Accurate wave equation modeling

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ABSTRACT

The study of complex wave fields requires precise modeling of the acoustic or elastic wave equation in two and three dimensions. I solve the elastic wave equation on a discrete grid using an accurate-time-update pseudospectral method. Spatial derivatives are calculated using the pseudospectral method; time evolution is based upon an orthogonal polynomial expansion of the formal solution of the wave equation. The resulting algorithm, like traditional finite-difference techniques, is a time-stepping solution to the wave equation. It differs from finite-difference methods because it is accurate to arbitrary precision for large time step sizes and all spatial frequencies up to Nyquist. Most importantly, numerical dispersion and numerical anisotropy are eliminated. For models with curved boundaries between regions of different material parameters, I construct an irregular grid that follows the boundaries, and a mapping that maps the irregular model grid onto a regularly sampled computational grid. The accurate-time-update pseudospectral method is used to calculate the solution of an appropriately modified wave equation on the computational grid. The resulting solution is mapped back onto the original irregular model grid. Mapping the interfaces to follow grid lines eliminates the errors associated with "stair-step" discretization of interfaces onto rectangular grids. The accurate-time-update pseudospectral method is useful whenever precise solutions to the elastic wave equation are needed in heterogeneous media.

INTRODUCTION

Historically, the acoustic or elastic wave equation was solved on a discrete grid using first or second-order differencing in time and space (Kelly et al., 1976); (Marfurt, 1984). The basic finite-difference method can be improved by using spatial differencing operators with more coefficients, while retaining second-order three-point time differencing. Commonly, these spatial difference operators are 5-33 points long

(Holberg, 1987), (Mora, 1986). Taking this approach to its limit, the pseudospectral method (Kosloff et al., 1984,1985) uses Fourier transformation, multiplication by ik, and inverse Fourier transformation to compute spatial derivatives. Note that since only derivatives are computed in the Fourier domain, these solutions to the wave equation are applicable in non-constant velocity media because all access to the velocity model occurs in the space domain. Pseudospectral spatial derivatives are accurate for all wavenumbers represented on the computational grid. Again, time-marching uses the three-point second-order time difference.

Dablain (1986) analyzed the error of the second-order second time difference and proposed a method for improving its accuracy by cascading the spatial derivatives of the wave equation operator. His innovation lights the way to wave equation modeling algorithms that have spectral accuracy in both space and time.

Tal-Ezer (1986) and Edwards et al. (1987) describe a new method for approximating the time dependence of solutions to hyperbolic partial differential equations such as the acoustic or elastic wave equation using orthogonal polynomials involving powers of the spatial differential operator of the equation. The orthogonal polynomial expression for the solution can be evaluated to arbitrary accuracy when pseudospectral spatial derivatives are used in the polynomial series. Rather than compute many time steps with a small time step size, Tal-Ezer's technique computes fewer time steps with a large time step size. This polynomial expression for the time evolution operator is a formal version of Dablain's heuristic of recursive application of spatial derivatives.

Fornberg (1988) gives another important contribution to accurate wave equation modeling. Curved interfaces between changes in material parameters cannot be adequately described on a rectangular grid, especially when models are sparsely sampled as allowed when using pseudospectral space derivatives. The "stair-step" discretization of boundaries on a rectangular grid leads to spurious diffractions and incorrect reflection coefficients versus angle of incidence. For boundaries that can be described by twice-differentiable curves, Fornberg builds an irregular grid model with grid lines aligned with the curved boundaries between material parameters. The irregular grid is mapped to a regular grid in a computation space where the pseudospectral method can be applied to an appropriately modified wave equation. This eliminates the discretization noise present in wave equation solutions when boundaries between regions of the model do not align with a rectangular grid.

I will briefly show how Dablain's notion of cascading spatial derivatives to improve the time derivative is equivalent to Tal-Ezer's orthogonal-polynomial expansion solution to the wave equation. I combine the techniques of Tal-Ezer and Fornberg to solve acoustic and elastic wave equations on irregular grid models with the accurate-time-update pseudospectral method. Algorithms based on this combined method resemble traditional finite-difference modeling algorithms in that they are explicit, time-marching solutions to wave equations.

HIGH-ORDER TIME DERIVATIVES

For simplicity, I will use a generic wave equation in the following derivations; the results are general and apply to 2-D and 3-D acoustic as well as elastic wave equations. Consider equation (1):

$$\frac{\partial^2 U}{\partial t^2} = -\mathcal{L}^2 U \ . \tag{1}$$

$-\mathcal{L}^2$ is a second-order spatial differential operator; equation (1) is a wave equation. We are interested in numerical solutions of this equation on a discrete grid; so $U = U(x,t)$ where x and t will be discrete variables. U can be a vector (elastic wave equation) or a scalar (acoustic wave equation). To solve the discretized version of equation (1), we must approximate the temporal and spatial derivatives in the equation. If we take the spatial derivatives by the pseudospectral method, the errors that remain must be due to our approximation to the second time derivative.

A convenient formula for time marching can be derived using the second-order finite-difference approximation to the second time derivative in equation (1).

$$\frac{\partial^2 U}{\partial t^2} \approx \frac{1}{\Delta t^2}(U(t+\Delta t) - 2U(t) + U(t-\Delta t)) \ . \tag{2}$$

The second-order difference is the sum of two Taylor series; its complete expression is given by:

$$\frac{1}{\Delta t^2}(U(t+\Delta t) - 2U(t) + U(t-\Delta t)) = 2[\frac{1}{2}\frac{\partial^2 U}{\partial t^2} + \frac{\Delta t^2}{4!}\frac{\partial^4 U}{\partial t^4} + \frac{\Delta t^4}{6!}\frac{\partial^6 U}{\partial t^6} + ...] \ . \tag{3}$$

The wave equation (equation (1)) relates second and higher-order even time derivatives $\partial^{2n}U/\partial t^{2n}$ to powers of the spatial differential operator $-\mathcal{L}^2$. Replace the time derivatives in equation (3) with powers of the spatial derivatives.

$$\frac{1}{\Delta t^2}[U(t+\Delta t) - 2U(t) + U(t-\Delta t)] = 2[-\frac{1}{2}\mathcal{L}^2 U + \frac{\Delta t^2}{4!}\mathcal{L}^4 U - \frac{\Delta t^4}{6!}\mathcal{L}^6 U + ...] \ . \tag{4}$$

Think of equation (4) as the basis for a time-marching scheme to compute $U(t+\Delta t)$ from $U(t)$ and $U(t-\Delta t)$. Find $U(t+\Delta t)$ by evaluating the right hand side of equation (4) and adding the terms from the previous time levels. Evaluating only the first spatial derivative term in equation (4) gives the standard second-order in time, arbitrary order in space (depending on how $-\mathcal{L}^2$ is evaluated), time-marching solution to the wave equation.

$$\frac{1}{\Delta t^2}[U(t+\Delta t) - 2U(t) + U(t-\Delta t)] \approx -\mathcal{L}^2 U \ . \tag{5}$$

However, it is possible to update the wave field to the new time level $U(t+\Delta t)$ to arbitrary accuracy by evaluating more terms on the right-hand side or equation (4).

