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

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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

TETHYS – Cluster Topology

Super-scale

Source: LRZ Munich

Source: Oeser et al., 2006

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: $O(100 \text{ TBytes})$
**Spatial Scales and Memory**  
*(back of the envelope)*

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Highest frequency</td>
<td>0.1 Hz</td>
<td></td>
</tr>
<tr>
<td>Shortest wavelength (crust)</td>
<td>20 km</td>
<td></td>
</tr>
<tr>
<td>Shortest wavelength (mantle)</td>
<td>50 km</td>
<td></td>
</tr>
<tr>
<td>Grid points per wavelength</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>Grid spacing (crust)</td>
<td>2000 m</td>
<td></td>
</tr>
<tr>
<td>Grid spacing (mantle)</td>
<td>5000 m</td>
<td></td>
</tr>
</tbody>
</table>

**Required grid points:** $O(10^9)$  
**Required memory:** $O(100 \text{ GBytes})$
Seismology and Geodynamics

Courtesy: G. Jahnke

Courtesy: H.P. Bunge, B. Schuberth
Numerical simulation of seismic wave propagation

Elastic wave equations

\[ \rho \partial_t^2 u_i = \partial_j (\sigma_{ij} + M_{ij}) + f_i \]
\[ \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \]
\[ \varepsilon_{kl} = \frac{1}{2} (\partial_k u_l + \partial_l u_k) \]

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)

Alluvial Basin

$V_S = 300 \text{ m/s}$

$f_{\text{max}} = 3 \text{ Hz}$

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

Bedrock

$V_S = 3200 \text{ m/s}$

$f_{\text{max}} = 3 \text{ Hz}$

$\lambda_{\text{min}} = V_S / f_{\text{max}} = 1066.7 \text{ m}$
Stupazzini et al. (2006)
The Courant Criterion

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

Largest velocity

Smallest grid size
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-or DER - Discontinuous Galerkin

- Combination of a discontinuous 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.


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 is possible without losing the accuracy of the scheme.
Mesh Partitioning and Parallel Computing

the problem of load balancing

Same color means same processor
Grenoble Basin Simulation

Time: 0 sec
Seismogram Comparison
Interactive Benchmarking

The SPICE Code Validation

To participate in the SPICE Code Validation (that is, calculate your solution for one or more defined models and compare it with solutions submitted by other participants), please follow these steps:

1. go to registration (do it only once for each method)
2. choose and download a model description
3. perform a computation with your code
4. convert your solution into a format appropriate for upload - see solution format
5. upload your solution (your solution will be stored on the server)
6. view/compare solutions

comments and suggestions to spice.cv@nuquake.eu

Moczo et al., 2006

www.spice-rtn.org
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
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

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 (diffraction 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)
Isosurfaces at -0.75% and +1.2%

Bunge and Schuberth, 2007
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

3-D synthetics for Model Earth
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
Adjoint methods - sensitivities

Quantification of sensitivities with 3D simulation technology

Tromp (2007)

Fichtner et al. (2007)
The kernel

- Earthquake scenarios
- Shaking hazard
- Sensitivities
- Experiment design
- Phenomenological studies
  - Model space studies
- Dynamic rupture
  - Source physics
- 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!”