An improved immersed boundary finite-difference method for seismic wave propagation modeling with arbitrary surface topography

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Seismic wave modeling with surface topography

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### ABSTRACT

To accurately simulate seismic wave propagation for the purpose of developing modern land data processing tools, especially the full waveform inversion (FWI), we developed an efficient high-order finite-difference forward modeling algorithm with the capability of handling arbitrarily shaped free surface topography. Unlike most of the existing forward modeling algorithms using curvilinear grids to fit irregular surface topography, this finite-difference algorithm, based on an improved immersed boundary (IB) method, employs a regular Cartesian grid system without suffering from staircasing error, which is inevitable in a conventional finite-difference method. In this improved immersed boundary finite-difference (IBFD) algorithm, arbitrarily curved surface topography is accounted for by imposing the free surface boundary conditions at exact boundary locations instead of using body-conforming grids or

refined grids near the boundaries, thus greatly reducing the complexity of its preprocessing procedures and the computational cost. Furthermore, local continuity, large curvatures, and sub-grid curvatures are represented precisely through the employment of the so-called dual coordinate system — a local cylindrical and a global Cartesian coordinate. In order to properly describe the wave behaviors near complex free surface boundaries (e.g., overhanging structures and thin plates, or other fine geometry features), the wavefields in a ghost zone required for the boundary condition enforcement are reconstructed accurately by introducing a special recursive interpolation technique into the algorithm, which substantially simplifies the boundary treatment procedures and further improves the numerical performance of the algorithm, as demonstrated by the numerical experiments. Numerical examples are presented to show the performance of the IBFD method in comparison with a conventional finite-difference method.

#### INTRODUCTION

Full waveform inversion (FWI) method developed rapidly in recent years because it is considered as a powerful tool for complex subsurface structure and geophysical property reconstruction (Tarantola, 1984; Pratt et al., 1998; Symes, 2008; Abubakar et al., 2009; Krebs et al., 2009; Hu et al., 2009; Virieux and Operto, 2009; Habashy et al., 2011; Hu et al., 2011; Ma et al., 2012; Li et al., 2013; Hu, 2014). Utilizing the full waveform information contained in recorded seismic data, FWI is able to provide high resolution velocity models and other geophysical property models such as anisotropic parameters, attenuation property (quality factor Q), mass density, etc. Unlike those conventional seismic processing tools, such as velocity tomography method using traveltime information only, the mechanism of FWI is mainly based on the waveform matching between simulated seismic data and recorded seismic data through minimizing a predefined objective function. Although many efforts have been made on elastic FWI research, most of the currently existing FWI algorithms in the industry are still based on the acoustic approximation. In spite of their acoustic approximation, these FWI algorithms have achieved various levels of success on both marine and land seismic data. An acoustic wave propagation engine is unable to produce shear waves, surface waves, etc., but the acoustic FWI algorithms can still practically reconstruct the subsurface P wave velocity models by matching the simulated data with the preprocessed field data. Consequently, a highly accurate forward modeling engine is required for successful FWI inversions. It is well known that free surface topography geometry has significant influences on seismic wave propagation modeling results (Lombard and Piraux, 2004; Bleibinhaus and Rondenay, 2009). Unfortunately, most existing FWI algorithms use a finite-difference-based forward modeling engine without the capability of accurate representation of irregular free surface topography (Li et al., 2010). With these conventional forward modeling engines, when grid lines and free surface boundaries are not conformal, staircasing errors will be induced, observed as the artificial scattering phenomena in the simulated data, severely contaminating the FWI inversion results.

A straightforward conventional finite-difference method for free surface modeling is the so-called image method (Levander, 1988). However, this method and its variants are accurate only for planar free surfaces. Robertsson (1996) extended the image method to more general problems with staircase approximation to irregular free surface geometry but staircase approximation induces artificial scattering effect. In order to eliminate these nonphysical scattering waves, grid refinement has to be applied near the free surface boundary, thus increasing the computational cost and the algorithm complexity dramatically. Empirically, 60 nodes per wavelength are required to effectively suppress the artificial scattering phenomenon (Bleibinhaus and Rondenay, 2009), which is unaffordable for large scale problems in exploration geophysics. Finite element methods (FEM) (Min et al., 2003) and spectral element methods (SEM) have been proposed to circumvent the difficulty brought by irregular surface topography (Komatitsch and Vilotte, 1998). In these weakform-based methods, grid lines are designed to be conformal to irregular surfaces, hence no grid refinement is required. However, the computational cost of an FEM can be prohibitive for typical 3D projects in exploration geophysics. On the other hand, the preprocessing procedure, mesh generation, is not a trivial task for SEM algorithms, preventing them from being a practical method for production use. Another category of approaches to irregular free surface topography adopts a transformation between a curvilinear coordinate system and a Cartesian coordinate system (Hestholm and Ruud, 1998; Appelö and Petersson, 2009; de la Puente et al., 2014). Combining coordinate mappings and differential geometry, Shragge (2014a,b) extended this approach to a 3D FDTD wave propagation engine and an RTM

algorithm on generalized structured meshes and explained their implementation strategy for efficient handling of the geometry related computation and memory overhead. These coordinate mapping based algorithms work effectively for simple topography geometry. For topography with high level of irregularity, many automated meshing algorithms commonly have difficulty in preventing locally small cells. In that case, the maximum allowable time stepping interval can be reduced significantly to maintain the algorithm stability, implying higher computational cost (Robertsson, 1996; Shragge, 2014b).

