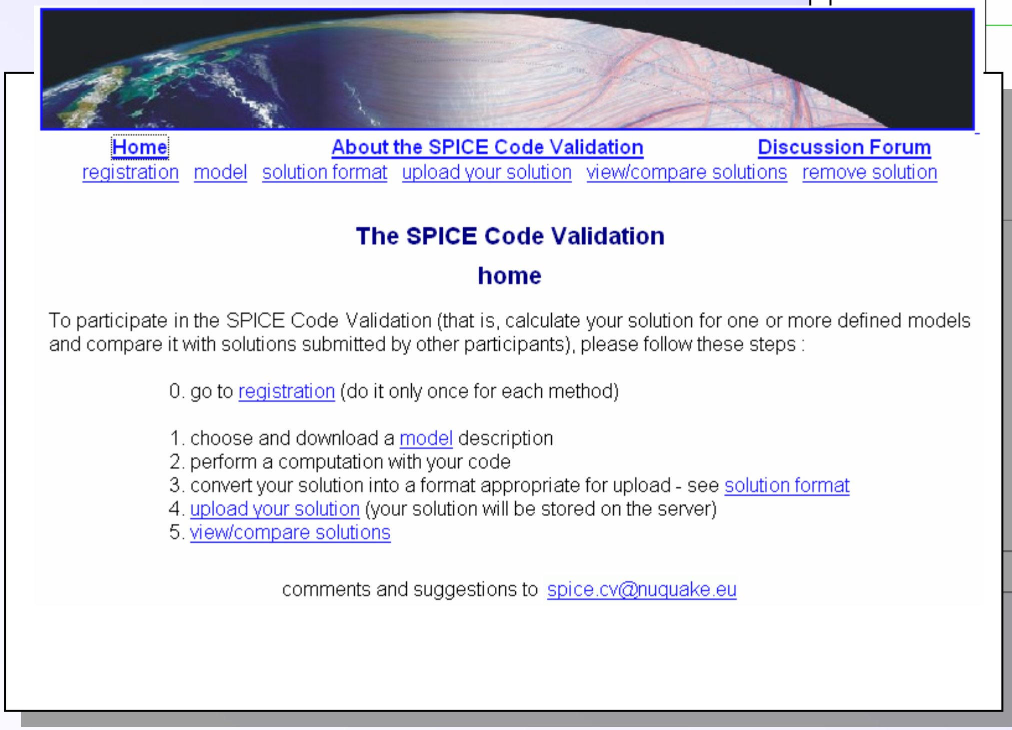
Seismogram Comparison





Interactive Benchmarking





Moczo et al., 2006

www.spice-rtn.org

SPICE Digital Library

- Software for wave propagation problems
- Training material – practicals
- Access to benchmarking (global tomography, kinematic source inversion, wave propagation and rupture)

-> 4th workshop in Cargese, Corsica, May 13-19, 2007

www.spice-rtn.org

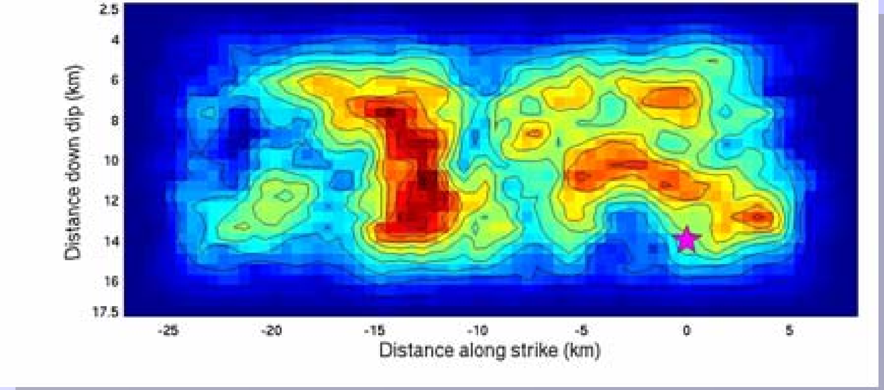
… more info on the SPICE stand …

Conclusions – Technical Challenges

- Strongly heterogeneous structures (or complex surfaces) still pose problems particularly when using hexahedral grids (e.g. oversampling, instabilities)
- Unstructured grids (triangles, tetrahedra) have advantages concerning grid generation but numerical operators often are less accurate, or expensive
- Efficient parallelization algorithms with heterogeneous time steps, accuracy and grid density requires substantial interaction with software engineers.

Dynamic rupture

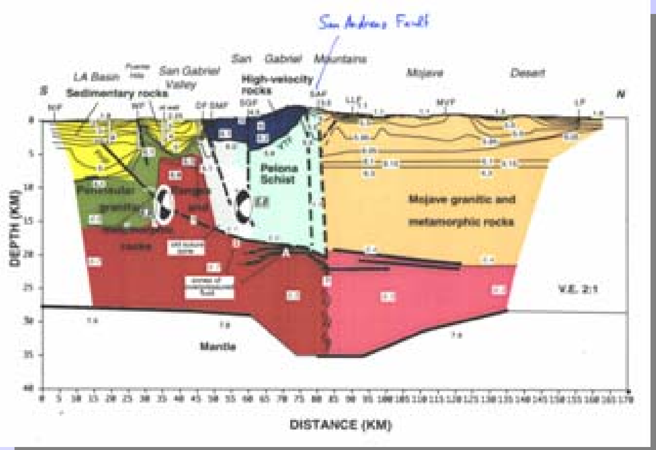
scientific objectives

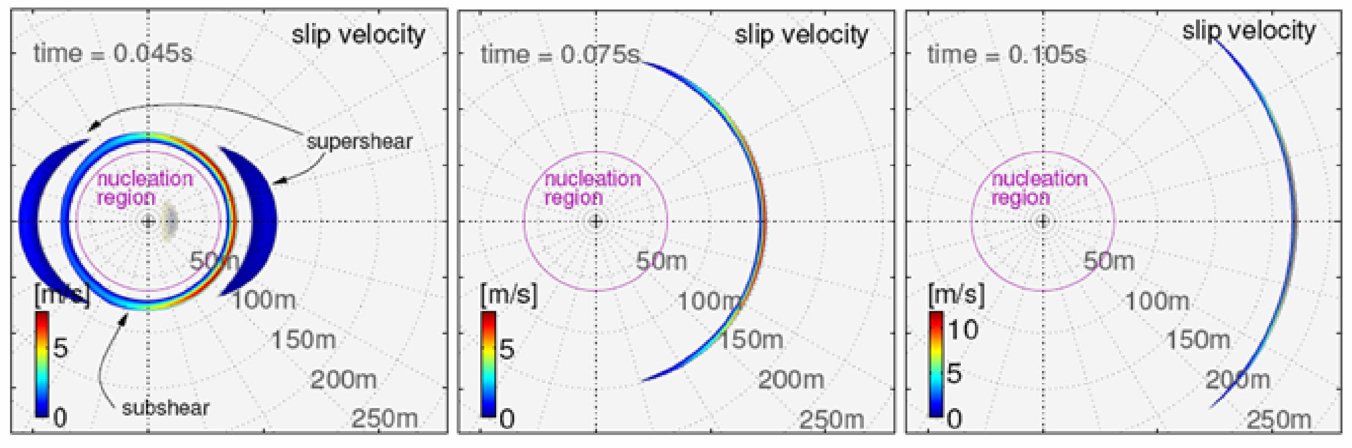


- Understanding the earthquake process
- Understanding the controlling mechanisms of earthquakes (frictional properties, strength heterogeneities, material interfaces, etc.)
- Resolving power of seismic observations with respect to (dynamic) source parameters
- Regional conditions (intraplate, interplate, subduction zones, normal, strike, etc.)

