Wave Propagation Project (WPP): A New Open-Source Tool Supporting Computational Seismology at LLNL

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Computational Seismology at LLNL

Nuclear explosion monitoring

- Modeling can help understand the complex seismic waves emerging from explosions
 - S-wave generation from explosions
 - Non-linear (hydrodynamic) wave propagation
 - Regional surface waves
- Hydroacoustic modeling
 - T-phase reflection off continental margin
- Strong earthquake ground motion
 - Large earthquakes and Performance-Based Design
 - GNEP (Global Nuclear Energy Partnership)
 - YMP (Yucca Mountain Project)
- Earth structure

Test 3D models inferred from various geophysical data

We Are A Multidisciplinary Team

- Applied Mathematicians
 - Anders Petersson, Bjorn Sjogreen, Daniel Appelo
 - Center for Applied Scientific computing
- Computer Scientist
 - Kathleen McCandless
 - Computer Applications and Research Dept.
- Seismologist
 - Arthur Rodgers
- Other experts
 - Geologist, Visualization, Mechanical/Structural Engineers

WPP Methodology



• Elastic wave equation in displacement formulation

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \mathbf{T} + \mathbf{F}(\mathbf{t})$$

- 2nd order system for displacements
 - Explicit time stepping
- Node-centered Cartesian mesh
 - Allows generalizations to embedded boundary methods for nonplanar topography & material discontinuities
 - Stable with free surface boundary condition for all V_P/V_S



WPP: Open source parallel code for 3D seismic wave propagation

- Code is open-source
 - Born parallel (uses mpich
 - But can run on single processor
 - Available for download
 - <u>http://www.llnl.gov/CASC/serpentine/software.html</u>
 - ~50 page user's guide & example input files
- Supported by LLNL institutional funds – LDRD (05-ERD-079)

WPP Current Features (version 1.0)

- 3D P- and S-wave velocity and density models
 - Block, vfile (binary raster) and etree models
 - Handles water regions (μ =0) accurately
- Purely elastic (no attenuation)
 - Handles acoustic case, where μ =0
 - Absorbing (Clayton and Enquist) boundary conditions
 - Free surface boundary conditions
- Models arbitrary number of sources
 - Point moment tensor
 - Point forces
 - Many source-time (moment) functions
- Writes time-series of motion as SAC files
- Writes 2D and 3D images

Building WPP



- You can build a wpp executable on your platform with source code:
 - wpp source code
 - mpich library, MPI-2 standard
 - blitz++ array class library
- To compile:
 - gcc, g++, g77
 - python scripting language
 - scons, python-based software construction tools
- Runs on Linux workstations/clusters & Mac OSX

The WPP Input file

- A (the?) simplest example Lamb's problem
 - Veritcal point force on free surface of homogeneous half-space

RRRR

```
grid x=10000.0 y=10000.0 z=5000.0 h=10
time t=5.
block vp=1732 vs=1000 r=1000
source x=5000 y=5000 z=0 fx=0 fy=0 fz=1e13 type=RickerInt \ Line continuation
   freq=1.0 t0=1.0
                                                  Vertical displacement
sac x=6000 z=0 y=5000 file=s1
                                                  Rec. 1
sac x=7000 z=0 y=5000 file=s2
                                             0.8
                                                  Rec. 2
                                                  Rec. 3
sac x=8000 z=0 y=5000 file=s3
                                             0.6
                                                  Rec. 4
sac x=9000 z=0 y=5000 file=s4
                                             0.4
```

0.2

-0.2

-0.4 0

1

2

Time [s]

3

4

5

Grid and Coordinates

- Can specify x,y,z grid x=10000.0 y=10000.0 z=5000.0 h=40
- Can specify nx,ny,nz grid nx=251 ny=251 nz=126 h=40
- Can specify (approximate!) geographic domain grid x=10e3 y=100e3 z=50e3 h=40 lat=38 lon=-117 az=144



WPP Scaling



Thunder: Linux Cluster, 4096 CPU's

A Few Words on FD Methods





 $\frac{\text{Courant}-\text{Friedrichs}-\text{Levy condition (CFL condition)}}{\text{For stability of solution}}$ $v_{max}^* \delta t/h < C \dots \delta t < C^*h/v_{max}$

So the high frequencies require small h and high velocities require small δt .

So you want high frequency ...

- Doubling the frequency content while maintaining the same resolution implies:
 - h -> h/2, halving the grid spacing
 - requires 2*2*2=8 more grid points in 3D
 - $-\delta t \rightarrow \delta t/2$, halving the time step
 - requires 2* more time steps
- So doubling
 - Once, 8x more memory
 - Twice, 64x
 - Thrice, 512x
- Large velocity differences lead to uneven sampling in terms of grid points/wavelength
 - Mesh refinement improves these problems

Planned Features

Mesh refinement

- Allows much more efficient calculations over fixed grid
 - Solve a problem faster with less memory
 - Higher frequency for the same resource
 - Use 4th order interpolation at mesh refinement boundaries

Attenuation

- Anelastic damping required for realistic simulations
 - Constant Q
- Perfectly Match Layer (PML) boundary conditions
 - Can make domain smaller
- Topography
 - Non-planar free surface
- Embedded boundaries
 - Internal material discontinuities

