Evaluating finite-difference operators applied to wave simulation

John T. Etgen

ABSTRACT

The continuous wave equation can be Fourier transformed over all spatial variables and over time, and then solved for ω as a function of spatial wavenumber. From the dispersion relation, phase velocity or group velocity can be obtained. This procedure can also be applied to discrete, finite-difference approximations to the acoustic or elastic wave equation. Finite-difference solutions to the wave equation have different dispersion relations than the continuous wave equation. The differences between the numerical and exact phase velocities lead to errors commonly observed in finite-difference generated wave fields. Understanding and counteracting these errors will lead to more accurate and efficient techniques for solving wave equations on discrete grids.

INTRODUCTION

The explicit in time finite-difference method has become a powerful tool for computing solutions to the acoustic and elastic wave equations. The accuracy and efficiency of these solutions can be enhanced by using high-order spatial differentiation operators (Dablain, 1986). The optimal temporal and spatial finite-difference solution to a wave equation depends on the characteristics of the velocity model, the spatial frequency content of the wave field, and also on the computer architecture used. For accuracy's sake one desires a difference equation that closely matches the desired continuous differential equation over all frequencies of interest. Also, the number of grid points required to model wave propagation in a given region should be as small as possible for economy's sake. In general, the accuracy of a spatial difference operator is directly related to the length of the operator. On many computers, the cost of the method is also directly related to the length of the operator. One is forced to compromise between the accuracy of the derivative operator and the cost of the implementation. On one extreme, the Fourier method (Kosloff et al., 1984,1985) can compute spatial derivatives accurate to spatial nyquist, but on many computers is more expensive than a convolutional operator 8 or 10 points long (Mora, 1986). On the other extreme the standard first-order finite-difference approximation to first derivatives (Kelly et al., 1976) can be inexpensive to apply, but its accuracy is poor if there are wavelengths present that are sampled fewer that 10-16 times per wavelength (Marfurt, 1984). The accuracy of the time differencing also plays an important role in the overall accuracy of the solution. Because of errors inherent in time differencing, even the Fourier method which has perfect space-difference operators cannot match the true differential equation at all spatial wavelengths. As more accurate spatial derivatives are used, the accuracy of the time differencing becomes paramount. One cannot simply ignore the errors caused by discrete time finite-difference methods.

The most common errors of finite-difference solutions to wave equations are known as grid dispersion and grid anisotropy. These errors are due to the deviation of the numerical phase velocity of a finite-difference method from the phase velocity of the wave equation one wishes to model. The continuous scalar acoustic wave equation and isotropic linear elastic wave equation both have phase velocities that are independent of direction or wavelength in a homogeneous medium. If a discrete approximation to these equations has a phase velocity spectrum that deviates from the constant phase velocity of the continuous equation, the wave field computed from the discrete equation will increasingly deviate from the continuous wave field as it propagates through the grid. The waveform distortion is known as grid dispersion. If the phase velocity is a function of wavelength the wave pulse will disperse as the distance it propagates through the grid increases. If phase velocity is a function of the direction the wave propagates through the grid, the wave field will be increasingly advanced or retarded from the true wave field as distance propagated through the grid increases depending on the direction the wave is traveling. The discrete solution will be anisotropic while the continuous, exact solution is isotropic. For explicit finite-difference techniques discussed here, phase velocities of waves propagated on a discrete grid are real, i.e., there is no attenuation or growth as long as the method is stable. For the remainder of this paper the accuracy criterion for a finite-difference algorithm is taken to be the deviation of the numerical phase velocities from the theoretical phase velocity as a function of wavelength and direction. I choose the phase velocity rather than the group velocity, because it is possible to model wave fields using the phase velocity spectrum. These modeled wave fields show the effect of propagating waves with a given numerical scheme for an arbitrary distance. The wave fields can then be examined for deviation from the analytical wave field in simple cases. It is also possible to do an analysis of finite-difference methods based on group velocities (Holberg, 1987).

Grid dispersion and grid anisotropy are not the only errors present when the finite-difference approximations to the wave equation are solved in inhomogeneous media. Depending on the implementation and the equation being solved, there can be errors in reflection coefficients at interfaces, errors in applying boundary conditions at the free surface, and instability due to rapid variations in velocity. None of these errors will be considered here; analyzing these errors requires detailed study of the complete algorithm for specific velocity models.

DISPERSION RELATIONS FOR DISCRETE WAVE EQUATIONS

By analyzing the phase velocity spectra of a given finite-difference scheme, one can decide if the method will produce results of the desired accuracy without having to implement the method and examine the results of calculations. Wave propagation through a homogeneous medium with a finite-difference method can be simulated by phase shifting the wavenumber components of the Fourier transform of the source pulse by the appropriate distance determined by the phase velocity spectrum. Determining the errors of wave propagation through an inhomogeneous medium, usually requires solving the difference equation and examining the results. To find the phase velocity one must find the numerical dispersion relation obeyed by waves propagated with the given finite-difference equation. For the 1-D, continuous scalar wave equation, the dispersion relation can be found by Fourier transforming the wave equation over x and t.

$$\frac{\partial^2 U}{\partial t^2} = C^2 \frac{\partial^2 U}{\partial x^2} \iff \omega^2 = C^2 k_x^2 \; . \tag{1}$$

The phase velocity is defined as

$$C_{phase}(k) = \frac{\omega(k)}{k} = C \; . \tag{2}$$

In a similar fashion, we can derive the dispersion relation and phase velocity for a given finite-difference approximation to the 1-D wave equation. Again, taking Fourier transforms in x and t we arrive at the double Fourier transform of the discrete wave equation. Let $\Omega(\omega)$ denote the temporal Fourier transform of the time difference operator D_t^2 and let $\kappa(k)$ denote the spatial Fourier transform of the spatial difference operator D_x^2.

$$D_t^2 U = C^2 D_x^2 U \iff \Omega(\omega) = C^2 \kappa(k) \; . \tag{3}$$

Solve for $\omega(k)$ and C_{phase},

$$\omega(k) = \Omega^{-1}(C^2\kappa(k)) \; ; \; C_{phase}(k) = \Omega^{-1}(C^2\kappa(k))/k \; . \tag{4}$$

For simple operators in space and time, the transformed operators can be found analytically; for more general operators the transforms can be found using an FFT. If we consider the standard second-order time derivative often used in explicit finite-difference schemes, the operator $\Omega(\omega)$ can be found analytically

$$D_t^2 * f(t) = \frac{1}{\Delta t^2}\left[f(t+\Delta t) - 2f(t) + f(t-\Delta t)\right] \; , \tag{5}$$

$$\frac{1}{\Delta t^2}\left[f(t+\Delta t) - 2f(t) + f(t-\Delta t)\right] \iff \Omega(\omega) = \frac{1}{\Delta t^2} 2\left[cos(\omega \Delta t) - 1\right] \ . \qquad (6)$$

When necessary, a similar analysis allows the computation of 2-D and 3-D phase velocity spectra. These phase velocity spectra will be a function of k_x and k_z or k_x, k_y, and k_z.

