Spectral-Element and Adjoint Methods in Seismology

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Governing Equations

Equation of motion:

$$
\rho \, \partial_t^2 \mathbf{s} - \mathbf{\nabla} \cdot \mathbf{T} = \mathbf{f}
$$

Boundary condition:

$$
|\hat{\mathbf{n}}\cdot\mathbf{T}=\mathbf{0}|
$$

Initial conditions:

$$
s(\mathbf{x},0) = \mathbf{0}, \qquad \partial_t s(\mathbf{x},0) = \mathbf{0}
$$

Earthquake source:

$$
\mathbf{f} = -\mathbf{M} \cdot \mathbf{\nabla} \delta(\mathbf{x} - \mathbf{x}_{\mathrm{s}}) S(t)
$$

Weak Form

$$
\int_{\Omega} \rho \mathbf{w} \cdot \partial_t^2 \mathbf{s} d^3 \mathbf{x} = -\int_{\Omega} \mathbf{\nabla} \mathbf{w} \cdot \mathbf{T} d^3 \mathbf{x} + \mathbf{M} \cdot \mathbf{\nabla} \mathbf{w}(\mathbf{x}_s) S(t)
$$

- Weak form valid for any test vector
- Boundary conditions automatically included
- Source term explicitly integrated

Finite-fault (kinematic) rupture:

$$
\mathbf{M} : \nabla \mathbf{w}(\mathbf{x}_{\mathrm{s}}) \, S(t) \rightarrow \int_{S_{\mathrm{s}}} \mathbf{m}(\mathbf{x}_{\mathrm{s}}, t) : \nabla \mathbf{w}(\mathbf{x}_{\mathrm{s}}) \, d^2 \mathbf{x}_{\mathrm{s}}
$$

 \mathbf{r}

The Diagonal Mass Matrix

Representation of the displacement:

$$
\mathbf{s}(\mathbf{x}(\xi,\eta,\zeta),t) = \sum_{i=1}^3 \hat{\mathbf{x}}_i \sum_{\sigma=0}^n \sum_{\tau=0}^n \sum_{\nu=0}^n s_i^{\sigma\tau\nu}(t) h_{\sigma}(\xi) h_{\tau}(\eta) h_{\nu}(\zeta)
$$

Representation of the test vector:

$$
\mathbf{w}(\mathbf{x}(\xi,\eta,\zeta)) = \sum_{i=j}^{3} \hat{\mathbf{x}}_j \sum_{\sigma=0}^{n} \sum_{\tau=0}^{n} \sum_{\nu=0}^{n} w_i^{\alpha\beta\gamma} h_{\alpha}(\xi) h_{\beta}(\eta) h_{\gamma}(\zeta)
$$

Weak form:

$$
\int_{\Omega} \rho \mathbf{w} \cdot \partial_t^2 \mathbf{s} d^3 \mathbf{x} = -\int_{\Omega} \mathbf{\nabla} \mathbf{w} \cdot \mathbf{T} d^3 \mathbf{x} + \mathbf{M} \cdot \mathbf{\nabla} \mathbf{w}(\mathbf{x}_s) S(t)
$$

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Degree 4 Lagrange polynomials:

Diagonal mass matrix:

$$
\int_{\Omega_e} \rho \, \mathbf{w} \cdot \partial_t^2 \mathbf{s} \, d^3 \mathbf{x} = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \rho(\mathbf{x}(\xi)) \, \mathbf{w}(\mathbf{x}(\xi)) \cdot \partial_t^2 \mathbf{s}(\mathbf{x}(\xi), t) \, J(\xi) \, d^3 \xi = \sum_{\alpha=0}^n \sum_{\beta=0}^n \sum_{\gamma=0}^n \omega_\alpha \omega_\beta \omega_\gamma J^{\alpha \beta \gamma} \rho^{\alpha \beta \gamma} \sum_{i=1}^3 w_i^{\alpha \beta \gamma} \tilde{s}_i^{\alpha \beta \gamma}
$$

- Integrations are pulled back to the reference cube
- In the SEM one uses:
	- interpolation on GLL points
	- GLL quadrature

June 12, 2005, M=5.1 Big Bear

QuickTime[™] and a YUV420 codec decompressor are needed to see this picture.