In this work, we developed a finite-difference algorithm, referred to as the improved immersed boundary finite-difference method (IBFD) for seismic wave propagation simulations with arbitrarily curved surface topography in presence. The distinguishing feature of the immersed boundary method is that a regular Cartesian grid system is employed and the grid lines under this system are not required to conform to the surface boundary. Instead, a surface boundary can cut through the grids and a special interpolation/extrapolation procedure is carried out to impose the free surface boundary conditions at the exact free surface boundary locations. Since the immersed boundary method was first developed by Peskin (1972), many variants of this method have been reported to address various issues (Tseng and Ferziger, 2003; Gao et al., 2007; Berthelsen and Faltinsen, 2008; Mittal et al., 2008; Pan and Shen, 2009; Shinn et al., 2009). It has also been introduced to exploration geophysics (Zhang and Symes, 1998; Lombard et al., 2008; Li et al., 2010). We improved this method by introducing some unique techniques. Our algorithm differentiates from the existing immersed boundary methods for seismic wave propagation modeling in the following aspects: 1) local continuity and sub-grid curvature are captured precisely through a dual coordinate system - a local cylindrical and a global Cartesian coordinate. The transformation between these two coordinate systems is straightforward and completely automatic; 2) a special

recursive interpolation scheme is designed for wavefield reconstruction in a ghost zone to suppress scattering artifacts effectively; 3) finite-difference stencil for ghost zone wavefield interpolation is adaptively adjusted by the algorithm, allowing one to avoid the numerical stability issue and treat geometrically complicated structures (overhanging structures, sharp corners, thin plates, etc.) accurately; 4) we use local explicit operators and there is no large linear system that needs to be solved for ghost zone wavefield reconstruction, thus avoiding the singularity issue in a matrix inversion.

# CONVENTIONAL FINITE-DIFFERENCE METHODS AND SURFACE TOPOGRAPHY

In this study, we only consider acoustic wave propagation whose governing equations are as follows

$$\nabla p + j\omega \rho \mathbf{v} = \mathbf{f}$$

$$\nabla \cdot \mathbf{v} + j\omega \frac{1}{K} p = q,$$
(1)

where  $\omega$  is the angular velocity,  $j = \sqrt{-1}$ , p is the pressure,  $\mathbf{v}$  is the particle velocity,  $\rho$  is the mass density,  $\mathbf{f}$  is the volume density of the body force, q is the volume density of mass, and K is the bulk modulus.

The method of vacuum is a straightforward conventional finite-difference method for airearth interface handling. It is simple to implement and its physical meaning is clear. The vacuum method updates the wavefields in the whole computational domain simultaneously in the same manner. However, above a free surface boundary, the mass densities are set to very small values while the seismic wave velocities are set to values comparable to the subsurface velocities. By doing this, the minimum finite-difference grid size in the air region remains relatively large without violating the finite-difference stability condition to save the computational expense. At the same time, the reflection coefficient values at the air-earth interface are honored by adjusting the mass density values in the air region because reflection coefficient is determined by wave impedance. When the grid lines and the free surface are conformal or very fine grids are used to correctly represent the irregular free surface topography, the vacuum method is an accurate method for the subsurface wave propagation simulation although the simulated wavefields above the air-earth interface are incorrect due to the wrong seismic wave velocities. If the air-earth interface is irregular, then the actual interface has to be approximated by a staircase boundary consisting of Cartesian grid lines because a conventional finite-difference method requires that the medium properties in each grid must be homogeneous, as shown in Figure 1a. With this rough staircase approximation to the actual smooth boundary, many nonphysical scattering points are generated, leading to a severe impact on the overall numerical performance including artifacts, accuracy order, and possibility of localized non-convergent behavior. Intuitively, these negative effects can be reduced by refining the finite-difference grids. Unfortunately, unless extremely small grid size (60 grid points per wavelength) is used, which is computationally unaffordable, it has been reported that using staircase approximation may have serious consequences and severely deteriorate simulation results (Bleibinhaus and Rondenay, 2009). A practical way to reduce the artificial scattering effect is to introduce a multi-grid approach (Hu and Cummer, 2006), where the original coarse grids located near an air-earth interface are refined to accurately describe the irregular free surface geometry, as shown in Figure 1b. To properly implement a multi-grid method, the information communication between coarse grids and fine grids has to be processed carefully through some advanced interpolation techniques. Nevertheless, artificial reflections at the interfaces between coarse grids and fine grids are often observed and a stability issue is commonly encountered (Venkatarayalu et al., 2007; Xiao et al., 2007).

# IMPROVED IMMERSED BOUNDARY FINITE-DIFFERENCE METHOD

Immersed boundary method (Peskin, 1972) offers a simple approach to an accurate representation of arbitrarily curved surface topography under a regular Cartesian grid system. Figure 2 is a diagram of the original immersed boundary method, where we observe that the grid lines are decoupled from the material interface. In order to honor the free surface without grid lines conformal to it, the free surface boundary condition is enforced on the wavefields across the material interface, i.e., at the boundary intercept point S. In Figure 2, the grids are classified into two categories. One category is called interior grid whose center is located in the subsurface region (grid 1 and grid 2) and the other category of grids is called ghost grid whose center is located in the air region. In the original immersed boundary method, a simple linear scheme is employed to estimate the wavefields at the ghost points based on the calculated wavefields at the associated interior points. As shown in Figure 2, a triangle is constructed with the ghost point and the two nearest interior points as the vertices. The wavefield at the ghost point G is estimated through a linear interpolation method using the known wavefield values at point 1 and point 2 with the stress-free boundary condition satisfied at the intercept point S. After the wavefield at point G is obtained, the algorithm is ready for the next temporal iteration. Mathematically,

$$\phi = w_0 + w_1 x + w_2 y,\tag{2}$$

where  $\phi$  is the wavefield, x and y are the coordinates, and  $w_0$ ,  $w_1$ , and  $w_2$  are the linear interpolation coefficients obtained by solving

$$\begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} 1 & x_S & y_S \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{pmatrix}^{-1} \begin{pmatrix} \phi_S \\ \phi_1 \\ \phi_2 \end{pmatrix}. \tag{3}$$

