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## **Making and Propagating Elastic Waves: Overview of the new wave propagation code WPP\***

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### **Abstract**

We are developing a new parallel 3D wave propagation code at LLNL called WPP (Wave Propagation Program). WPP is being designed to incorporate the latest developments in embedded boundary and mesh refinement technology for finite difference methods, as well as having an efficient portable implementation to run on the latest supercomputers at LLNL. We are currently exploring seismic wave applications, including a recent effort to compute ground motions for the 1906 Great San Francisco Earthquake. This paper will briefly describe the wave propagation problem, features of our numerical method to model it, implementation of the wave propagation code, and results from the 1906 Great San Francisco Earthquake simulation.

### **I. Motivation**

Wave propagation phenomena arise in many applications of interest to scientists at Lawrence Livermore National Laboratory (LLNL): evaluation of seismic event scenarios and damage from earthquakes, non-destructive evaluation of materials, underground facility detection, oil and gas exploration, predicting the electro-magnetic fields in accelerators, and acoustic noise generation.<sup>1</sup> The initial target application for our code Wave Propagation Program (WPP) is seismology, and future plans include participation in the research efforts of other application areas at LLNL.

### **II. Background: wave propagation**

When an external force is applied to a solid body, it deforms and changes shape. If it is a perfectly elastic material, once the force is removed it will return back to its original shape. Most solids are characterized by the elastic limit, which is the amount of force that can be applied to a solid without permanently damaging it. Elastic wave propagation is a study of the vibrational motion about the equilibrium position of a solid body.<sup>2</sup>

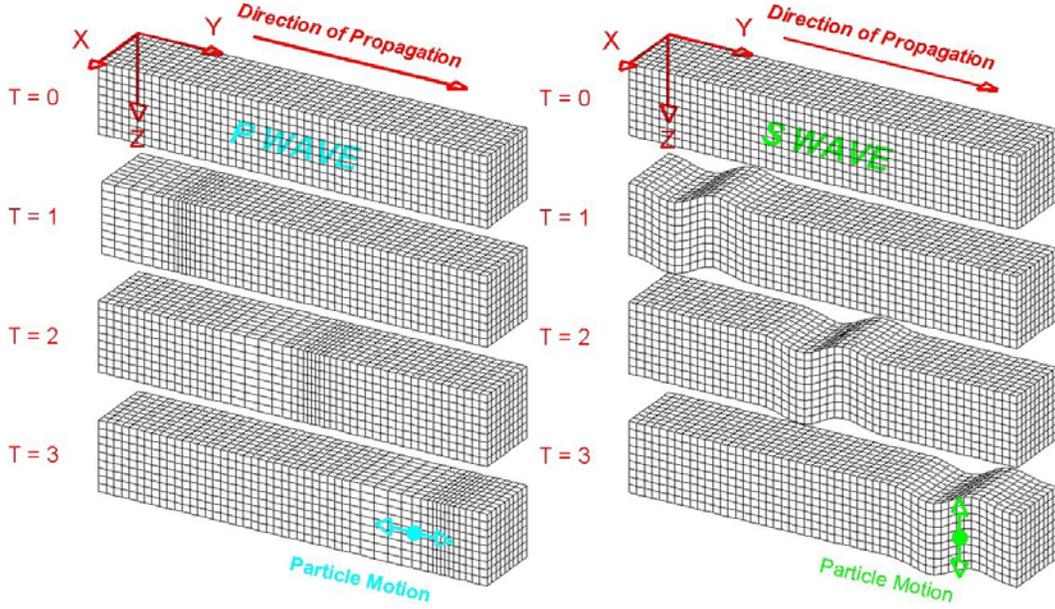
When an external force causes a deformation of a solid, internal forces in the material arise to restore the solid to its equilibrium position. It is these forces, along with the inertia of the material particles themselves, which lead to the wave like motion in the solid.<sup>2</sup>

Waves are produced in several modes depending on the way the particles are forced to oscillate including longitudinal, shear and surface waves. Surface waves cause the most commotion during an earthquake, but seismologists generally only need to evaluate the longitudinal (P-wave) and shear wave (S-wave) response to determine the epicenter and magnitude of an earthquake. For the purposes of our discussion, we will only consider the P- and S-waves.