3D Regional Forward Simulations

June 12, 2005, M=5.1 Big Bear

Qinya Liu

Near Real-Time Applications

- •Automated near real-time simulations of all M>3.5 events
- •ShakeMovies at http://www.shakemovie.caltech.edu/
- • Soon:
	- CMT source solutions
	- –Synthetic seismograms

SPECFEM3D_BASIN: Future Plans

- • Switch to a (parallel) CUBIT hexahedral finite-element mesher (Casarotti, Lee)
	- Topography & bathymetry
	- Major geological interfaces
	- –**Basins**
	- –Fault surfaces
- •Use ParMETIS or SCOTCH for mesh partitioning & load-balancing
- •Retain the SPECFEM3D_BASIN solver (takes ParMETIS meshes; Komatitsch)
- •Add dynamic rupture capabilities (Ampuero, Lapusta, Kaneko)

Global Simulations

S20RTS (Ritsema et al. 1999)

Cubed sphere mesh

Great 2004 Sumatra-Andaman Earthquake

 5°

 0°

 -5° 80°

 85°

 90°

 95°

 100°

 105°

 110°

Finite slip model (Chen et al., 2005)

Sumatra Surface Waves

QuickTime™ and a YUV420 codec decompressor are needed to see this picture.

Surface-Wave Fits

Vala Hjorleifsdottir

SPECFEM3D_GLOBE: Future Plans

On-demand TeraGrid applications:

- •Automated, near real-time simulations of all M>6 earthquakes
- •Analysis of past events (more than 20,000 events)
- •Seismology Web Portal

Petascale simulations:

- •Global simulations at 1-2 Hz
- \bullet New doubling brick (perfect load-balancing)

Adjoint Spectral-Element Simulations

Adjoint Tomography

PDE-constrained waveform tomography:

$$
\chi = \frac{1}{2} \sum_{r} \int_{0}^{T} \left[\mathbf{s}(\mathbf{x}_{r}, t) - \mathbf{d}(\mathbf{x}_{r}, t) \right]^{2} dt - \int_{0}^{T} \int_{\Omega} \boldsymbol{\lambda} \cdot (\rho \, \partial_{t}^{2} \mathbf{s} - \boldsymbol{\nabla} \cdot \mathbf{T} - \mathbf{f}) d^{3} \mathbf{x} dt
$$

Change in the waveform misfit function:

$$
\delta \chi = \int_0^T \int_{\Omega} \sum_r [\mathbf{s}(\mathbf{x}_r, t) - \mathbf{d}(\mathbf{x}_r, t)] \delta(\mathbf{x} - \mathbf{x}_r) \cdot \delta \mathbf{s}(\mathbf{x}, t) d^3 \mathbf{x} dt \n- \int_0^T \int_{\Omega} (\delta \rho \lambda \cdot \partial_t^2 \mathbf{s} + \nabla \lambda \cdot \delta \mathbf{c} \cdot \nabla \mathbf{s} - \lambda \cdot \delta \mathbf{f}) d^3 \mathbf{x} dt - \int_0^T \int_{\Omega} [\rho \partial_t^2 \lambda - \nabla \cdot (\mathbf{c} \cdot \nabla \lambda)] \cdot \delta \mathbf{s} d^3 \mathbf{x} dt \n- \int_{\Omega} [\rho (\lambda \cdot \partial_t \delta \mathbf{s} - \partial_t \lambda \cdot \delta \mathbf{s})]_T d^3 \mathbf{x} - \int_0^T \int_{\partial \Omega} \hat{\mathbf{n}} \cdot (\mathbf{c} \cdot \nabla \lambda) \cdot \delta \mathbf{s} d^2 \mathbf{x} dt,
$$