The most important advantage of the immerse boundary method over other numerical methods is that its grid complexity and numerical computation quality are not significantly affected by boundary geometry complexity. In addition, compared with curvilinear body-conformal grid methods, the Cartesian grid system used by the immersed boundary method reduces the per-grid-point operation cost due to the absence of extra terms brought by grid transformations.

Although the original immersed boundary method is simple to implement, it is a low order accuracy method due to its simple linear interpolation scheme. Furthermore, when the boundary intercept point is close to one of the interior points used in the extrapolation, extremely large weighting coefficient can be generated even if the surface topography geometry is simple, leading to a numerical instability issue. This issue becomes even more serious when high order reconstruction polynomials are used for the ghost wavefield interpolation. Besides, ramifications of boundary treatment have severe impact on accuracy. In order to overcome these drawbacks, we developed an improved immersed boundary finite-difference method (IBFD) by introducing some special techniques. In this section, we will discuss the technical details of these new features.

#### Multi-Level Ghost Grid Scheme

Figure 3 is a diagram of the IBFD grid system. Similar to the original immersed boundary method scheme shown in Figure 2, there is no approximated staircase surface boundary required in this method. Here, the actual free surface boundary is allowed to cut through the Cartesian grids. Furthermore, unlike the method of vacuum, the material property above an actual surface boundary is no longer defined as air, because the surface boundary conditions in the IBFD method are not enforced through medium property contrasts. Instead, the stress-free (p=0) boundary condition at an actual air-earth interface is incorporated implicitly by reconstructing the wavefields at the ghost grids through interpolation and extrapolation. In other words, the wavefields in a ghost zone are extrapolated from the associated interior grids with the constraint that the stress at the air-earth interface vanishes. By doing this, Cartesian grid lines and the actual free surface boundary are decoupled while the free surface boundary conditions are satisfied at the exact air-earth interface locations.

To achieve high order finite-difference accuracy, a multi-level ghost grid scheme is introduced. With this scheme, grids in a ghost zone are classified into 1st-level ghost grids (defined as grids that have at least one neighboring interior grid), 2nd-level ghost grids (defined as grids that have at least one neighboring 1st-level ghost grid), and so on. In practice, wavefields at 1st-level ghost grids are updated through extrapolation using the associated interior point wavefields only. Then, 2nd-level ghost grid wavefields are obtained from the associated interior point wavefields only or from the combination of the interior point wavefields and the updated 1st-level ghost grid wavefields. For higher order finite-difference schemes, more levels of ghost grids need to be included in this procedure. After all the levels in the ghost zone are updated, we can update the wavefields in the whole computational

domain as a conventional finite-difference method for time marching purpose.

## Ray-Casting Ghost Wavefield Extrapolation

In this subsection, we discuss the approach of ghost grid wavefield extrapolation, which plays an important role in the IBFD method and directly affects its accuracy order and numerical stability. There are a number of options available for ghost wavefield extrapolation. We follow the approach proposed by Zhao (2010), the ray-casting extrapolation method. The main idea is to use a set of local fictitious points along the normal direction to the free surface to approximate the spatial derivatives of wavefields at the intercept point by finite-difference methods. Each ghost point has its own set of local fictitious points.

Let us first consider a general scenario shown in Figure 4 to illustrate the idea of how we reconstruct wavefield p at the 1st-level ghost point G. To carry out the extrapolation for wavefield p at the ghost point G (i.e., p (G)), a normal line is generated, passing the ghost point G, perpendicular to the free surface boundary  $\Gamma$  at an intercept point S. In order to achieve high order accuracy, multiple fictitious points (denoted as  $F_1$ ,  $F_2$ , and  $F_3$  in Figure 4 are picked to apply the free surface boundary condition at S. In the case shown in Figure 4, the three fictitious points, combined with the ghost point G, define a 4-point stencil for the evaluation of wavefield p at S. Consequently, the wavefield p at point G is reconstructed by solving the following equation with the stress-free boundary condition implicitly enforced at S, as follows

$$p(S) = c_0^G p(G) + \sum_{i=1}^N c_i^F p(F_i) = 0,$$
(4)

where  $c_i^F$  are the interpolation coefficients associated with the fictitious points,  $c_0^G$  is the interpolation coefficient associated with the ghost point, and N is the number of fictitious

points. Wavefield p at a fictitious point is evaluated by interpolation using the four neighboring auxiliary points as shown in Figure 4, as follows

$$p(F_i) = \sum_{j=1}^{M} c_j^A p(A_{ij}),$$
 (5)

where  $c_j^A$  are the interpolation coefficients associated with the auxiliary points, and M is the number of the auxiliary points. By solving (4) and (5), one may reconstruct the ghost point wavefield using

$$p(G) = -\frac{1}{c_0^G} \sum_{i=1}^{N} c_i^F \sum_{j=1}^{M} c_j^A p(A_{ij}).$$
(6)

After reconstruction of the 1st-level ghost grid point wavefields, similar procedures are implemented to update the 2nd-level ghost grid point wavefields. In this study, the 1st-level ghost grid point G is not included in the finite-difference stencil for the 2nd-level ghost grid point wavefield evaluation. Thus, these two levels are obtained independently. The number of ghost grid levels is dependent on the finite-difference accuracy order employed. For 8th-order accuracy, 4 levels are needed to handle the free surface boundary conditions. The 3rd- and 4th-level ghost wavefields are estimated in a similar way using equation (6). Finally, the multiple layer ghost wavefields are all updated to coat the free surface and are ready for a regular whole domain finite-difference update.

