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An Open-Source High-Performance Computing Software for 3D Geophysical Modeling and Inversion

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Short Abstract

Geophysical seismic applications typically involve extensive computations, large volumes of data, and diverse methodological approaches, making their development highly demanding. It is common for research efforts to focus on creating tools tailored to specific applications. Although techniques developed for one application could, in principle, be adapted to others, their design rooted in a particular context often makes it difficult to generalize them for broader use.

In addition to the efforts dedicated to ensuring consistency with physical theory, the development of geophysical applications usually prioritizes computational performance. This emphasis compels developers to apply high-performance computing (HPC) techniques to make certain experiments feasible. HPC is indispensable for addressing complex problems; however, given the multiple possibilities for parallelizing an application, it becomes crucial to analyze several factors to optimize resource utilization. These factors include the available environment's characteristics, the problem's size to be solved, the likelihood of system failures, and the efficient strategies for task distribution.

Developing software that delivers geophysical applications while incorporating HPC techniques presents various challenges, from ensuring consistency with physical theory to optimizing available HPC resources. We have developed an open-source software to address these challenges, released under the MIT license, specifically designed to develop HPC solutions for geophysical applications. Implemented in C++, the software supports 3D acoustic and visco-acoustic modeling, reverse time migration (RTM), full-waveform inversion (FWI), and least-squares reverse time migration (LSRTM). These applications leverage HPC methods already integrated into the software, such as distributed and shared memory task scheduling, fault tolerance mechanisms, and GPU acceleration.

We designed the software to support FWI and LSRTM workflows by integrating advanced optimization algorithms. In particular, we apply the quasi-Newton limited-memory Broyden- Fletcher-Goldfarb–Shanno (L-BFGS) method to efficiently approximate the inverse of the Hessian matrix, accelerating convergence while minimizing memory requirements. We also incorporated a conjugate gradient method tailored for high-dimensional parameter spaces. To further enhance stability and computational efficiency, we consider adaptive step-length selection in the optimization algorithms and gradient preconditioning strategies, such as a smoothing strategy based on the Bessel filter, which reduces acquisition-related footprints in the final estimated model parameters.

Finally, the software's development has been guided by concerns for physical consistency, computational efficiency, and ease of maintenance, as well as by adopting best practices in software engineering and are committed to providing accessible, high-quality documentation. The platform has been validated on small-scale experiments and is currently being tested on more complex problems, aiming to support experienced researchers and new users. This open-source initiative represents a flexible and extensible solution for the next generation of large-scale geophysical applications in high-performance computing environments.