For a P-wave (P is for primary), the oscillations occur in the direction of wave propagation as noted in Figure 1. They compress and dilatate the material as they propagate and can propagate both in fluids and solids as the energy travels through the structure. These are the first waves to arrive on the scene, but their effect is quite small and not the shaking and rumbling which causes the most damage.<sup>3</sup>

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**Figure 1: P and S wave propagation through a grid presenting an elastic material <sup>4</sup>**

For an S-wave (S is for secondary), the particles oscillate at a right angle to the direction of wave propagation as seen in Figure 1. These waves do not propagate in fluids, because fluids cannot produce a restoring force due to shearing motion.

### III. New numerical method for solving the wave equation

The WPP code includes an accurate and stable second order finite difference numerical kernel which solves the elastic wave equation, in terms of the displacement vector  $\mathbf{u}$ :

$$\rho \frac{\partial^2 \bar{\mathbf{u}}}{\partial t^2} = \nabla(\lambda \nabla \cdot \bar{\mathbf{u}}) + \nabla \cdot (\mu \nabla \bar{\mathbf{u}}) + \nabla \cdot (\mu (\nabla \bar{\mathbf{u}})^T) + \bar{\mathbf{f}}$$

where  $\rho$  is the material density, vector  $\mathbf{f}$  is the external force, and the terms with coefficients  $\mu$  and  $\lambda$  represent the restoring forces due to deformations of the material. Here  $\mu$  and  $\lambda$  are called the Lamé parameters and completely determine the stress tensor, describing the relation between deformation and stresses in the material. In WPP, the source term can be specified by a variety of time forcing functions acting at point locations; values for  $\rho$ ,  $\mu$ ,  $\lambda$  are determined by the material properties. In terms of the material parameters, the P and S velocities are:

$$V_p = \sqrt{\frac{3\mu + \lambda}{\rho}} \quad V_s = \sqrt{\frac{\mu}{\rho}}$$

Early finite difference approximations of the elastic wave equation went unstable for materials where the ratio of  $V_p/V_s$  exceeded about 3. To compensate, simulation codes would typically use alternate methods with staggered grids together with a first-order system formulation involving the velocity and stress tensor components. The new method being developed at LLNL, and implemented into WPP, solves the elastic wave equation directly in second order formulation for the displacements. We use a second order formulation because we plan to include embedded boundaries in the future. For seismic applications, embedded boundaries will allow us to include topography as well as other geometrical features. Nilsson, et al.<sup>5</sup> describes the new finite difference method that avoids the stability problems that plagued earlier discretizations of the elastic wave equation.

### IV. WPP code architecture

WPP is a 3D, massively parallel, finite difference code, architected using C++ with select computational

kernels written in Fortran for efficiency. WPP uses several supporting libraries including:

- The blitz++ array class for its numerical abstractions and encapsulation ([www.oonumerics.org/blitz](http://www.oonumerics.org/blitz))
- The brick of wavelet compression library to compress volumetric data for visualization ([www.cognigraph.org/LibGen](http://www.cognigraph.org/LibGen))
- The central California velocity model query software for querying Etree databases written by the USGS using the Euclid project's Etree library ([www.cs.cmu.edu/~euclid](http://www.cs.cmu.edu/~euclid))
- The tuning analysis utilities (TAU) library for diagnosing and measuring performance ([www.cs.uoregon.edu/research/tau](http://www.cs.uoregon.edu/research/tau))
- The MPI-2 and MPI-IO libraries for the parallel decomposition, communication and IO
- Scons, a Python based software construction build system enabling specification of "Makefiles" as object-based Python configuration files ([www.scons.org](http://www.scons.org))

The user interface consists of simple line identifier, key-value pairs to specify the material properties, time step advance information, and output options. It was purposely designed to be similar to Larsen's E3D code, another wave propagation code at LLNL.<sup>6</sup> While our first target application is seismology, in the future we may incorporate additional interfaces as we pursue other applications.

