Spectral-Element and Adjoint Methods in Seismology



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Governing Equations



Equation of motion:

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

Boundary condition:

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

Initial conditions:

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

Earthquake source:

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

Weak Form



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

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

Finite-fault (kinematic) rupture:

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

e

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:

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

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Degree 4 Lagrange polynomials:



Diagonal mass matrix:

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

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

Degree 4 GLL points:







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 <u>http://www.shakemovie.caltech.edu/</u>
- 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)



Great 2004 Sumatra-Andaman Earthquake







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
- New doubling brick (perfect load-balancing)







Adjoint Spectral-Element Simulations

Adjoint Tomography



PDE-constrained waveform tomography:

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

Change in the waveform misfit function:

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

Adjoint EquationsAdjoint wavefield:
$$\mathbf{s}^{\dagger}(\mathbf{x},t) \equiv \boldsymbol{\lambda}(\mathbf{x},T-t)$$
Adjoint equation of motion: $\rho \partial_t^2 \mathbf{s}^{\dagger} = \nabla \cdot \mathbf{T}^{\dagger} + \mathbf{f}^{\dagger}$ Adjoint boundary conditions: $\mathbf{\hat{n}} \cdot \mathbf{T}^{\dagger} = \mathbf{0}$ Adjoint initial conditions: $\mathbf{s}^{\dagger}(\mathbf{x},0) = \mathbf{0}, \qquad \partial_t \mathbf{s}^{\dagger}(\mathbf{x},0) = \mathbf{0}$ Adjoint 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:

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

Density and elastic tensor kernels:

$$K_{\rho}(\mathbf{x}) = -\int_{0}^{T} \mathbf{s}^{\dagger}(\mathbf{x}, T-t) \cdot \partial_{t}^{2} \mathbf{s}(\mathbf{x}, t) \,\mathrm{d}t$$

$$\mathbf{K}_{\mathbf{c}}(\mathbf{x}) = -\int_{0}^{T} \boldsymbol{\nabla} \mathbf{s}^{\dagger}(\mathbf{x}, T - t) \, \boldsymbol{\nabla} \mathbf{s}(\mathbf{x}, t) \, \mathrm{d}t$$

Numerical Implementation



$$K_{\rho}(\mathbf{x}) = -\int_{0}^{T} \mathbf{s}^{\dagger}(\mathbf{x}, T-t) \cdot \partial_{t}^{2} \mathbf{s}(\mathbf{x}, t) \,\mathrm{d}t$$

Need simultaneous access to $\mathbf{s}^{\dagger}(\mathbf{x}, T-t)$ and $\mathbf{s}(\mathbf{x}, t)$

 During calculation of adjoint field s[†], reconstruct s by solving the `backward' wave equation

Need to store from a previous forward simulation:

- Last snapshot $\mathbf{s}(\mathbf{x},T)$
- 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