The higher powers of the spatial derivatives acting on U are computed by recursive application of $-\mathcal{L}^2$, e.g. $\mathcal{L}^4 U = -\mathcal{L}^2[-\mathcal{L}^2 U]$. Dablain (1986) used this technique to compute solutions to the acoustic wave equation to fourth-order accuracy in time by using the first two spatial derivative terms in equation (4) to compute the time updated wave field.

An interesting result is that the infinite series on the right-hand side of equation (4) is part of the power series for the cosine.

$$2[\cos \Delta t\mathcal{L} - 1]U = 2[-\frac{\Delta t^2}{2!}\mathcal{L}^2 U + \frac{\Delta t^4}{4!}\mathcal{L}^4 U - \frac{\Delta t^6}{6!}\mathcal{L}^6 U + ...] \ . \tag{6}$$

The formal solution for the updated wave field $U(t + \Delta t)$ can be seen by rewriting equation (4) above as:

$$U(t + \Delta t) - 2U(t) + U(t - \Delta t) = 2[\cos \Delta t\mathcal{L} - 1]U \ . \tag{7}$$

There is no closed form expression for the cosine of a differential operator acting on a function; a series expansion like the Taylor series in equation (4) above must be used. We could use the Taylor series above, and the truncation order of the time-update operator would be determined by where the series was truncated. The Taylor series is not always the most efficient representation of cosine because it requires many terms for large values of the argument of the cosine. Tal-Ezer (1987) presents a more efficient orthogonal polynomial series expansion for the cosine that can be used in time-marching schemes:

$$\cos t\mathcal{L} = \sum_{k=0}^{\infty} C_{2k} J_{2k}(tR) Q_{2k}(\frac{i\mathcal{L}}{R}) \ ; \tag{8}$$

where $C_{2k} = 1$ for $k = 0$ and $C_{2k} = 2$ for $k > 0$. R is chosen to bring the eigenvalues of $\mathcal{L}$ inside $(-i, i)$. The largest eigenvalue of $\mathcal{L}$ is the product of the maximum velocity, the highest spatial frequency, and $\sqrt{n}$ where n is the number of spatial dimensions. J_{2k} are the Bessel functions of the first kind of order $2k$. Q_{2k} are modified Chebychev polynomials that satisfy the following recurrence relation:

$$Q_0(\frac{i\mathcal{L}}{R}) = I \quad (\textit{the identity operator}) \ ;$$

$$Q_2(\frac{i\mathcal{L}}{R}) = I - \frac{2\mathcal{L}^2}{R^2} \ ;$$

$$Q_{2k+2}(\frac{i\mathcal{L}}{R}) = (-\frac{4\mathcal{L}^2}{R^2} + 2I)Q_{2k} - Q_{2k-2} \ . \tag{9}$$

In practice, the infinite series is truncated when additional terms only add numerical noise to the solution. Notice that equation (8) is evaluated just like equation (6), by recursive application of the spatial derivatives of the wave equation.

Adding a forcing function

In equation (1) no forcing function was present; and if no source term is active, the derivation of the previous section is valid for time stepping. However, when source terms are active, we need an alternate derivation. Consider the forced wave equation:

$$\frac{\partial^2 U}{\partial t^2} = -\mathcal{L}^2 U + F \quad . \tag{10}$$

The forcing function $F = f(x,t)$. As in equation (3), write the expansion for the second-order time difference:

$$\frac{1}{\Delta t^2}(U(t+\Delta t) - 2U(t) + U(t-\Delta t)) = 2[\frac{1}{2}\frac{\partial^2 U}{\partial t^2} + \frac{\Delta t^2}{4!}\frac{\partial^4 U}{\partial t^4} + \frac{\Delta t^4}{6!}\frac{\partial^6 U}{\partial t^6} + ...] \ . \tag{11}$$

Now write a different relation between the second and higher-order time derivatives and the spatial differential operator plus forcing function. Consider the fourth time derivative:

$$\frac{\partial^4 U}{\partial t^4} = \frac{\partial^2}{\partial t^2}\Big[-\mathcal{L}^2 U + F\Big] = -\mathcal{L}^2\Big[-\mathcal{L}^2 U + F\Big] + \frac{\partial^2 F}{\partial t^2} \quad . \tag{12}$$

Recursive application of $\partial^2/\partial t^2$ leads to a general formula for the spatial operator plus forcing function recursion that can be used to calculate the solution $U(t+\Delta t)$ from $U(t)$ and $U(t-\Delta t)$ using equation (11):

$$\frac{\partial^{2n+2} U}{\partial^{2n+2}} = -\mathcal{L}^2\Big[\frac{\partial^{2n} U}{\partial^{2n}}\Big] + \frac{\partial^{2n} F}{\partial t^{2n}} \quad . \tag{13}$$

Rewriting equation (11) with appropriate substitutions from equation (13) for all n does not lead to a cosine series, so I do not see an "clever" replacement series for the Taylor series in computing the time-marching operator like equation (8). However, when the source term is separable $F = f(t)g(x)$, and the initial conditions in equation (10) are zero, Edwards et al. (1987) present an orthogonal polynomial series similar to equation (8) that replaces equation (11).