WPP supports several source time functions for specifying the time dependence of the external forcing, including: Ricker, Brune, Sawtooth, and Triangle.<sup>7</sup> In addition to one or more source terms, users also specify material properties either by using a binary raster file or an Etree database.

There are several output options for validating and visualizing the computation. For visualization, WPP supports 2D image slices of the 3D volume along any coordinate plane, and compressed 3D volumetric data which can be directly visualized using LLNL's parallel visualization tool Visit ([www.llnl.gov/visit](http://www.llnl.gov/visit)). WPP also outputs time series data for the displacement (SAC files), which are used to compare to both synthetic and actual recorded seismograms at particular stations on the surface of the domain.

## V. Verification and Validation

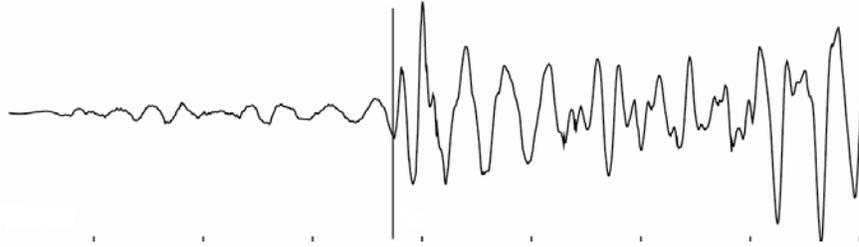
We have employed several means of verifying the WPP code, including: unit tests of infrastructure components, convergence studies of the numerical kernel employing the method of analytical solutions to verify the accuracy<sup>8</sup>, and several analytic and semi analytic tests varying the source options and material properties.

We have now completed enough of the verification to move towards a more rigorous validation of the physical modeling. To validate the code for seismic applications, we have modeled several smaller earthquakes in the San Francisco bay area and most recently the 1906 Great San Francisco Earthquake.

## VI. 1906 Great San Francisco Earthquake

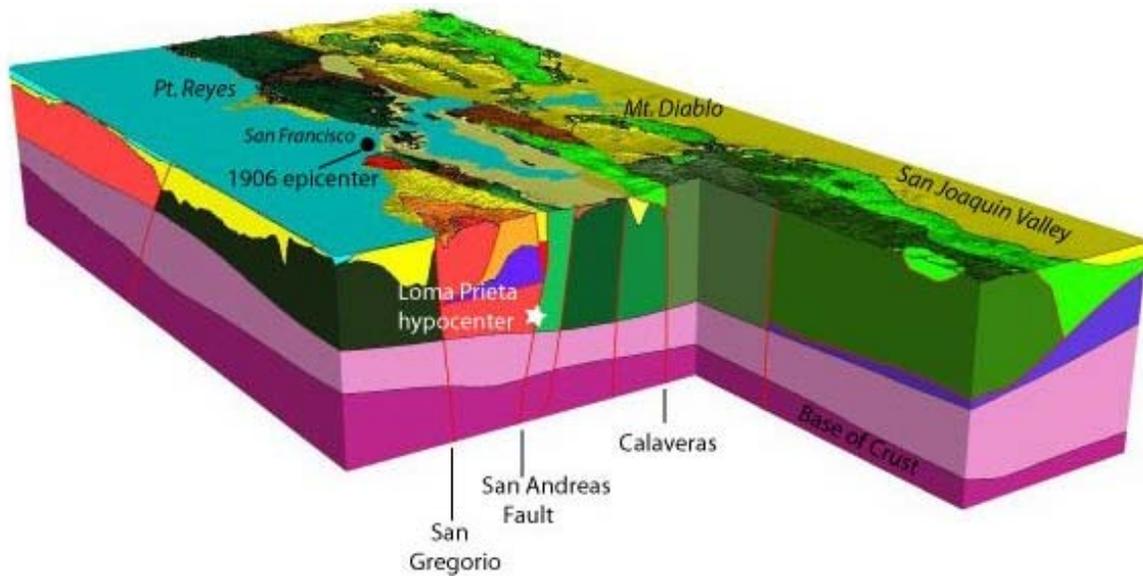
The 1906 San Francisco Earthquake is an important event to study, not just because LLNL is located near the same San Andreas fault which ruptured along 480 km in one of the most significant earthquakes in California's recorded history, but also because there is a great deal of scientific knowledge derived from it.<sup>9</sup> After the 1906 quake, the field of seismology really began to take shape and expand as seismologists studied the displacements and strain in the Earth's crust, leading to a deeper understanding of the nature of the earthquake cycle.<sup>10</sup> There are only a few seismic recordings from this event, including the seismogram from Germany shown in Fig. 2.

