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FY08 LDRD Final Report A New Method for Wave Propagation in Elastic Media LDRD Project Tracking Code: 05-ERD-079

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Abstract

The LDRD project "A New Method for Wave Propagation in Elastic Media" developed several improvements to the traditional finite difference technique for seismic wave propagation, including a summation-by-parts discretization which is provably stable for arbitrary heterogeneous materials, an accurate treatment of non-planar topography, local mesh refinement, and stable outflow boundary conditions. This project also implemented these techniques in a parallel open source computer code called WPP, and participated in several seismic modeling efforts to simulate ground motion due to earthquakes in Northern California. This research has been documented in six individual publications which are summarized in this report. Of these publications, four are published refereed journal articles, one is an accepted refereed journal article which has not yet been published, and one is a non-refereed software manual. The report concludes with a discussion of future research directions and exit plan.

1 Introduction

Computational modeling of elastic wave propagation phenomena is essential for the success of many LLNL programs, such as strong ground motion prediction for the Enhanced Test Site Readiness Program, the Yucca Mountain Program, underground explosion monitoring, and undergound facilities characterization. Simulation of elastic wave propagation is also important in non-destructive evaluation, for example to locate material imperfections in National Ignition Facility optics. There are other programs and future LLNL applications that also could benefit from elastic wave simulations, such as sub-surface charaterization for carbon sequestration as well as geothermal energy applications.

Traditionally, linear elastic wave propagation has been simulated using staggered grid finite difference (FD) methods on a Cartesian grid with uniform grid spacing throughout the entire computational domain. This technique is reasonably efficient, both in terms of computational effort and memory requirements and it also produces accurate solutions for box-shaped domains, as long as the boundary conditions can be applied along a flat surface. However, the traditional FD method is difficult to apply to complex geometries whose boundaries are not planar. For free-surface boundaries, an ad-hoc density tapering approach has been proposed to replace a non-planar boundary by a narrow region where the density is artificially tapered to a small value outside, but the accuracy of this approach is not well understood.

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Furthermore, the uniform grid spacing in the traditional method leads to sub-optimal performance when the wave speed varies across the domain, because the spatial grid size is dictated by the smallest wave speed in the domain, while the temporal step size is determined by the spatial grid size divided by the largest wave speed through the Courant stability condition. An additional complication in the traditional FD method is that strong material heterogeneities can de-stabilize the time-stepping, which completely destroys the accuracy of the numerical solution. To stabilize the traditional scheme, some implementations apply an ad-hoc averaging scheme to the material properties before the time integration is started, thus modifying the orginal problem.

This LDRD project has developed several improvements to the traditional FD technique for seismic wave propagation, including a summation-by-parts discretization which is provably stable for arbitrary heterogeneous materials, an accurate treatment of non-planar topography, local mesh refinement, and stable outflow boundary conditions. This project also implemented these techniques in a parallel open source computer code called WPP, and participated in several seismic modeling efforts to simulate ground motion due to earthquakes in Northern California. This research has been documented in six individual publications [59, 9, 65, 66, 69, 4], which are summarized in the following sections. Of these publications, [59, 9, 69, 4] are published refereed journal articles, [65] is an accepted refereed journal article which has not yet been published, and [66] is a non-refereed software manual. This project also produced several conference abstracts, e.g. [64, 70, 68], which are not summarized below because their content is covered in the summaries of [69, 4]. Section 8 concludes this report with a discussion of future research directions and exit plan.

2 Stable difference approximations for the elastic wave equation in second order formulation [59]

As a model for seismic wave propagation, we consider the elastic wave equation for an isotropic inhomogeneous material in a three-dimensional domain Ω,

$$\begin{aligned} \rho\frac{\partial^2 \mathbf{u}}{\partial t^2} &= \nabla\cdot\mathfrak{T} + \mathbf{f}, \quad \boldsymbol{x}\in\Omega,\ t\geq 0, \\ \mathfrak{T} &= \lambda(\nabla\cdot\mathbf{u})\mathbf{I} + \mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right), \end{aligned} \tag{1}$$

subject to initial data

$$\boldsymbol{u}(\boldsymbol{x},0) = \boldsymbol{U}_0(\boldsymbol{x}), \quad \boldsymbol{u}_t(\boldsymbol{x},0) = \boldsymbol{U}_1(\boldsymbol{x}), \quad \boldsymbol{x}\in\Omega.$$

Here $\mathfrak{T}$ is the stress tensor, $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x},t)$ is the displacement vector with Cartesian components $\boldsymbol{u} = (u,v,w)^T$, where $\boldsymbol{x} = (x,y,z)^T$ is the location and t is time. $\mathbf{f}$ is the external (volume) forcing and the material properties are characterized by the density $\rho(\boldsymbol{x}) > 0$, and the Lamé parameters $\lambda(\boldsymbol{x}) > 0$ and $\mu(\boldsymbol{x}) \geq 0$. The degenerate case $\mu = 0$ corresponds to acoustic wave propagation and will not be discussed here. We henceforth assume $\mu(\boldsymbol{x}) > 0$. In seismic applications, the material parameters ρ, μ, and λ often vary on a length scale which is significantly smaller than the wave length of the elastic waves.

