Title: Higher-order mass-lumped wave propagators on variable resolution, triangular meshes

Introduction

Numerical models that simulate wave propagation are powerful tools that help scientists explore the subsurface of the earth (Lines and Newrick, 2004). Many seismic research activities consist of iteratively updating an initial model to better fit recorded seismic signals through the simulation of wave propagation through the ground. The primary computational expense of this process is associated with the numerical simulation of the wave propagation. It is thus important to advance and develop methodologies to reduce the associated computational cost of wave propagation.

There are several ways to numerically simulate waves for seismic applications including finite difference methods and the comparatively more complex finite element method (FEM). The additional complexity associated with FEM comes with more challenges, but a key advantage of FEM is that they can utilize unstructured, variable resolution meshes to discretize seismic domains (van Driel et al., 2020, Thrastarson et al., 2020, Trinh et al., 2019). Despite this advantage, mesh adaptation is infrequently used in seismic applications because the generation of unstructured meshes can be potentially laborious (Peter et al., 2011) and more readily-generated triangular meshes result in a non-diagonal system of equations that are computationally expensive to solve. In this work, we help reduce these issues by implementing open-source, wave propagators that use stable and numerically accurate higher-order (up to P=5) mass-lumped triangular elements (Chin-Joe-Kong et al., 1999, Geevers et al., 2018a). In a similar manner to spectral element discretization with quadrilateral elements, these triangular elements lead to diagonal mass matrices and thus can be efficiently time-marched in fully-explicit numerical wave simulations.

Ongoing work and open-source code developments (Roberts et al. 2021a, Roberts et al. 2021b) in the Firedrake programming environment (Rathgeber et al., 2016) have demonstrated that the combination of automatically generated, variable resolution triangular meshes with higher-order mass lumped elements of Chin-Joe-Kong et al. (1999) represent a powerful methodology to efficiently simulate wave propagations at scale in both 2D and 3D for seismic applications. Here we briefly illustrate some of our developments applying FEM to wave propagation for seismic applications by using recently developed automatic mesh generation technology and the Firedrake computing environment.

Mass-lumped wave propagators in Firedrake

We have implemented 2D/3D acoustic wave propagators and an implementation of a Perfectly Matched Layer (PML) along with their discrete adjoints using these higher-order mass lumped elements of Chin-Joe-Kong et al. (1999) and Geevers et al. (2018a) into an open-source and user-friendly Python package called spyro (Roberts et al. 2021b). These elements rely on enriching the basis functions with higher-order bubble functions and integrating with special quadrature rules so that mass-lumping can be achieved. As a result, higher-order mass lumped elements contain a greater density of nodes per space. The spyro package utilizes the automatic code generation capabilities of Firedrake enabling concise expression of variational forms symbolically through a code lowering process. It also provides great flexibility with regard to how the user wants to solve the wave equations numerically and leads to a representation of complex algorithms (e.g., full waveform inversion) in a few dozen lines of code. Systems of equations are solved via calls to PETSc solvers and parallelism is implemented using the message passing interface.

Mesh design: cells per wavelength

When performing wave simulations on meshes, a minimum number of degrees-of-freedom density otherwise referred to as grid points per minimum wavelength are required to inhibit numerical error. The spatial polynomial order of the method will determine the number of degrees-of-freedom (DoF) inside the element and each element has a different distribution of DoFs. This translates to a cell density per wavelength restriction in mesh generation. A dispersion analysis of KMV elements has already been done by Geevers et al. (2018b) for the acoustic wave equation without the PML in a homogenous domain discretized with a uniform resolution mesh. However, necessary cell density may also be affected by conditions such as point receiver location and mesh heterogeneity. Here we measure the number of cells-per-minimum wavelength that are required to keep the normalized error below a given threshold, based on work by Lyu et al. (2020) (Figure 1a) with the addition of a PML layer and measurements occurring at non-grid points. Figure 1 demonstrates that higher-order methods can provide more accuracy with comparatively fewer overall DoF, thus potentially accelerating simulations. Ongoing work is analysing these grid point requirements for additionally 3D domains with heterogeneous velocity fields using these higher-order mass lumped elements.