→ phenomenological studies

Rupture at a bi-material interface

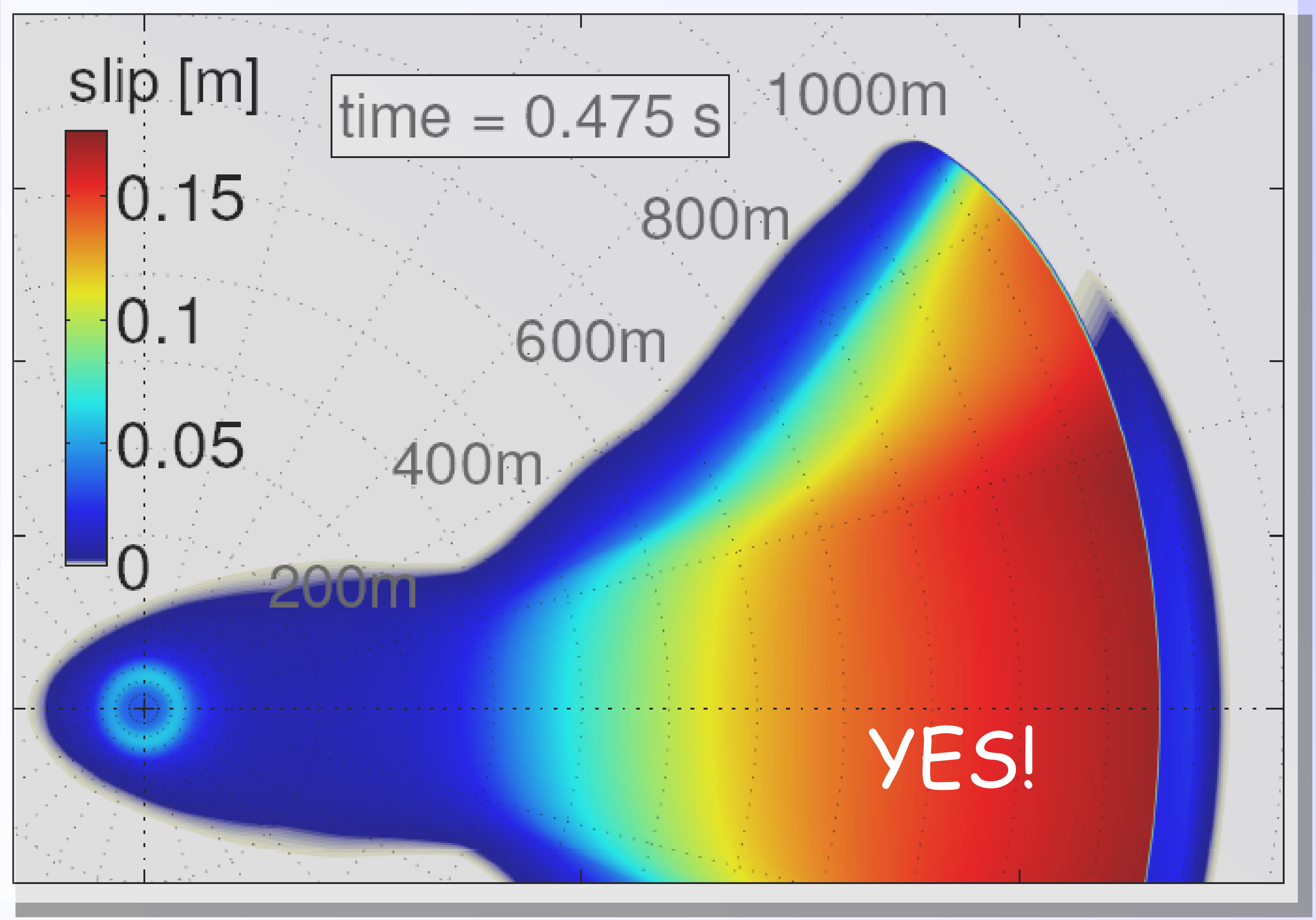




Convergence tests with high-resolution models

- Grid size 500x3200x3200
- 12.5 cm grid spacing
- High-order staggered-grid finite differences

Self-sustained pulse in 3D?



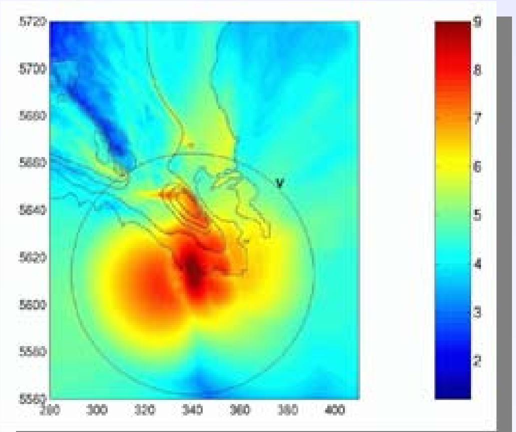
Brietzke, Cochard, Igel, GRL 2007, submitted

Earthquake scenarios

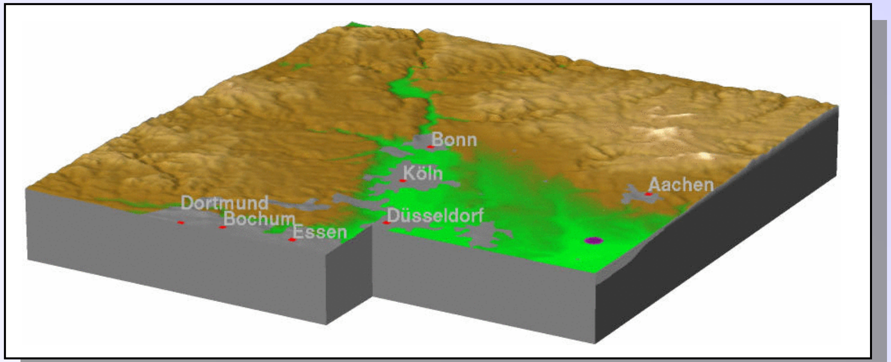
scientific objectives

- Accurate forecasting of hazard and risk scenarios for specific regions and time intervals
- Incorporation of earthquake scenario simulations into probabilistic hazard analysis

