Difference Approximations for Forward Modelling Problems

David Brown and Robert Clayton

In this paper, difference approximations for forward modelling problems of interest in reflection seismology are discussed. After reviewing the standard second-order accurate differencing schemes for the acoustic wave equation and for the displacement equations of motion in two dimensions for elastic waves, more accurate explicit fourth-order approximations are given. The accuracy of the various approximations is compared by looking at the theoretical phase error for each approximation. It is seen that the advantages afforded by the greater accuracy of the fourth-order schemes can greatly outweigh the disadvantages of the slight increase in computational expense for the methods. The possibility of adding dissipative terms (numerical viscosity) to the approximations to attenuate the inaccurately modelled frequencies is also discussed. Finally, examples are given in which the second-order and fourth-order schemes with and without dissipation for the acoustic case are compared for a simple model.

I. The Differential Equations

The differential equations of interest for forward modelling in reflection seismology are relatively simple to derive beginning with the stress equations of motion (Newton's second law) and using Hooke's law for an isotropic medium. Hooke's law expressed in vector notation is given by:

$$\tau = \lambda \nabla \cdot u I + \mu [\nabla u + (\nabla u)^T] \tag{1}$$

and the stress equations of motion are:

$$\rho (\partial^2 u / \partial t^2) = \nabla \cdot \tau \quad . \tag{2}$$

Here, τ is the stress tensor, u is the displacement vector, I = diag(1,1,1) is the unit tensor, ρ is the density of the medium, and λ and μ are the Lamé parameters.

In an acoustic medium, the rigidity, μ, vanishes, so the stress tensor is diagonal, and $\tau_{xx} = \tau_{yy} = \tau_{zz} = -p$, where p is the hydrostatic pressure. Equation (1) becomes:

$$-p = \lambda \nabla \cdot u \tag{3}$$

and equation (2) becomes:

$$\rho(\partial^2 u/\partial t^2) \quad = \quad -\nabla p \quad . \qquad (4)$$

If u is eliminated between these two equations, the acoustic wave equation results with pressure as the dependent variable:

$$\partial^2 p/\partial t^2 \quad = \quad K\nabla\cdot(\rho^{-1}\nabla p) \quad , \qquad (5)$$

where $K \; = \; \lambda + 2\mu/3$ is the incompressibility of the medium. For the special case of a homogeneous medium, this equation reduces to:

$$\partial^2 p/\partial t^2 \quad = \quad c^2\nabla^2 p \quad , \qquad (6)$$

where $c = (K/\rho)^{1/2}$ is the (constant) velocity of the medium. Often, in an inhomogeneous medum, it is quite reasonable to assume that ρ is approximately constant, and that the variation in velocity can be attributed to variations in the incompressibility. In this case, the acoustic wave equation can be expressed:

$$\partial^2 p/\partial t^2 \quad = \quad c^2(x,y,z)\nabla^2 p \quad . \qquad (6a)$$

In an elastic medium, equations (1) and (2) may be combined to obtain the displacement equations of motion:

$$\rho(\partial^2 u/\partial t^2) \quad = \quad \nabla(\lambda\nabla\cdot u) \quad + \quad \nabla\cdot\{\mu[(\nabla u + (\nabla u)^T\,]\} \quad . \qquad (7)$$

When the motion is restricted to be in the x-z plane, and the displacements are further restricted to depend only on x,z, and t, equation (7) reduces to the form:

$$\rho U_{tt} \; = \partial_x[A(x,z)\partial_x U] \;\; + \;\; \partial_z[B(x,z)\partial_x U] \;\; + \;\; \partial_x[C(x,z)\partial_z U] \;\; + \;\; \partial_z[E(x,z)\partial_z U] \quad . \qquad (8)$$

Here, $U = (u,w)^T$, where u and w are the horizontal and vertical dispacements, respectively, and the matrices A,B,C, and E are given by

$$A = \begin{pmatrix} \lambda+2\mu & 0 \\ 0 & \mu \end{pmatrix} \quad B = \begin{pmatrix} 0 & \mu \\ \lambda & 0 \end{pmatrix} \quad C = \begin{pmatrix} 0 & \lambda \\ \mu & 0 \end{pmatrix} \quad E = \begin{pmatrix} \mu & 0 \\ 0 & \lambda+2\mu \end{pmatrix} .$$

Physically, this corresponds to treating P and SV-waves, but neglecting SH-wave motion. For a homogeneous medium (i.e. when A,B,C, and E are constant), equation (8) reduces to:

$$\rho U_{tt} = AU_{xx} + (B+C)U_{xz} + EU_{zz} . \qquad (8a)$$

Difference approximations for equations (6), (8), and (8a) are discussed in the next two sections.

