ANL/ALCF/ESP-13/8

Using Multi-scale Dynamic Rupture Models to Improve Ground Motion Estimates

ALCF-2 Early Science Program Technical Report

Argonne Leadership Computing Facility

ANL/ALCF/ESP-13/8

Using Multi-scale Dynamic Rupture Models to Improve Ground Motion Estimates

ALCF-2 Early Science Program Technical Report

prepared by
Geoffrey Ely
Argonne Leadership Computing Facility, Argonne National Laboratory

June 7, 2013

Using Multi-scale Dynamic Rupture Models to Improve Ground Motion Estimates

PI: Thomas Jordan
ESP Postdoc: Geoffrey Ely

Science Overview

This project uses dynamic rupture simulations to investigate high-frequency seismic energy generation. The relevant phenomena (frictional breakdown, shear heating, effective normal-stress fluctuations, material damage, etc.) controlling rupture are strongly interacting and span many orders of magnitude in spatial scale, requiring high-resolution simulations that couple disparate physical processes (e.g., elastodynamics, thermal weakening, pore-fluid transport, and heat conduction). Compounding the computational challenge, we know that natural faults are not planar, but instead have roughness that can be approximated by power laws potentially leading to large, multiscale fluctuations in normal stress. The capacity to perform 3D rupture simulations that couple these processes will provide guidance for constructing appropriate source models for high-frequency ground motion simulations. The improved rupture models from our multi-scale dynamic rupture simulations will be used to conduct physics-based (3D waveform modeling-based) probabilistic seismic hazard analysis (PSHA) for California. These calculation will provide numerous important seismic hazard results, including a state-wide extended earthquake rupture forecast with rupture variations for all significant events, a synthetic seismogram catalog for thousands of scenario events and more than 5000 physics-based seismic hazard curves for California.

Numerical Method

We simulates spontaneous rupture within a 3D isotropic viscoelastic solid. Wave motions are computed on a logically rectangular hexahedral mesh, using the generalized finite difference method of support operators. Stiffness and viscous hourglass corrections are employed to suppress suppress zero-energy grid oscillation modes. The fault surface is modeled by coupled double nodes, where the strength of the coupling is determined by a linear slip-weakening friction law. External boundaries may be reflective or absorbing, where absorbing boundaries are handled using the method of perfectly matched layers (PML). The hexahedral mesh can accommodate non-planar ruptures and surface topography. Details are described in Ely *et al.* (2008, 2009).

Code

The numerical Method is implemented in the Support Operator Rupture Dynamics code (SORD). SORD is a component of the open-source Computational Seismology Tools (Coseis) which includes other requirements for performing earthquake simulations such as mesh generation, velocity model specification, and visualization. The SORD numerical engine is implemented in Fortran 95, with multi-threaded numerical kernels using OpenMP, domain decomposition using MPI, and parallel I/O using MPI-IO. SORD jobs are configured and launched through the Coseis Python Interface.

Porting to Blue Gene

Prior to ALCF Mira, SORD was first ported to ALCF Intrepid. The Fortran numerical engine required very little modification to run. Substantial effort was required for the supporting utility codes however. Many of these tools required a custom Python install with multiple package dependencies running on the compute nodes; a cumbersome and poorly performing arrangement for Blue Gene. This was improved by reorganized the codes into a two-step process where initial Python-based data processing is performed on the login nodes, with any heavy processing performed by compiled codes on the compute nodes. Additional modifications were needed to the Coseis work-flow tools to adjust to the ACLF Cobalt scheduling environment. Cobalt is a significant departure from prior systems used to run Coseis, such as LoadLeveler, PBS, and SGE. Although the initial porting process required substantial effort, the outcome is highly satisfactory: cleaner, portable, and better performing code.