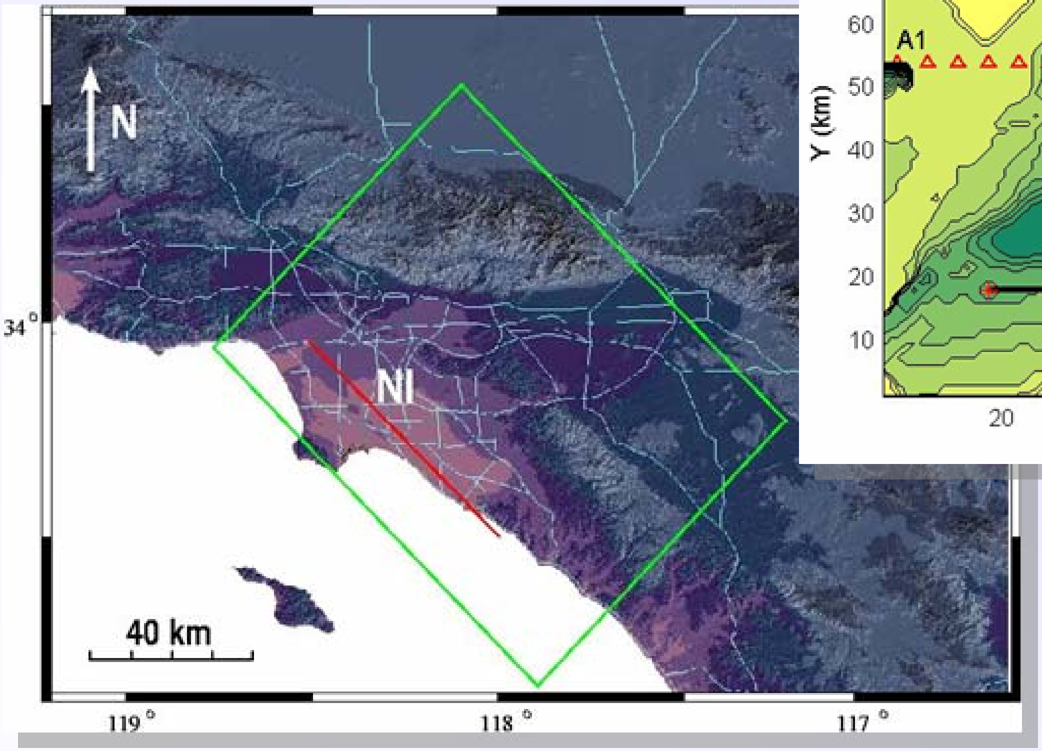
Shaking hazard

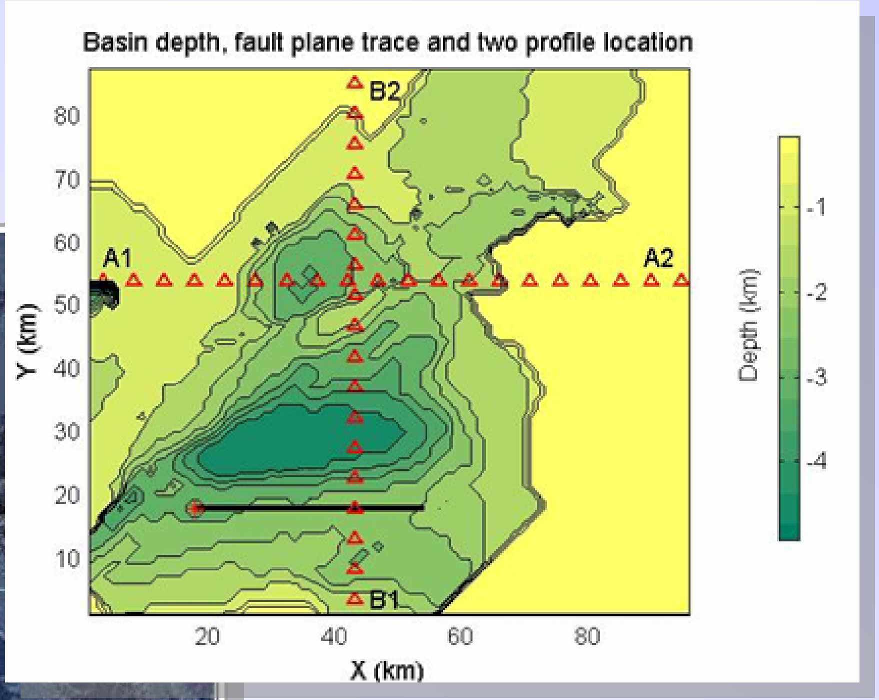


M5.9 Roermond 1992



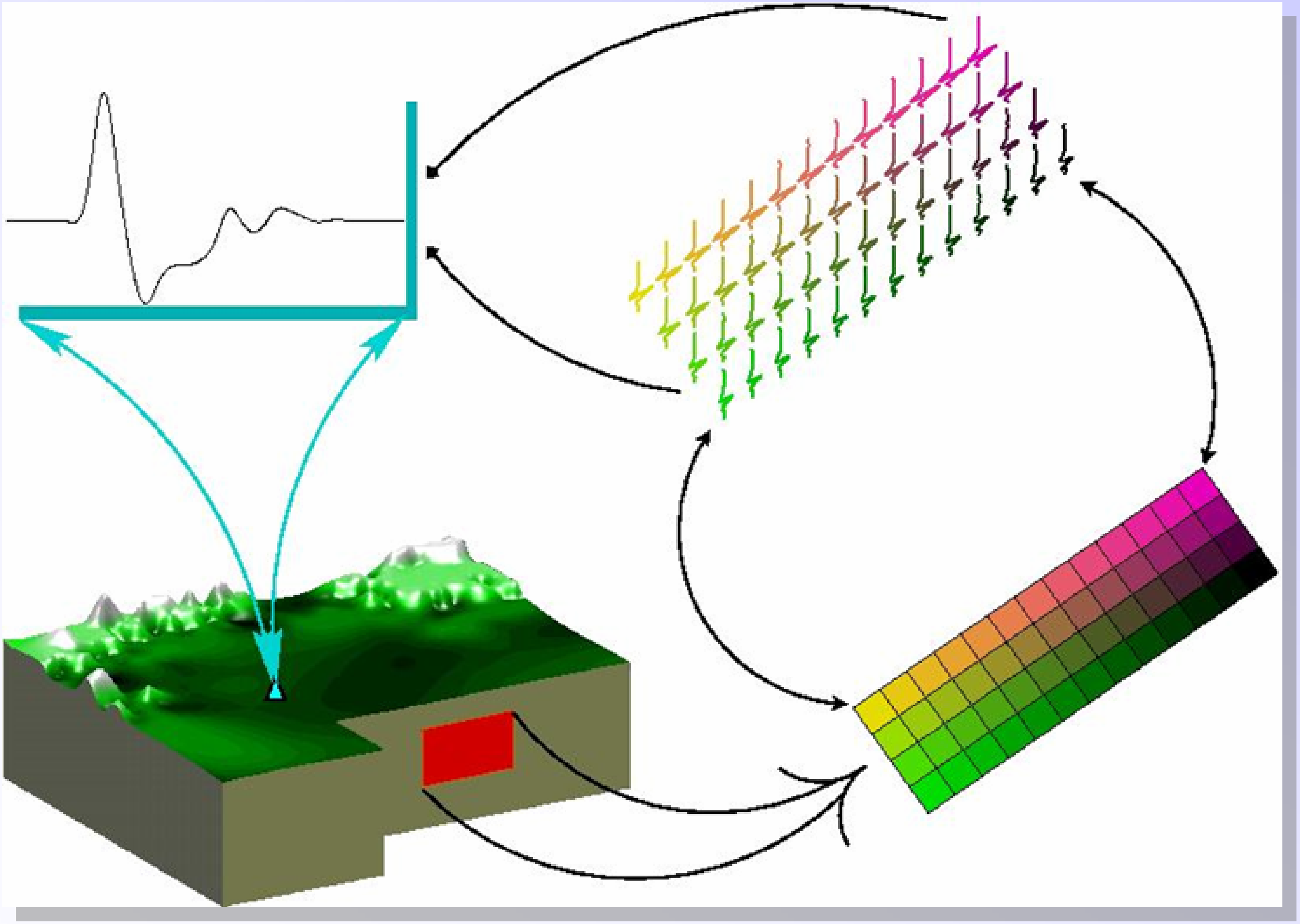
Example: Newport-Ingelwood Fault, Los Angeles Basin



