Spectral-Element and Adjoint Methods in Seismology

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Introduction to the Spectral-Element Method (SEM)
Governing Equations

Equation of motion:

\[ \rho \frac{\partial^2 s}{\partial t^2} - \nabla \cdot T = f \]

Boundary condition:

\[ \hat{n} \cdot T = 0 \]

Initial conditions:

\[ s(x, 0) = 0, \quad \partial_t s(x, 0) = 0 \]

Earthquake source:

\[ f = -M \cdot \nabla \delta(x - x_S) S(t) \]
Weak Form

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

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

Finite-fault (kinematic) rupture:

\[ \mathbf{M} : \nabla \mathbf{w}(x_s) S(t) \rightarrow \int_{S_s} \mathbf{m}(x_s, t) : \nabla \mathbf{w}(x_s) \, d^2 x_s \]
Finite-Elements

Mapping from reference cube to hexahedral elements:

\[ \mathbf{x}(\xi) = \sum_{a=1}^{M} \mathbf{x}_a N_a(\xi) \]

Volume relationship:

\[ d^3 \mathbf{x} = dx \, dy \, dz = J \, d\xi \, d\eta \, d\zeta = J \, d^3 \xi \]

Jacobian of the mapping:

\[ J = \left| \frac{\partial (x, y, z)}{\partial (\xi, \eta, \zeta)} \right| \]

Jacobian matrix:

\[ \frac{\partial \mathbf{x}}{\partial \xi} = \sum_{a=1}^{M} \mathbf{x}_a \frac{\partial N_a}{\partial \xi} \]
Lagrange Polynomials and Gauss-Lobatto-Legendre (GLL) Points

The 5 degree 4 Lagrange polynomials:

Degree 4 GLL points:

GLL points are $n+1$ roots of:

$$ (1 - \xi^2) \frac{P'_n(\xi)}{P_n(\xi)} = 0 $$

General definition:

$$ h_\alpha(\xi) = \frac{(\xi - \xi_0) \cdots (\xi - \xi_{\alpha-1})(\xi - \xi_{\alpha+1}) \cdots (\xi - \xi_n)}{(\xi_{\alpha} - \xi_0) \cdots (\xi_{\alpha} - \xi_{\alpha-1})(\xi_{\alpha} - \xi_{\alpha+1}) \cdots (\xi_{\alpha} - \xi_n) } $$

Note that at a GLL point:  \[ h_\alpha(\xi_\beta) = \delta_{\alpha\beta} \]
Interpolation

Representation of functions on an element in terms of Lagrange polynomials:

\[ f(\mathbf{x}(\xi, \eta, \zeta)) = \sum_{\alpha=0}^{n} \sum_{\beta=0}^{n} \sum_{\gamma=0}^{n} f^{\alpha\beta\gamma} h_{\alpha}(\xi) h_{\beta}(\eta) h_{\gamma}(\zeta) \]

Gradient on an element:

\[ \nabla f(\mathbf{x}(\xi, \eta, \zeta)) = \sum_{i=1}^{3} \hat{x}_i \sum_{\alpha=0}^{n} \sum_{\beta=0}^{n} \sum_{\gamma=0}^{n} f^{\alpha\beta\gamma} \left[ h_{\alpha}'(\xi) h_{\beta}(\eta) h_{\gamma}(\zeta) \partial_i \xi + h_{\alpha}(\xi) h_{\beta}'(\eta) h_{\gamma}(\zeta) \partial_i \eta + h_{\alpha}(\xi) h_{\beta}(\eta) h_{\gamma}'(\zeta) \partial_i \zeta \right] \]
Integration of functions over an element based upon GLL quadrature:

\[
\int_{\Omega_e} f(x) \, d^3x = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} f(x(\xi, \eta, \zeta)) \, J(\xi, \eta, \zeta) \, d\xi \, d\eta \, d\zeta = \sum_{\alpha=0}^{n} \sum_{\beta=0}^{n} \sum_{\gamma=0}^{n} \omega_\alpha \omega_\beta \omega_\gamma f^{\alpha\beta\gamma} J^{\alpha\beta\gamma}
\]