EXACT SOLUTION TO THE WAVE EQUATION

It is also possible to derive the expression for accurate time marching by abandoning numerical analysis and starting afresh with an analytical approach (which is what Tal-Ezer did). The formal solution to the wave equation (equation (1)) for an initial value problem in an infinite or periodic medium can be written as:

$$U(t) = \cos(t\mathcal{L})U(0) + \frac{\sin(t\mathcal{L})}{\mathcal{L}}\frac{\partial U}{\partial t}(0) \ . \tag{14}$$

If U were simply a function of a single variable (and likewise, $\mathcal{L}$ =constant), this is easily recognized as the general solution to a homogeneous second-order ordinary differential equation. In the continuous case, U is a function of the continuous variables x and t, and $\mathcal{L}$ is a differential operator. When the solution is computed on a discrete grid, $U(t)$ is a vector function of x, and $\mathcal{L}$ is a matrix. Symbolically, equation (14) is still the solution to equation (1) for the continuous or discrete wave equation. To use equation (14) to advance a solution to the wave equation in time, add the solutions from equation (14) for $t = +T$ and $t = -T$:

$$U(T) = -U(-T) + 2\cos(T\mathcal{L})U(0) \quad . \tag{15}$$

This removes the odd part in time of the solution and leaves only the even part of the solution resembling the leap-frog time update operator derived from second-order time differencing. The time update operator for any time level can be found by shifting the initial conditions to other values of t:

$$U(t + \Delta t) = -U(t - \Delta t) + 2\cos(\Delta t\mathcal{L})U(t) \quad . \tag{16}$$

Equation (16) is the same expression we derived in equation (7) that describes how to propagate a solution at a given time level to another time level with arbitrary precision. All that remains is to evaluate numerically the solution using a truncated infinite series for the cosine.

IRREGULAR GRID PSEUDOSPECTRAL METHOD

The previous sections describe how to compute solutions to wave equations for general models on regular grids with no grid dispersion errors. However, grid dispersion is not the only source of error in wave equation models. Boundaries between changes in material parameters in a model are forced to be discretized onto a rectangular grid when pseudospectral spatial derivatives are used. When curved boundaries are present, they are discretized into a rough "stair-step" approximation of their desired shape. The wave field senses these rough boundaries which produce diffractions and incorrect reflection coefficients versus angle. The error in the solution is solely due to the incorrect representation of curved boundaries between materials. Fornberg (1988) shows how to compute wave fields for models with curved boundaries that are not aligned with a rectangular grid. His method is summarized here.

An irregular model grid that follows the curved reflector boundaries is constructed out of twice differentiable functions of the spatial variables. These functions provide a mapping from the irregular model grid to a regularly sampled computational grid. A modified wave equation is solved using the pseudospectral method on the regular grid and the solution is mapped back to the irregular grid by interpolation.

Write a mapping between the x, z coordinates of an irregularly sampled model and the coordinates ξ, η as:

$$x = X(\xi, \eta) \quad ; \quad z = Z(\xi, \eta). \tag{17}$$

Then choose the mapping functions $(X(\xi,\eta), Z(\xi,\eta))$ such that boundaries between regions of different material parameters in (x,z) follow the grid lines for regularly sampled (ξ,η). $(X(\xi,\eta), Z(\xi,\eta))$ defines a mapping from the irregular model grid to a rectangularly sampled computational grid. We can solve a wave equation on the irregular grid in (x,z) by mapping the model to the regular grid in (ξ,η) and solving a modified version of the wave equation in (ξ,η) space using the accurate-time-update pseudospectral method.

The modifications to the spatial derivatives in the wave equation are found by applying the chain rule. All spatial derivatives of the original wave equation in the model space are replaced with the derivatives shown in equations (18) and (19).

$$\frac{\partial U}{\partial x} = \frac{\partial U}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial U}{\partial \eta}\frac{\partial \eta}{\partial x} \quad ; \tag{18}$$

$$\frac{\partial U}{\partial z} = \frac{\partial U}{\partial \xi}\frac{\partial \xi}{\partial z} + \frac{\partial U}{\partial \eta}\frac{\partial \eta}{\partial z} \quad . \tag{19}$$

The derivatives of U with respect to ξ and η are calculated on the regular computational grid by Fourier transformation with respect to ξ or η, multiplication by ik_ξ of ik_η, and inverse Fourier transformation. The terms needed to apply the chain rule can be found by differentiating $X(\xi,\eta)$ and $Z(\xi,\eta)$ each with respect to both x and z and solving for the 4 unknowns.

$$\frac{dx}{dx} = 1 = \frac{\partial X}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial X}{\partial \eta}\frac{\partial \eta}{\partial x} \quad ; \tag{20}$$

$$\frac{dx}{dz} = 0 = \frac{\partial X}{\partial \xi}\frac{\partial \xi}{\partial z} + \frac{\partial X}{\partial \eta}\frac{\partial \eta}{\partial z} \quad ; \tag{21}$$

$$\frac{dz}{dx} = 0 = \frac{\partial Z}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial Z}{\partial \eta}\frac{\partial \eta}{\partial x} \quad ; \tag{22}$$

$$\frac{dz}{dz} = 1 = \frac{\partial Z}{\partial \xi}\frac{\partial \xi}{\partial z} + \frac{\partial Z}{\partial \eta}\frac{\partial \eta}{\partial z} \quad . \tag{23}$$

Solving for the four chain rule terms $\xi_x = \partial\xi/\partial x$, $\xi_z = \partial\xi/\partial z$, $\eta_x = \partial\eta/\partial x$, and $\eta_z = \partial\eta/\partial z$ in terms of the known quantities $X_\xi = \partial X/\partial\xi$, $X_\eta = \partial X/\partial\eta$, $Z_\xi = \partial Z/\partial\xi$, and $Z_\eta = \partial Z/\partial\eta$ gives:

$$\xi_x = \frac{Z_\eta}{X_\xi Z_\eta - X_\eta Z_\xi} \; ; \; \xi_z = \frac{-X_\eta}{X_\xi Z_\eta - X_\eta Z_\xi} \; . \tag{24}$$

$$\eta_x = \frac{-Z_\xi}{X_\xi Z_\eta - X_\eta Z_\xi} \; ; \; \eta_z = \frac{X_\xi}{X_\xi Z_\eta - X_\eta Z_\xi} \; . \tag{25}$$

To solve the wave equation on the irregular model grid, make the substitutions in equations (18) and (19) and solve this modified equation using the accurate-time-update pseudospectral method described in the previous section on the regular (ξ,η)

grid. The solution to the modified wave equation can be returned to the original model grid by inverse interpolation of the mapping from (x, z) to (ξ, η).