Performance Tuning

Tests show very good scalability for the MPI domain decomposition scheme on Blue Gene/Q (Fig. 1). However, the initial port achieved only four percent of peak FLOPS performance on Blue Gene/Q. Profiling with Walkup's HPM library revealed memory bandwidth bottlenecks cause by multiple stencil kernel operations sweeping through arrays larger than cache memory. We implemented a cache titling scheme to make better reuse of arrays in cache. We also added OpenMP multi-threading for the kernels. The optimizations achieve a 2.5 times per-core speedup. Taken with the increase core count and bus speed for BG/Q, gives a total of 20 times per-node speedup over the initial BG/P port. QPX-vectorized versions of the computational kernels have been tested, but not integrated into the production code yet.

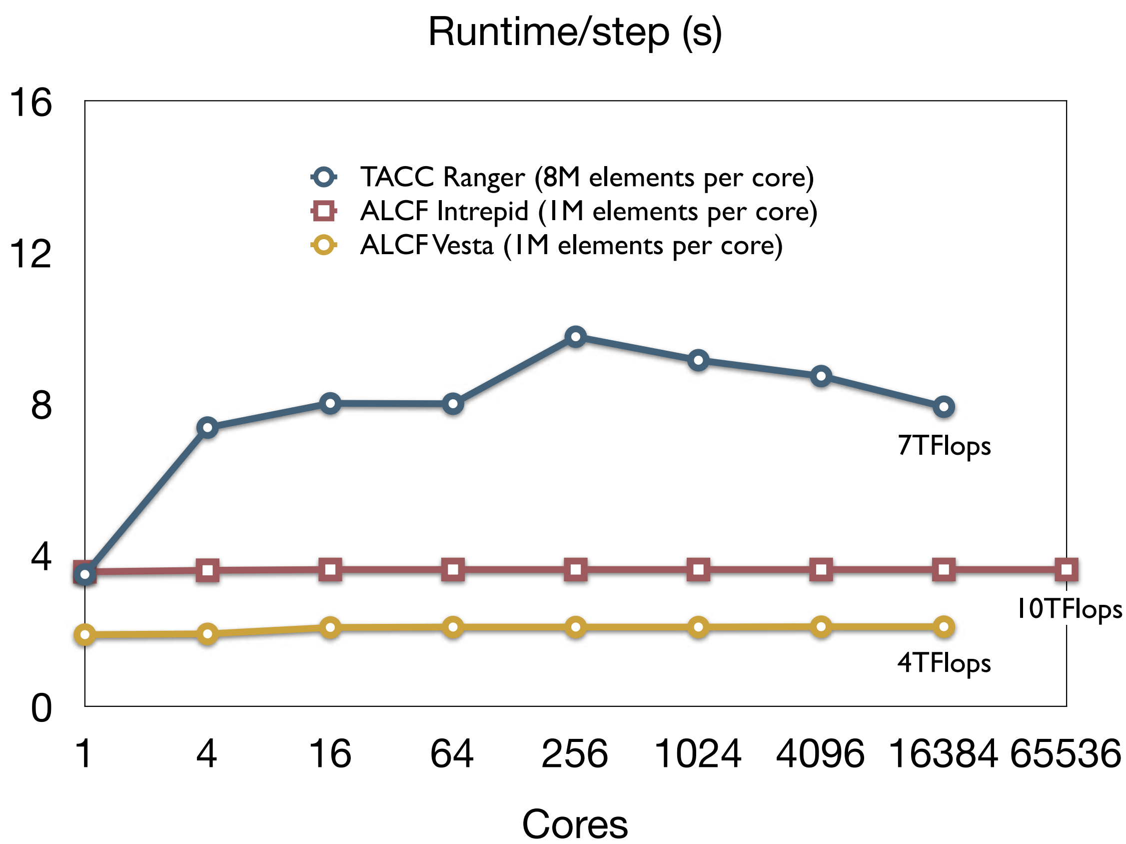
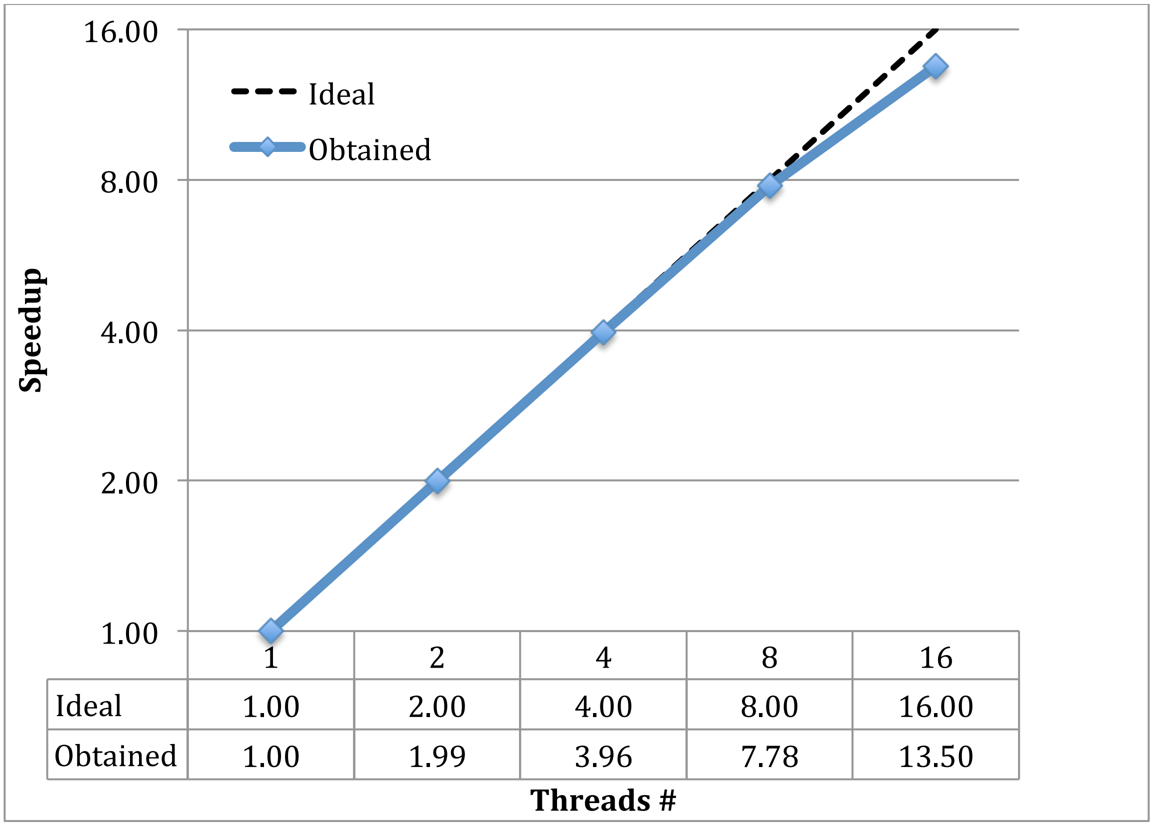