In this ray-casting discretization scheme, each ghost point wavefield value depends on a set of local auxiliary interior points. Therefore, although all ghost point wavefields and interior point wavefields are actually coupled, this local operator approach avoids solving a large linear system to mitigate instability issues while keeping the computational overhead at a negligible level.

# Recursive Ghost Wavefield Reconstruction

Under some circumstances, we may encounter more complicated situations in which some auxiliary points also act as ghost points whose wavefields are unknown. For example, in Figure 5, G' is a ghost point but it also belongs to the auxiliary point set for evaluation of wavefields at the fictitious point  $F_1$ . In such a case, Zhao (2010) proposed an approach where the fictitious point set is shifted downward by one grid. In other words,  $F_1$  is skipped and an extra fictitious point  $F_4$  is appended to the stencil (Scheme B in Figure 5). Consequently, all the auxiliary points are now sitting below the free surface boundary and the ghost wavefield reconstruction can be implemented by equation (6). An alternative approach is to shift the first line of the auxiliary points to the left by one grid to exclude point G' from the stencil for  $F_1$  interpolation (Scheme A in Figure 5). In spite of more complicated preprocessing procedures, both of these approaches work well for slowly varying surface topography. However, for highly irregular surface topography, these methods are no longer effective, as will be discussed later.

Instead of using the grid down-shifting or lateral-shifting methods, we keep point G' in the auxiliary point set for the wavefield reconstruction at the ghost point G. One of the advantages of doing this is that no special treatment is needed in the selection of auxiliary points, which simplifies the preprocessing procedure. However, if we simply use the wavefield value at G' obtained from the previous temporal iteration to estimate the ghost wavefield at G, a certain level of artificial scattering energy is generated that deteriorates the simulation results. To address this issue, we developed a special recursive interpolation scheme for this type of ghost wavefield reconstruction. First, we set all ghost wavefields to be 0. Then, we update the ghost wavefields one by one using equation (6) in a recursive manner until

convergence is achieved. Mathematically, this procedure can be described in a matrix form as

$$\mathbf{P}^{n+1}(G) = \mathbf{C}^A \mathbf{P}(A) + \mathbf{C}^G \mathbf{P}^n(G), \tag{7}$$

where  $\mathbf{P}^n(G)$  are the wavefields at ghost point at n-th iteration,  $\mathbf{P}(A)$  are the wavefields at the auxiliary points located below the free surface boundary, and  $\mathbf{C}^A$  and  $\mathbf{C}^G$  are the corresponding interpolation coefficient matrices. This strategy removes most of the remaining artificial scattering energy, as will be demonstrated by the numerical example. According to equation (7),  $\mathbf{P}(A)$  does not change during the iteration but  $\mathbf{P}(G)$  is updated at each iteration. In our experiments,  $\mathbf{P}(G)$  converges quickly in approximately 10 iterations. As we employ a local operator for the ghost wavefield reconstruction, the coefficient matrices  $\mathbf{C}^A$  and  $\mathbf{C}^G$  are highly sparse. In addition, the number of ghost grids is usually very limited even for a multi-level ghost grid scheme. As a result, the computational cost of solving equation (7) is negligible, in comparison with the cost of a whole domain finite-difference update.

### Local Continuity and Sub-grid Curvature Capture

For geometrically complex free surface topography featuring large curvatures, the zeroth order stress-free Dirichlet boundary condition might not be accurate enough. In order to accurately simulate the rapid wavefield variations near a free surface, higher order surface boundary conditions are required, i.e., the normal and tangential derivative conditions. In a conventional immersed boundary method based on a Cartesian coordinate system x-z, with the aid of an auxiliary rotated Cartesian coordinate system x-z' shown in Figure 6,

these Dirichlet and Neumann boundary conditions can be formulated as

$$\begin{cases} v_{x'}|_{\Gamma} = 0\\ \frac{\partial v_{z'}}{\partial z'}|_{\Gamma} = 0. \end{cases}$$
(8)

Unfortunately, boundary condition (8) is derived from the acoustic wave propagation governing equation under a rotated Cartesian coordinate system x'-z' and this approach fails to capture local continuity and sub-grid curvatures of surface topography.

In our approach, instead of rotating the Cartesian coordinate, we introduce an extra local cylindrical coordinate  $\phi$ -r as shown in Figure 6, to form a dual coordinate system. Under this local cylindrical coordinate, the original wave propagation governing equations are reformulated as

$$\begin{cases}
\frac{\partial v_r}{\partial t} = \frac{1}{\rho} \frac{\partial p}{\partial r} \\
\frac{\partial v_{\phi}}{\partial t} = \frac{1}{\rho} \left( \frac{1}{r} \frac{\partial p}{\partial \phi} \right) \\
\frac{\partial p}{\partial t} = -K \left( \frac{1}{r} v_r + \frac{\partial v_r}{\partial r} + \frac{1}{r} \frac{\partial v_{\phi}}{\partial \phi} \right).
\end{cases} \tag{9}$$