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

Degree 4 GLL points:
The Diagonal Mass Matrix

Representation of the displacement:
\[
\mathbf{s}(\mathbf{x}(\xi, \eta, \zeta), t) = \sum_{i=1}^{3} \sum_{\sigma=0}^{n} \sum_{r=0}^{n} \sum_{\nu=0}^{n} s_i^{\sigma r \nu}(t) h_{\sigma}(\xi) h_{\tau}(\eta) h_{\nu}(\zeta)
\]

Representation of the test vector:
\[
\mathbf{w}(\mathbf{x}(\xi, \eta, \zeta)) = \sum_{i=j}^{3} \sum_{\alpha=0}^{n} \sum_{\beta=0}^{n} \sum_{\gamma=0}^{n} w_i^{\alpha \beta \gamma} h_{\alpha}(\xi) h_{\beta}(\eta) h_{\gamma}(\zeta)
\]

Weak form:
\[
\int_{\Omega} \rho \mathbf{w} \cdot \partial_t^2 \mathbf{s} \, d^3 x = - \int_{\Omega} \nabla \mathbf{w} : \mathbf{T} \, d^3 x + \mathbf{M} : \nabla \mathbf{w}(\mathbf{x}_s) S(t)
\]

Diagonal mass matrix:
\[
\int_{\Omega_c} \rho \mathbf{w} \cdot \partial_t^2 \mathbf{s} \, d^3 x = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \rho(x(\xi)) \mathbf{w}(x(\xi)) \cdot \partial_t^2 \mathbf{s}(x(\xi), t) \, J(\xi) \, d^3 \xi = \sum_{\alpha=0}^{n} \sum_{\beta=0}^{n} \sum_{\gamma=0}^{n} \omega_{\alpha} \omega_{\beta} \omega_{\gamma} J^{\alpha \beta \gamma} \rho^{\alpha \beta \gamma} \sum_{i=1}^{3} w_i^{\alpha \beta \gamma} s_i^{\alpha \beta \gamma}
\]

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

Need to distinguish:
- local mesh
- global mesh

Efficient routines available from FEM applications

Global equations:

\[ M \ddot{U} = -KU + F \]

Global SEM time-marching is based upon an explicit second-order time scheme
Parallel Implementation

Global mesh partitioning:

Cubed Sphere: $6 \times n^2$ mesh slices

Regional mesh partitioning:

$n \times m$ mesh slices
Basin Code: SPECFEM3D_BASIN

- Freely available for non-commercial use from geodynamics.org
- Manual available at geodynamics.org
- 3D Attenuation
- 3D Anisotropy
- Ocean load
- Topography & bathymetry
- Kinematic ruptures
- Movies
- Models:
  - Harvard 3D Southern California model
  - SOCAL 1D model
  - Homogeneous half-space model
- Adjoint capabilities
Southern California Simulations

n x m mesh slices
Periods $> 2$ s

Komatitsch et al. 2004
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
San Andreas Rupture Scenario

QuickTime™ and a YUV420 codec decompressor are needed to see this picture.
San Andreas Rupture Scenario: Quantitative Seismic Hazard Assessment

Title: San Andreas M_w 7.9
Site: Thousand Oaks
Amplification Factor: 10

Existing Building: Isometric View, Elevations, Plan, and Penthouse Displacement Time Histories

Ground Velocity & Displacement
System Clock: 0.09s

Redesigned Building: Isometric View, Elevations, Plan, and Penthouse Displacement Time Histories

Swami Krishnan
Near Real-Time Applications

- Automated near real-time simulations of all M>3.5 events
- ShakeMovies at [http://www.shakemovie.caltech.edu/](http://www.shakemovie.caltech.edu/
- Soon:
  - CMT 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 Code: SPECFEM3D_GLOBE

- Freely available for non-commercial use from geodynamics.org
- Manual available at geodynamics.org
- 3D Attenuation
- 3D Anisotropy
- Ocean load
- Topography & bathymetry
- Rotation
- Self-gravitation (Cowling approximation)
- Kinematic ruptures
- Movies
- Models:
  - 1D models: isotropic PREM, transversely isotropic PREM, AK135, IASP91, 1066A
  - S20RTS
  - Crust2.0
- Adjoint capabilities
Global Simulations

PREM benchmarks

Cubed sphere mesh

Parallel implementation: 6 $n^2$ mesh slices
SEM Implementation of Attenuation

Anelastic, anisotropic constitutive relationship:

\[ T(t) = \int_{-\infty}^{\infty} \partial_{t} \mathbf{c}(t-t') : \nabla \mathbf{s}(t') \, dt' \]