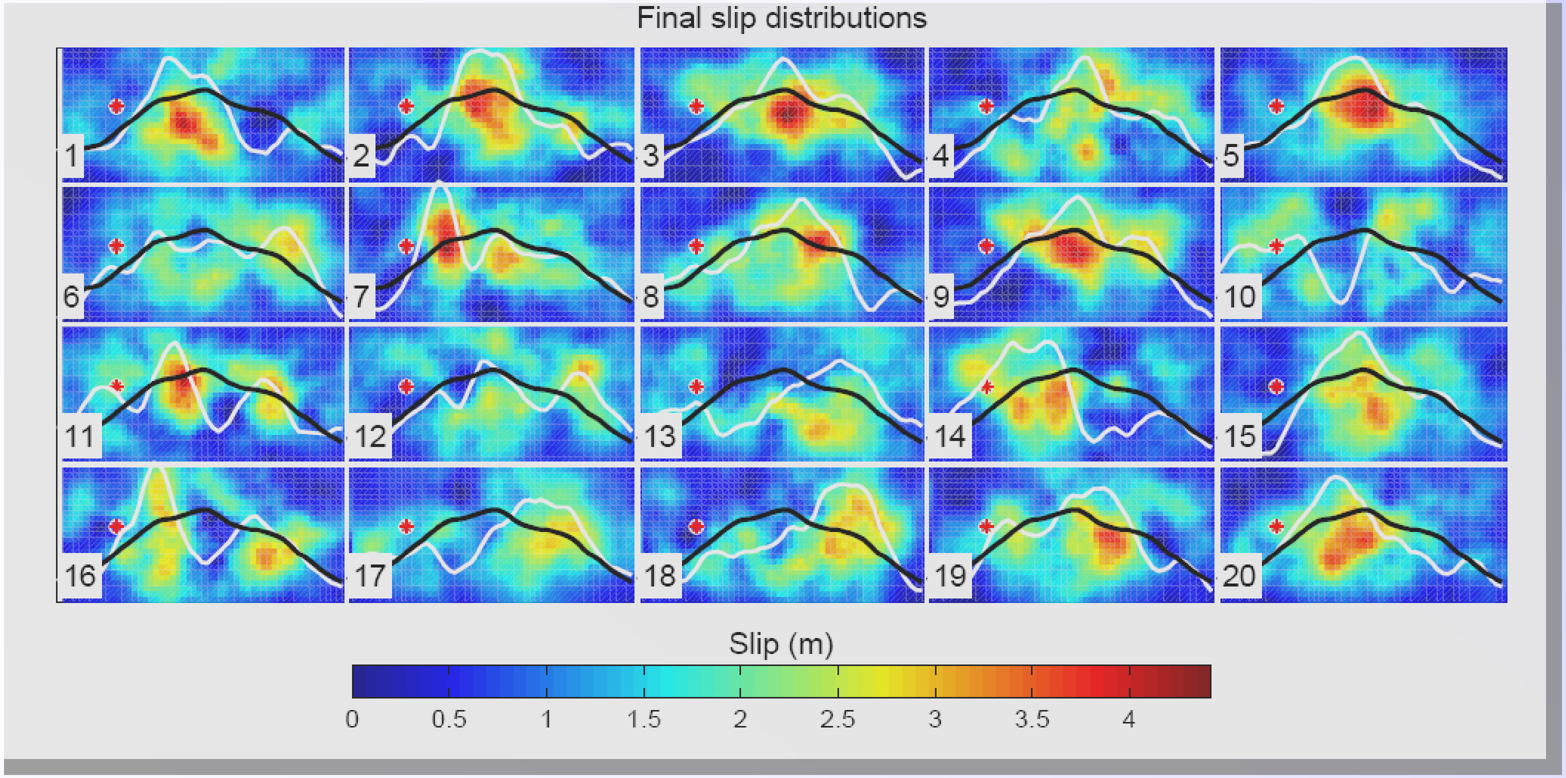


Wang, Igel, Cochard, Ewald (2006)