Common boundary conditions include a Dirichlet condition for $\boldsymbol{u}$ or a normal stress condition

$$\mathfrak{T}\cdot\hat{\boldsymbol{n}} = \lambda(\nabla\cdot\mathbf{u})\hat{\mathbf{n}} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\cdot\hat{\mathbf{n}} = \mathbf{g}, \tag{2}$$

which prescribes the stresses on a boundary with unit normal $\hat{\mathbf{n}}$. When $\mathbf{g} = \mathbf{0}$, this boundary condition is often called a free surface or stress-free condition. The system (1) admits longitudinal (P, or primary) and transverse (S, or secondary) waves which propagate at phase velocities

$$c_p = \sqrt{(2\mu+\lambda)/\rho}, \quad \text{and} \quad c_s = \sqrt{\mu/\rho},$$

respectively. There can also be surface waves, which travel along a free surface, as well as waves which travel along internal material discontinuities.

Finite difference approximations of the elastodynamic equations in second order formulation have been around for a long time [6]. Early methods, based on explicit centered difference approximations, were initially very successful but suffered from instability problems when a free surface boundary condition was imposed, and the ratio between the P- and S-wave velocities,

$$\nu = \frac{c_p}{c_s}$$

became too large [35] (note that $\nu > \sqrt{2}$). Ilan [34] proposed a remedy which only applied to materials with constant properties normal to the boundary, and an implicit boundary update technique was suggested by Vidale and Clayton [80]. However, no generally applicable, stable, explicit discretization was found for the second order formulation which worked for high values of ν. Due to the instability problems, alternative formulations were explored where the elastic wave equation was rewritten as a larger first order system for the three velocity and six stress components, and discretized on a staggered grid [57]. Most current finite difference methods for seismic wave propagation are based on the staggered grid technique. It is however difficult to handle complex geometry (e.g., topography) with these staggered grid methods, so there has been recent interest in more expensive methods based on unstructured meshes, such as the spectral element technique described by Komatisch and Tromp [42].

In this paper we revisit the problem of devising an explicit finite difference method for the elastic wave equation in second order formulation. Building on our recently developed theory for difference methods for second order hyperbolic systems [48], we develop a technique which is stable for all ratios c_p/c_s. The first step to consider is stress-free boundary conditions on a surface which is aligned with a grid direction. However, our longer term goal is to extend the embedded boundary technique [49, 47, 46] to the elastic wave equation for handling general domains. Since we are interested in seismic applications where the material parameters can vary rapidly on the computational grid, it is desirable to develop a numerical method which satisfies an energy estimate. For a hyperbolic system in second order formulation, the key to an energy estimate is a spatial discretization which is self-adjoint, i.e., corresponds to a symmetric or symmetrizable matrix. In this paper, we present a discretization which makes the spatial approximation second order accurate, self-adjoint, and explicit. The self-adjoint property also implies that the method is conservative.

Seismic events (for example, earthquakes) are often modeled using singular source terms applied at points, along lines, or over surfaces in the three-dimensional domain. To avoid stair-stepping errors, we device a technique to place sources independently of the grid while retaining second order accuracy away from the source. We also study how the temporal smoothness of a point source effects the spatial smoothness of the solution.

In seismic applications it is common to have water (i.e., a lake or an ocean) in parts of the domain. Only compressional P-waves can travel through water and the acoustic wave propagation can be modeled by setting $\mu = 0$ in the elastic wave equation. We have generalized our scheme to handle the mixed elastic/acoustic case, and an early version of this scheme was used to model ground motions during the great 1906 San Francisco earthquake [4].

3 A stable finite difference method for the elastic wave equation on complex geometries with free surfaces [9]

The isotropic elastic wave equation governs the propagation of seismic waves caused by earthquakes and other seismic events. It also governs the propagation of waves in solid material structures and devices, such as gas pipes, wave guides, railroad rails and disc brakes. In the vast majority of wave propagation problems arising in seismology and solid mechanics there are free surfaces, i.e. boundaries with vanishing normal stresses. These free surfaces have, in general, complicated shapes and are rarely flat.