EXAMPLES

The phase velocities for a numerical solution to the 1-D wave equation are useful for studying grid dispersion. Figure 1 shows the numerical phase velocity for a second-order in time, high-order in space finite-difference method; a second-order in time, pseudospectral method; and the correct phase velocity for the model. Note that although the pseudospectral method has spatial derivatives accurate to Nyquist, the numerical phase velocity is not equal to the correct phase velocity. This error is due to the second-order time differencing. The phase velocity error in the finite-difference method becomes a function of propagation angle in 2-D and 3-D; this is called grid anisotropy. As I noted in SEP–57 (Etgen, 1988), the phase velocity error of the pseudospectral method is independent of propagation angle; thus, there is no grid anisotropy in any method that uses the pseudospectral method to calculate spatial derivatives.

Figure 2 shows the numerical phase velocity for the accurate-time-update pseudospectral method. The phase velocity is equal to the true phase velocity for all spatial wavenumbers. The small bump in phase velocity near $k_x = 0$ is due numerical difficulty in obtaining phase velocities near $k_x = 0$, and not due to inaccuracy in the time-update method. The Courant number, $v\ t/dx$ assumed for this phase velocity spectrum is $v\ dt/dx = 2$, where v is the wave propagation speed; dt is the time step size; and dx is the grid spacing. The increased accuracy of the time evolution operator allows time steps much larger than the Courant stability limit of any method that uses second-order time differencing. The stability limit $v\ dt/dx$ for finite-difference or pseudospectral methods using second-order time differences is .5 or less.

To illustrate the method, the acoustic and isotropic-elastic wave equations were solved for a model that has curved reflector boundaries. The curved boundaries were mapped to lines of constant η in a computational domain using equation (17). There was a sinusoidal reflector in the middle of the model and a hard boundary at the bottom. Figure 3 shows the irregular model grid; light lines denote grid lines of constant η ($x = \xi$ for this example); the heavy lines represent interfaces between regions of different material parameters. The modified wave equations (acoustic and elastic) were solved on the regular computational grid and the results were interpolated back onto the irregular grid for display. Note that mapping the wave field back to the irregular grid is not part of the time evolution of the wave equation. Mapping the computations back to the irregular grid is only needed for displaying time snapshots.

Figures 4 and 5 show time snapshots of an acoustic wave field computed for the irregular-grid model. Figures 6 and 7 show time snapshots of the horizontal

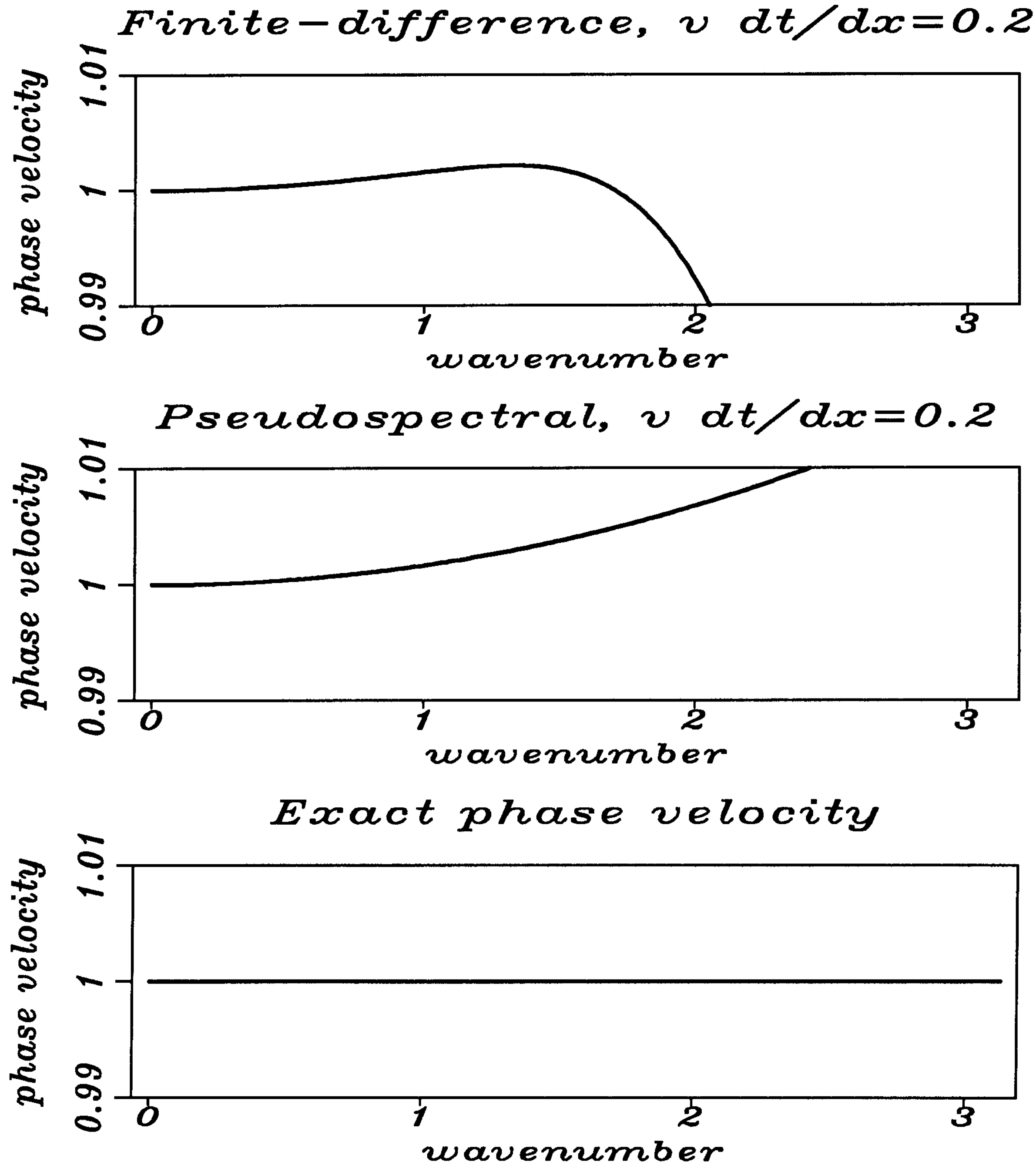

FIG. 1. Phase velocity versus wavenumber for a high-order finite-difference method, a pseudospectral method, and the correct phase velocity. The high-order finite-difference method has errors in the representation of both the time derivative and the space derivative. The pseudospectral method has error only in the time derivative.