Numerical Green's Functions



Varying slip histories
M7 earthquakes



… while keeping the hypocenter location fixed …

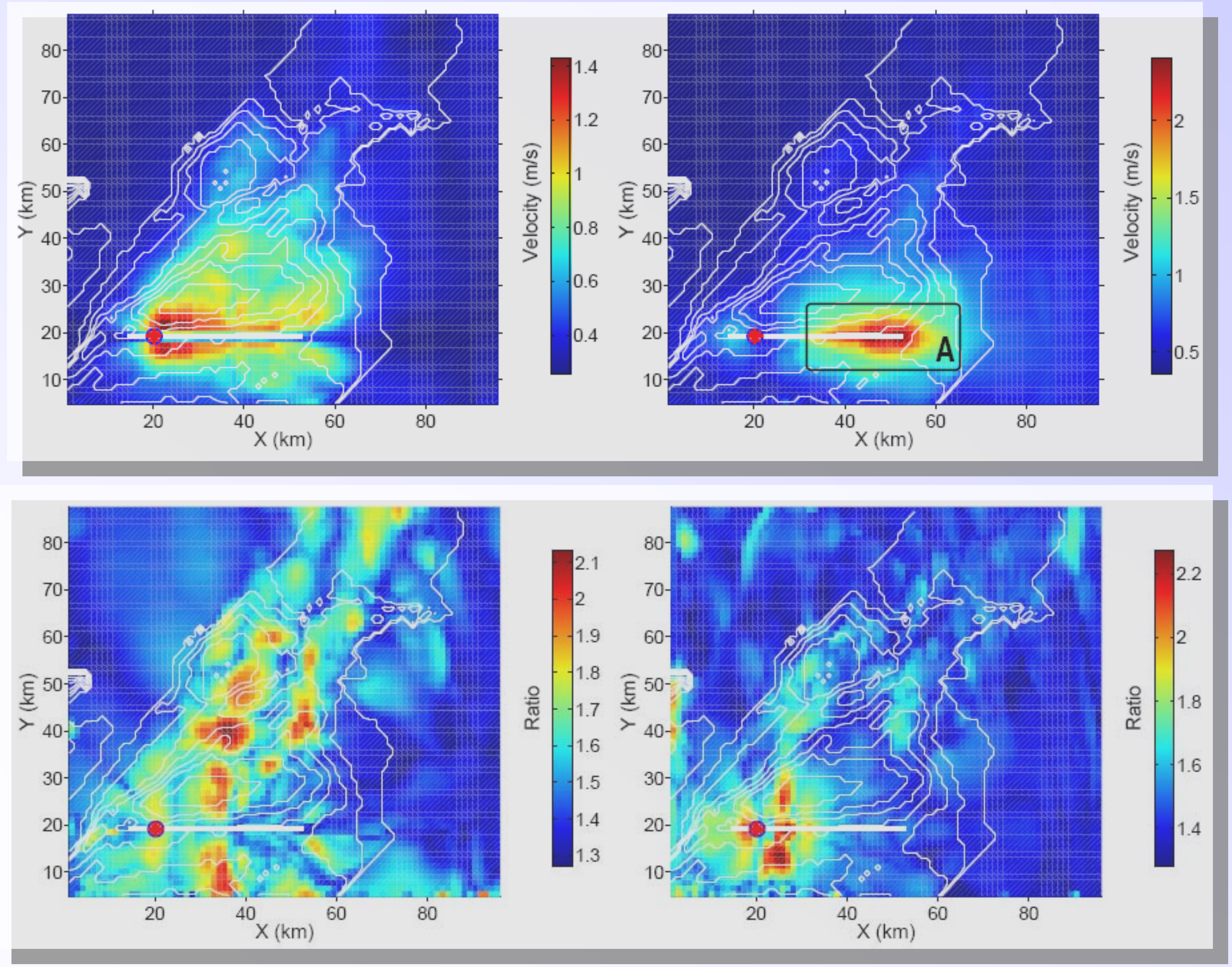
Variations due to slip history

20 scenarios

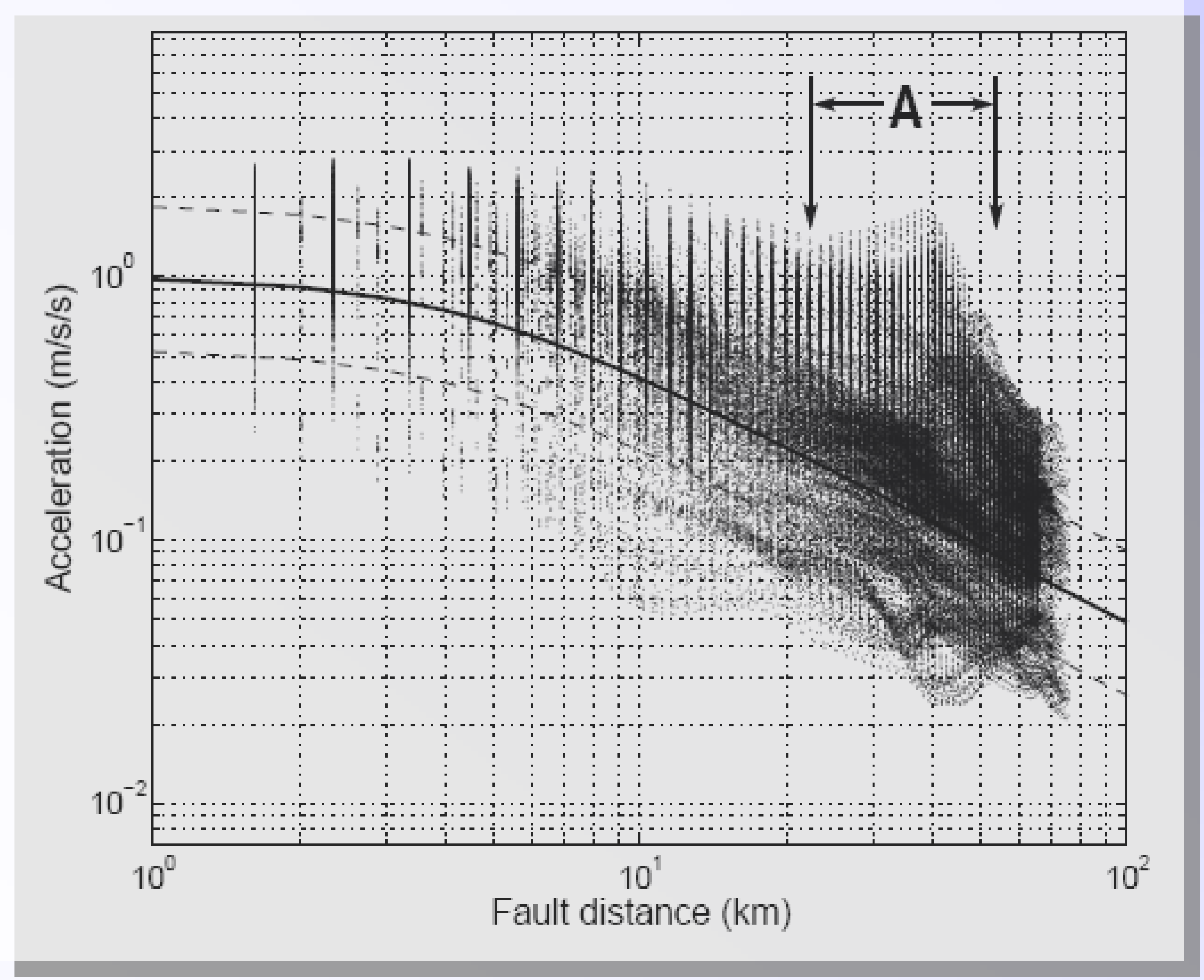
Fault || — Fault ⊥

PGV

Max / Mean



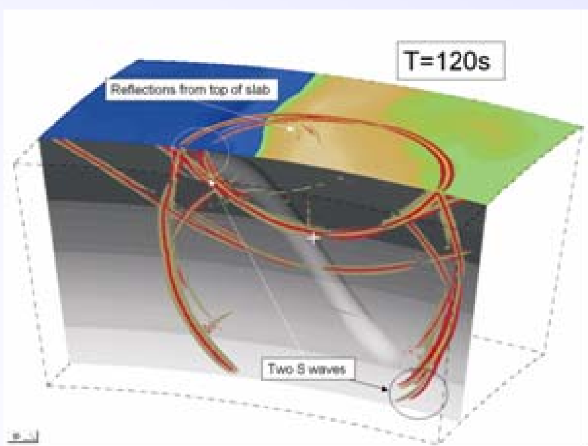
Compatible with Attenuation Relations?

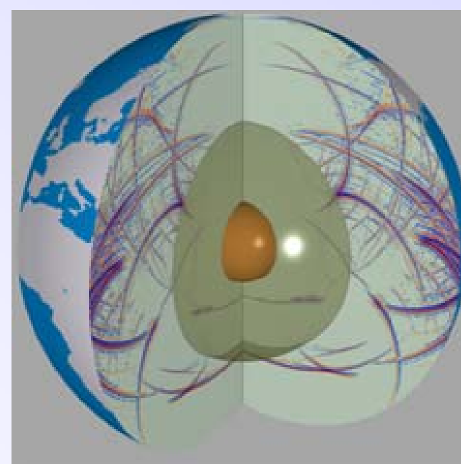


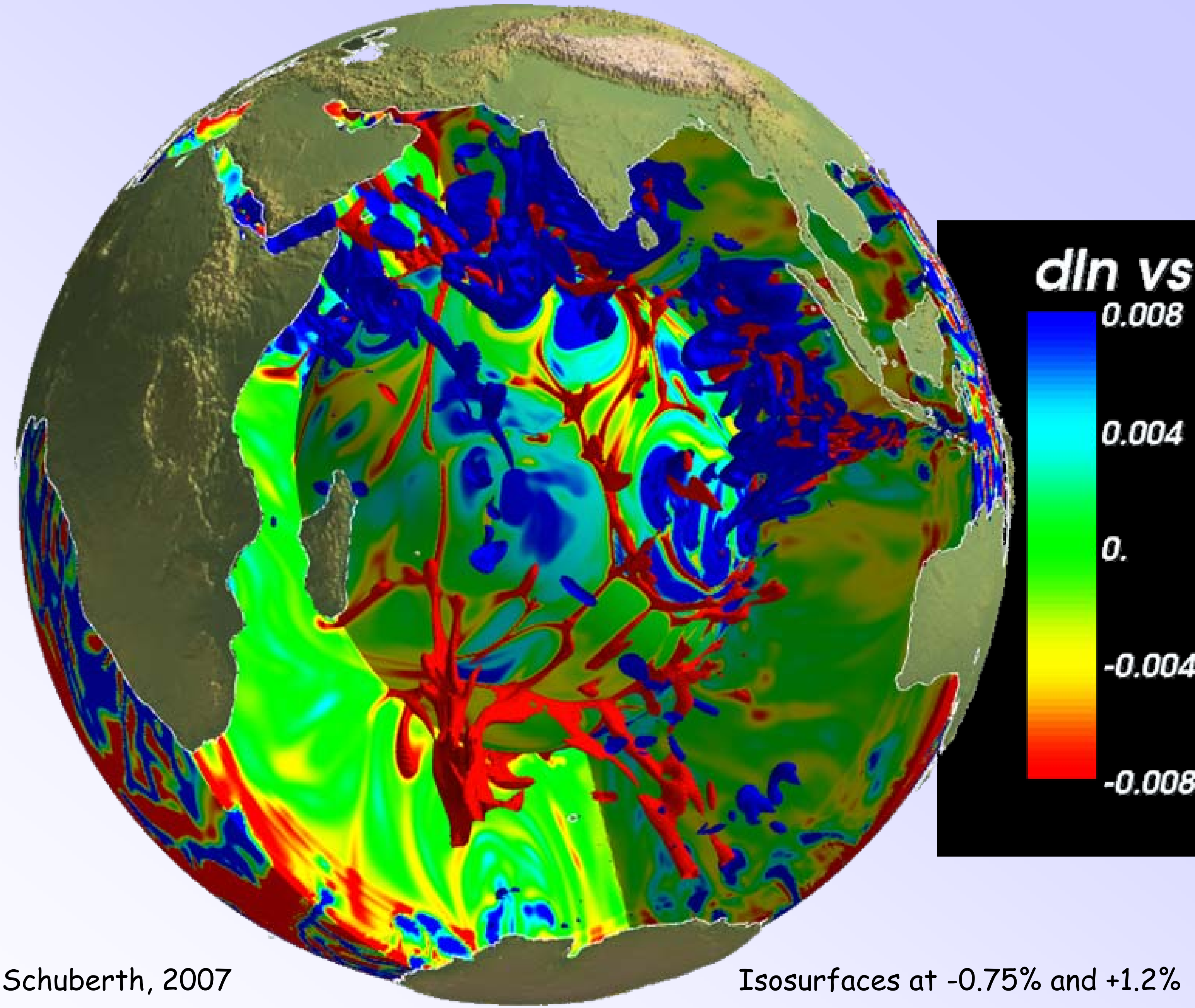
Global and regional seismology

scientific objectives

- High resolution imaging (diffration tomography) of global earth structure (geodynamics)
- 3D wave effects of structures like plumes, subduction zones, D'' -> geodynamic issues
- Development of 3D reference models (e.g. European reference model)