Another feature, characterizing problems arising in these areas, is the strong heterogeneity of the media, in which the problems are posed. For example, on the characteristic length scales of seismological problems, the geological structures of the earth can be described by piecewise smooth functions with jump discontinuities. However, compared to the wavelengths which can be resolved in computations, the material properties vary rapidly. Large spatial contrasts are also found in solid mechanics devices composed of different materials welded together.

The presence of curved free surfaces, together with the typical strong material heterogeneity, makes the design of stable, efficient and accurate numerical methods for the elastic wave equation challenging. Today, many different classes of numerical methods are used for the simulation of elastic waves. Early on, most of the methods were based on finite difference approximations of space and time derivatives of the equations in second order differential form (displacement formulation), see for example [5, 6]. The main problem with these early discretizations were their inability to approximate free surface boundary conditions in a stable and fully explicit manner, see e.g. [35, 34, 80, 75]. The instabilities of these early methods were especially bad for problems with materials with high ratios between the P-wave (C_p) and S-wave (C_s) velocities.

For rectangular domains, a stable and explicit discretization of the free surface boundary conditions is presented in the paper [59] by Nilsson et al. In summary, they introduce a discretization that use boundary-modified difference operators for the mixed derivatives in the governing equations. Nilsson et al. show that the method is second order accurate for problems with smoothly varying material properties and stable under standard CFL constraints, for *arbitrarily* varying material properties.

In this paper we generalize the results of Nilsson et al. to curvilinear coordinate systems, allowing for simulations on non-rectangular domains. Using summation by parts techniques, we show how to construct a corresponding stable discretization of the free surface boundary condition on curvilinear grids. We also prove that the discretization is stable and energy conserving both in semi-discrete and fully discrete form. As for the Cartesian method in [59], the stability and conservation results holds for *arbitrarily varying material properties*. By numerical experiments it is established that the method is second order accurate.

The strengths of the proposed method are its ease of implementation, its (relative to low order unstructured grid methods) efficiency, its geometric flexibility, and, most importantly, its "bullet-proof" stability. The proposed method is second order accurate for materials with smoothly varying properties. However, it has been known for a long time [45] that second order methods are less efficient than higher (4th or more) order methods. When the material properties are only piecewise smooth (as e.g. in seismology), the difference in efficiency between high and low order accurate methods is not as pronounced, see e.g. [19, 27]. For such problems the formal order of accuracy (for both high and low order methods) is reduced to one, but as has been shown in [19], the higher order methods produce more accurate results. Although we believe that the present method is reasonably competitive for strongly heterogeneous materials, it would be of great interest to derive a similarly "bullet-proof" fourth or higher order accurate method.

There are of course many other numerical methods capable of handling general geometries. Two recent finite difference methods are the traction image method for curvilinear grids [85], and the embedded boundary method by Lombard et al. described in [56]. Both these methods use dissipative time-integration schemes while our method is non-dissipative and energy conserving. In comparison to the embedded boundary method of Lombard et al., our method works best for problems where most of the computations take place close to a surface (where an embedded boundary method has large overhead), while the embedded boundary method is more efficient for problems with large volume to surface ratio. Regarding the stability of the methods in [85, 56], no theoretical results are provided in the papers (in the latter paper stability is tested in a long-time simulation).

Other methods include the well-established spectral element method [25, 44, 78], the pseudospectral method [26] and the discontinuous Galerkin method [38]. For homogeneous materials these methods can, in principle, be made arbitrary accurate as the order n of the polynomial approximation increases. This property together with the geometrical flexibility of unstructured methods make spectral element and discontinuous Galerkin methods attractive for simulation of elastic waves in complex geometries. A drawback of spectral elements, pseudospectral methods and discontinuous Galerkin methods is that the maximum time step (when an explicit time stepping method is used) decrease as $1/n$, thus when the order of the polynomial approximation go up the time step becomes smaller. In addition, to fully utilize the high order approximations, the unstructured grids must be of high quality. The construction of such high quality grids, based on quad/hex elements, can be labor intensive and is not easily automated. As for finite difference methods, the formal order of these methods will be reduced to first order if material discontinuities are not aligned with element boundaries, see [21, 27].

It would be of great interest to develop a higher (4th or more) order self-adjoint discretization of the elastic wave equation. The possibilities of using summation by parts techniques to extend the present method to such a high order discretization is currently under investigation.

The curvilinear formulation of the elastic wave equation contains many more terms than the Cartesian formulation, making the present method more expensive than a method on a Cartesian grid. A way to increase the efficiency is to use a hybrid approach where the equations close to curved boundaries are solved on body fitted curvilinear grids while the equations in the interior are solved on Cartesian grids.