EXAMPLES

It is possible to evaluate the dispersion properties of many different explicit finite-difference methods for both the acoustic and elastic wave equations, by considering simple 1-D and 2-D scalar wave equations. The behavior of the more complicated equations can be inferred from the simple results. To study grid dispersion, a 1-D scalar wave equation will suffice. To study grid anisotropy it is necessary to examine the behavior of a 2-D scalar wave equation. As a canonical example, I will consider scalar wave propagation on a grid with $\Delta x = \Delta z = 1$, $C = 1$, for various Δt's and various different spatial finite-difference operators. The correct phase velocity is the phase velocity for the corresponding continuous equation which is a constant $= 1$ for all wavenumbers.

Specification of an accuracy criterion is arbitrary for finite-difference methods, a method that may suffice for one size model will be inappropriate for a larger model. In general, for increasing distances the waves will propagate (in number of grid points) the greater the absolute accuracy of the phase velocity must be to obtain satisfactory results. Common models encountered usually have several hundred grid points in each direction, so absolute deviation of the numerical phase velocity from the correct phase velocity of 1 per cent or fractions of a per cent will usually ensure that no wave number component is shifted more than a grid point or fractions of a grid point from the exact solution. This translates to less than a wavelength shift for all spatial frequencies that can be represented on the grid. The resulting wave form can still be distorted if there is oscillation of the phase velocity curve; different spatial frequencies bands will "beat" together to produce a distorted wave form even though the absolute deviation from the correct phase velocity is small.

1-D phase velocities

Figure 1 shows a waveform in space that will be used for propagation in the Fourier domain with the phase velocity spectrum from each derivative operator. Also shown is the spectrum of the wavelet. Figure 2 shows the phase velocity spectra and resulting wave fields after propagation with the 1-D, second-order in space and time finite-difference method, for various time step sizes. It is interesting to note that the accuracy of the standard second-order in space and time method increases as the stability limit of the method, $v\Delta t/\Delta x = 1$ is approached. At the stability limit, the time and space discretization errors exactly cancel each other and the resulting solution is exact. At smaller time step sizes, the phase velocity decreases

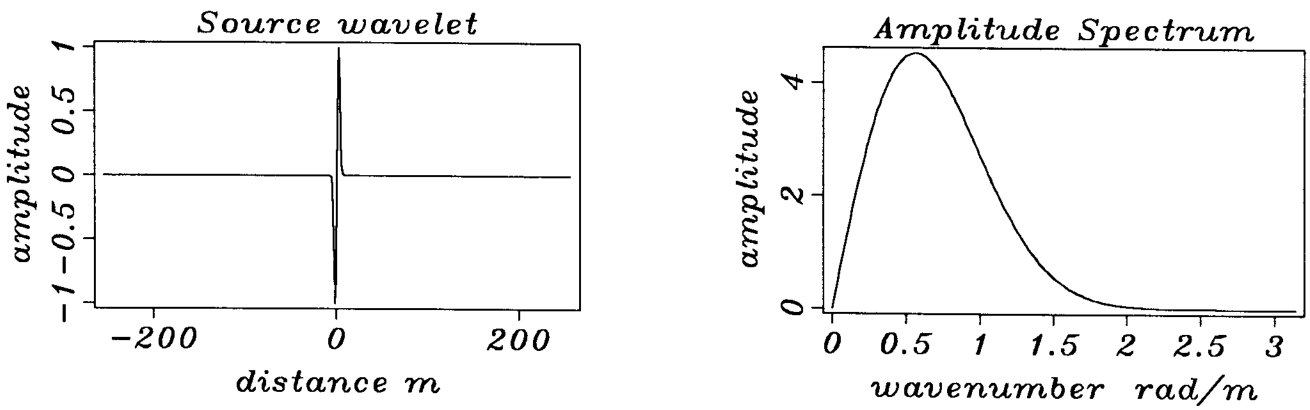

FIG. 1. Spatial wavelet used for dispersion studies and its spectrum. Most of the energy is below 1/2 nyquist, but there is energy up to almost nyquist.

with increasing wavenumber. The wavelet shape shows the higher wavenumber components of the source wave trailing the lower wavenumbers, the pulse is highly dispersed. Since the phase velocity curve does not oscillate, the dispersion is simply an increasing delay of the higher wavenumbers.

Figure 3 shows phase velocity spectra and resulting wave fields after propagation with a finite-difference method that uses second-order in time differencing and space operators designed by inverse transforming ik and windowing with a gaussian taper (Mora, 1986). The first derivative operator was 8 points long, giving a second derivative that is effectively 15 points long. The results of using three different time step sizes are shown. Increasing the time step size raises the phase velocity more at increasing wavenumbers. For this finite-difference method, there are phase velocities above and below the correct phase velocity. The distortion of the modeled pulse is mainly due to the middle and high wavenumbers traveling faster than the low wavenumbers, but the oscillation of the phase velocity curves also contributes to the dispersion of the pulse. The oscillation is aggravated by increasing time step size. There is no long tail as in Figure 1, but the results are inadequate at the distances used in this example.

