Technical report, SCEC Award 17192, Stable and Accurate Fault and Free Surface Boundary Conditions in Staggered Grid Wave Propagation Codes

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This work focuses on the development and testing of free surface boundary condition implementations for the elastic wave equation. In recent work, we showed how to extend the so-called summation-by-parts (SBP) finite difference method and simultaneous approximation term penalty method (SAT) to staggered grids for the acoustic wave equation [1]. Here, we investigate how applicable this method is for solving the elastic wave equation. In particular, we study the accuracy of the method for some challenging problems featuring surface waves. We make a detailed comparison to the more conventional free surface boundary condition (FS2) [2, 3, 4], which is implemented in SCEC's wave propagation code (AWP)[5, 6]. In this study, we show that SBP-SAT delivers comparable accuracy to FS2, is capable of solving both forward and reciprocal problems (of particular relevance to Cybershake), is provably stable and energy conserving regardless of material properties, and is also extensible to other types of problems and methods. However, the implementation of the SBP-SAT approach is slightly more complicated and computationally expensive compared to FS2, and does also require a factor of two reduction in the timestep.

Our work is motivated by several factors. First, since the resolution requirements are typically set by surface waves, an improvement in the accuracy of the free surface boundary condition could imply that fewer grid points per minimum wavelength (ppw) are needed to maintain the same desirable accuracy as before. Second, the current free surface boundary condition (FS2) may be non-trivial to extend to non-planar free surface (i.e., topography) without introducing instability. However, we believe that a curvilinear method based on SBP-SAT could be developed. Third, we are interested in understanding if the SBP-SAT approach is applicable to Cybershake-related work. For this purpose it becomes necessary to solve the reciprocal problem by placing point forces on the free surface. The solution to adjoint problems is also elegantly expressed using SBP-SAT, and could therefore be beneficial for tomography applications that rely on full-waveform inversion.

The SBP-SAT method is a systematic way of designing a numerical scheme such that it is energy conserving (or slightly dissipative), and hence stable [7, 8, 9]. This property makes the SBP-SAT method generally applicable to many types of numerical schemes (not necessarily finite difference-based) and problems. For example, a SBP-SAT on curvilinear grids has been developed for studying earthquake rupture dynamics [10, 11, 12]. A notable difference between this SBP-SAT method and the one presented here is that we use a staggered grid instead of a collocated grid. More recently, the SBP-SAT has also been used to develop an energy conserving coupling procedure for nonconforming grids (also known as discontinuous meshes). A key ingredient in the SBP-SAT method is the weak enforcement of boundary conditions using so-called SAT terms. This weak enforcement provides automatic error control on the boundary because the boundary condition is not exactly satisfied (error can be defined by comparing the numerical solution on the boundary to the known boundary condition). The SBP operators themselves are typically designed by satisfying accuracy and stability conditions for a few stencils near the boundary. There are usually free parameters present that can be tuned to improve accuracy. There are also many ways to construct the operators such as allowing grid points to be non-equidistantly spaced, or by placing the boundary inside the domain. Some of these techniques