4 An energy absorbing far-field boundary condition for the elastic wave equation [65]

In regional simulations of seismic wave propagation, the extent of the computational domain must be limited to make the problem computationally tractable. Some form of far-field absorbing boundary condition needs to be imposed where the computational domain is truncated such that waves can propagate out of the computational domain without being reflected due to the artificial boundary. For a material with constant wave speeds, and a domain with a single planar boundary, it is possible to derive a boundary condition which allows all waves to exit the domain without any artificial reflection. However, such a boundary condition involves a pseudo-differential operator and is therefore non-local in space and unsuitable for numerical computations.

One of the first practically useful far-field boundary condition for the elastic wave equation was derived by Clayton and Engquist [20], where the authors presented a hierarchy of boundary conditions by approximating the exact pseudo-differential operator to increasing order of accuracy in the angle of incidence. (All boundary conditions in the hierarchy are perfectly non-reflecting for waves of normal incidence.) A slightly different approach was suggested by Higdon in [33], where the boundary condition is obtained by component wise application of a scalar non-reflecting boundary condition. Higdon also derived a hierarchy of boundary conditions with increasingly absorbing properties. In the case of a scalar wave equation, the Higdon and Clayton-Engquist boundary conditions are equivalent. First order Clayton-Engquist conditions have been used extensively in large scale computations of seismic wave propagation, see [22]. However, instabilities have been reported for the third order condition for some values of the wave speeds [58].

The perfectly matched layer (PML) is a more modern boundary condition which was originally developed for Maxwell's equations by Berenger [10] and has been studied in numerous subsequent papers, see for example [72] and the references therein. Perfectly matched layers have superior non-reflecting properties compared to low order Clayton-Engquist or Higdon conditions, but they are also more complicated to implement and require correct tuning of the size and strength of the absorbing layer. PMLs for the elastic wave equation were developed in [43, 8]. Unfortunately, the PML boundary condition can become unstable when it interacts with surface waves along material discontinuities [73].

Higdon [32] performed a normal-mode stability analysis for a class of discretized non-reflecting boundary conditions for the elastic wave equation, which includes the first order Clayton-Engquist condition as a special case. In particular, Higdon showed stability for a first order accurate discretization of the Clayton-Engquist condition. Note that the normal mode analysis is only valid for half-space problems with homogeneous materials and does not take corners or edges into account. Furthermore, the stability concept in the normal mode analysis only guarentees the solution to be bounded independently of the grid size for a fixed, finite, interval in time. It does not exclude the possibility that the solution may grow as the time interval is made longer. We remark that the discretization given in the original paper by Clayton and Engquist [20] is second order accurate and is therefore not covered by Higdon's analysis.

In seismic simulations, the material properties are not known very precisely and there are often uncertainties associated with the source terms modeling the spatial distribution and temporal variation of the slip during an earthquake. We therefore believe that in many realistic seismic simulations, adequate accuracy can be obtained by using low order outflow boundary conditions as long as they are stable. Often the material properties vary rapidly on the computational grid and this can cause stability problems for the Clayton-Engquist conditions, which are derived under the assumption of constant coefficients. Additonal stability problems occur for large ratios between the compressional and shear wave speeds: c_p/c_s.

In this paper we propose an alternative non-reflecting boundary condition based on summation by part operators, which is stable for all values of c_p/c_s. Since the stability follows from an energy estimate for the fully discretized problem, the propsed boundary condition is stable in realistic situations with strongly variable coefficients. Furthermore, our theory shows how to discretize the non-reflecting boundary condition at edges and corners of a logically cubical three-dimensional domain and also extends to the case where free surface boundary conditions are imposed on some sides of the computational domain.

When implementing a production code for use by application experts, who seldomly have any interest in tuning numerical stabilizing parameters, we believe it is extremely valuable to use techniques where there is a mathematical proof of the stability of the underlying numerical method. Hence, the main advantage of the method proposed in this article lies in the stability proof for heterogeneous materials including corners and edges. Furthermore, the stability follows from an energy estimate which shows that the energy is bounded as time goes to infinity on a fixed grid.

While the Clayton-Engquist condition works well in most practical situations, there are cases where it makes the simulation go unstable. The instability appears to occur when the outflow boundary cuts through a heterogeneous material with high c_p/c_s ratio. As a motivating example, consider the synthetic seismograms in [65] (Figure 1) from two simulations of the magnitude 5.4 earthquake which occured in Alum Rock, CA, in October of 2007. Both calculations were performed using the WPP code [66] and a modified version of the material model from the U.S. Geological Survey [15]. The first, displayed in blue, uses the first order Clayton-Engquist non-reflecting boundary condition. This computation is unstable and the solution starts growing exponentially after time ≈ 60 seconds. The second computation, displayed in red, uses the stable energy absorbing non-reflecting boundary condition proposed in this paper. In this case the solution remains bounded for long times.