Equivalent Standard Linear Solid (SLS) formulation:

\[ T = \mathbf{c}^{U} : \nabla \mathbf{s} - \sum_{\ell=1}^{L} \mathbf{R}^{\ell} \]

Memory variable equation:

\[ \partial_{t} \mathbf{R}^{\ell} = -\mathbf{R}^{\ell} / \tau_s^{\ell} + \delta \mathbf{c}^{\ell} : \nabla \mathbf{s} / \tau_s^{\ell} \]

Unrelaxed modulus:

\[ c_{ijkl}^{U} = c_{ijkl}^{R} \left[ 1 - \sum_{\ell=1}^{L} \left( 1 - \tau_{ijkl}^{\ell} / \tau_s^{\ell} \right) \right] \]

Modulus defect:

\[ \delta c_{ijkl}^{\ell} = -c_{ijkl}^{R} \left( 1 - \tau_{ijkl}^{\ell} / \tau_s^{\ell} \right) \]
Effect of Attenuation
Attenuation
Effect of Anisotropy

![Graph showing the effect of anisotropy](image_url)
SEM Implementation of Anisotropy
Antipodal Transverse Record
Vertical PKP
Rotation & Self-Gravitation

Wave equation solved by SPECFEM3D_GLOBE in crust, mantle and inner core:

$$\rho \left( \frac{\partial^2 s}{\partial t^2} + 2\Omega \times \frac{\partial s}{\partial t} \right) = \nabla \cdot T + \nabla(\rho s \cdot g) - \nabla \cdot (\rho s)g + f$$

Wave equation solved by SPECFEM3D_GLOBE in fluid outer core:

$$\frac{\partial^2 s}{\partial t^2} + 2\Omega \times \frac{\partial s}{\partial t} = \nabla(\rho^{-1} \kappa \nabla \cdot s + s \cdot g)$$

SPECFEM3D_GLOBE uses domain decomposition between the fluid outer core and the solid inner core and mantle matching exactly:

- continuity of traction
- continuity of the normal component of displacement
Full Gravity Versus Cowling
SEM Implementation of Gravity

![Graph showing displacement and time with SEM and Modes lines]

- **Displacement (mm)**
- **Time (s)**
- **R1**
- **Modes**
- **SEM**
Effect of Ocean

![Graph showing displacement over time with two lines: one labeled "Modes ocean" and the other labeled "SEM no ocean".]
SEM Implementation of Ocean

Modified boundary condition: \[ p = \rho_w h \hat{n} \cdot \partial_t^2 s \]
3D Mantle Models

S20RTS (Ritsema et al. 1999)
Crustal and Topographic Models

Crust 2.0 (Bassin et al. 2000)  
ETOPO5

[Images of crustal and topographic models]
Great 2004 Sumatra-Andaman Earthquake

Main shock & aftershocks (Harvard)

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 (prototype available at this meeting)

Petascale simulations:
- Global simulations at 1-2 Hz
- New doubling brick (perfect load-balancing)
Adjoint Spectral-Element Simulations (ASEM)
Adjoint Tomography

PDE-constrained waveform tomography:

$$\chi = \frac{1}{2} \sum_r \int_0^T [s(x_r, t) - d(x_r, t)]^2 dt - \int_0^T \int_\Omega \lambda \cdot (\rho \partial_t^2 s - \nabla \cdot T - f) \, d^3 x \, dt$$

Change in the waveform misfit function:

$$\delta \chi = \int_0^T \int_\Omega \sum_r [s(x_r, t) - d(x_r, t)] \delta(x - x_r) \cdot \delta s(x, t) \, d^3 x \, dt$$

$$- \int_0^T \int_\Omega (\delta \rho \lambda \cdot \partial_t^2 s + \nabla \lambda : \delta c \cdot \nabla s - \lambda \cdot \delta f) \, d^3 x \, dt - \int_0^T \int_\Omega [\rho \partial_t^2 \lambda - \nabla \cdot (c \cdot \nabla \lambda)] \cdot \delta s \, d^3 x \, dt$$

$$- \int_\Omega [\rho (\lambda \cdot \partial_t \delta s - \partial_t \lambda \cdot \delta s)]_T \, d^3 x - \int_0^T \int_{\partial \Omega} \hat{n} \cdot (c \cdot \nabla \lambda) \cdot \delta s \, d^2 x \, dt,$$
Adjoint Equations