Figure 4 displays the phase velocity spectra and wave fields after propagation with a finite-difference method similar to the one used to produce Figure 2. Again the first derivative is 8 points long. The derivative operator was constructed by Francis Muir using his "beat the central limit theorem" method (Dellinger and Muir, 1986). Unlike the derivative operator of Figure 2, the phase velocity spectrum of this operator is flat for low wavenumbers and diverges from the correct phase

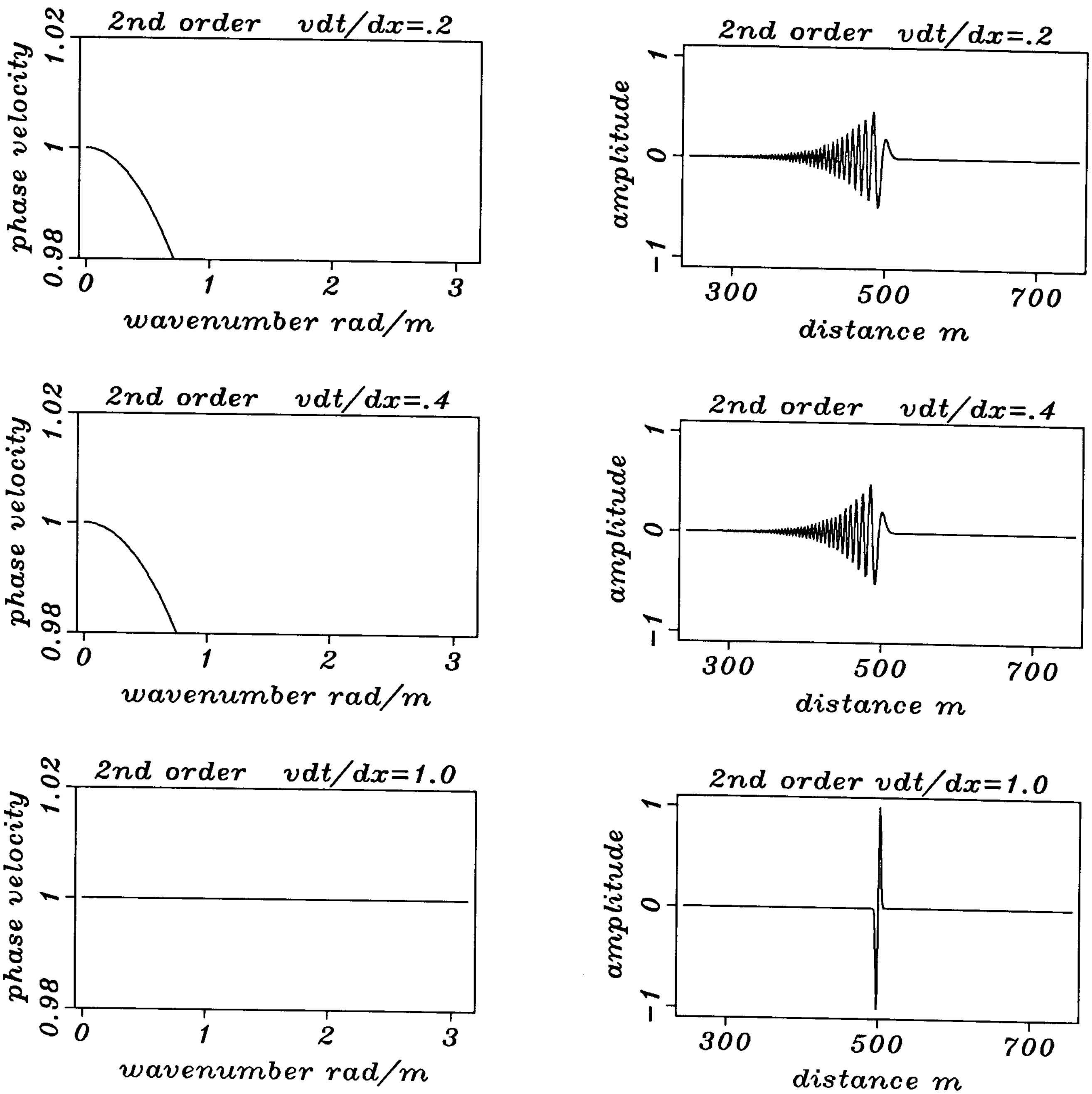

FIG. 2. Phase velocity spectra for 1-D acoustic wave equation using second-order in space and time differencing. The plots on the left are the phase velocities as a function of wavenumber for different time step sizes. On the right are the corresponding wave fields after propagation for the number of time steps required to take the exact solution 500 normalized meters. The upper and lower bounds of the phase velocity plots are the two percent relative error lines.