Starting from (9), the normal and tangential derivative boundary conditions under this local cylindrical coordinate system can be derived as

$$\begin{cases} v_{\phi}|_{\Gamma} = 0\\ (\frac{1}{r}v_r + \frac{\partial v_r}{\partial r})|_{\Gamma} = 0. \end{cases}$$
 (10)

The curvature  $\kappa|_{\Gamma} = (1/r)|_{\Gamma}$  defines the local cylindrical coordinate system and the corresponding osculating circle at the intercept point S. The boundary condition (10) describes the differentiation along the osculating circle assumed to be a more accurate approximation of the actual curved free surface boundary. When the curvature tends to be 0 (i.e.,  $r \to \infty$  at the intercept point), the surface boundary becomes flat and the corresponding boundary condition (10) is reduced to (8). From this observation, boundary condition (8) is a special case of (10) where the curved free surface is approximated by an infinite tangential plane.

As a result, using the conventional Neumann boundary condition in (8) to approximate the Robin boundary condition in (10) can lead to significant errors for geometrically complex surface topography.

Combining equation (10) and the Cartesian-cylindrical transformation formulation, the particle velocity  $v_x$  defined at ghost point G can be calculated using

$$v_{x}(G) = -\sum_{i=1}^{N} \left[ \frac{\cos^{2}\theta c_{i}^{0}}{c_{0}^{0}} + \frac{\sin^{2}\theta \left(\kappa c_{i}^{0} + c_{i}^{1}\right)}{\kappa c_{0}^{0} + c_{0}^{1}} \right] v_{x}\left(F_{i}\right) + \sin\theta \cos\theta \sum_{i=1}^{N} \left( \frac{c_{i}^{0}}{c_{0}^{0}} - \frac{\kappa c_{i}^{0} + c_{i}^{1}}{\kappa c_{0}^{0} + c_{0}^{1}} \right) v_{z}\left(F_{i}\right),$$

$$(11)$$

where  $\kappa$  is the local curvature at the intercept point S,  $\theta$  is the angle between the vertical direction and the normal direction to the surface at the intercept point S,  $c_i^m$  represents the interpolation coefficient (for m=0) and the first order derivative approximation coefficient (for m=1) for the associated fictitious points (Fornberg, 1988). Similarly, we are able to calculate  $v_z$  defined at point G,

$$v_{z}(G) = \sin\theta \cos\theta \sum_{i=1}^{N} \left( \frac{c_{i}^{0}}{c_{0}^{0}} - \frac{\kappa c_{i}^{0} + c_{i}^{1}}{\kappa c_{0}^{0} + c_{0}^{1}} \right) v_{x}(F_{i}) - \sum_{i=1}^{N} \left[ \frac{\sin^{2}\theta c_{i}^{0}}{c_{0}^{0}} + \frac{\cos^{2}\theta \left(\kappa c_{i}^{0} + c_{i}^{1}\right)}{\kappa c_{0}^{0} + c_{0}^{1}} \right] v_{z}(F_{i}).$$

$$(12)$$

#### **IBFD** Workflow

The workflow of the IBFD method is summarized as follows:

- 1. Input free surface topography geometry to determine the multiple layers of ghost grids; for each ghost grid point, estimate the corresponding surface curvature, find the associated auxiliary interior grid points, and calculate the interpolation coefficients;
- 2. implement a conventional finite-difference update of wavefields p in the whole computation domain;

- 3. extrapolate from the interior auxiliary grid points to estimate the 1st-level ghost wavefields  $p^G$  by applying the stress-free boundary condition  $p|_{\Gamma} = 0$ ;
- 4. repeat the procedure described in step 3 for the remaining levels;
- 5. implement a conventional finite-difference update of wavefields  $v_x$  and  $v_z$  in the whole computation domain;
- 6. decompose  $v_x$  to obtain  $v_r$  and  $v_\phi$  for each ghost point and the associated auxiliary interior points;
- 7. extrapolate to estimate the 1st-level ghost wavefield  $v_{\phi}^{G}$  by enforcing the boundary condition  $v_{\phi}|_{\Gamma} = 0$ ;
- 8. extrapolate to estimate the 1st-level ghost wavefield  $v_r^G$  by enforcing the boundary condition  $\left(\frac{1}{r}v_r + \frac{\partial v_r}{\partial r}\right)|_{\Gamma} = 0;$
- 9. repeat step 7 and 8 to finish the remaining levels;
- 10. combine  $v_{\phi}^{G}$  and  $v_{r}^{G}$  to reconstruct  $v_{x}^{G}$  at all ghost point locations;
- 11. similarly, step 6 to step 10 are implemented to reconstruct  $v_z^G$  at all ghost points;
- 12. go to step 2 to start the next finite-difference iteration and this procedure is repeated until all the finite-difference temporal iterations are finished.