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

Adjoint equation of motion: \( \rho \partial_t^2 s^\dagger = \nabla \cdot T^\dagger + f^\dagger \)

Adjoint boundary conditions: \( \hat{n} \cdot T^\dagger = 0 \)

Adjoint initial conditions: \( s^\dagger(x, 0) = 0, \quad \partial_t s^\dagger(x, 0) = 0 \)

Adjoint source: \( f^\dagger(x, t) = \sum_{r=1}^{N} [s(x_r, T - t) - d(x_r, T - t)] \delta(x - x_r) \)
The Frechet derivative may be expressed as:

$$\delta \chi = \int_{\Omega} (\delta \rho K_{\rho} + \delta c \cdot \mathbf{K}_c) \, d^3x + \int_0^T \int_{\Omega} \mathbf{s}^\dagger \cdot \delta \mathbf{f} \, d^3x \, dt$$

Density and elastic tensor kernels:

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

$$\mathbf{K}_c(x) = -\int_0^T \nabla \mathbf{s}^\dagger(x, T-t) \nabla \mathbf{s}(x, t) \, dt$$
Isotropic Kernels

For isotropic perturbations we have:

\[ \delta \mathbf{c} \cdot \mathbf{K}_c = \delta \ln \mu K_\mu + \delta \ln \kappa K_\kappa \]

where

\[ K_\mu (\mathbf{x}) = - \int_0^T 2\mu(\mathbf{x}) \mathbf{D}^\dagger (\mathbf{x}, T - t) : \mathbf{D}(\mathbf{x}, t) \, dt \]

and \[ K_\kappa (\mathbf{x}) = - \int_0^T \kappa(\mathbf{x}) [\nabla \cdot \mathbf{s}^\dagger (\mathbf{x}, T - t)] [\nabla \cdot \mathbf{s}(\mathbf{x}, t)] \, dt \]

and we have defined the strain deviators

\[ \mathbf{D} = \frac{1}{2} [\nabla \mathbf{s} + (\nabla \mathbf{s})^T] - \frac{1}{3} (\nabla \cdot \mathbf{s}) \mathbf{I}, \]

\[ \mathbf{D}^\dagger = \frac{1}{2} [\nabla \mathbf{s}^\dagger + (\nabla \mathbf{s}^\dagger)^T] - \frac{1}{3} (\nabla \cdot \mathbf{s}^\dagger) \mathbf{I} \]

In terms of wave speeds:

\[ \delta \ln \rho K_\rho + \delta \ln \mu K_\mu + \delta \ln \kappa K_\kappa = \delta \ln \rho K_\rho' + \delta \ln \beta K_\beta + \delta \ln \alpha K_\alpha \]

where

\[ K_\rho' = K_\rho + K_\kappa + K_\mu \]

\[ K_\beta = 2 \left( K_\mu - \frac{4}{3} \frac{\mu}{\kappa} K_\kappa \right) \]

\[ K_\alpha = 2 \left( \frac{\kappa + \frac{4}{3} \mu}{\kappa} \right) K_\kappa \]
Traveltime Frechet Derivatives

Traveltime tomography:

\[ \chi(m) = \frac{1}{2} \sum_{r=1}^{N} [T_r(m) - T_r^{\text{obs}}]^2 \]

Change in the misfit function:

\[ \delta \chi = \sum_{r=1}^{N} [T_r(m) - T_r^{\text{obs}}] \delta T_r = \int K(\mathbf{x}) \delta \ln m(\mathbf{x}) \, d^3 \mathbf{x} \]

Traveltime anomaly in terms of banana-donut kernel (Dahlen):

\[ \delta T_r = \int K_r(\mathbf{x}) \delta \ln m(\mathbf{x}) \, d^3 \mathbf{x} \]

The kernel \( K \) is a weighted sum of banana-donut kernels \( K_r \):

\[ K(\mathbf{x}) = \sum_{r=1}^{N} [T_r(m) - T_r^{\text{obs}}] K_r(\mathbf{x}) \]
Adjoint Wavefield

Kernel in terms of the *adjoint* wavefield:

\[
K(x) = \sum_{r=1}^{N} [T_r(m) - T_r^{\text{obs}}] K_r(x) = \int_0^T D(x, t) : D^\dagger(x, T - t) \, dt
\]