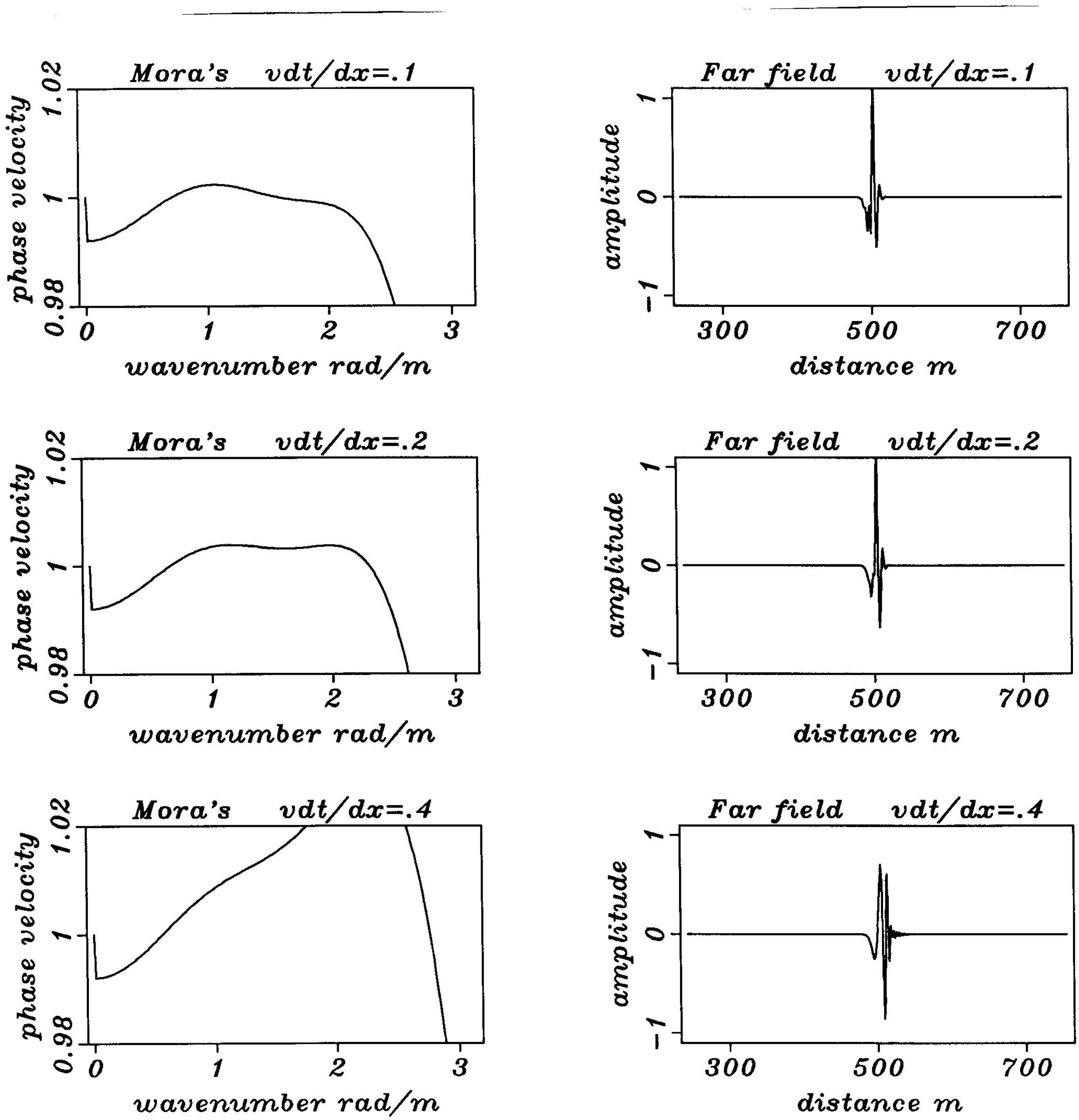

FIG. 3. Phase velocity spectra for 1-D acoustic wave equation using second-order in time differencing with space operators designed by Pete Mora, obtained by inverse transform and windowing ik. The plots on the left are the phase velocities as a function of wavenumber for different time step sizes. On the right are the corresponding wave fields after propagation for the number of time steps required to take the exact solution 500 normalized meters. The upper and lower bounds of the phase velocity plots are the two percent relative error lines.

velocity only at high wavenumbers. The effect of the time step size is to pull the phase velocity spectrum increasingly above the correct value as wavenumber increases until the increasing error of the space operator causes the phase velocity to decrease as nyquist is approached. The phase velocity curve does oscillate if large time step sizes are used, but the oscillation is not a severe as Figure 2. For small time step sizes, the phase velocity curve matches the exact phase velocity curve over the middle and low wavenumbers and becomes less than the exact phase velocity at high wavenumbers. The only dispersion is the highest frequencies trailing the main pulse. As time step size increases, a band of middle and higher wavenumbers travels with greater phase velocity. The dispersion then becomes those wavenumbers preceding the main pulse and distorting it.

Figure 5 shows the phase velocity spectra obtained using a second-order in time differencing combined with spectral space derivatives (Kosloff et al., 1984). For a small time step size the method is accurate for all wavenumbers that can be represented on the grid. As the time step size increases, the accuracy of this scheme deteriorates more and more because the time differencing error dominates. There is no error in the space derivatives to cancel the time error. The dispersion is always due to the highest wavenumbers preceding the main pulse and eventually distorting the main pulse.

Spatial finite-difference operators usually lead to numerical phase velocities that are less than the correct phase velocity. The error increases as nyquist wavenumber is approached. Time finite-difference operators lead to numerical phase velocities that are greater than the correct phase velocity. This error also increases as nyquist is approached. The advantage of using imperfect space operators is now apparent. The errors caused by time and space differencing have opposite effects and the error due to the space differencing can be canceled by the error of time differencing to some degree. The cancellation is best when the space and time discretization is the same order. This was apparent in Figure 1 when the space and time errors exactly canceled at the stability limit.

2-D phase velocities

A 2-D finite-difference wave equation can have a phase velocity spectrum that is not only a function of wavenumber, but also a function of direction of propagation through the grid. If the phase velocity only depends on wavelength of the wave, but not on direction, the wave equation is isotropic. In general, finite-difference wave equations will not be isotropic, but will have phase velocities that vary with angle through the grid. This anisotropy is purely numerical and undesirable, just as the dependence of the phase velocity on wavelength was undesirable, because the computed solution will differ from the solution of the continuous wave equation.

Figure 6 shows a contour plot of the phase velocity of the second-order in space and time finite-difference method for two different time step sizes. In 2-D the stability limit decreases to $1/\sqrt{2}$ times the 1-D stability limit, so it is impossible