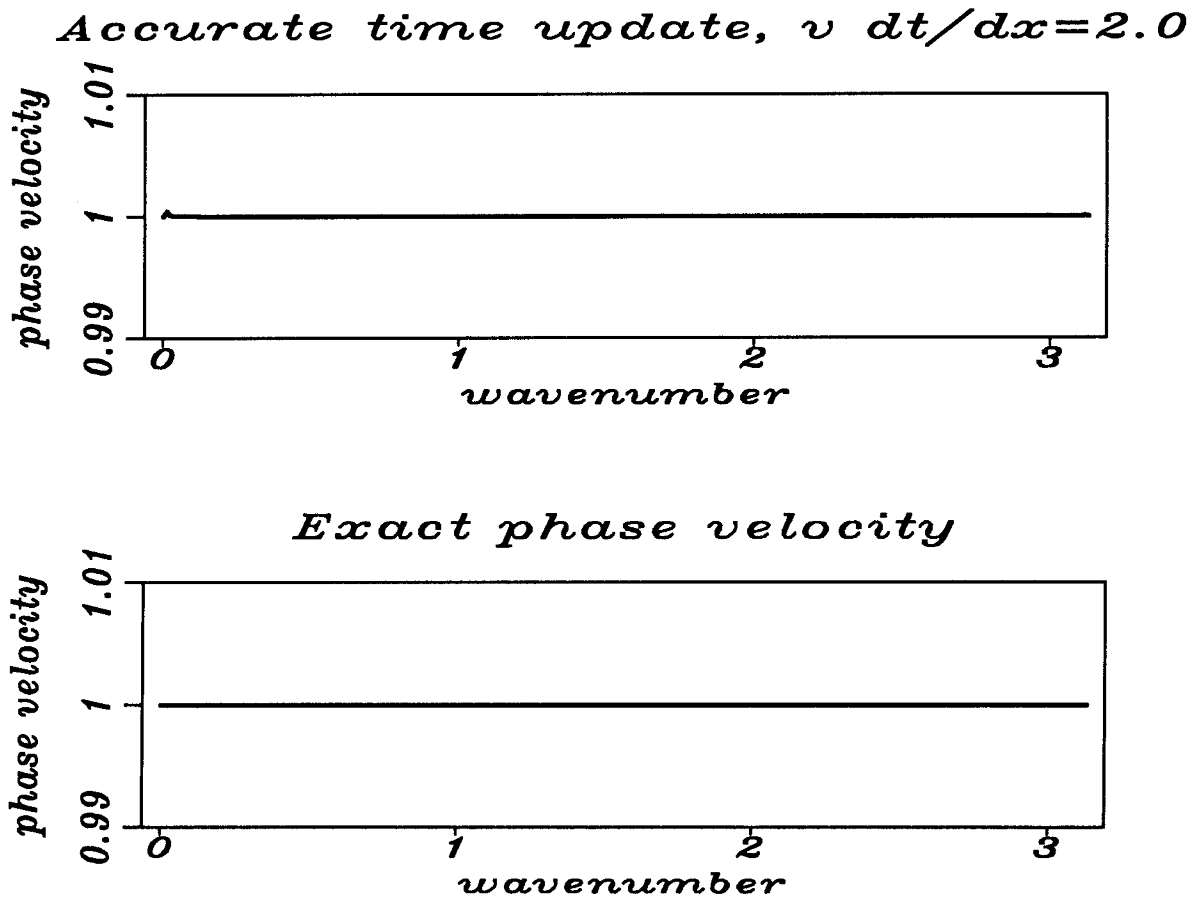

FIG. 2. Phase velocity spectrum for the accurate time update pseudospectral method. The numerical phase velocity is almost exactly equal to the true phase velocity. The small bump near $k_x = 0$ is due to numerical difficulty in computing v_{phase} near $k_x = 0$.

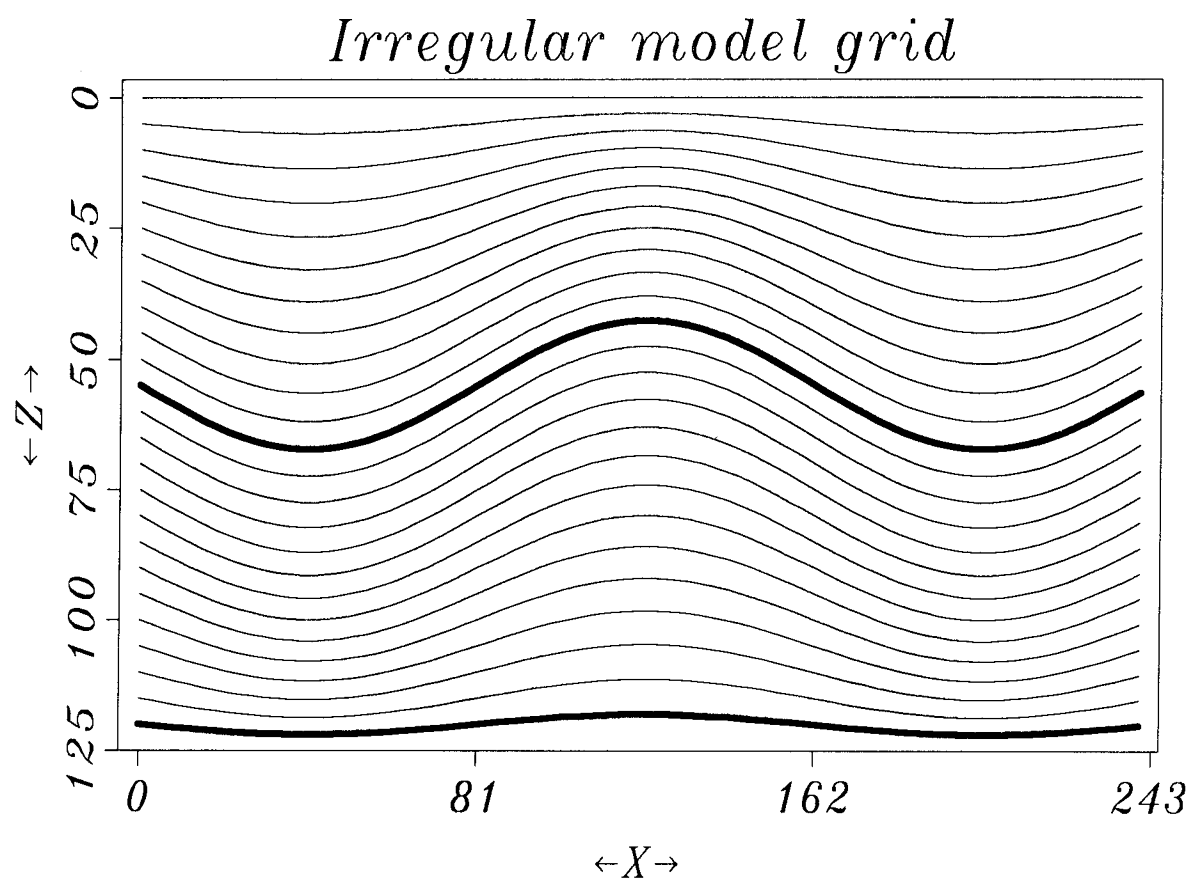

FIG. 3. Irregular grid used for 2-D acoustic and elastic wave simulations. The light lines are grid lines of constant η. The heavy lines are the reflector boundaries.