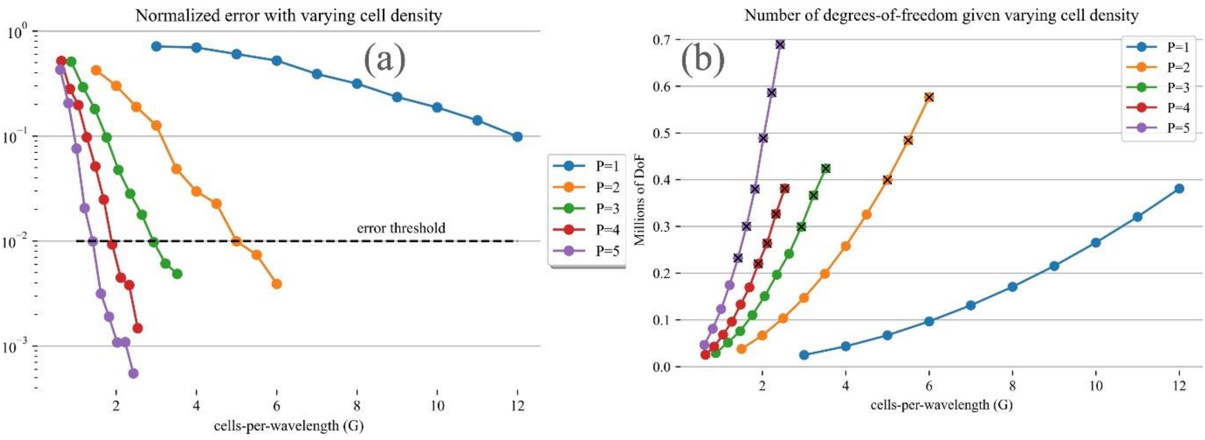

Figure 1 *(a) Normalized error when increasing cell density for different degrees of 2D mass-lumped KMV elements. The error threshold of 0.01 is also shown in the graph as the black dotted line. (b) Using the G from (a), the number of degrees-of-freedom (DoF) in 2D meshes with resolution adapted to the P-wave velocity field of the BP2004 model. Meshes are built using SeismicMesh with a size gradation bound of 15%. Black x's in (b) indicate solutions which satisfy the error threshold of 0.01.*

Automatic mesh generation and mesh adaptation

Using automatic mesh generation technology called SeismicMesh (Roberts et al. 2021a), the complexity to discretize a domain with a graded triangular mesh is reduced. The software creates a graded mesh-density function from seismological data taking a number of parameters into account. Using the results from the dispersion analysis gives us insight into what a cost-effective value for G should be to distribute mesh resolution (Figure 1a). Here we build a sequence of meshes for the BP2004 synthetic P-wave velocity model each with local mesh resolution adapted to the local wavelength divided by G for a 5 Hz Ricker wavelet with a constant mesh gradation rate of 15%. From Figure 1b, P=4 with ~2 G satisfies our error threshold with the fewest number of DoF thus representing a cost-effective solution.

Degenerate elements and performance

Distorted triangular and tetrahedral elements have significant impacts on numerical stability for fully-explicit numerical methods as the maximum eigenvalues of the operator increase greatly with thinly shaped elements. In 3D, distorted flat elements are referred to as slivers and are characterized by a small angle between two adjacent faces of a tetrahedral (minimum dihedral angle). In SeismicMesh, a sliver-removal algorithm is thus implemented to ensure the worst quality tetrahedral elements can be bounded below. Here we mesh a subset of the Overthrust 3D model for G=5 and P=2 incrementally increasing the minimum dihedral angle bound. One can see there is a substantial improvement (~140x increase) in the maximum stable timestep when simulation is attempted on the 3D mesh with a dihedral angle bound of 17.5 degree. When this optimized 3D mesh with a minimum dihedral angle bound of 17.5 degree is then simulated on both Intel and AMD nodes, overall excellent performance is observed with near ideal strong scalability. Higher-mass lumped elements require far less intercommunication between compute nodes as the solution to the system of the equations require only simple pointwise division.

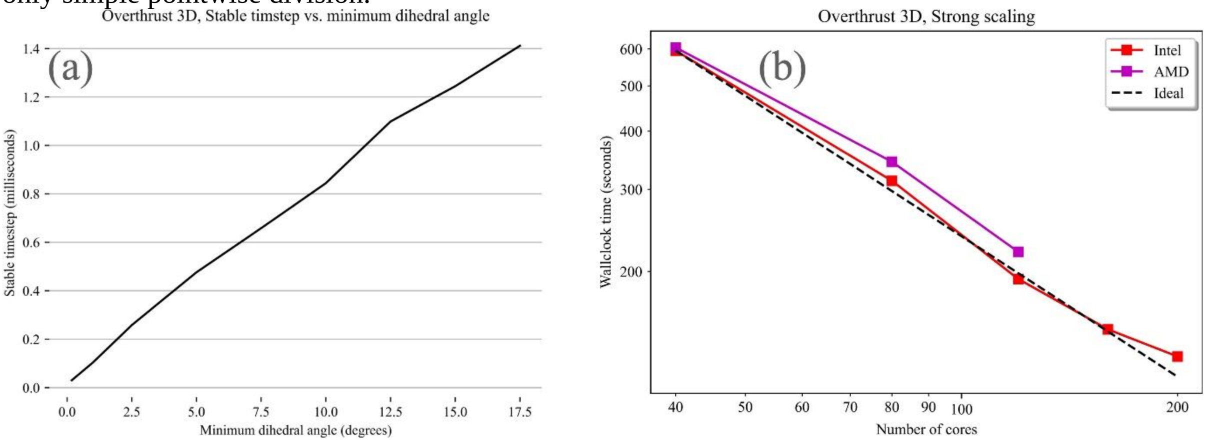

Figure 2 *(a) An example of the effect on the maximum stable timestep to simulate a 3D wave simulation on the 3D Overthrust model after applying the sliver removal technique as documented in Roberts et al. (2021a). Note a 2nd order in time timestepping scheme is used. (b) A strong scaling curve when simulating for 3 simulation seconds with a 11 million DoF mesh of the Overthrust 3D model given a minimum dihedral angle of 17.5 degrees to boost the maximum stable timestep. Both Intel and AMD compute nodes were used.*

Conclusions

Wave propagators that utilize the higher-order mass-lumped triangular elements are available via an open-source Python package spyro that can take advantage of variable resolution triangular meshes with an open source automatic mesh generation tool called SeismicMesh. We highlighted the necessity for a high-quality mesh and a reliable mesh generation tool and showed how one can use automatic mesh generation software to greatly increase the throughput of seismic wave simulations with the FEM. Together these two open-source tools can be used to script full waveform inversion algorithms that can operate at scale in both 2D and 3D.

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