The main advantage of the proposed non-reflecting boundary condition is its guarenteed stability property for strongly heterogeneous materials. The proposed boundary condition is first order accurate in the incident wave angle, and it would be desirable to generalize the energy absorbing principle to derive an outflow boundary condition with improved transmission properties for larger angles of incidence.

5 User's guide to the Wave Propagation Program (WPP) version 1.2 [66]

WPP is a parallel computer program for simulating time-dependent elastic and viscoelastic wave propagation, with some provisions for acoustic wave propagation. *WPP* solves the governing equations in displacement formulation using a node-based finite difference approach on a Cartesian grid, see [59] for details. *WPP* implements substantial capabilities for 3-D seismic modeling, with a free surface condition on the top boundary, non-reflective far-field boundary conditions on the other boundaries, (many) point force and point moment tensor source terms with many time dependencies, fully 3-D material model specification, output of synthetic seismograms in the *SAC* [28] format, output of *GMT* [84] scripts for laying out simulation information on a map, and output of 2-D slices of (derived quantites of) the solution field as well as the material model.

To allow the user to locally refine the computational mesh in areas where finer resolution is needed, version 1.2 of *WPP* implements local mesh refinement. The resolution of the solution is often charaterized in terms of the number of grid points per wave length. For a signal of frequency f, the wave length is V_s/f, where V_s is the wave speed in the material. Hence the grid size needs to be small where the wave speed is small, and vice versa. A locally refined mesh can therefore be used to reduce the variations in resolution in terms of grid points per wave length, which otherwise occur when a mesh with constant grid spacing discretizes a heterogeneous material model. For seismic applications, the savings in computational effort can be significant, since the wave speed often is an order of magnitude smaller in sedimentary basins near the surface than in the mantle below the MoHo.

In seismic applications, viscoelastic behavior is often significant for modeling the dissipative nature of realistic materials, especially for higher frequencies. Version 1.2 of *WPP* implements the eight term viscoelastic model described in [54], and models quality factors Q_p and Q_s for the attenuation of P- and S-waves. These quality factors can vary from grid point to grid point over the computational domain and are read in the same way as the elastic properties of the material model.

The tests/examples subdirectory of the *WPP* source distribution contains several examples and validation tests, see [66] for a detailed discussion.

6 Broadband waveform modeling of moderate earthquakes in the San Francisco bay area and preliminary assessment of the USGS 3D seismic velocity model [69]

Strong ground motions are the result of the combined effects of the earthquake source and interaction of the seismic wavefield with complex three-dimensional geologic structure. An accurate three-dimensional (3D) seismic velocity model is required to predict ground motion for scenario earthquakes and to account for propagation and site effects when imaging earthquake ruptures from strong motion waveforms. Advances in numerical methods and computational power are facilitating simulations of large (MW > 6.0) scenario earthquakes for the purposes of strong ground motion prediction. Pioneering studies (e.g. Vidale and Helmberger [79], Kawase and Aki [39], Dreger and Helmberger [23], Schrivner and Helmberger [71]) demonstrated that two-dimensional elastic finite difference modeling can be used to predict ground motions in the presence of strong heterogeneity, including basin edge effects. Several more recent studies reveal the power of simulations to predict ground motions in complex three-dimensional (3D) structure of southern California (e.g., Olsen et al. [60, 61, 62], Wald and Graves [81], Olsen [63], Komatitsch et al. [41]) and the San Francisco Bay Area (Graves [29], Stidham et al. [76]). While advances in methods and computational power facilitate the simulation of ground motions, the accuracy of the resulting predictions are limited by the accuracy of the 3D earth model and ignorance of detailed earthquake rupture kinematics.