The computational overhead of the IBFD method includes two parts. The first part, described in step 1, is populating the ghost grids, finding the corresponding fictitious points and auxiliary grids, and calculating the associated interpolation coefficients. Because this part is a one-time preprocessing procedure and it is completely automatic, it barely affects the overall efficiency. The second part, consisting of step 3, 4, 6, 7, 8, 9, 10, and

11, is the ghost wavefield estimation, which needs to be implemented at each IBFD iteration. Therefore, this part has some impact on the efficiency. Here, we will evaluate the overall computational complexity of the IBFD algorithm. The computational complexity of a conventional FDTD algorithm, steps 2 and 6, is  $O(N^{1+1/d})$  for N grid points and d spatial dimensions (Taflove et al., 2013)(p.560), where the extra factor of  $O(N^{1/d})$  is due to the number of time steps. The ghost wavefield estimation is carried out only near a free surface at  $O(N^{(d-1)/d})$  grid points for  $N^{1/d}$  time steps. Consequently, the approximate extra computational complexity introduced by the ghost wavefield estimation procedure is  $O(k*(m/2)*N^{(d-1)/d}*N^{1/d})$ , i.e., O(k\*(m/2)\*N), where k is the iteration number of the recursive ghost wavefield reconstruction and m is the finite-difference accuracy order (Oğuz and Gürel, 1997). Because k is a relatively small number ( $\sim 10$ ), this extra computational cost brought by the ghost wavefield estimation is much lower than the cost of a conventional FDTD algorithm. The computation time measured in the second numerical example presented in this work validated this computational complexity analysis. In that numerical experiment, the CPU time for the conventional FDTD is 6.75 s; the CPU time for the IBFD is 7.02 s when k = 5 and m = 4; the CPU time for the IBFD is 7.35 s when k=10 and m=4; the CPU time for the IBFD is 7.64 s for k=15 and m=4. The measured computation overhead for these three cases are 4%, 8.8%, and 13.2% respectively. This experiment result is generally consistent to the computational complexity analysis. Based on the above analysis and the experiment result, we believe that the efficiency of IBFD is comparable to a conventional FDTD algorithm.

# Some Implementation Strategies on Topography Treatment

Figure 7 shows a highly irregular surface boundary including an overhanging structure. For the ghost point  $G^A$ , there are not enough interior auxiliary points that can be found for the extrapolation procedure due to the local fine geometry structure. In such a case, either the grid-down-shifting or grid-lateral-shifting strategy suggested by Zhao (2010) does not work. On the other hand, the recursive ghost wavefield reconstruction approach proposed in this work can easily solve this problem without any tedious special treatment, because this approach does not differentiate between interior points and ghost points during the procedure of selecting auxiliary points to form an extrapolation stencil. In other words, some ghost points can participate in the reconstruction process of another ghost point wavefield. The initial wavefields at the ghost points can be set to 0. Although these inaccurate initial wavefields may introduce some errors in the beginning of a ghost wavefield reconstruction process, these errors are reduced to a minimum level through the recursive wavefield interpolation according to our numerical experiments.

In practice, sometimes we encounter situations where more than one normal-intercept points are found, such as the points  $S_1$  and  $S_2$  shown in Figure 7. In this case, the intercept point that has the shortest intercept,  $S_1$ , is chosen. In some other cases, if a fictitious point is very close to an intercept point as shown in Figure 8, its associated interpolation coefficient becomes extremely large in comparison with that associated with the ghost point. As a result, equation (6) will result in a highly overestimated wavefield value at the ghost point, causing a numerical instability issue. Therefore, the algorithm automatically removes these singularity points by setting a normal intercept distance threshold  $\alpha \min(\Delta x, \Delta z)$ , where  $\alpha$  is a small number.

### NUMERICAL EXAMPLES

Three numerical simulations involving irregularly shaped free surface topography are conducted to validate the proposed IBFD algorithm. The surface topography geometry of the first example is shown in Figure 9a, where the hill in the middle is constructed by a partially buried circle. The source is buried deep in the subsurface while the receivers are distributed evenly at the sea level. Figure 9b shows the shot gather generated by a conventional finite-difference method, in which many scattering artifacts are observed due to the staircase approximation to the curved free surface boundary. On the other hand, the IBFD algorithm (in this simulation, without the recursive ghost wavefield reconstruction scheme) removes most of the artificial scattering effect, as presented in Figure 9c. As a matter of fact, the simulation result plotted in Figure 9c still has some remaining artifacts although they are very weak compared with the signal. To visually boost these remaining artifacts, we re-plotted Figure 9c result in Figure 10a using a different plotting clip parameter. After that, we performed the numerical simulation again with the recursive ghost wavefield reconstruction scheme and presented the simulation result in Figure 10b. Comparing Figure 10a and Figure 10b, we note that the artificial scattering effects are further suppressed to an extremely low level, indicating that an IBFD algorithm featuring the recursive ghost wavefield reconstruction technique is immune to the staircasing errors. The scattering energy observed in Figure 10b is real, caused by the surface boundary discontinuity, which can be clearly seen in Figure 9a. To further validate the accuracy and the scattering artifact removal capability of the IBFD method, the simulation results generated by the conventional finite-difference method with refined grids are compared with the IBFD result. Figure 11a to Figure 11c show the shot gathers produced by the conventional finite-difference with grid size of 10 m, 2 m, and 1.11 m respectively. With the decrease of the grid size, the

artifacts in the shot gathers become weaker and weaker. In this numerical experiment, the source wavelet is a Ricker wavelet with the dominant frequency of 15 Hz and the P wave velocity is 2000 m/s, hence the point-per-wavelength (PPW) for the shortest wavelength is approximately 50 for the case  $\Delta x = \Delta z = 1.11$  m. In Figure 11e, a sample trace extracted from the shot gathers is plotted to rigorously compare the algorithm performances, showing that the IBFD result with the grid size of 10 m is very close to the conventional finite-difference result with  $\Delta x = \Delta z = 1.11$  m, which serves as the reference solution here. On the other hand, the trace obtained using the conventional finite-difference method with  $\Delta x = \Delta z = 10$  m significantly deviates from the reference solution.