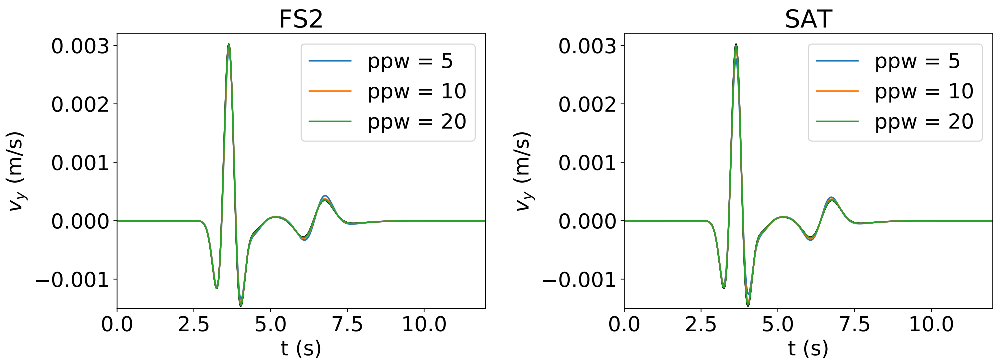


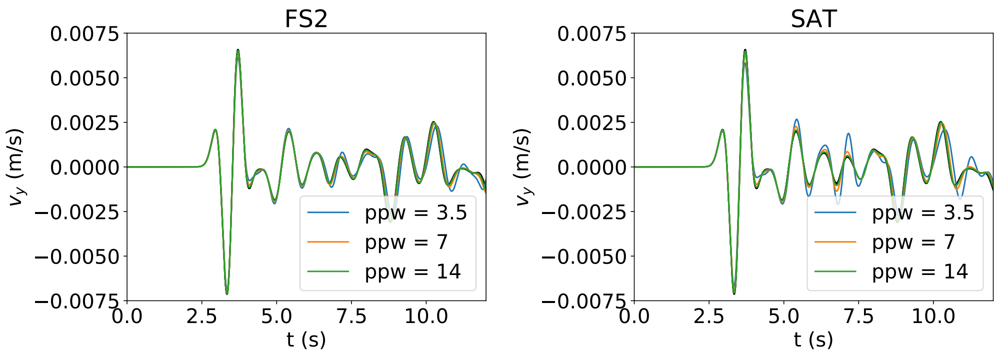
Figure 1: Vertical component of the velocity at the receiver on the free surface, 5 km away from the compressional source, showing the numerical solution at different resolutions. Homogeneous material properties are used in this test. The barely visible black line is the reference solution computed using 40 ppw.

could potentially be used to develop more accurate operators than what we present here.

In this study, we investigate the accuracy and stability properties of the FS2 and SBP-SAT implementations of the free surface boundary condition for the elastic wave equation in two dimensions. We stress that the only difference between these two methods is in how the free surface boundary condition is implemented. That is, in the interior both methods reduce to the same fourth order in space finite difference method and second order time (leap frog) on staggered grids. Although it is possible to implement the material properties in certain ways, we have chosen to refrain from using interpolation (and thereby storing a material parameter such as the density at each velocity component). We also don't take any harmonic averaging, or geometric averaging to improve the method's ability to represent material discontinuities. The reason being that we are primarily interested in the performance of the free surface implementation. All of our numerical solutions in the accuracy tests have been verified against FDMAP [10, 11]. Implementation details for the SBP-SAT approach on staggered grids can be found in [1].

Our first test involves solving Garvin's problem which features a compressional source buried at depth. We use a Ricker wavelet as the source time function, and set the peak frequency to 0.96 Hz and its duration to 2 s. The Amplitude is set to unity for self-consistent units. We set the source depth $y_s = 1$ km. The source is deliberately placed close to the free surface to excite large-amplitude surfaces waves. The receiver location is placed on the free surface, $x_r = 5$ km to the right of the epicenter of the source. The material parameters are taken to be $\rho = 2.8$ g/cm^3 for density, $c_s = 1.2$ km/s for s-wave speed, and $c_p = 3$ km/s for the p-wave speed. Using a grid spacing of $h = 100$ m gives 5 ppw. This definition sets the maximum frequency f_{max} that must be resolved to 5% of peak amplitude of the spectrum of the Ricker wavelet. In this case, $f_{max} = 2.4$ Hz. Since the horizontal component of the velocity field is not available at the free surface for FS2, one should use the average of the two nearest points [4]. For convenience, we have chosen to compare the vertical components only. That said, no averaging is needed for SBP-SAT (both velocity components are available, but staggered relative to each other on the free surface). Figure 1 shows the vertical component of velocity, and that both free surface implementations give comparable accuracy. We have also tested using a double-couple moment tensor source, which is typical for earthquake seismology. Again, we find comparable accuracy between the two methods (result not shown).

Our second test features a layered material structure with piecewise constant material properties. These properties are listed in the table in Figure 2. This setup is motivated by a typical geological setting, where soft sediments of soil rest on top of layer of rock. The soil layer is a low velocity layer that acts as a wave guide and causes surface wave amplification. In the seismogram shown in Figure 2, we can see multiple reflections from waves trapped within the soil layer. In terms of numerical accuracy, we note that SBP-SAT exhibits slightly larger overshoots compared FS2 at the lowest resolution, but otherwise the two methods produce comparable results.



	Layer (km)	ρ (g/cm^3)	c_p (km/s)	c_s (km/s)
1	$1.5 \le y \le 0$	1.0	0.8	3.6
2	$3 \le y < 1.5$	1.5	1.0	4.0
3	$7 \le y < 3$	2.3	2.7	5.0
4	$y > 7$	2.8	3.464	6.0

Figure 2: Vertical velocity component at the receiver on the free surface, 5 km away from the compressional source, showing the numerical solution at different resolutions. The barely visible black line is the reference solution computed using 28 ppw. The material properties are piecewise constant, modeling soil over rock. The free surface is at $y = 0$.