We chose to model the 1906 SF earthquake for reasons other than its historical significance. The United States Geological Survey (USGS) coordinated a massive effort for modeling the earthquake during its centennial year. By joining their effort, we gained access to state of the art material models and were then able to further validate our code against other current wave propagation ground motion simulation codes. The goal of the simulation project was to improve our understanding of the three dimensional structure of the earth's crust in northern California, the fault rupture that occurred during the quake, and to simulate the ground motions from the magnitude 7.8 quake.<sup>11</sup>



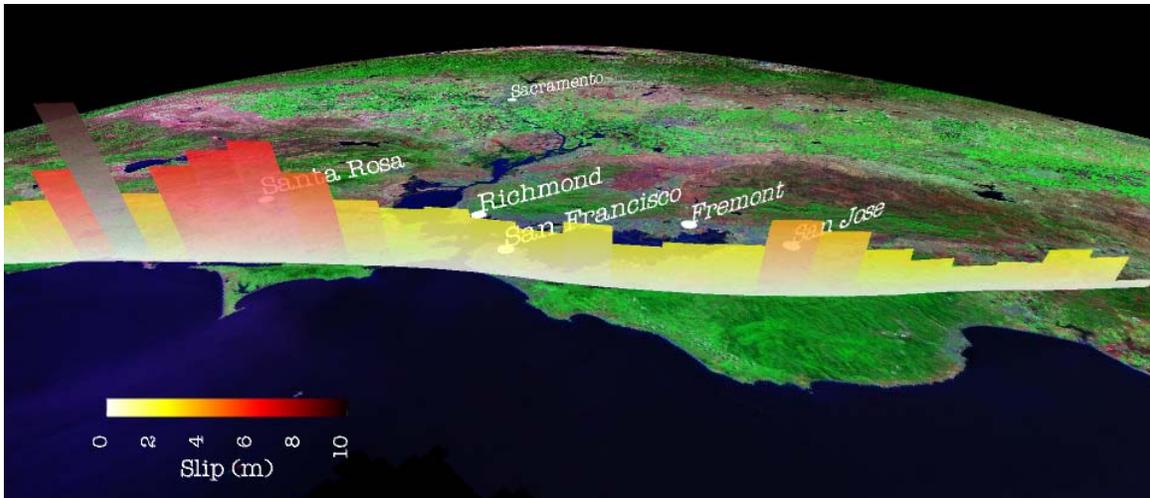
**Figure 2: Seismogram from Germany, ~9000km from the epicenter. Time spans 26 minutes moving from left to right: small wiggles signal the arrival of the first P-waves, larger wiggles represent arrival of the slower S-waves, the instrument went off-scale when the surface waves arrived<sup>12</sup>**

It is important to have an accurate geologic model for the simulation, because waves propagate at different speeds through different materials. To improve our understanding of the earth's crust in northern California, a joint effort between the USGS Earthquake Hazards Program and the USGS National Cooperative Geologic Mapping Program was formed. The new 3D geologic model (Fig. 3), which was developed for the SF bay area, has taken into account over 100 years of surface geologic mapping, decades of research into the seismic properties of rocks, information from boreholes into the Earth's crust, and variations in the Earth's gravity and magnetic fields. Taking this new geologic model, Brocher, et al.<sup>13</sup> then derived empirical elastic wave velocities versus depth for the various rock types in the bay area and produced an Etree database file which contained all the material properties required to setup our calculation.