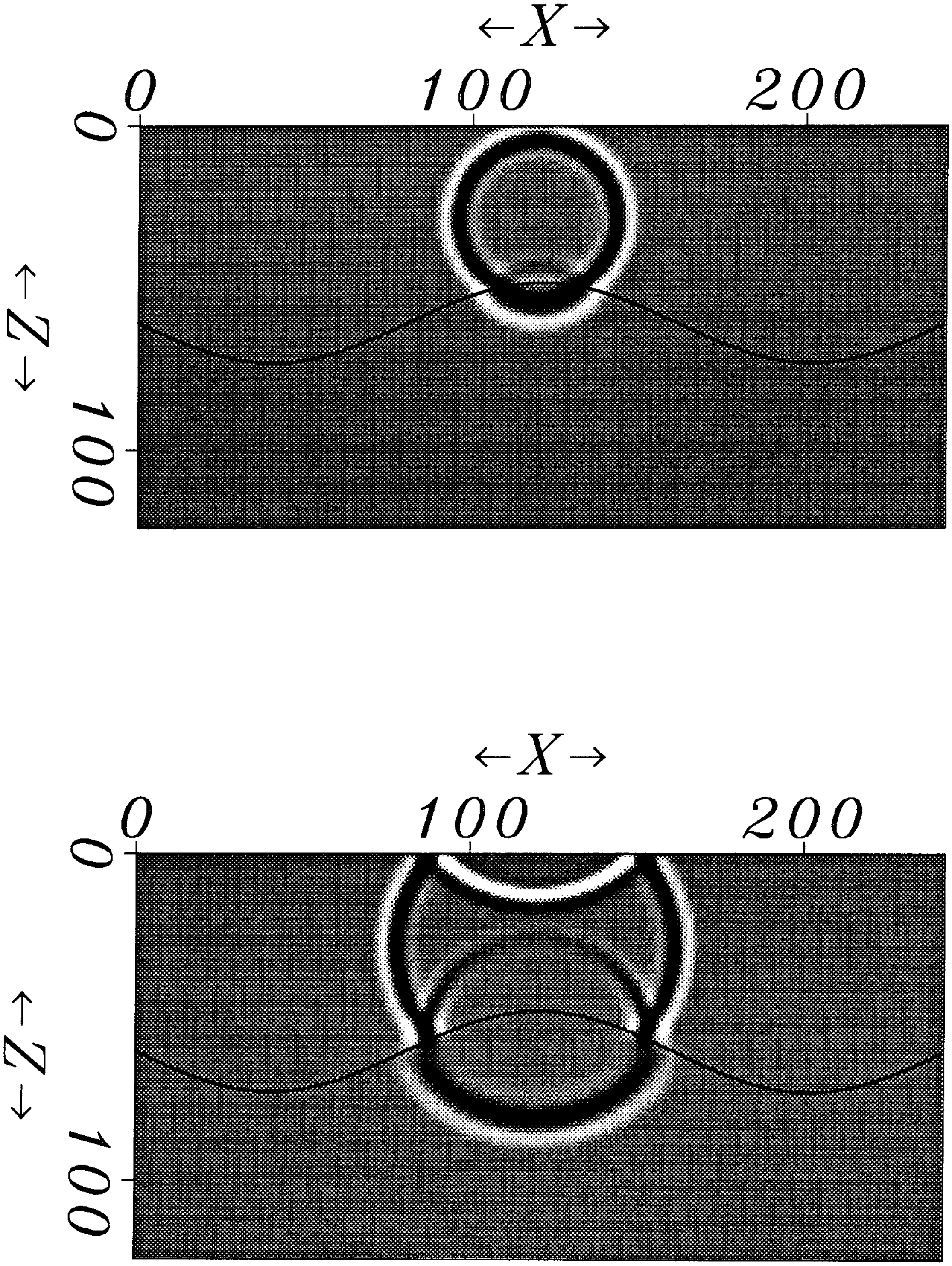

FIG. 4. First set of time snapshots of the solution to the acoustic wave equation on the irregular grid of Figure 3. The computations used the mapping of equation (17) and modified the acoustic wave equation using equations (18)–(19).