II. Difference Approximations for Acoustic Waves

The usual explicit approximation for the acoustic wave equation in two dimensions with constant density (6a) is given by:

$$D_+^t D_-^t P_{j,k}^n = (c_k^n)^2 (D_+^x D_-^x + D_+^z D_-^z) P_{j,k}^n . \quad * \qquad (9)$$

This scheme is accurate to second order in $\Delta t, \Delta x$, and Δz. The necessary conditions for the stability of the method are quite straightforward to derive (Mitchell, p.206). First equation (9) is Fourier transformed with respect to x, and z, assuming that c is a constant to get:

$$D_+^t D_-^t \hat{P}_j = -(4c^2/h^2)[\sin^2(\eta/2) + \sin^2(\phi/2)]\hat{P}_j . \qquad (10)$$

(Here $\eta = k_x \Delta x$, $\phi = k_z \Delta z$, and $\Delta x = \Delta z = h$.) For the method to be stable with t as the evolution direction, it is necessary that the discrete L_2-norm of the solution at any time, $t>0$, be uniformly bounded in terms of the initial conditions, i.e., an estimate of the form

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*This differencing notation has been used throughout most of the recent SEP reports. A review is given in the appendix to this paper. In addition, most of the difference operators are given schematically in the appendix.

$$||P^n_{j,k}|| \le ||e^{\alpha t}P^n_{0,k}|| \qquad (11)$$

is desired, where α is a constant. By Parseval's relationship, it is clear that

$$|\hat{P}_k| \le |e^{\alpha t}\hat{P}_0| \qquad (11a)$$

is an equivalent bound. If the solution to (10) is assumed to be of the form

$$\hat{P}_j = \hat{P}_0 e^{ij\theta} , \qquad (12)$$

where $\theta = \omega\Delta t$, then a bound of the form (11a) can only be obtained if $Im(\theta) = 0$. Substituting (12) into (10), the following relationship results:

$$\sin^2(\theta/2) = (c^2\Delta t^2/h^2)[\sin^2(\eta/2) + \sin^2(\phi/2)] .$$

If $Im(\theta) = 0$, then the following inequality must hold:

$$(c^2\Delta t^2/h^2)[\sin^2(\eta/2) + \sin^2(\phi/2)] \le 1,$$

which ==> $(c\Delta t/h) \le 2^{-1/2}$. (13)

When c is variable, the stability requirement will be

$$(c_{max}\Delta t/h) \le 2^{-1/2} \cong .707 . \qquad (13a)$$

A scheme which is accurate to fourth order in Δx and Δz can be obtained by modifying the approximations for the x and z derivatives. The resulting difference equation is given by

$$D^t_+D^t_-P^n_{j,k} = (c^n_k)^2\{D^x_+D^x_-[1 - (h^2/12)D^x_+D^x_-] + D^z_+D^z_-[1 - (h^2/12)D^z_+D^z_-]\}P^n_{j,k} . \qquad (14)$$

The stability limit is given by

$$(c_{max}\Delta t/h) \le (3/8)^{1/2} \cong .612 . \qquad (15)$$

This scheme has a difference star which uses nine points at the j'th level. This is to be compared with the second-order scheme which uses five points at the j'th level. Both schemes use one grid point at the j-1'th and j+1'th levels.

The accuracy of the two methods can be compared by calculating the phase error associated with each approximation. If the differencing in the t-direction is ignored, and the solution to the differential equation can be written as

$$\hat{P}(t) = \hat{P}(t=0)e^{i\omega t} ,$$

and the solution to the difference equation is written

$$\hat{P}_j = \hat{P}_0 e^{i\tilde{\omega} j\Delta t} ,$$

then $\omega - \tilde{\omega}$ is the phase error. The dispersion relationship for the differential equation (with constant velocity) is

$$\omega^2 = c^2(k_x^2 + k_z^2) . \qquad (16)$$

The dispersion relationship for the difference equations will be slightly different from equation (16). Ignoring time differencing, the second-order scheme gives

$$\tilde{\omega}_2^2 = (4c^2/h^2)[\sin^2(\eta/2) + \sin^2(\phi/2)] , \qquad (16a)$$

and the fourth-order scheme gives

$$\tilde{\omega}^2_4 = (4c^2/h^2)(\sin^2(\eta/2)[1 + (1/3)\sin^2(\eta/2)] + \sin^2(\phi/2)[1 + (1/3)\sin^2(\phi/2)]) . \qquad (16b)$$

The phase error for the second-order scheme is then

$$e_2 = \omega(1 - [\frac{\sin^2(\eta/2) + \sin^2(\phi/2)}{(\eta/2)^2 + (\phi/2)^2}]^{1/2}) , \qquad (17a)$$

and the phase error for the fourth-order scheme is given by

$$e_4 = \omega\left(1 - \left[\frac{\sin^2(\eta/2)[1+(1/3)\sin^2(\eta/2)] + \sin^2(\phi/2)[1+(1/3)\sin^2(\phi/2)]}{(\eta/2)^2 + (\phi/2)^2}\right]^{1/2}\right) \quad (17b)$$

Contour plots of e_2 and e_4 vs. horizontal wavenumber η and vertical wavenumber ϕ are given in figure 1. It is seen that a relative phase error of 1% can be obtained if η and ϕ are less that $.16\pi$ for the second-order scheme, but η and ϕ need only be less than $.38\pi$ for the fourth order scheme to obtain the same degree of accuracy. In terms of points per wavelength, this means that the principal wavelengths must be sampled at 76 points per wavelength for the second order scheme, but only at 6.2 points per wavelength for the fourth-order scheme to get one-percent accuracy!

