Toward Exascale Seismic Imaging & Inversion

Jeroen Tromp
Department of Geosciences
Program in Applied & Computational Mathematics
Princeton Institute for Computational Science & Engineering

Ebru Bozdağ, Dimitri Komatitsch, Lion Krischer, Matthieu Lefebvre, Wenjie Lei, Daniel Peter & James Smith
ORNL: Judy Hill, Norbert Podhorszki & David Pugmire
Software

SPECFEM3D_Cartesian

SPECFEM3D_GLOBE
Spectral-Element M

- Hexahedral finite-elements
- Gauss-Lobatto-Legendre quadrature
- Diagonal mass matrix
- Explicit time-marching scheme
Open-Source

- Unstructured meshes
- Load-balanced mesh partitioning
- Fluid-solid coupling
- Anisotropy
- Attenuation
- Adjoint capabilities

www.geodynamics.org
Seismic Imaging
Open-Source

- 3D crust & mantle models
- Topography & bathymetry
- Rotation
- Ellipticity
- Gravitation
- Anisotropy
- Attenuation
- Adjoint capabilities

www.geodynamics.org
Automatically triggered by global earthquakes

1D & 3D synthetics

Public outreach movies

Provided by Incorporated Research Institutions for Seismology (IRIS)

http://global.shakemovie.princeton.edu
Global Seismic Tomography

Assimilation of ~100 million data
High-performance computing
GPU C

Titan

Piz Daint

Top500.org - June 2015
SPECFEM3D
~70,000 lines of code
Fortran90 / C / Cuda

GPU C

SPECFEM3D_GLOBE
~100,000 lines of code
Fortran90 / C / Cuda / OpenCL
Initial implementation: CUDA

- In collaboration with NVIDIA (Peter Messmer & Cyril Zeller)

Current implementation:

- **BOAST**: Bringing Optimization through Automatic Source-to-Source Transformations

- Kernels written in Ruby

- Generates CUDA and OpenCL

- Calls to kernels in C

- Tuned for Fermi and Kepler architectures
Test Drive the World’s Fastest GPU Accelerators

Your GPU-Accelerated Code Just Got Even Faster

Accelerate your code with NVIDIA® Kepler™ GPUs, the world’s fastest accelerators. The Tesla® K40 GPU is our latest and fastest accelerator. With powerful features like GPU Boost and 12 GB of memory, Tesla K40 delivers up to 40% more performance compared to the Tesla K20X.
February 05, 2013
Four Applications Sustain One Petaflop on Blue Waters

July 18, 2012
Researchers Squeeze GPU Performance from 11 Big Science Apps
2015 **K computer simulation > 1.24 PFlops** (shortest period ~ 1.2 s)
on 82,134 nodes, 82,134 MPI ranks w/ 8 OpenMP threads, 657,072 cores

2013 **Blue Waters XE6 simulation > 1 PFlops** (shortest period < 2 s)
on 21,675 XE nodes, 693,600 MPI ranks, 693,600 cores

2008 **Kraken XT5 simulation > 160 TFlops** (shortest period ~1.72 s)
on 149,784 cores

2003 **Earth Simulator simulation > 5 TFlops** (shortest period ~5 s)
on 243 nodes, 1,944 MPI ranks, 1,944 cores
Titan

2013 - 2015 SPECFEM3D_GLOBE allocation: 250M core hours
Next Generation Machine: Summit

ORNL’s Center for Accelerated Application Readiness (CAAR)

Code: SPECFEM
Science Domain: Seismology
Title: Mapping the Earth’s Interior Using Big Data
PI: Jeroen Tromp, Princeton University

OLCF partnership with IBM, NVIDIA & Mellanox
Exascale Challenges
Taming Workflow Issues

1. Request observed data
2. Extract SEED files
3. Convert to ADIOS
4. N observed ADIOS data
5. Run mesher: 1 ADIOS mesh file
6. Run N forward simulations
7. Compute adjoint sources
8. Process data, select windows, make measurements & compute adjoint sources
9. Run N adjoint simulations
10. Sum kernels: 1 ADIOS gradient file
11. Pre-condition & smooth the gradient
12. Determine step length
13. Update model: 1 ADIOS model file
14. N synthetic ADIOS data
15. Convergence?
16. No
17. Iterate
18. Finish
Seismic Tomography Workflow

1. Current data formats are inadequate for fast, parallel I/O; ASDF: an Adaptable Seismic Data Format
   - Convert to ASDF
   - Pre-processing (embarrassingly parallel)

2. Storage & visualization of Earth models: ADIOS with VisIt

3. Workflow stabilization: Kepler, Swift & Pegasus
   - L-BFGS Quasi-Newton

N observed data

- Request observed data
- Extract SEED files
- Process data, select windows, make measurements & compute adjoint sources
- Run N adjoint simulations
- Sum kernels: 1 ADIOS gradient file
- Pre-condition & smooth the gradient
- Determine step length
- Update model: 1 ADIOS model file

N ADIOS data

- N observed ADIOS data
- N synthetic ADIOS data

N selected earthquakes

- Run mesher: 1 ADIOS mesh file
- Run N forward simulations

N ADIOS adjoint source files

- N ADIOS kernel files

Finish

Convergence?

No
Seismic Imaging & Inversion Challenges

- Cheap, abundant sensors
- Massive amounts of data
  - Industry data sets
  - Regional & global seismology data sets
  - Cross-correlation data sets for seismic interferometry
- On HPC systems, I/O is the bottleneck
- Adopt new data formats for fast parallel I/O (e.g., NetCDF, HDF5 & ADIOS)
- Data culling tools to reduce preprocessing time
- A standard for the exchange of Earth models
- Adopt workflow management tools (e.g., Kepler, Pegasus & Swift)
- Tools for data mining, feature extraction, visualization & virtualization (e.g., ParaView, VisIt)
Taming I/O Issues: Adaptable Seismic Data Format
Data in Regional & Global Seismology

[www.iris.edu]

MERMAID/MariScope

[Simons et al, 2006]
Data in Exploration Seismology

3D marine survey can involve 5,000 shots and 50,000 recorders

- Petabytes of data
- SEG-Y is the current standard
- Variable SEG-Y file structure
- SEG-Y programs do not always follow specifications
ASDF: Adaptable Seismic Data Format

- Collaboration involving Princeton University, Munich University (ObsPy) and Oak Ridge National Laboratory
- Increase I/O performance by combining all the time series for a single shot or earthquake into one file
- Take advantage of parallel processing
- Use modern file format as container (HDF5)
- Store provenance inside the file for reproducibility
- Use existing standards when possible (e.g., XML)
- Open wiki for development
Development Team

2010 **BULL Joseph Fourier Prize winner**
for the partial GPU port of SPECFEM3D_GLOBE

2008 **ACM Gordon Bell Finalist**
for SPECFEM3D_GLOBE simulation reaching resolution of 1.72s shortest period

2003 **ACM Gordon Bell Award for Best Performance**
for SPECFEM3D_GLOBE simulation on the Earth Simulator