The adjoint wavefield \( s^\dagger \) is generated by the adjoint source

\[
f^\dagger(x, t) = \sum_{r=1}^{N} [T_r(m) - T_r^{\text{obs}}] \partial_t s(x_r, T - t) \delta(x - x_r)
\]

Notes:
- Need simultaneous access to the regular wavefield at time \( t \) and the adjoint wavefield at time \( T - t \)
- Use of the time-reversed velocity as the source for the adjoint wavefield
Need simultaneous access to $s^\dagger(x, T - t)$ and $s(x, t)$

- During calculation of adjoint field $s^\dagger$, reconstruct $s$ by solving the `backward’ wave equation

Need to store from a previous forward simulation:
- Last snapshot $s(x, T)$
- Wavefield absorb on artificial boundaries

Challenge:
- `Undoing’ attenuation
2D Adjoint Tomography
Construction of a Banana-Donut Kernel

\[ \delta T_r = \int K_r(x) \delta \ln m(x) \, d^3x \]

Tape et al. 2006
Adjoint Tomography

Phase velocity for data

Phase velocity for synthetics

% pert. from 3.50 km/s
Construction of an Event Kernel

\[ K(x) = \int_0^T D(x, t) : D^\dagger(x, T-t) \, dt \]

Event Kernel:
- Sum of weighted banana-donut kernels
- Two simulations per event

\[ K(x) = \sum_{r=1}^{N} [(T_r(m) - T_r^{\text{obs}}) K_r(x)] \]
Construction of the Misfit Kernel

Misfit kernel:

- Sum of all the event kernels
- Two simulations per event
- Gradient of misfit function
Conjugate Gradient Algorithm
Conjugate Gradient Algorithm
Joint Structure-Source Inversion

(a) Misfit, $\chi^2 (m^k)$ ($s^2$)

(b) Structure model $m^{16}$

(c) Error in source parameters (zero)

(d) Misfit, $\chi^2 (m^k)$ ($s^2$)

(e) Structure model $m^{16}$

(f) Error in source parameters

% pert. from 3.50 km/s

Origin time error (s)

Source mislocation (km)
A Southern California example
Southern California Rayleigh Waves

Phase velocity model $m^0$

Phase velocity model $m^1$

Phase velocity model $m^2$

Phase velocity model $m^3$

Phase velocity model $m^6$

Phase velocity for data

25 events
Toward 3D Tomography: SPECFEM3D
Adjoint Capabilities
3D Sensitivity Kernels

Liu & Tromp 2006

SPECFEM3D_BASIN
3D Body-Wave Sensitivity Kernels

September 3, 2002, M=4.2 Yorba Linda
3D Surface-Wave Sensitivity Kernels

Rayleigh (HEC)

Love (HEC)
Our First 3D Event Kernels!

P-wave speed Event Kernels at various depths for Yorba Linda event

S-wave speed Event Kernel for the Yorba Linda Event
Global 3D Body-Wave Sensitivity Kernels

Finite-Frequency effects

20 second P wave

9 second P wave

SPECFEM3D_GLOBE

Qinya Liu
Global 3D Body-Wave Sensitivity Kernels

Pdiff

K_{alpha}

PKP

K_{alpha}

ScS

K_{beta}

SKS

SKS kernel
PKP Kernel

\[ T = 9s, \Delta = 170^\circ \]
Global 3D Transversely Isotropic Kernels

\[ \alpha_h, \beta_h, \eta, \rho, \alpha_v, \beta_v, \eta, \rho \]
Rayleigh wave fundamental mode (100 s - 180 s)

Transversely Isotropic Parameters: A, C, L, N, F
1 $\zeta$: J, K, M
2 $\zeta$: G, B, H
3 $\zeta$: D
4 $\zeta$: E

Anne Sieminski
1D Versus 3D Kernels

(a) 15-mHz Love wave

(b) 5-mHz Love wave

Ying Zhou
Time-Reversal Imaging: Glacial Earthquakes

Vertical component; 118 stations; 55s-90s

Greenland

t = 0 s

Velocity Norm

-5.00e-07 -2.72e-02 5.00e-07

Carene Larmat
Measuring all available Phase & Amplitude Anomalies
Measure all suitable phases
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: $3 \times (\#\text{ earthquakes}) \times (\#\text{ iterations})$
- 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