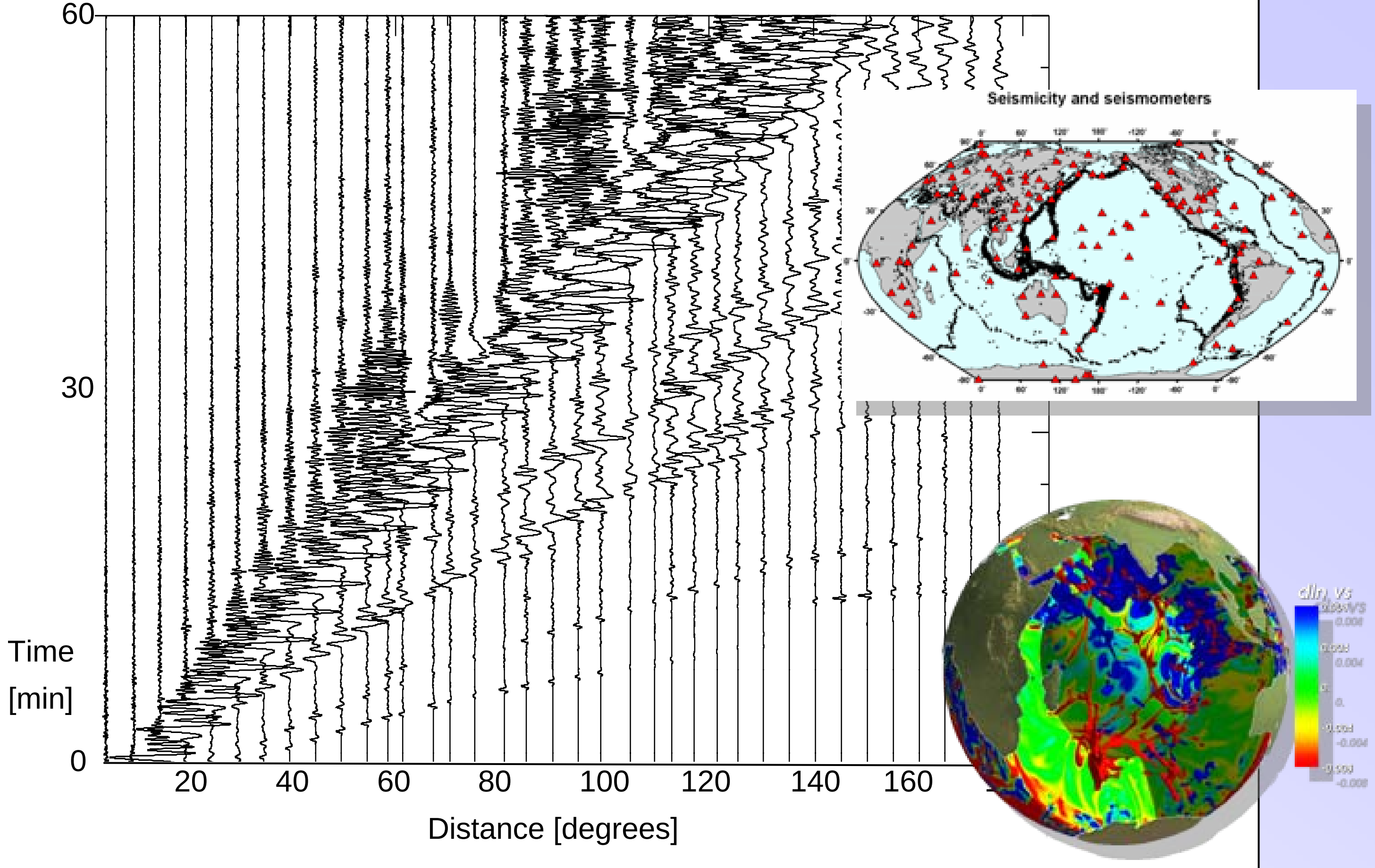




Bunge and Schuberth, 2007

Isosurfaces at -0.75% and +1.2%

Spectral Element Simulations

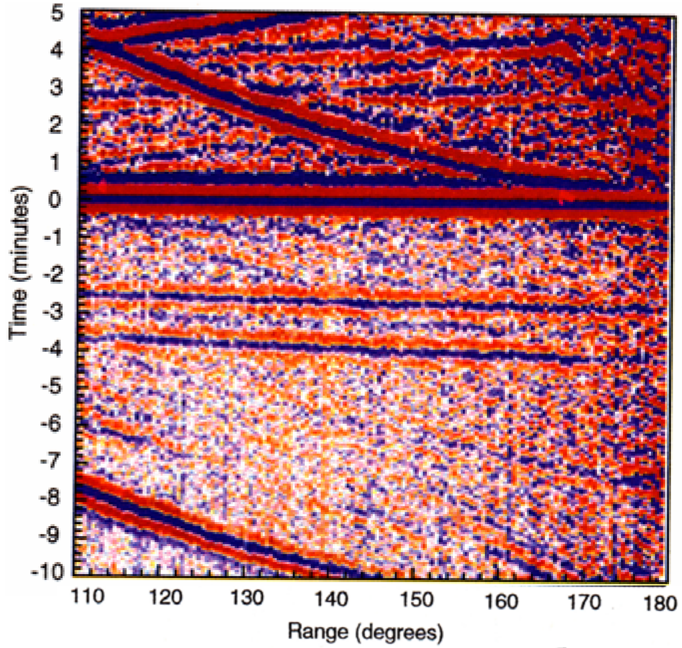


(SPECFEM3D, Komatitsch and Tromp)

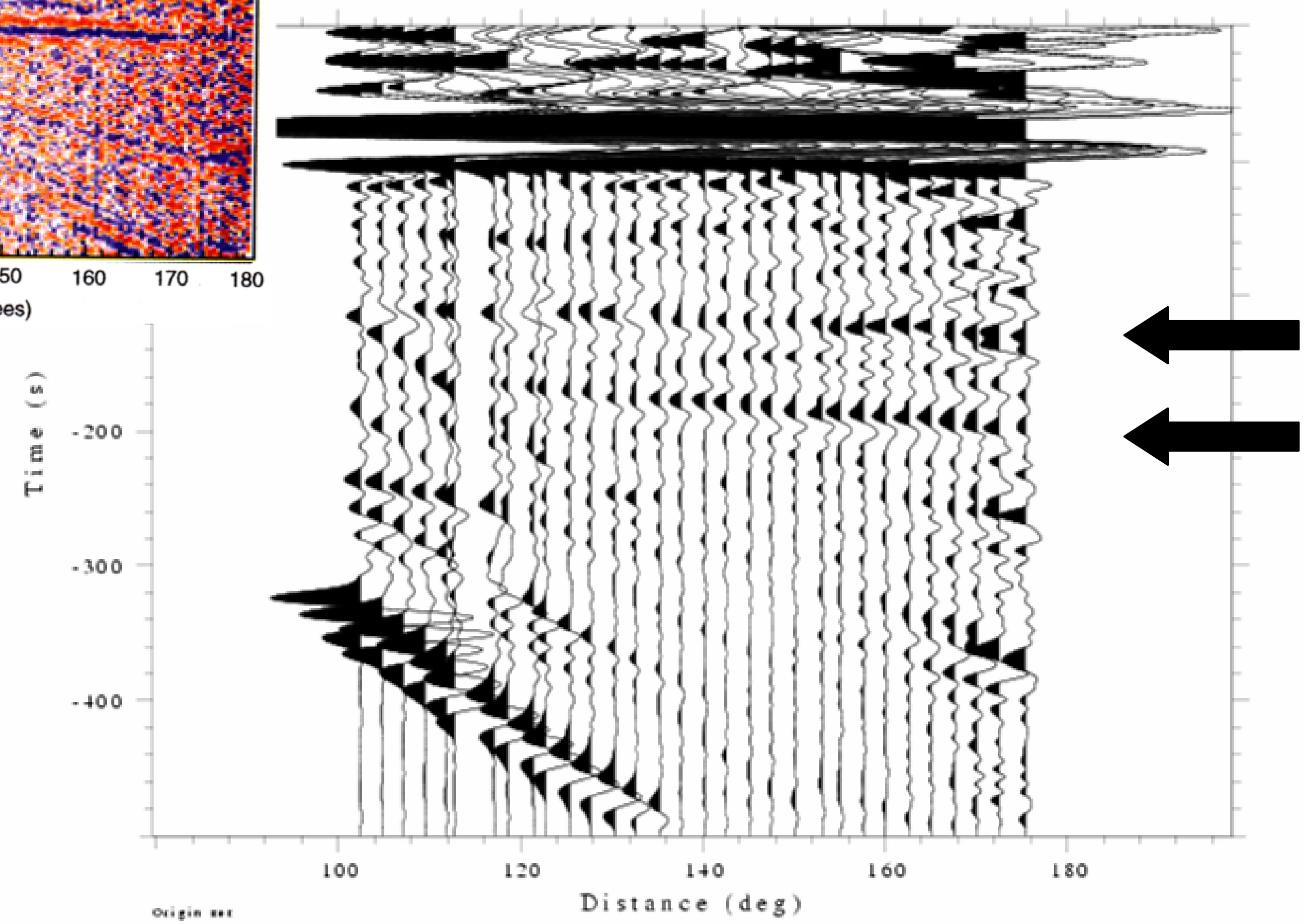
14.5 billion DOF on 1944 procs, down to 5 secs period! 50 h runtime