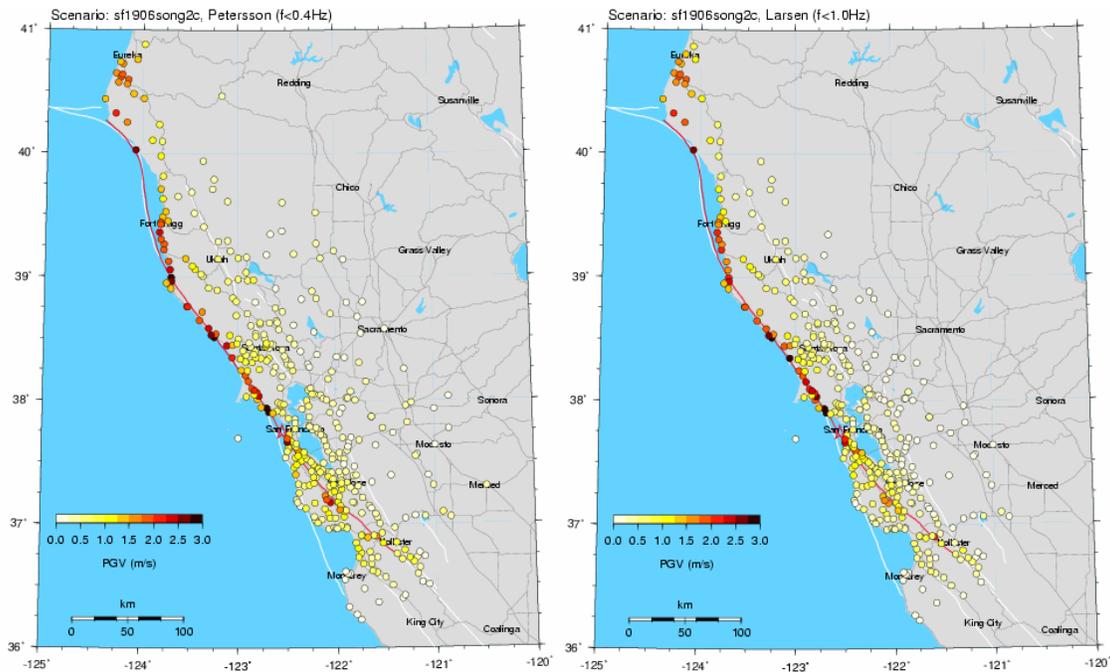
**Figure 3: Geologic block model of the SF bay area provided by the USGS**

To better understand the rupture that occurred during the 1906 quake, Song, et al.<sup>14</sup> devised a new slip and rupture velocity distribution which satisfactorily fit the seismic and geodetic data available. To generate this rupture model, a careful study of the triangulation measurements were made – i.e., measures of actual physical displacements around the SF bay area before and after the earthquake (Fig. 4).



**Figure 4: Bar graph of Song's slip in source model zoomed into SF bay area (B.Aagaard, USGS)**

Using these two new models, we setup WPP to simulate a the 1906 Great San Francisco Earthquake. The simulation ran on 1024 processors on LLNL's MCR Linux machine for 12 hours. We simulated a domain that spanned 550 km x 200 km x 40 km, divided into cubical computational units with side 125 m, yielding 2.26 billion grid points and a total of 27,500 time steps reaching a simulation time of 300 seconds. During the simulation we generated over 2 terabytes of volumetric visualization data, and computed the peak ground velocities (PGV) for over 600 sites in and around the bay area. The PGV values were then compared against other ground motion simulation codes (see Figure 5), and with maps of shaking intensity determined from historical records



**Figure 5: Our PGV results compare well to other codes (WPP (left) and Larsen (right))**

## VII. Conclusion

WPP has now established itself as a contender for modeling seismic activity by delivering results from the 1906 Great San Francisco Earthquake simulation. In the future, we plan to introduce the embedded boundary technology to enable the inclusion of topography. We are also currently implementing local mesh refinement to model larger domains with less memory requirements.

## Acknowledgements

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