Advanced Scientific Computing Research
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Serpentine – Embedded boundary methods for wave propagation in complex geometries

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Summary

This project advances computational science by developing and analyzing numerical methods for wave propagation in complex materials and geometries. We explore methods which discretize hyperbolic systems of partial differential equations in second order differential form by using efficient finite difference methods on regular Cartesian grids combined with embedded boundary technology to handle complex geometrical shapes.

Simulation of wave propagation phenomena is essential for the success of many DOE programs such as strong ground motion prediction for the Enhanced Test Site Readiness Program, the Yucca Mountain Program, the Global Nuclear Energy Partnership, underground explosion monitoring and underground facilities characterization. Simulating wave propagation is also important in non-destructive testing, with application to locating imperfections in National Ignition Facility optics. There are also future applications that could benefit from elastic wave simulations, such as sub-surface characterization for carbon sequestration via seismic reflection and geothermal energy applications.

LLNL researchers have recently developed new numerical simulation capabilities for seismic wave propagation modeled by the three-dimensional elastic wave equation in domains with complex material properties and subject to stress-free boundary conditions. The second order formulation of the elastic wave equation was discretized using a summation-by-parts technique which guarantees a robust numerical scheme that is stable even when the material properties vary arbitrarily from point to point in the computational mesh. The new technique improves on previous numerical schemes by being second order accurate, energy conserving, and stable for all ratios between the longitudinal and transverse wave speeds.

To allow realistic seismic simulations that include water (oceans or lakes), we generalized the basic elastic scheme to handle acoustic regions that have zero rigidity and no shear waves. The slip along an earthquake fault surface (such as the San Andreas fault in California), is commonly modeled by distributing force double-couples along the fault surface. No forces are applied before an earthquake starts. During the earthquake, the forces are gradually ramped up in time starting at the hypocenter of the quake. The start time of each double couple is determined by the distance from the hypocenter and the rupture velocity of the slip. The duration of the slip is determined by empirical relations derived from measurements, but the magnitude of each double-couple is proportional to the

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slip at each point along the fault. One important improvement over previous methods is that we developed an accurate spatial discretization of the force double-couple which allows them to be placed anywhere in the domain, independently of where the grid points are located. Hence, using the new discretization, we can respect the three-dimensional shape of the fault surface which allows more accurate simulations of large earthquakes which generally cause the fault to slip over an extended area. This technique was used to simulate the 475 km (300 miles) long rupture on the San Andreas fault modeling the great San Francisco earthquake in 1906. The calculations, which were run on up to 1024 processors on a LLNL Linux cluster, produced state-of-the-art predictions of the ground motion using up to 4 Billion grid points covering all of Northern California, see Figure 1. Results from our simulations were presented at the Seismological Society of America meeting commemorating the centennial of the great San Francisco earthquake which occurred on April 18th, 1906.

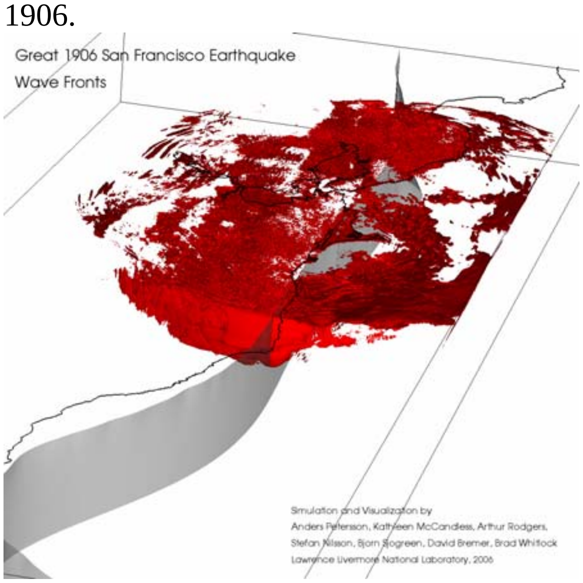

Figure 1: Wave fronts during the 1906 San Francisco earthquake. The San Andreas fault surface is shown in grey and the coast line of northern California in black.

During next year we plan to extend our embedded boundary capability (see Figure 2) to satisfy stress-free boundary conditions on complex geometrical shapes in the elastic wave equation, first in 2D and later in 3D. The embedded boundary approach will allow modeling of topography in seismology, which is important to handle seismic waves of shorter wave length. Shorter wave lengths are important to accurately predict the safety of structures such as buildings, bridges, dams and levees. The embedded boundary technique will also enable the study of how elastic waves are modified by internal voids and defects in a material, which is important to non-destructive evaluation techniques with applications to detecting imperfections in National Ignition Facility (NIF) optics.

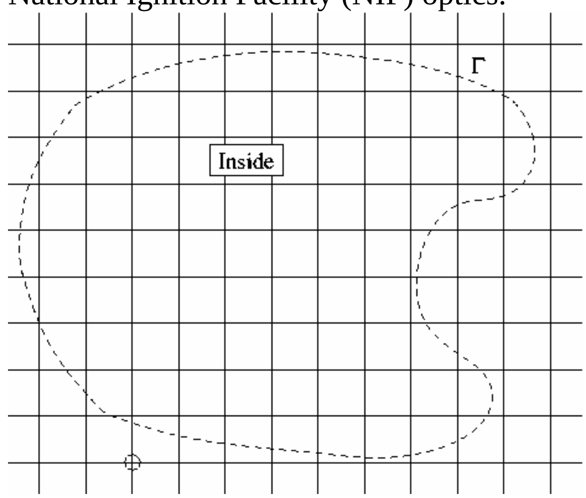

Figure 2: In the embedded boundary method, the boundary intersects the regular mesh in an arbitrary way. The differential equation is solved in the interior, and the grid points just outside the boundary (marked by "o") are used to satisfy the boundary conditions.

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