High-frequency simulations of seismic wave propagation in the whole Earth on 150,000 processor cores of a petaflop machine

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Abstract

SPECFEM3D_GLOBE is a spectral-element application enabling the simulation of global seismic wave propagation in the 3D Earth at unprecedented resolution. A fundamental challenge in global seismology is to model the propagation of waves with periods between 1 and 2 seconds, the highest frequency signals that can propagate clear across the Earth. These waves help reveal the 3D structure of the Earth's deep interior and can be compared to seismographic recordings. We broke the 2 second barrier using the 62K processor Ranger system at TACC. We obtained similar results on the XT4 Franklin system at NERSC and the XT4 Kraken system at University of Tennessee Knoxville, while a similar run on the 28K processor Jaguar system at ORNL, which has more memory per processor, sustained 35.7 teraflops (a higher flops rate) with a 1.94 shortest period. For the final run we obtained access to the ORNL Petaflop System, a new very large Cray XT5, and achieved 1.72 shortest period and 161 teraflops using 149,784 processor cores.

Introduction

The calculation of accurate synthetic seismograms for 3D global Earth models poses a significant computational challenge, both in terms of the demands on the numerical algorithm and with regards to computer hardware (i.e., memory and CPU requirements). Global seismologists routinely analyze recorded seismic signals with period between 1 and 2 seconds. Previous large-scale simulations in 3D Earth models have only been capable of reaching 3.5 seconds [5]. Therefore, our objective is to simulate global seismic wave propagation down to periods between 1 and 2 seconds, the highest frequency signals that can propagate clear across the Earth. Shorter periods get attenuated before reaching the other side of the Earth. These waves at periods of 1 to 2 seconds, generated when large earthquakes (typically of magnitude 6.5 or above) occur in the Earth, help reveal the detailed 3D structure of the Earth's deep interior and image its complex structures, an endeavor that will enhance our understanding of the physics and chemistry of the Earth's interior. The SPECFEM3D_GLOBE package has been designed to compute these simulations.

Since the record-breaking 3.5 second frequency run of 2003 which used the Earth Simulator [5], our team has expended a major R&D effort towards breaking the 2 second barrier. Achieving this goal required radical algorithmic changes to SPECFEM3D enabling peta-scalability (beyond 10Ks of processors) and incorporation of new algorithms that are both more scientifically accurate and more computationally scalable. The code includes optimizations to reduce cache misses, a new mesh design to improve spatial resolution for the seismic waves and to nearly eliminate load imbalance, and improvements to the inner Earth core resolution based upon an inflated central cube instead of a real cube with flat faces; reduction of the 'central cube' bottleneck by cutting the cube in two, and reduction of MPI messages by 33% inside each chunk by handling crust mantle and inner core simultaneously.

1 Description of the method and of the SPECFEM3D_GLOBE package

To simulate global seismic wave propagation in 3D anelastic, anisotropic, rotating and self-gravitating Earth models we have developed and implemented a spectral-element method (SEM). The SEM was introduced more than twenty years ago in computational fluid dynamics [7]. It has gained interest for problems related to 3-D seismic wave propagation, for instance following a large earthquake [6], [3], [1].

The method accurately represents the propagation of both body waves and surface waves, and lends itself well to parallel computation with distributed memory.

The SPECFEM3D_GLOBE package was designed to simulate three-dimensional global and regional seismic wave propagation based upon the SEM [4], [2]. The package has been extensively benchmarked against semi-analytical normal-mode synthetic seismograms (i.e., curves showing the evolution of displacement with time after the earthquake at a given mesh point) for spherically-symmetric Earth models. These benchmarks are very challenging because they involve solid-fluid domain decomposition and coupling, attenuation, anisotropy, self-gravitation, and the effect of the ocean layer located at the surface of the Earth. Our simulations incorporate effects due to topography and bathymetry as well as fluid-solid boundaries, such as the ocean floor, the core-mantle boundary (CMB), and the inner-core boundary (ICB). Thus far, only SPECFEM3D_GLOBE has been capable of accurately incorporating all of these effects.

SPECFEM3D_GLOBE consists of two major subprograms: meshfem3D, the mesher, which generates the spectral-element mesh and specfem3D, the solver, which uses the generated mesh to run the simulation. The mesher is designed to generate a spectral-element mesh for either regional or entire globe simulations. Our work focuses on simulations of the entire globe, which are the most expensive and therefore by far the most challenging. These simulations use a spectral-element mesh which is based upon an analytical mapping from the cube to the sphere called the 'gnomonic mapping' or the 'cubed sphere', which splits the globe into 6 chunks, each of which is further subdivided into N $\times$ N mesh slices for a total of 6 $\times$ N $\times$ N slices. The work for the mesher code is distributed to a parallel system by distributing the slices.

Given the shortest desired period, the grid spacing is determined by a requirement of at least 5 grid points (GLL points) per shortest seismic wavelength that we want to accurately model, and the Courant stability condition determines the upper bound of the associated time step. Current tomographic models reveal only large-scale features of the Earth's interior, features with dimensions much larger than the wavelengths of 1-second to 2-second waves.

For the final run we obtained access to the ORNL Petaflop System, a new very large Cray XT5 system, and achieved 1.72 shortest period and 161 teraflops using 149,784 processor cores. With this landmark calculation we have enabled a powerful new tool for seismic wave simulation, one that operates in the same frequency regimes as in the real Earth; in seismology there is no need to pursue periods much smaller because higher frequency signals do not propagate across the entire globe. We employed performance modeling methods to identify performance bottlenecks and worked through issues of parallel I/O and scalability. Improved mesh design and mesh numbering results in excellent load balancing and few cache misses.

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