Study of SS-precursors
Mantle discontinuities

From Flanagan & Shearer JGR 1998



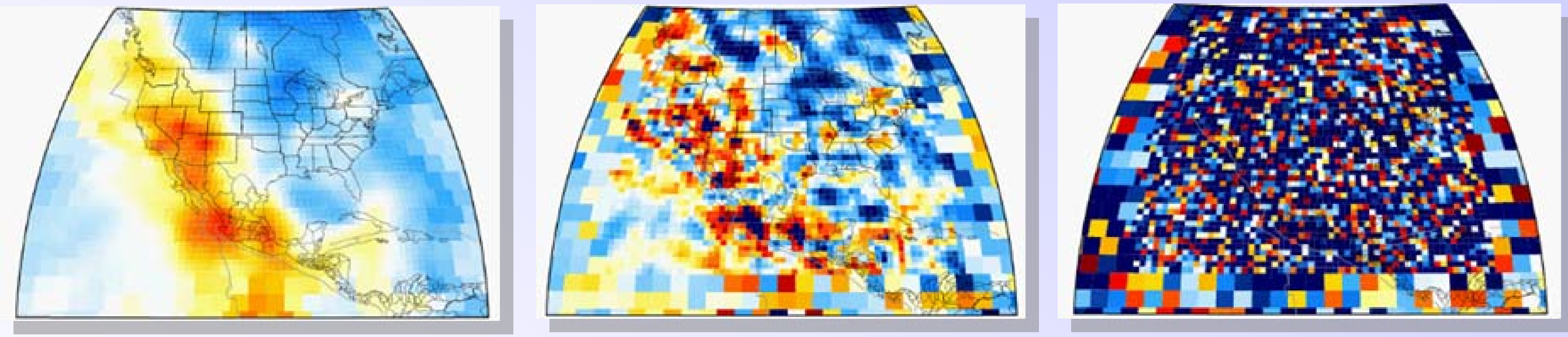
3-D synthetics for Model Earth




A. Tarantola

Model Uncertainties – Degrees of Freedom

Decreasing misfit

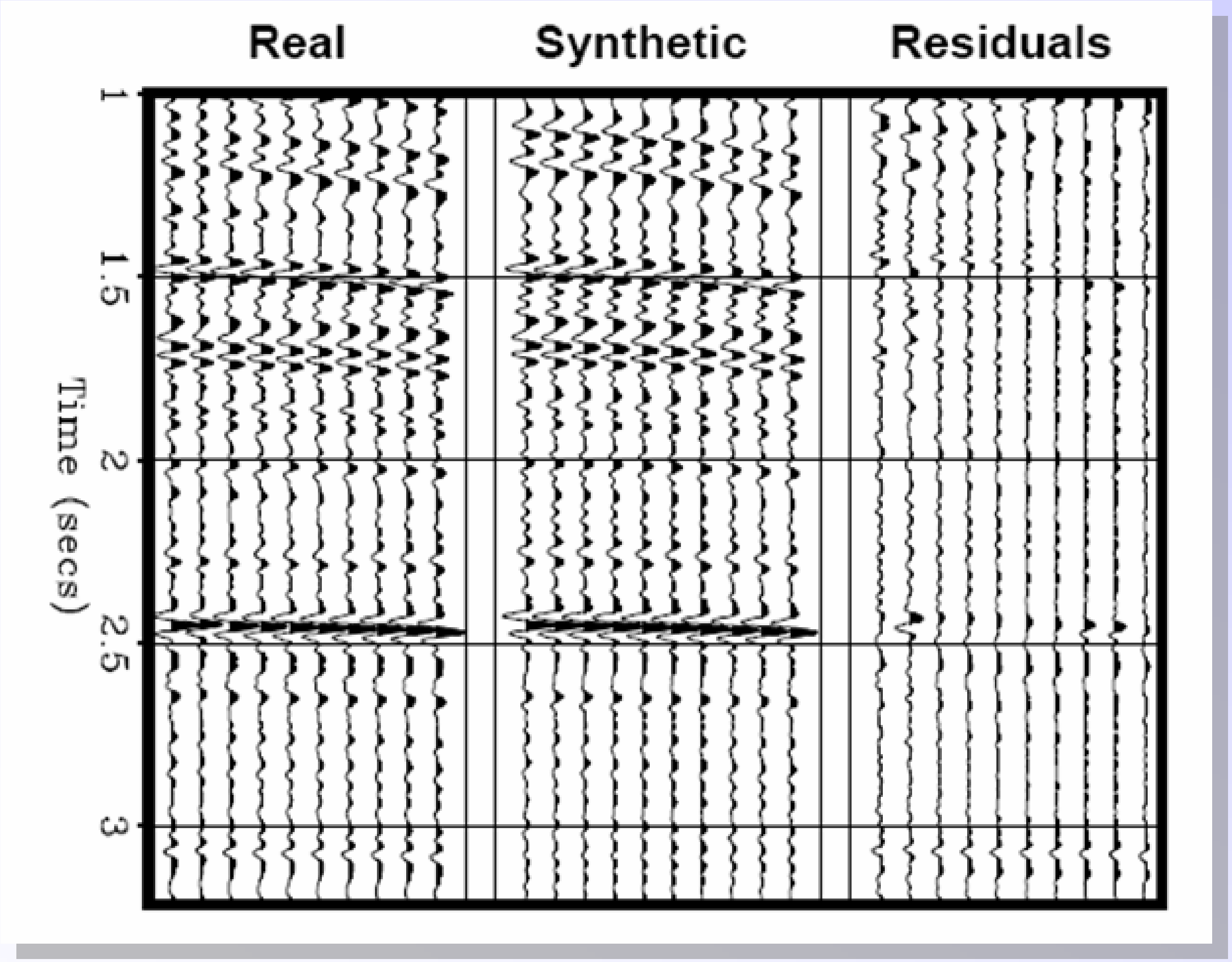


Increasing model complexity

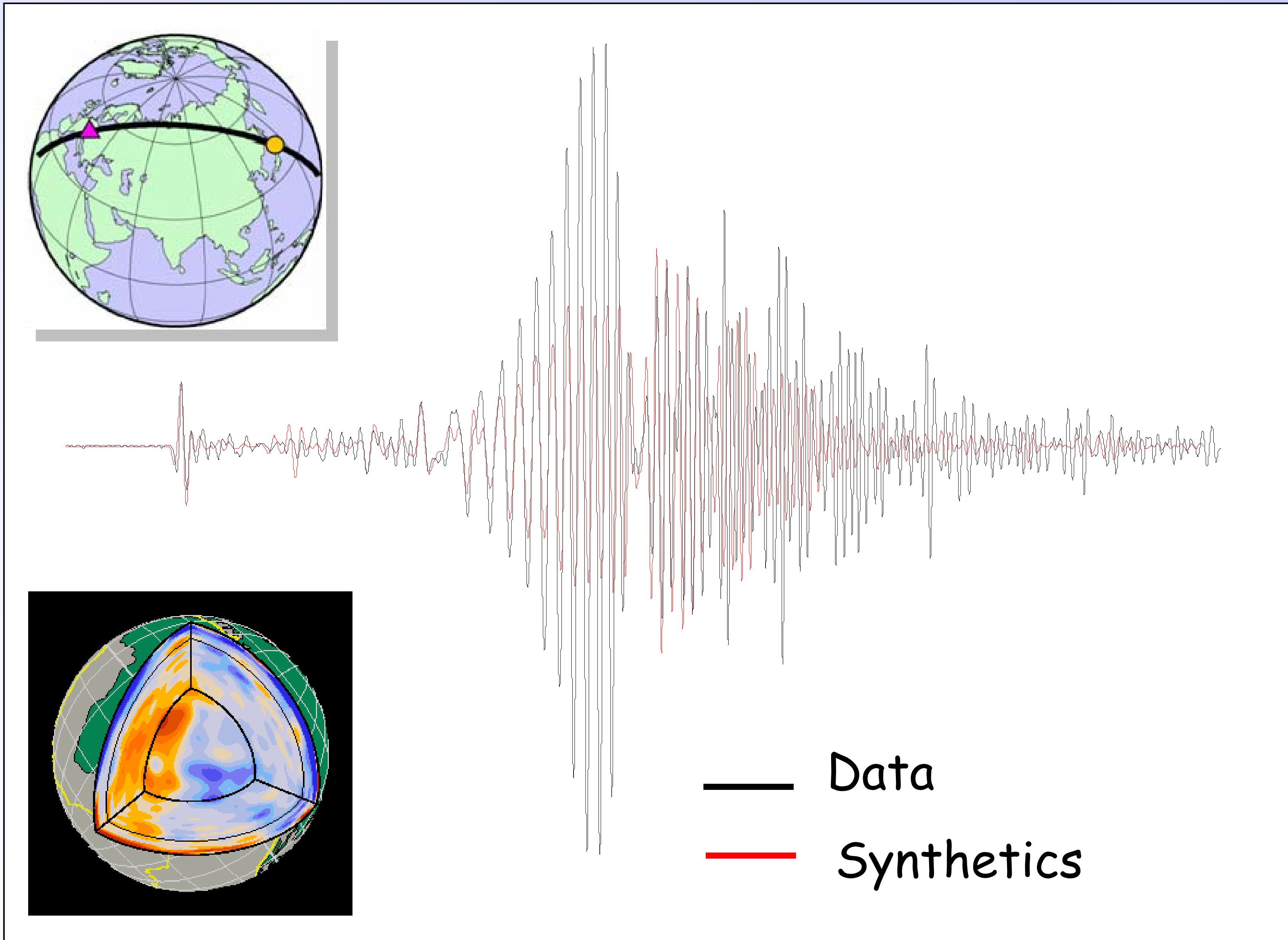
Increasing number of degrees of freedom

after L. Boschi (2007)

Diffraction tomography – Adjoint Methods

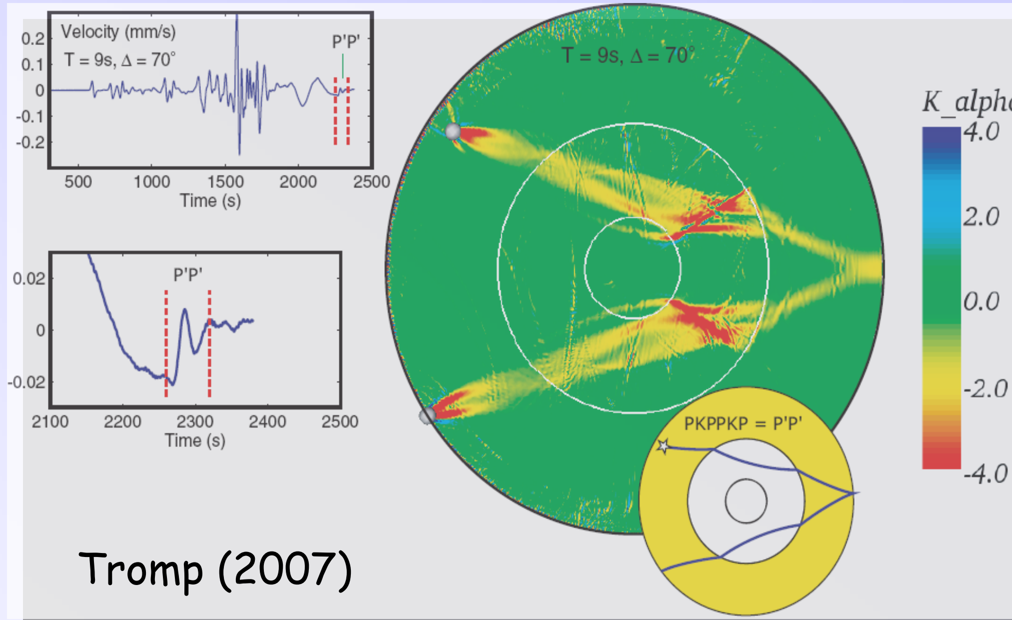


2D finite-difference waveform inversion on CM-5

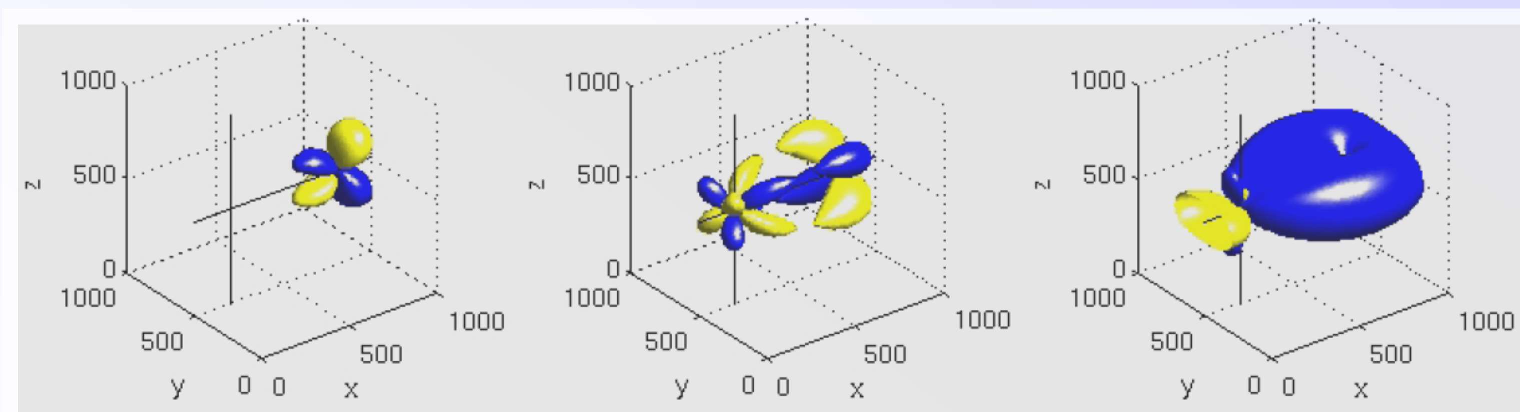

Data
Synthetics

Adjoint methods - sensitivities

Quantification of sensitivities with 3D simulation technology



Tromp (2007)

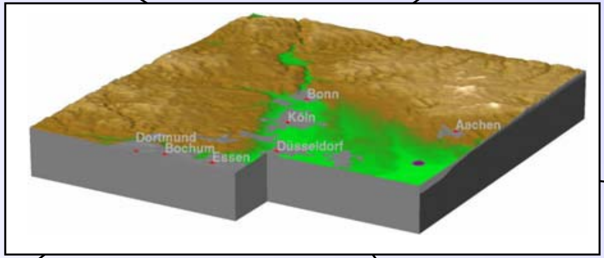


Fichtner et al. (2007)

The kernel

Earthquake scenarios
Shaking hazard

Phenomenological studies
Model space studies



Dynamic rupture
Source physics

Sensitivities
Experiment design