The second numerical simulation was conducted on a model featuring a ramp and a steep cliff on the free surface shown in Figure 12a. The misalignment between the grid lines and the cliff makes it an extreme topographic model, which is challenging for the coordinate mapping methods to treat efficiently. The velocity is homogeneous (2000 m/s) and the source is a Ricker wavelet whose dominant frequency is 15 Hz. In the conventional finite-difference simulation result shown in Figure 12b, the artificial scattering effect caused by the ramp edge and the cliff approximated by the staircases reaches a significant level. In contrast, the result produced by the IBFD method, which is shown in Figure 12c, is almost immune to these artifacts.

To demonstrate the capability and the performance of the IBFD algorithm on treating a more realistic case, we implemented another wave propagation simulation in a large scale model shown in Figure 13, where the velocity ranges from 3500 m/s to 6300 m/s. The model size is 21 km in lateral direction and 9 km in vertical direction. The shot and the associated receivers are located near the surface as shown in Figure 13. The maximum offset is 6 km and the 600 receivers are uniformly distributed every 20 m on both sides of the

shot. The velocity model is discretized using uniform grids with 10 m grid size. A Ricker wavelet with a dominant frequency of 30 Hz is used to excite the simulation. With the 8th order spatial accuracy and the 2nd order temporal accuracy finite-difference scheme, we believe that numerical dispersion is not an issue because the number of grids per minimum wavelength is approximately 5. A shot gather generated by a conventional finite-difference method is shown in Figure 14a to Figure 14c, where Figure 14a and Figure 14b are the zoom-in images of the shot gather for display purpose. Compared with the first numerical example, the highly irregular free surface topography combined with the multilayered velocity model produces a much more complicated wave pattern due to multiple reflections and scattering. In Figure 14d to 14f, the recorded wavefields using the IBFD method are presented. Apparently, almost all of the scattering artifacts due to the staircasing error vanish (note the regions highlighted by the circles in the figures).

# **CONCLUSIONS**

We report an improved immersed-boundary finite-difference method (IBFD) for seismic wave propagation modeling with arbitrarily curved free surface topography in presence. Unlike FEM, SEM, and some finite-difference algorithms employing structured curvilinear body-fitted grids, the IBFD method uses a regular Cartesian grid system, which greatly simplifies mesh generation and other related preprocessing procedures. Enforcing the free surface boundary conditions at actual surface locations through a recursive ghost wavefield reconstruction technique, the IBFD method is able to represent irregular free surface geometry accurately. Numerical experiments demonstrated that this algorithm is immune to the notorious staircasing error, which is inevitable in conventional finite-difference methods. Furthermore, by introducing a dual coordinate system, the IBFD algorithm is able to pre-

cisely capture the effects of local continuity and large curvatures on the wave propagation behaviors near a surface boundary, significantly improving the overall accuracy. In this method, irregular surface topography is treated with high order accuracy with a multi-level ghost wavefield extrapolation scheme that is completely automatic. Because the ghost zone wavefield extrapolation procedure is only required in the vicinity of a free surface, the additional computational cost of the IBFD algorithm is negligible even for very high-order finite-difference schemes. According to our numerical experiments, the efficiency of the IBFD method remains at the same level as a conventional finite-difference method. Extension to 3D scenarios is straightforward by replacing the local cylindrical coordinate system with a local spherical coordinate. Generalization of this method to elastic cases is under investigation. The main idea remains the same for elastic scenarios, some modifications need to be made to the algorithm because the normal direction wavefield derivative and the tangential direction wavefield derivative are numerically coupled to accommodate the elastic free surface boundary conditions. Because this algorithm can handle any arbitrarily curved surface topography automatically under a regular Cartesian grid system, we believe that IBFD has a great potential to become a powerful forward modeling engine for FWI land data processing.

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### REFERENCES

- Abubakar, A., W. Hu, T. M. Habashy, and P. M. van den Berg, 2009, Application of the finite-difference contrast-source inversion algorithm to seismic full-waveform data: Geophysics, 74, WCC47–WCC58.
- Appelö, D., and N. A. Petersson, 2009, A stable finite difference method for the elastic wave equation on complex geometries with free surfaces: Communications in Computational Physics, 5, 84–107.
- Berthelsen, P. A., and O. M. Faltinsen, 2008, A local directional ghost cell approach for incompressible viscous flow problems with irregular boundaries: Journal of computational physics, 227, 4354–4397.
- Bleibinhaus, F., and S. Rondenay, 2009, Effects of surface scattering in full-waveform inversion: Geophysics, **74**, WCC69–WCC77.
- de la Puente, J., M. Ferrer, M. Hanzich, J. E. Castillo, and J. M. Cela, 2014, Mimetic seismic wave modeling including topography on deformed staggered grids: Geophysics, 79, T125–T141.
- Fornberg, B., 1988, Generation of finite difference formulas on arbitrarily spaced grids: Mathematics of computation, **51**, 699–706.
- Gao, T., Y.-H. Tseng, and X.-Y. Lu, 2007, An improved hybrid cartesian/immersed boundary method for fluid-solid flows: International Journal for Numerical Methods in Fluids, 55, 1189–1211.
- Habashy, T., A. Abubakar, G. Pan, and A. Belani, 2011, Source-receiver compression scheme for full-waveform seismic inversion: Geophysics, 76, R95–R108.
- Hestholm, S., and B. Ruud, 1998, 3-D finite-difference elastic wave modeling including surface topography: Geophysics, **63**, 613–622.