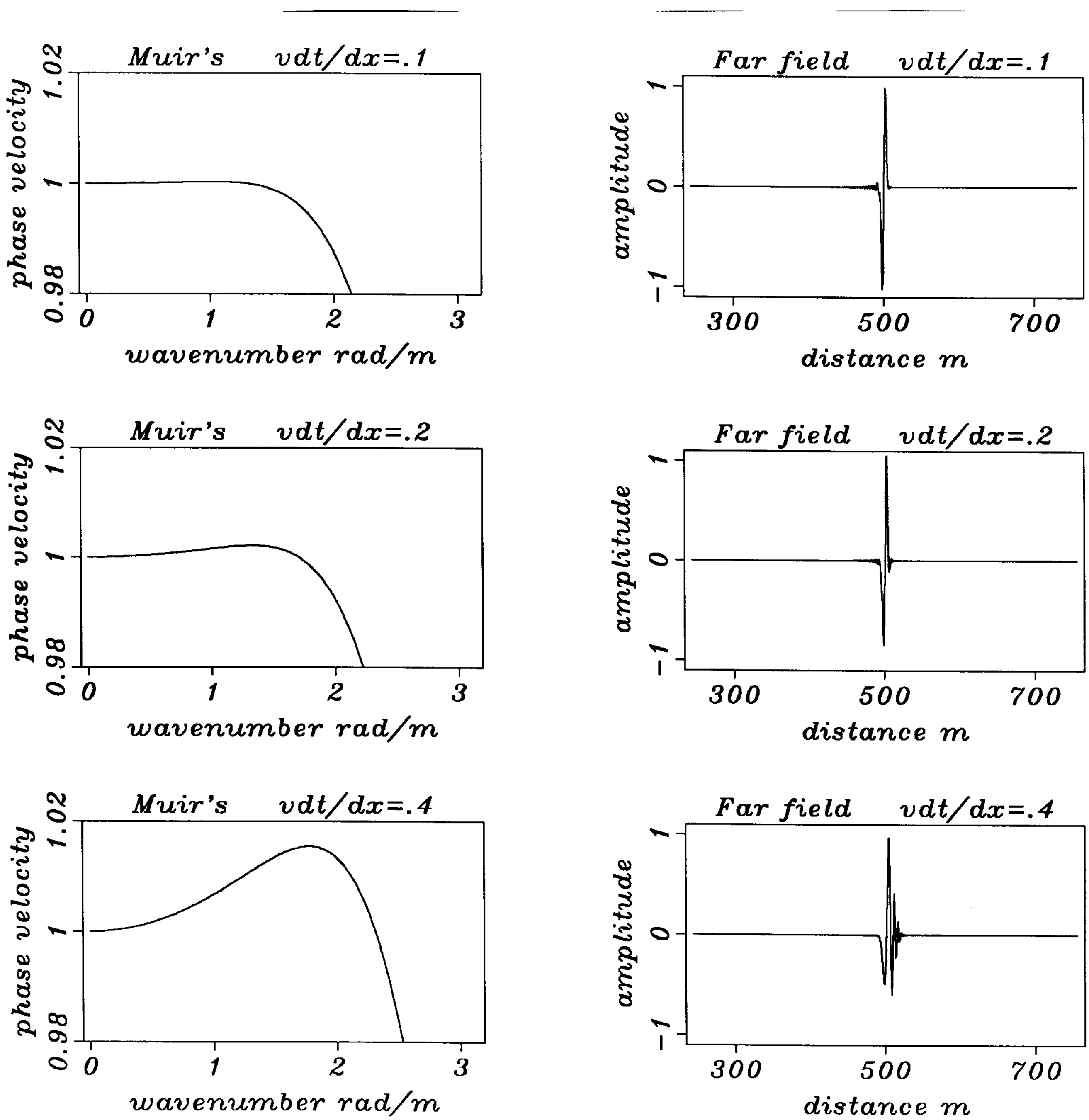

FIG. 4. Phase velocity spectra for 1-D acoustic wave equation using second-order in time differencing with space operators obtained by Muir and Dellinger's "Beat the central limit theorem" method. The plots on the left are the phase velocities as a function of wavenumber for different time step sizes. On the right are the corresponding wave fields after propagation for the number of time steps required to take the exact solution 500 normalized meters. The upper and lower bounds of the phase velocity plots are the two percent relative error lines.

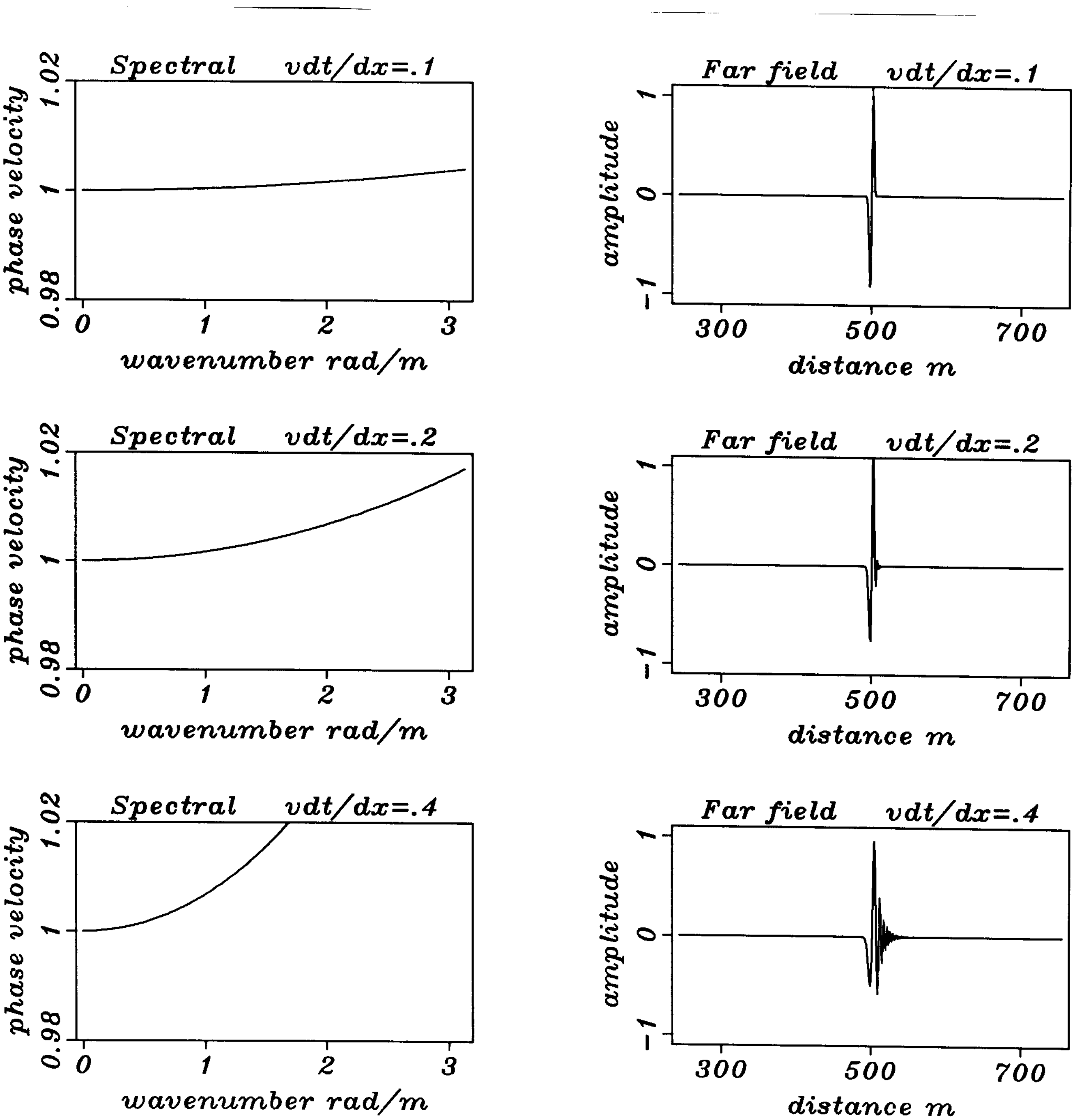

FIG. 5. Phase velocity spectra for 1-D acoustic wave equation using second-order in time differencing with spectral space derivatives. The plots on the left are the phase velocities as a function of wavenumber for different time step sizes. On the right are the corresponding wave fields after propagation for the number of time steps required to take the exact solution 500 normalized meters. The upper and lower bounds of the phase velocity plots are the two percent relative error lines.

to use the time differencing error to cancel exactly the space differencing error for all directions through the grid. The contours are not circular indicating the method is not isotropic. The phase velocity along a 45 degree line through the grid is significantly higher than along the coordinate axes. The grid anisotropy arises because the Fourier spectrum of the 1-D spatial operator is not exactly flat.