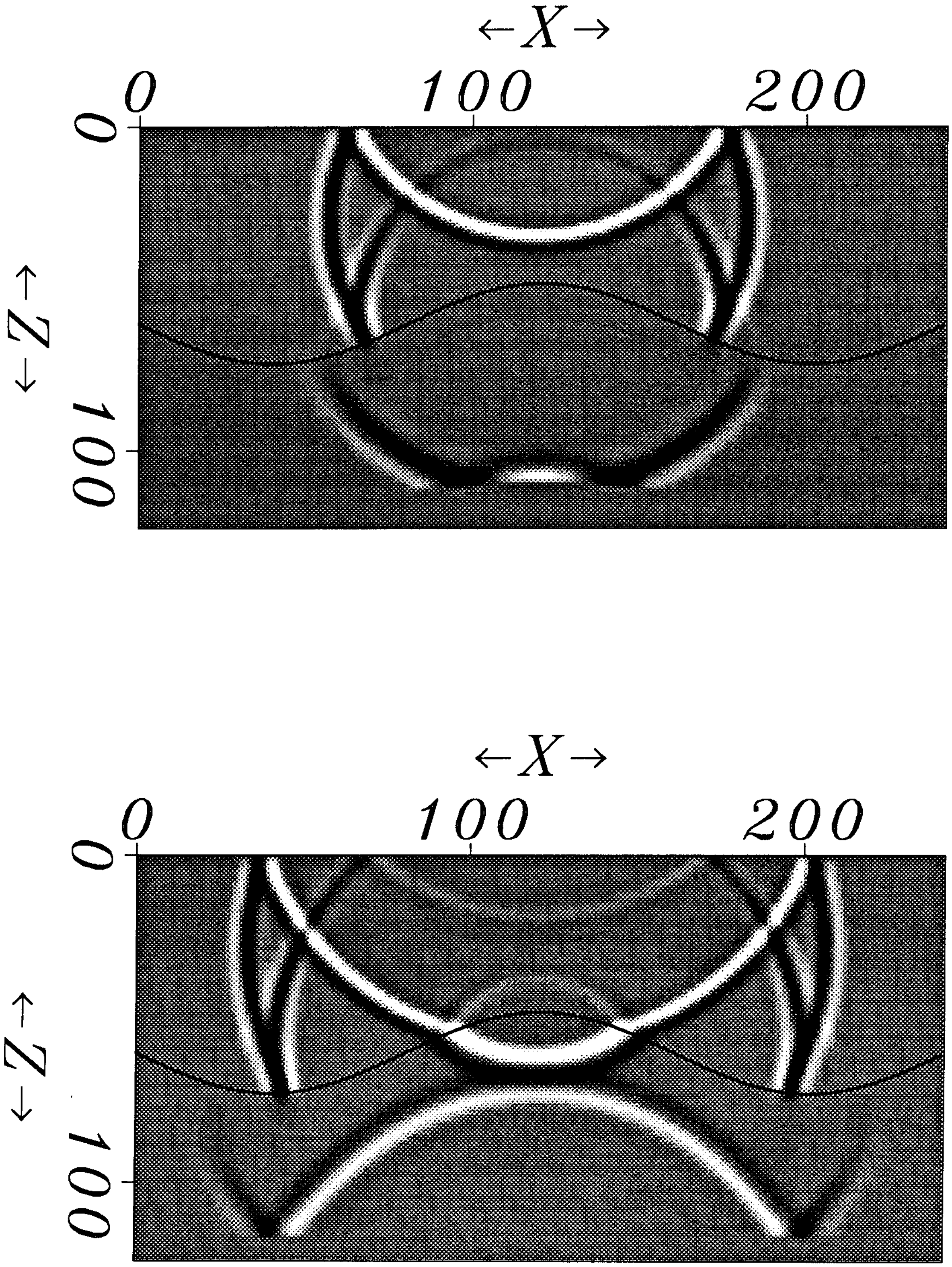

FIG. 5. Second set of time snapshots of the solution to the acoustic wave equation on the irregular grid of Figure 3. The computations used the mapping of equation (17) and modified the acoustic wave equation using equations (18)–(19).

(x) component of displacement computed using the elastic wave equation on the irregular-grid model. In Figures 4–7 the wave fields propagate with no grid dispersion and there are no spurious diffractions or irregularities in the wave field reflected from the curved reflectors.

SUMMARY

Wave equation modeling with the accurate-time-update pseudospectral method does not suffer from grid dispersion. For models with curved boundaries between layers, a smoothly varying irregular grid is constructed that follows the boundaries. The irregular grid is mapped to a regularly sampled grid where a modified version of the desired wave equation is solved using the accurate-time-update pseudospectral method. In the computational domain, boundaries between regions of different material parameters align with the grid eliminating errors due to misrepresentation of the curved boundary on a rectangular grid.

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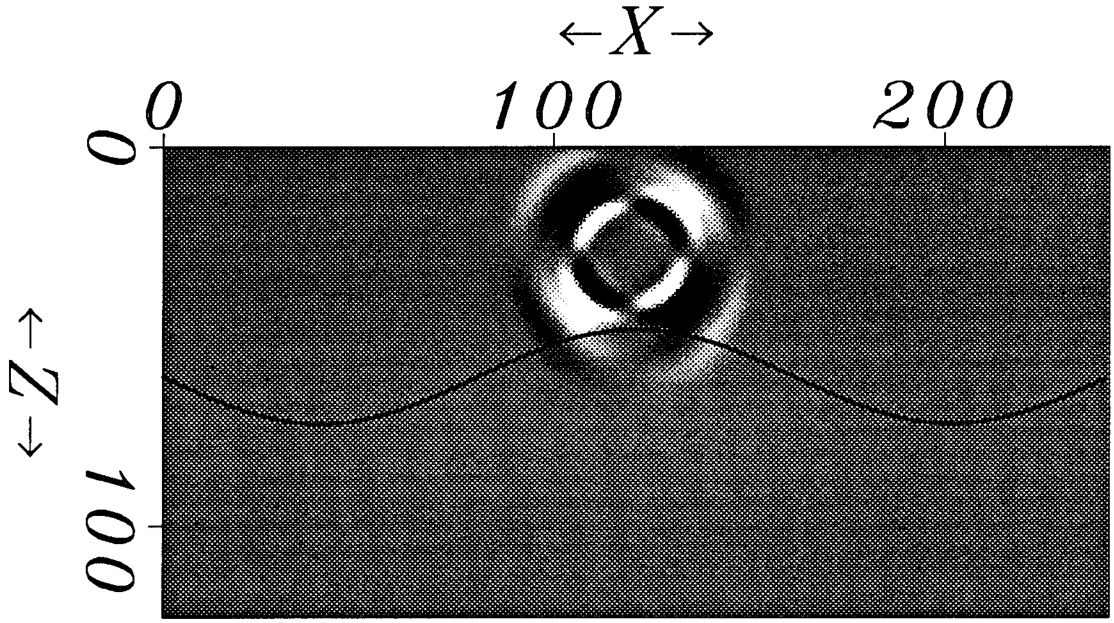