This study focuses on ground motion prediction in the San Francisco Bay area using a new 3D earth model developed by the United States Geological Survey (USGS) Earthquake Hazards Program. The model (USGS [24], Brocher et al. [15], Jachens et al. [36], hereafter referred to as the USGS 3D model) has been used for an investigation of the 1906 San Francisco earthquake at its centenary (Aagaard [1], Petersson et al. [64], Rodgers et al. [70, 68], Larsen et al. [50], Graves [30], Aagaard et al. [4]) as well as the 1989 Loma Prieta earthquake (Aagaard et al. [2]). It is based on detailed geologic and geophysical mapping of the region and rules for converting lithologic properties to density, seismic compressional and shear wave speeds and attenuation (Brocher [17, 16]) and represents an improvement in detail over a previous model reported by Stidham et al. [76]. We compared ground motions observed from moderate earthquakes (MW = 4.0-5.1) to those computed with an elastic finite difference computer code using the 3D model. These events have well determined locations, depths and focal mechanisms and should be well represented as simple point sources for the periods considered. These factors help to eliminate the variability in ground motion due to earthquake source complexity and isolate the effects of three-dimensional structure. We focus on modeling the frequency band 0.03-0.25 Hz in order to determine if the 3D model reproduces the main features of seismograms. While these frequencies are lower than is typically calculated in scenario earthquake simulations, the goal is to assess the model in this frequency band before increasing the bandwidth and hoping to resolve more subtle differences possibly due to smaller scale structure. For the highest frequencies we considered (0.2-0.25 Hz), the wavelengths of surface waves within the Bay Area (shear velocities 1-3 km/s) are about 4-15 km, allowing for sampling of features on the same scale-length. Results indicate that the USGS 3D model predicts many important features of the observed broadband seismograms. However, the model can be improved by reducing the shear velocities in order to predict the observed surface wave arrival times. In this paper we describe the data, 3D model and simulation algorithm used in the analysis, results are presented and summarized, and we conclude with a discussion of the implications of this analysis for improved modeling of ground motions in the region.

7 Ground-motion modeling of the 1906 San Francisco earthquake, Part II: Ground-motion estimates for the 1906 earthquake and scenario events [4]

The 18 April 1906 magnitude 7.9 San Francisco earthquake ruptured the San Andreas fault for nearly 500 km with a mean slip of 4-5 m (Thatcher et al. [77], Song et al.[74]). The occurrence and subsequent scientific investigation of this earthquake marked the birth of modern earthquake science in the United States. For the first time, a large earthquake and its effects were systematically documented, and the shaking was properly interpreted as resulting from slip on an active fault and as part of a recurring tectonic process of strain accumulation and release (Lawson [52]). To commemorate the centennial of the 1906 earthquake, a two year collaborative effort was launched to recreate the strong ground motion produced by this event and the 1989 magnitude 6.9 Loma Prieta earthquake. By utilizing modern computational methods and taking advantage of new data and constraints, we are able to characterize both the amplitude and duration of shaking in 1906 across central and northern California. Aagaard et al. [2] discusses our efforts to validate the 3D geologic and seismic velocities models used in this study with data from the 1989 Loma Prieta earthquake.

The 1906 earthquake was felt throughout California, in southern Oregon, and as far east as central Nevada. It also wrote the first useful strong-motion record, a three component seismograph from a duplex pendulum recording at Mount Hamilton, about 90 km from the epicenter. More than 600 detailed reports of shaking intensity and damage were compiled in the two-volume landmark document, The Report of the State Earthquake Investigation Commission. Volume I was edited by A. Lawson and was published in 1908 (Lawson [52]), and volume II was edited by H. F. Reid and was published in 1910 (Reid [67]). Hereafter, we will refer to the report using the volume number as appropriate.

Based on these data, the commission investigators concluded that, in general, shaking intensity diminished with distance from the fault. They also recognized the importance of site effects, noting that the "amount of damage produced by the earthquake ...depended chiefly on the geological character of the ground" (H. O. Wood, vol. I, p. 241), and, in particular, commented that "areas that suffered most severely were those upon filled ground" (vol. I, p. 253). H. F. Reid applied elasticity theory to extend the application of F. J. Rogers' vibrating sand box experiments (vol. I, pp. 326-335). Reid properly concluded that (1) the response of basins depended on their size relative to the wavelength of the seismic waves, (2) in large basins, internal reflections could result in increased amplification (vol. II, p. 54), and (3) variations in amplitude within and between large basins were related to "differences in the character and depth of the alluvium" (vol. II, p. 56). Our groundmotion modeling results demonstrate all of these effects, indicating the robustness of these early observations, modeling, and interpretations.

Reid (vol. II, p. 11) used four local timing observations of ground shaking and an assumed crustal velocity to compute a least-squares hypocenter located near Olema, the site of the largest recorded surface displacement. Bolt [12] showed that a hypocenter 50 km to the southwest, coincident with the 22 March 1957 magnitude 5.3 Daly City earthquake, could satisfy both the local observations as well as teleseismic P and S recordings, although he could not preclude Reid's Olema location. Boore [13] interpreted phases in the sole strong-motion recording at Mt. Hamilton to constrain the epicentral location to lie somewhere offshore from San Francisco and likely much farther south than the previously presumed epicenter near Olema. More recently, Lomax [55] reevaluated the arrival-time observations and applied modern event-location techniques to determine a maximum-likelihood hypocenter of 37.78 N, 122.51 W at a depth of around 12 km. Wald et al. [82] combined the preserved teleseismic records with empirical Greens functions to construct a finite-source model for the 1906 earthquake; however, the slip distribution differs markedly from the one Thatcher et al. [77] developed based on triangulation surveys. A new source model (Song et al. [74]) that combines both datasets resolves many of the discrepancies between the two.