Figure 7 shows the phase velocity of the finite-difference operators of Figure 2 applied to the 2-D scalar wave equation for two different time step sizes. This operator has an oscillatory 1-D phase velocity spectrum, that causes an anisotropic 2-D phase velocity spectrum. Note however, that there is a large region of middle wave numbers for which the phase velocity spectrum is nearly flat.

Figure 8 shows the phase velocity spectra of the finite-difference of Figure 3 by Muir. Because there is less oscillation of the 1-D phase velocity spectrum, the resulting 2-D velocity spectrum is closer to isotropic. The operator is flat near zero in k_x, k_z. Middle wavenumbers are pulled above the correct phase velocity by the time derivative error. Finally at higher wavenumbers, the phase velocities drop below the correct value. At high wavenumbers there is also significant anisotropy.

Finally, Figure 9 shows the phase velocity spectra for the second-order in time, spectral derivative in space method for two different time step sizes. Because the phase velocity of the 1-D method has no oscillation (perfect ik was used for space derivatives), the resulting 2-D scheme is exactly isotropic, although still dispersive. The Fourier method for space derivative suffers mainly from the inaccuracy of the time derivative. The other spatial finite-difference methods gain some advantage (even if only slight) because the time error is canceled by the space error to some degree at the higher wavenumbers. The Fourier method could be the method of choice if an accurate and stable time derivative existed that was better than the standard second-order time derivative.

CONCLUSIONS

The dispersion properties of finite-difference methods applied to the wave equation can be analyzed using phase velocities computed by Fourier transforming the difference equation. It is hoped that the ability to evaluate the properties of a finite-difference method rapidly will lead to better numerical modeling of acoustic and elastic wave equations.

ACKNOWLEDGMENTS

Special thanks to Francis Muir for challenging me to look at finite-difference operators one more time.

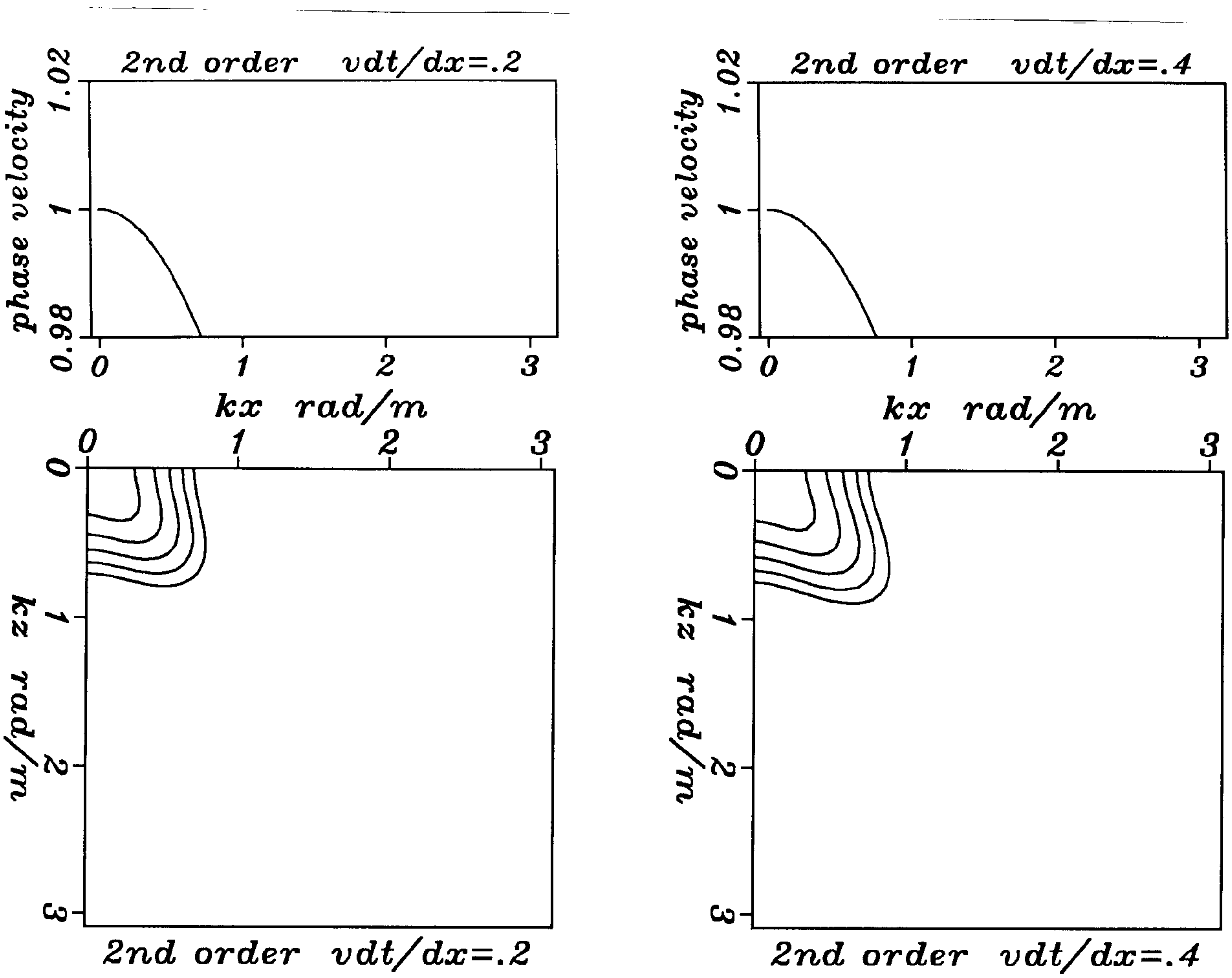

FIG. 6. 2-D phase velocity spectra for the second-order in space and time finite-difference method for 2 different time step sizes. The error is worse than the 1-D implementation of this method, since it is impossible to cancel all the space error in all directions with the time error. The outermost contour is the two percent relative phase velocity error curve.