Imaging (source and structure)
Adjoint methods

What's missing?

... easy access for data modellers to well tested simulation tools ...

... easy (e.g., hidden) access to HPC infrastructure (GRIDs, EU-HPC)

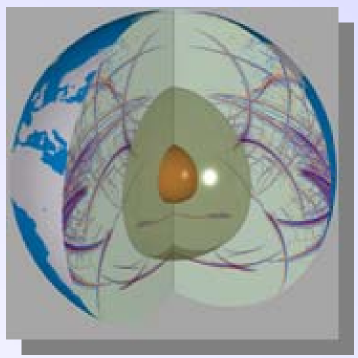
... community codes for wave propagation problems

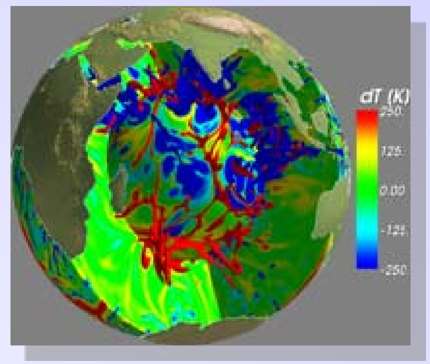
... software engineering support

General conclusions

- 3D wave simulation technology is about to enter routine seismic processing and inversion
- High-Performance Computing and parallel programming will remain an essential issue
- Infrastructure is developing (GRIDs, EU-HPC) that may revolutionize the way we process and simulate data, the soft infrastructure is missing
- Most Earth science institutions (and in part the whole community) are/is ill-prepared for these developments

Thank you for your attention! *





* "… if you don't know what MPI stands for, you 're in trouble !"