Figure 1: Weak scaling benchmark for SORD in pure MPI mode (no multi-threading). ALCF Intrepid (Blue Gene/P) and Vesta (BG/Q) demonstrate near ideal weak scaling, with BG/Q clock speak increase giving a factor of two speedup relative to BG/P.



	1	2	4	8	16
Ideal	1.00	2.00	4.00	8.00	16.00
Obtained	1.00	1.99	3.96	7.78	13.50

Figure 2: SORD OpenMP strong scaling benchmark for single node Blue Gene/Q.

References

Ely, G. P., S. M. Day, and J.-B. Minster (2008), A support-operator method for visco-elastic wave modeling in 3D heterogeneous media, *Geophys. J. Int.*, *172*(1), 331–344, doi:10.1111/j.1365-246X.2007.03633.x.

Ely, G. P., S. M. Day, and J.-B. Minster (2009), A support-operator method for 3D rupture dynamics, *Geophys. J. Int.*, *177*(3), 1140–1150, doi:10.1111/j.1365-246X.2009.04117.x.

Argonne Leadership Computing Facility
Argonne National Laboratory
9700 South Cass Avenue, Bldg. 240
Argonne, IL 60439

www.anl.gov

Argonne National Laboratory is a U.S. Department of Energy
laboratory managed by UChicago Argonne, LLC