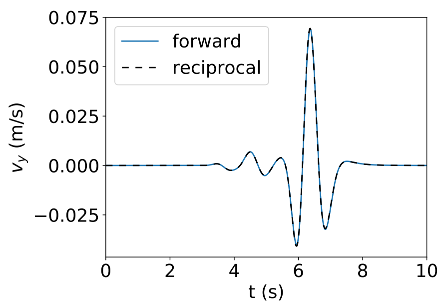


Figure 3: Reciprocity test in which the SBP-SAT method is used to solve the forward problem using reciprocity (dashed line). This solution is compared to the numerical solution of the forward problem (solid line).

In our third test we demonstrate that SBP-SAT method can be used to solve the reciprocal problem using the representation theorem [13]. The need to solve this problem is at the heart of the Cybershake project. Cybershake relies on reciprocity to reverse the role of source and receivers, and thereby reducing the number of expensive wave propagation simulations by at least two orders of magnitude. To numerically test reciprocity, we reconstruct the result the forward solution obtained by using the double-couple source in the first test. Instead of placing a moment tensor source at depth, we place a directional point force on the free surface at the previous receiver location. We follow [14] and record the stress tensor at the previous source location (1 km below depth). This process is repeated for each component of the particle velocity field that we wish to obtain. Then by the computing the strain Green's tensor we can recover the solution to the forward problem. Figure 3 shows the result of the reciprocity test for SBP-SAT. There is excellent agreement between the forward calculation and recovered forward calculation using reciprocity (less than one percent error).

Finally, we investigate the long-term stability behavior of both implementations. To perform this test, we modify the heterogeneous material properties such that instead of having layers stacked on top of each other, we have layers stacked side by side. In this way, the material discontinuities intersect with the free surface. We use a low velocity layer surrounded by a high velocity layer (properties of layers 3-4 in Figure 2 are used for this test). The source is placed

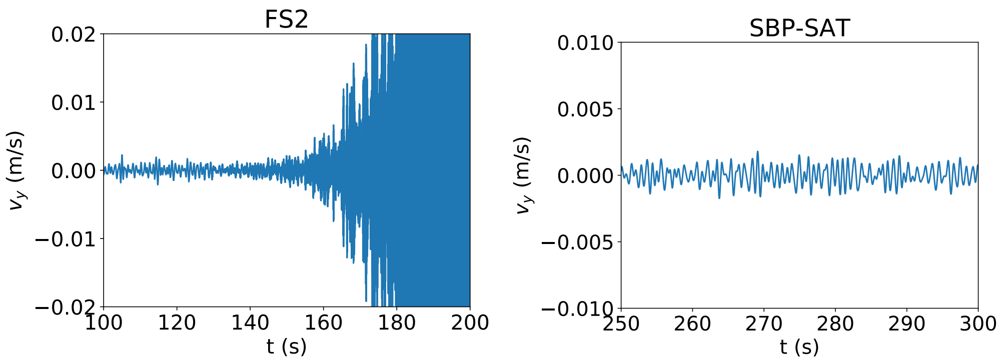


Figure 4: Long-time stability test using a low velocity layer that intersects the free surface.

in the center of the low velocity layer. Some of the surface wave energy that is generated is trapped inside the low velocity layer. As waves reflect against the material contrast, numerical error in the form of low amplitude surface waves that grow in time are generated for FS2. Since there is no filtering or artificial dissipation present in the numerical scheme, this growth will inevitably cause the onset of a long-term instability (Figure 4). On the other hand, the SBP-SAT implementation is stable as it does not allow for any energy growth in time. A stable result will always be produced regardless of the simulation duration and choice of material structure.

It should be noted that we are not aware of any reports, or work in the literature, that have previously documented this instability. At this point in time, we cannot rule out an implementation error on our side.

In conclusion, we have shown that the SBP-SAT method can be used to discretize the free surface boundary condition in the elastic wave equation and deliver comparable accuracy to conventional approaches (FS2). In our investigation we have considered both homogeneous, heterogeneous material properties, compressional, and double-couple sources. Both the forward and reciprocal problems have been solved. Furthermore, we have showed that for certain material structures the FS2 implementation in susceptible to long-term instabilities. In contrast, the SBP-SAT approach is provably stable for any type of material structure provided by the problem is well-posed (i.e., Lame‘s first parameter is non-negative). We are currently investigating how to extend the method to curvilinear, staggered grids. We also hope to improve the accuracy of the free surface boundary condition by allowing for non-equidistant points near the boundary (requiring the need to solve a highly non-linear and constrained optimization problem), and by enforcing the free surface boundary conditions by alternative means, as done in for example [15].

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