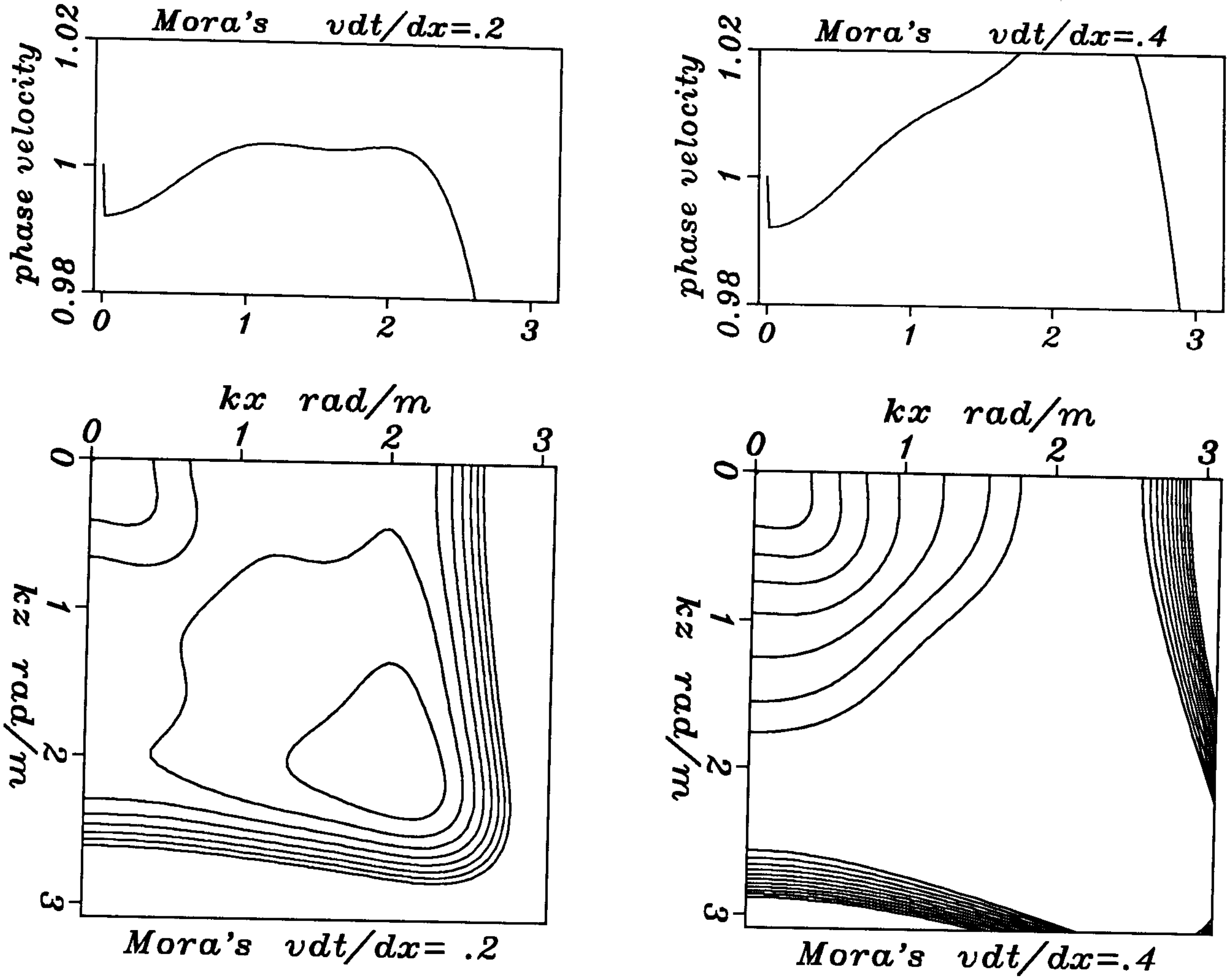

FIG. 7. 2-D phase velocity spectra for Mora's derivative operators at two different time step sizes. The wiggliness of the operator's response causes anisotropy. Although the contours show significant departure from circles, there is an area that is nearly flat. The outermost contour is the two percent error curve. There are regions above and below the correct phase velocity. The 1-D phase velocity spectra are included to show where contours are above or below the correct phase velocity.