In the last few decades several studies have attempted to characterize the ground motions in the 1906 earthquake. Borcherdt and Gibbs [14] combined modern site-response data with intensity mapping in Lawson [52] to estimate the variability in response for various geologic units and quantify the dependencies of the 1906 shaking intensities with distance from the rupture and site conditions. Anooshehpoor et al. [7] calculated a lower bound for the peak acceleration of about 1g at frequencies less than 2 Hz at the Point Reyes train station based, in part, on the conductors description of the ground motions that overturned the train, as documented in Lawson [52]. Ward [83] combined a quasi-static model of the 1906 earthquake and modified whole-space Greens functions with the geodetic slip model from Thatcher et al. [77] to compute a very rough estimate of the variability of shaking. The simulated ground motions were limited to a few stations and included directivity, but not 2D or 3D Earth structure. As a result, these simulations fail to capture the dynamics (i.e., rise time) of the source. None of these studies provide a regional perspective of the spatial variations in the intensity, duration, and character of the ground motions.

Boatwright and Bundock [11] constructed a Shake-Map for the 1906 earthquake by carefully examining more than 600 reports of shaking and damage compiled in Lawson [52] and reinterpreting them in terms of the modern Modified Mercalli Intensity (MMI) scale. This Shake-Map provides a comprehensive picture of the shaking intensities and serves as the primary independent constraint for our ground-motion simulations. Shaking intensities, such as those in a Shake-Map, however, lack information about the duration and character of the ground motion. Our ground-motion simulations utilize up-to-date information on the 3D crustal structure and our experience in generating realistic kinematic source models to produce ground-motion time histories over the San Francisco Bay Area and the surrounding region extending more than 500 km along the San Andreas fault. We also investigate the variability in ground motions for similarly sized events on this portion of the San Andreas fault due to changes in the hypocenter, rupture directivity, and differences in the distribution of slip. Instead of focusing on a particular geologic structure (e.g., one of the sedimentary basins) or geographic location (e.g., San Francisco), we examine Shake-Maps displaying the spatial distributions of shaking over the San Francisco Bay Area and entire rupture extent as well as velocity time histories at a number of sites.We also estimate the relative impact each scenario would have on todays infrastructure in the context of the analysis by Kircher et al. [40], who calculated the expected impact of a repeat of the 1906 earthquake.

For our ground-motion modeling of the 1906 earthquake, we use the Song et al. [74] source model, which uses both teleseismic records and triangulation surveys to constrain the slip distribution, and teleseismic records to constrain the rupture speed. Even with these combined datasets, many important details and source parameters are missing from the rupture model. We fill in the missing details, such as short-length scale variations in slip and rise time, based on empirical observations and parameter searches in which we attempt to fit the Boatwright and Bundock [11] shaking intensities. Given the large uncertainty in the source parameters, we employed five different ground-motion modeling groups to search the parameter space and constrain the missing details, yielding our preferred source model for generating strong ground motions from the 1906 earthquake.

The five ground-motion modeling groups include (1) Aagaard, (2) Graves, (3) Harmsen et al. (consisting of Harmsen and Hartzell), (4) Larsen et al. (consisting of Larsen, Dreger, and Dolenc), and (5) Petersson et al. (consisting of Petersson, Rodgers, McCandless, Nilsson, and Sjögreen). Each group employs a different modeling code to solve the elastic-wave equation. Four of these codes (Larsen and Schultz [51], Graves [31], Aagaard et al. [3], Liu and Archuleta [53]) were used in our efforts to model the Loma Prieta earthquake (Aagaard et al. [2]). The other one, called the wave propagation project (WPP), used by Petersson et al. and developed by Nilsson et al. [59], relies on node-centered (nonstaggered) finite differences with a displacement formulation to discretize the elastic-wave equation.

Simulating wave propagation through the 3D structure in the volume surrounding the entire rupture length of the 1906 earthquake at periods of 1-2 seconds and longer requires extensive computational resources. As a result, Aagaard and Harmsen et al. model only portions of the rupture, whereas the domains for Graves, Larsen et al., and Petersson et al. cover the entire rupture. Many of the features and parameters match those used in modeling the Loma Prieta earthquake, including the use of a recently developed 3D geologic model (Jachens et al. [37]) and the seismic velocity model, U.S. Geological Survey Bay Area Velocity Model 05.1.0 (USGS 05.1.0) (Brocher [15, 18]). Some notable exceptions include the bounding boxes of the domains of the Graves and Larsen et al. modeling groups and the inclusion of topography and attenuation in the Larsen et al. simulations.