Mesh Refinement Will Allow Higher Frequency Simulations

Test problem LOH-2: Layer over half-space: unit slip over planar fault



Results agree well:



Refined calculation about 70 times faster and uses 5.5 times less memory

	Grid	Grid points	Processors	CPU [hours]
1 mesh	h = 50	1.24e8	984	0.445 x 984 = 437.9
Refined mesh	h ₁ = 50 h ₂ = 100	2.27e7	32	0.197 x 32 = 6.3

Embedded Boundary Method for Topography

2D slices



3D sphere response to point force

- Cartesian w/ embedded boundary method for stress-free bc
- Includes all cases of topography geometry

Handling 3D Models: EarthVision to Etree





EarthVision Geologic Models

Lithology -> Material properties -> Etree file ->

Wave propagation

The Euclid library utilizes an octant tree like data structure (Etree) which has an efficient addressing scheme allowing for improved flexibility in problem setup.



d's left-lower corner (2, 2) binary form (010, 010) interleave the bits to obtain Morton code 010 010

00 11 00

append the level of *d* 001100_11

3D Model for the San Francisco Bay Area and Northern CA

- USGS developed model of SF region
- We performed simulations of moderate earthquakes were used to validate the model

• We performed large simulations of the 1906 earthquake





SF Bay Area Geology is Complex





Pieces For Earthquake Ground Motion Modeling

Etree Model(s) (USGS or other)



WPP Code



Livermore Computing LINUX parallel machines Thunder - 22 Tflop, 4096 CPU's Zeus - 11 Tflop, 2304 CPU's Thunder GC 50,000 CPU-hours/week Weekend DAT ~ 65,000 CPU-hours



Scaling Up to Big Problems

Seismic modeling requires significant computer resources

 You won't run any significant 1906 simulations on your workstation!



Simulating 300 seconds on 1024 processors on MCR with the WPP code:

freq	Grid size	# grid points	Time step	# time steps	CPU [h]
0.2	250	256e6	2.2e-2	13,600	2
0.4	125	2e9	1.1e-2	27,300	26
0.5	100	4e9	8.7e-3	34,500	67
1.0	50	32e9	4.4e-3	68,200	1;061

MCR: 2304 proc Linux cluster 7.6 Tflop/s on Linpack benchmark



SF1906 Waveform Comparison





Moderate Earthquakes Allow Us To Test the USGS Model

Moderate (M_W 4-5) earthquakes are useful for evaluating velocity model

12 events (circles)15 stations (triangles)

Coverage uneven, many paths along Hayward-Rodgers Creek Fault

Events, BB Stations & Paths



2000/09/03 Yountville Earthquake Broadband (BDSN) Stations BKS - Berkeley WENL - Livermore

red = higher res. domain





Absolute timing and amplitude

2002/05/14 Gilroy Earthquake Broadband (BDSN) Stations



Frequencies = 0.03-0.15 Hz Periods = 7-33 seconds Delays increase with distance ...

Aug. 3 2006, Glen Ellen Earthquake



Snapshot of vertical displacement

Note distortion of wavefronts

San Pablo Bay generates surface wave coda

Waveform Fits for August 3 2006, Glen Ellen



80

80

Green's Functions From Ambient Noise Provide New Constraints on Model

Empirical GF's provide more balanced path coverage of the SF Bay Area.

Vertical-to-vertical component cross-correlations between stations provided by Morgan Moschetti and Mike Ritzwoller (University of Colorado, Boulder).

Part of an NSF-Earthscope project to estimate lithospheric structure across the western US.



Empirical GF's in Four Period Bands



GF's for all available inter-station pairs plotted as record section.

Rayleigh waves are clearly observed, but phase is variable. Noise appears to be variable as well.

We Modeled GF's With WPP and the USGS 3D Model



MCCM



10-14 s







Note: require at least three wavelengths

Phase Delays Between Observed and Modeled GF's Show Systematics



The delays decrease with distance suggesting USGS 3D model is too fast, consistent with earthquake observations. Scatter provides path-specific constraints on structure.

Ground Motions For M_W 7.0 Hayward Fault Scenario



Future Effort - Consider Stochastic Rupture Models

Following Liu, Archuleta and Hartzell (2006) pseudodynamic rupture models generated stochastically with correlated slip, rise time, rupture velocity and rake

Hypocenter at star $M_W = 7.0$ L = 60 km; H = 20 km

Correlation structure of **slip** based on empirical relations on M_0

Remainder from based on relationships between slip, rise time, rupture velocity and rake



Ground Motions For Three Stochastic Rupture Models



These calculations valid to 1 Hz.

M_w 7.0 Hayward Fault SF Bay Bridge Response



Development Plans

- Complete current development
 - Mesh refinement & attenuation (later in 2007)
 - Topography & PML (early 2008)
- Domain Reduction/Representation Theorem
 - Pass motions from non-linear (hydrodynamic) code to WPP (explosion modeling)
 - Introduce plane-wave to 3D structure in WPP
 - Pass motions from WPP to 1D (ω -k, Cagniard) codes
 - Pass motions from WPP to non-FE code (GNEP & YMP)
 - Include soil/structure interaction
 - Please download and use the code!