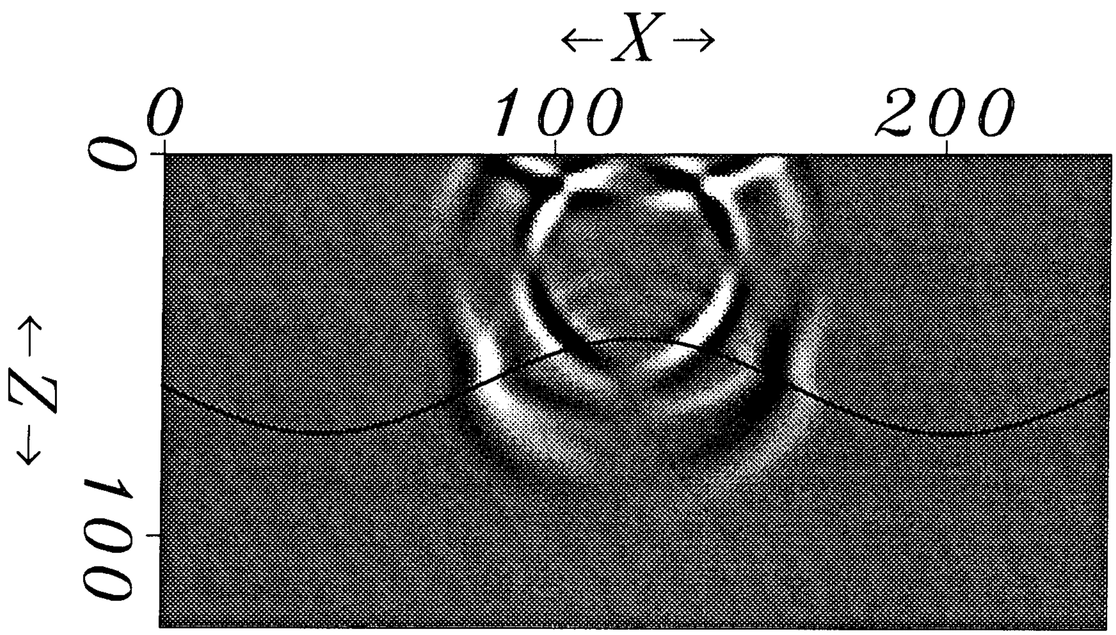

FIG. 6. First set of time snapshots of the solution to the elastic wave equation (x component of displacement) on the irregular grid of Figure 3. The computations used the mapping of equation (17) and modified the elastic wave equation using equations (18)–(19).

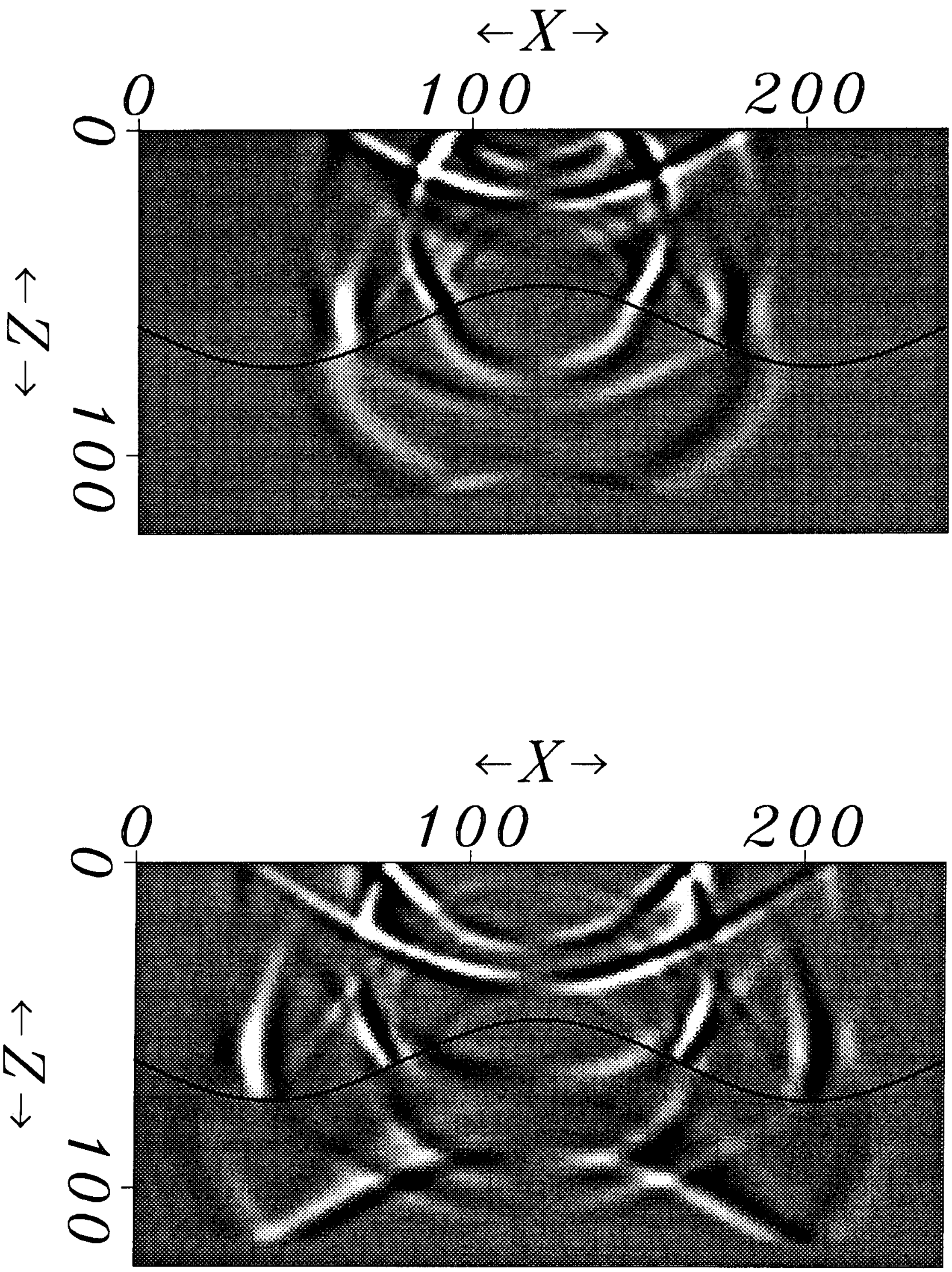

FIG. 7. Second set of time snapshots of the solution to the elastic wave equation (x component of displacement) on the irregular grid of Figure 3. The computations used the mapping of equation (17) and modified the elastic wave equation using equations (18)–(19).

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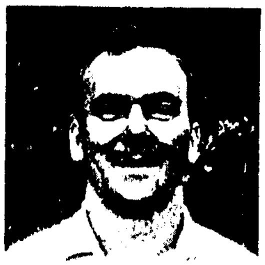

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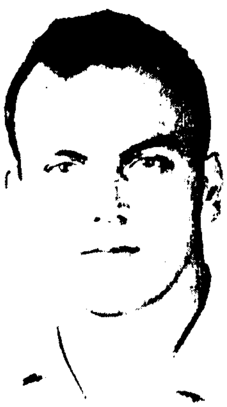

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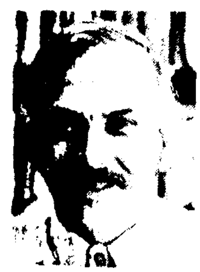

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