Because the 3D geologic and seismic velocity models include topography, the ground-motion simulations must account for it when querying the velocity model for material properties. The finite-difference wave-propagation codes that do not include topography directly either bulldoze the surface of the Earth by stripping away any material above some elevation and filling in voids below this elevation with some generic material, or they squash the surface of the Earth by deforming the near-surface material in the vertical direction so that the free surface is flat and aligned at some elevation. The bulldozing method tends to remove shallow, low-velocity layers but retains the geometry of the geologic units, whereas squashing includes shallow, low-velocity layers but tends to distort the geometry of the geologic units. Graves and Petersson et al. employ variations of the bulldozing approach: Petersson et al. include water while Graves fills areas below sea level with a generic sediment (Vp: 2200 m/sec, Vs: 760 m/sec, density: 2100 kg/m^3). Harmsen et al. employ the squashing approach. Our simulations of the Loma Prieta earthquake (Aagaard et al. [2]) indicate that including topography is the preferred approach, followed by squashing and then bulldozing. Bulldozing often removes shallow, low-velocity layers that are important for capturing basin effects.

Another difference with respect to the Loma Prieta simulations is that in this study, the Graves, Larsen et al., and Petersson et al. domains extend well beyond the boundaries of the detailed portion of the velocity model and into the coarser resolution regional portion. While there is a smooth transition from the detailed portion to the regional portion, the regional portion contains only the major geologic units (mantle, mafic lower crust, major Mesozoic units, and a representation of the Great Valley fill). As a result, we expect to capture much less detail in the spatial distribution of shaking and the waveforms in the areas of the simulation domains that lie in the regional portion of the velocity model.

8 Exit plan and future research directions

After the conclusion of the LDRD project in March of 2008, we recieved ASC funding to port WPP to the BG/L system at LLNL. After modifying the coding to run more efficiently on the IBM system, we performed our largest to date seismic simulation using about 26 Billion grid points (78 Billion degrees of freedom) integrated about 41,000 time steps on 32,768 cores on BG/L. We have thereafter also ported WPP to the BG/P system at the Argonne leadership computing facility (ALCF).

Our research project was focused on solving the linear elastic wave equation, where the rupture model can be described by source terms. The underlying assumptions when deriving the linear elastic wave equation are that the deformations are small relative to the wave length of the elastic waves, and that the material stress levels are small enough for the linear Hook's law to be valid. Unfortunately, both of these assumptions are invalid near an explosion. We are therefore currently developing a coupling technique between the GEODYN code, which solves the non-linear near-field problem, and WPP to propagate the seismic signal to regional distances. This work is currently supported by NA-22.

The implementation of mesh refinement in WPP version 1.2 allowed for very general placement of refinement patches to allow the grid size to closely follow the variations of the velocity structure in the material model. But in a practical three-dimensional model, it has turned out to be cumbersome to precisely specify the location of these patches. Instead, the mesh refinement is often only performed in the vertical direction such that the finest grid is near the top surface, and the grid is coarsened three or four times towards the bottom of the computational domain, where less resolution is needed. Based on the actual usage of mesh refinement in WPP, next version of the code will only allow vertical refinements, which will allow for significant simplifications in the software. Furthermore, the original approach for coupling the solution across mesh refinement boundaries used high order interpolation to preserve the overall accuracy, together with an artificial stabilizing term to keep the solution smooth. Unfortunately, this coupling approach can lead to instabilities if the mesh refinement boundary is too close to significant material heterogeneities. Using ASC funding, an improved mesh refinement coupling strategy is currently under development which satisfies energy conservation, and therefore is stable without artificial dissipation.

This project was focused on solving the forward problem, i.e., predicting ground motions given the material properties and rupture model (seismic forcing terms). Recently, there has been a growing interest in the inverse problem, which aims at improving the material and/or rupture model, based on the discrepancies between simulated and measured ground motions. Since elastic wave propagation is governed by a self-adjoint partial differential equation, a solver for the forward problem can be used as a building block for the inverse problem, where the material and rupture model are iteratively modified based on the interaction between the solutions of the forward and adjoint problems. There are several important applications of this technique including material characterization, underground facitilites detection, determination of source mechanism for underground explosion monitoring, as well as oil and gas exploration. We are currently crafting proposals to support the development of inverse methods applied to these problems.

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