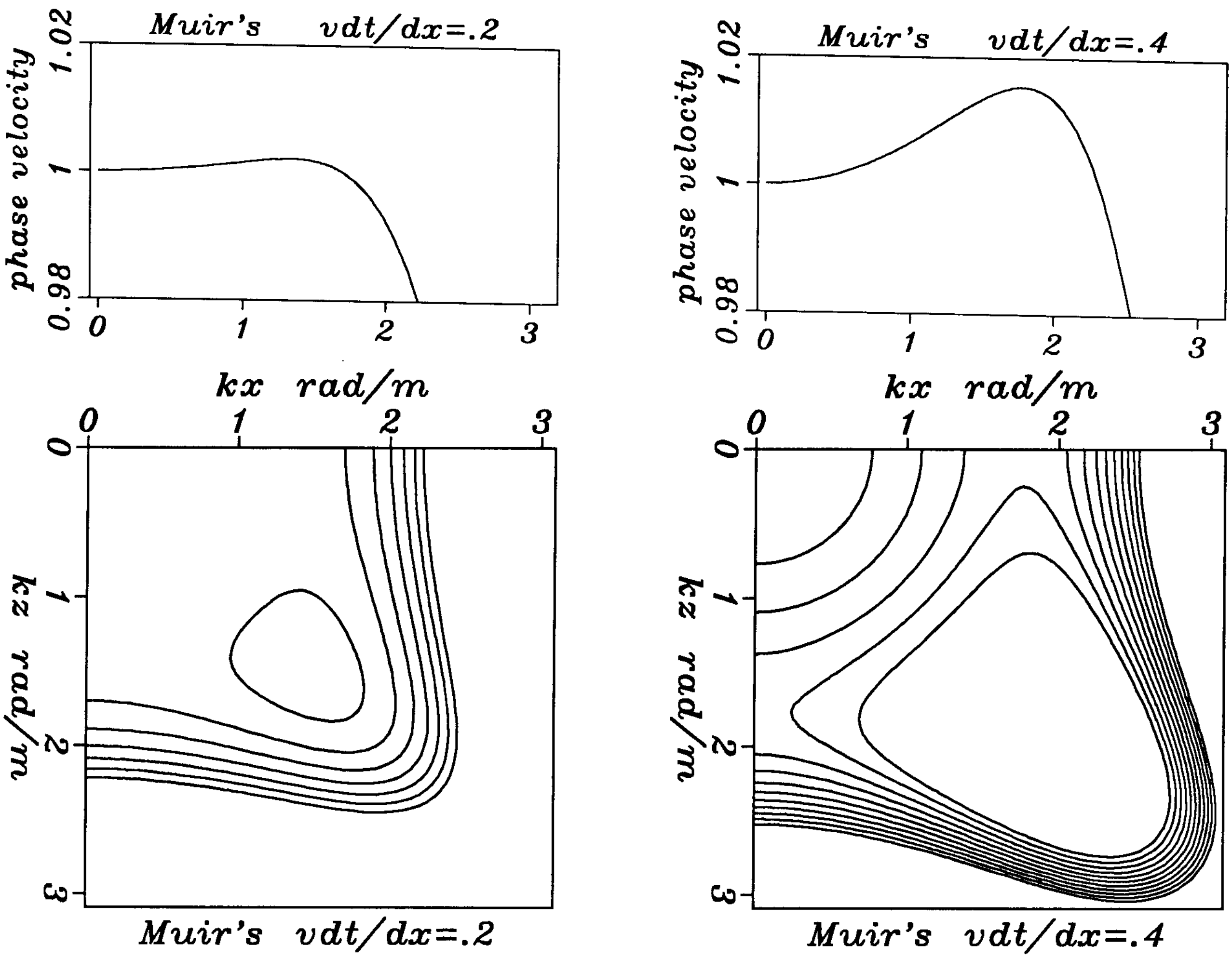

FIG. 8. 2-D phase velocity spectra for Muir's operators at two different phase velocities. This operator is much flatter near the origin than that of Figure 7, and only suffers from anisotropy at high wavenumbers. The outermost contour is the two percent error line. The 1-D phase velocity spectra are included to show where contours are above or below the correct phase velocity.

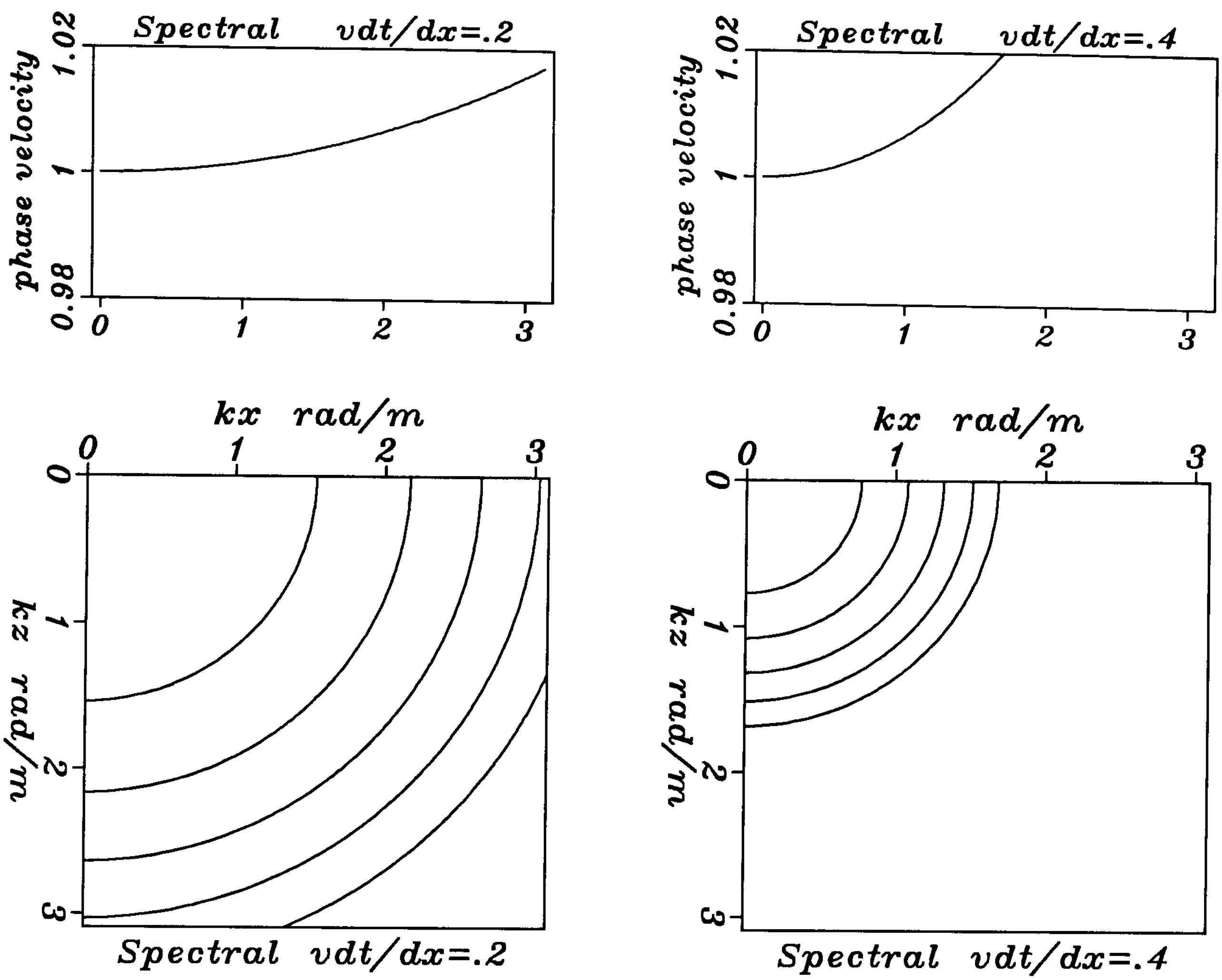

FIG. 9. 2-D phase velocity spectra for the second-order in time Fourier method in space for two different time step sizes. The Fourier method is exactly isotropic for all values of the time step size. The outermost contour is the two percent error line. The 1-D phase velocity spectra are included to show where contours are above or below the correct phase velocity.

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