Adjoint wavefield:
$$
\mathbf{s}^{\dagger}(\mathbf{x},t) \equiv \lambda(\mathbf{x},T-t)
$$

\nAdjoint equation of motion:
$$
\rho \frac{\partial^2 \mathbf{s}^{\dagger}}{\partial t} = \nabla \cdot \mathbf{T}^{\dagger} + \mathbf{f}^{\dagger}
$$

\nAdjoint boundary conditions:
$$
\hat{\mathbf{n}} \cdot \mathbf{T}^{\dagger} = \mathbf{0}
$$

\nAdjoint initial conditions:
$$
\mathbf{s}^{\dagger}(\mathbf{x},0) = \mathbf{0}, \qquad \frac{\partial_t \mathbf{s}^{\dagger}(\mathbf{x},0) = \mathbf{0}}{\partial t}
$$

\nAdjoint source:
$$
\mathbf{f}^{\dagger}(\mathbf{x},t) = \sum_{r=1}^{N} [\mathbf{s}(\mathbf{x}_r, T-t) - \mathbf{d}(\mathbf{x}_r, T-t)] \delta(\mathbf{x} - \mathbf{x}_r)
$$

Frechet derivative

The Frechet derivative may be expressed as:

$$
\delta \chi = \int_{\Omega} (\delta \rho K_{\rho} + \delta \mathbf{c} \, \therefore \, \mathbf{K}_{\mathbf{c}}) \, d^3 \mathbf{x} + \int_{0}^{T} \int_{\Omega} \mathbf{s}^{\dagger} \cdot \delta \mathbf{f} \, d^3 \mathbf{x} \, dt
$$

Density and elastic tensor kernels:

$$
K_{\rho}(\mathbf{x}) = -\int_0^T \mathbf{s}^\dagger(\mathbf{x}, T - t) \cdot \partial_t^2 \mathbf{s}(\mathbf{x}, t) dt
$$

$$
\mathbf{K_c}(\mathbf{x}) = -\int_0^T \mathbf{\nabla s}^\dagger(\mathbf{x}, T - t) \mathbf{\nabla s}(\mathbf{x}, t) dt
$$

Numerical Implementation

$$
K_{\rho}(\mathbf{x}) = -\int_0^T \mathbf{s}^\dagger(\mathbf{x}, T - t) \cdot \partial_t^2 \mathbf{s}(\mathbf{x}, t) dt
$$

Need simultaneous access to $\left|\mathbf{s}^\intercal(\mathbf{x},T-t)\right|$ and

 \bullet During calculation of adjoint field \mathbf{s}^{\dagger} , reconstruct **s** by solving the `backward' wave equation

Need to store from a previous forward simulation:

- Last snapshot
- Wavefield absorb on artificial boundaries
- Challenge:
- `Undoing' attenuation

Toward 3D Tomography: SPECFEM3D Adjoint Capabilities

Conclusions

Adjoint methods:

- •Choose an observable, e.g., waveforms or cross-correlation traveltimes
- •Choose a measure of misfit, e.g., least-squares
- •Determine the appropriate adjoint source for this observable & measurement
- •Use fully 3D reference models
- •Any arrival suitable for measurement
- •No dependence on the number of stations, components, or measurements
- •3D sensitivity kernels may be calculated based upon two forward simulations for each earthquake
- •Number of simulations: 3 * (# earthquakes) * (# iterations)
- •Full anisotropy for the same cost
- •Attenuation remains a challenge

Regional simulations:

- •One 3 minute forward simulation accurate to 1.5 seconds takes 45 minutes on a 75 node cluster
- • 150 events and 3 iterations would require 1800 simulations, i.e., three weeks of dedicated CPU time on 75 nodes
- •Near real-time simulations

Global simulations:

- •One 1 hour forward simulation accurate to 20 seconds takes 4 hours on a 75 node cluster
- •500 events and 3 iterations would require 6,000 simulations, i.e., 100 days on a 750 node cluster
- •Near real-time simulations
- •On-demand global seismology
- •Petascale application