- Hu, W., 2014, Fwi without low frequency data beat tone inversion: SEG Technical Program Expanded Abstracts 2014, Society of Exploration Geophysicists, 1116–1120.
- Hu, W., A. Abubakar, T. Habashy, and J. Liu, 2011, Preconditioned non-linear conjugate gradient method for frequency domain full-waveform seismic inversion: Geophysical Prospecting, 59, 477–491.
- Hu, W., A. Abubakar, and T. M. Habashy, 2009, Simultaneous multifrequency inversion of full-waveform seismic data: Geophysics, 74, R1–R14.
- Hu, W., and S. A. Cummer, 2006, An FDTD model for low and high altitude lightninggenerated em fields: Antennas and Propagation, IEEE Transactions on, **54**, 1513–1522.
- Komatitsch, D., and J. P. Vilotte, 1998, The spectral element method: an efficient tool to simulate the seismic response of 2D and 3D geological structures: Bulletin of the Seismological Society of America, 88, 368–392.
- Krebs, J. R., J. E. Anderson, D. Hinkley, R. Neelamani, S. Lee, A. Baumstein, and M.-D. Lacasse, 2009, Fast full-wavefield seismic inversion using encoded sources: Geophysics, 74, WCC177–WCC188.
- Levander, A. R., 1988, Fourth-order finite-difference p-sv seismograms: Geophysics, **53**, 142501436.
- Li, J., Y. Zhang, and M. N. Toksoz, 2010, Frequency-domain finite-difference acoustic modeling with free surface topography using embedded boundary method: Massachusetts Institue of Technology, Earth Resources Laboratory.
- Li, M., J. Rickett, and A. Abubakar, 2013, Application of the variable projection scheme for frequency-domain full-waveform inversion: Geophysics, 78, R249–R257.
- Lombard, B., and J. Piraux, 2004, Numerical treatment of two-dimensional interfaces for acoustic and elastic waves: Journal of Computational Physics, **195**, 90–116.

- Lombard, B., J. Piraux, C. Gélis, and J. Virieux, 2008, Free and smooth boundaries in 2-D finite-difference schemes for transient elastic waves: Geophysical Journal International, 172, 252–261.
- Ma, Y., D. Hale, B. Gong, and Z. Meng, 2012, Image-guided sparse-model full waveform inversion: Geophysics, 77, R189–R198.
- Min, D. J., C. Shin, R. G. Pratt, and H. S. Yoo, 2003, Weighted-averaging finite-element method for 2D elastic wave equations in the frequency domain: Bulletin of the Seismological Society of America, 93, 904–921.
- Mittal, R., H. Dong, M. Bozkurttas, F. Najjar, A. Vargas, and A. von Loebbecke, 2008, A versatile sharp interface immersed boundary method for incompressible flows with complex boundaries: Journal of computational physics, 227, 4825–4852.
- Oğuz, U., and L. Gürel, 1997, Interpolation techniques to improve the accuracy of the plane wave excitations in the finite difference time domain method: Radio Science, **32**, 2189–2199.
- Pan, D., and T.-T. Shen, 2009, Computation of incompressible flows with immersed bodies by a simple ghost cell method: International journal for numerical methods in fluids, **60**, 1378–1401.
- Peskin, C. S., 1972, Flow patterns around heart valves: a digital computer method for solving the equations of motion: UMI.
- Pratt, R. G., C. Shin, and G. Hick, 1998, Gauss–Newton and full Newton methods in frequency–space seismic waveform inversion: Geophysical Journal International, 133, 341–362.
- Robertsson, J. O., 1996, A numerical free-surface condition for elastic/viscoelastic finite-difference modeling in the presence of topography: Geophysics, **61**, 1921–1934.

- Shinn, A., M. Goodwin, and S. Vanka, 2009, Immersed boundary computations of shearand buoyancy-driven flows in complex enclosures: International Journal of Heat and Mass Transfer, **52**, 4082–4089.
- Shragge, J., 2014a, Reverse time migration from topography: Geophysics, 79, S141–S152.
- ——, 2014b, Solving the 3D acoustic wave equation on generalized structured meshes: A finite-difference time-domain approach: Geophysics, **79**, T363–T378.
- Symes, W. W., 2008, Migration velocity analysis and waveform inversion: Geophysical prospecting, **56**, 765–790.
- Taflove, A., A. Oskooi, and S. G. Johnson, 2013, Advances in FDTD computational electrodynamics: photonics and nanotechnology: Artech house.
- Tarantola, A., 1984, Inversion of seismic reflection data in the acoustic approximation: Geophysics, 49, 1259–1266.
- Tseng, Y.-H., and J. H. Ferziger, 2003, A ghost-cell immersed boundary method for flow in complex geometry: Journal of computational physics, 192, 593–623.
- Venkatarayalu, N. V., R. Lee, Y.-B. Gan, and L.-W. Li, 2007, A stable FDTD subgridding method based on finite element formulation with hanging variables: Antennas and Propagation, IEEE Transactions on, **55**, 907–915.
- Virieux, J., and S. Operto, 2009, An overview of full-waveform inversion in exploration geophysics: Geophysics, **74**, WCC1–WCC26.
- Xiao, K., D. J. Pommerenke, and J. L. Drewniak, 2007, A three-dimensional FDTD subgridding algorithm with separated temporal and spatial interfaces and related stability analysis: Antennas and Propagation, IEEE Transactions on, 55, 1981–1990.
- Zhang, C., and W. W. Symes, 1998, Fourth-order, full-stencil immersed interface method for elastic waves with discontinuous coefficients: SEG Technical Program Expanded Ab-

stracts 1998, 1929–1932.

Zhao, S., 2010, A fourth order finite difference method for waveguides with curved perfectly conducting boundaries: Computer Methods in Applied Mechanics and Engineering, 199, 2655–2662.