The result of undersampling will be dispersion of the higher wavenumbers since a non-zero phase error implies that the effective phase velocity is incorrect. It is possible to attenuate this dispersion by the addition of dissipative terms to the differencing scheme. This is discussed later on in section IV.

III. Difference Approximations for Elastic Waves

A second order accurate difference approximation method for equation (8) is given by Kelly et. al. (1976), and is repeated below:

$$\rho^n_k D^t_+ D^t_- U^n_{j,k} = (D^x_{1/2} A^n_k) D^x_o U^n_{j,k} + {}^{x}\bar{A}^n_k D^x_+ D^x_- U^n_{j,k}$$

$$+ (D^z_{1/2} E^n_k) D^z_o U^n_{j,k} + {}^{z}\bar{E}^n_k D^z_+ D^z_- U^n_{j,k} + (D^z_o B^n_k) D^x_o U^n_{j,k}$$

$$+ {}^{zo}\bar{B}^n_k D^z_o D^x_o U^n_{j,k} + (D^x_o C^n_k) D^z_o U^n_{j,k} + {}^{xo}\bar{C}^n_k D^z_o D^x_o U^n_{j,k} \quad . \quad (18)$$

In a homogeneous medium, this reduces to

$$\rho D^t_+ D^t_- U^n_{j,k} = A D^x_+ D^x_- U^n_{j,k} + (B + C) D^z_o D^x_o U^n_{j,k} + E D^z_+ D^z_- U^n_{j,k} \quad . \quad (18a)$$

A scheme accurate to fourth-order in Δx and Δz can be gotten by replacing D_+D_- by $D_+D_-[1 - (h^2/12)D_+D_-)$, replacing $D^z_o D^x_o$ with

$D_o^zD_o^x[1 - (h^2/6)(D_+^xD_-^x + D_+^zD_-^z)]$, D_o with

$D_o[1 - (h^2/6)D_+D_-)$, and $D_{1/2}$ with $D_{1/2}[1 - (h^2/24)D_{+1/2}D_{-1/2}]$.

For the homogeneous case, the resulting differencing scheme is:

$$\rho D_+^tD_-^tU_{j,k}^n = AD_+^xD_-^x[1 - (h^2/12)D_+^xD_-^x]U_{j,k}^n$$
$$+ (B+C)D_o^zD_o^x[1 - (h^2/6)(D_+^xD_-^x + D_+^zD_-^z)]U_{j,k}^n$$
$$+ ED_+^zD_-^z[1 - (h^2/12)D_+^zD_-^z]U_{j,k}^n \quad . \qquad (19)$$

In order to calculate the phase error for the elastic wave approximations, it is first necessary to determine the dispersion relationships. Again, consideration is limited to the constant-coefficient case, although the conclusions drawn apply to the variable-coefficient case as well. Fourier-transforming equation (8a) gives:

$$MU = \begin{pmatrix} (\lambda+2\mu)k_x^2 + \mu k_z^2 - \rho\omega^2 & (\lambda+\mu)k_xk_z \\ (\lambda+\mu)k_xk_z & \mu k_x^2 + (\lambda+2\mu)k_z^2 - \rho\omega^2 \end{pmatrix} U = 0 \quad . \qquad (20)$$

The dispersion relations are defined by det(M) = 0:

$$\omega^2 = [(\lambda+2\mu)/\rho](k_x^2 + k_z^2) \qquad (21a)$$

and

$$\omega^2 = [\mu/\rho](k_x^2 + k_z^2), \qquad (21b)$$

or in terms of the compressional and shear wave velocities, α and β,

$$\omega^2 = \alpha(k_x^2 + k_z^2), \qquad (22a)$$

and

$$\omega^2 = \beta(k_x^2 + k_z^2) \quad . \qquad (22b)$$

The dispersion relations for the approximation equations can also be derived. For the second-order case,

$$\tilde{\omega}^2_2 = (1/h^2)\{[\alpha+\beta](2\sin^2(\eta/2) + 2\sin^2(\phi/2))]$$

$$\pm (\alpha-\beta)[4(\sin^2(\eta/2)-\sin^2(\phi/2))^2 + \sin^2\eta\sin^2\phi]^{1/2}\}, \quad (23)$$

and for the fourth-order case,

$$\tilde{\omega}^2_4 = (1/h^2)\{(\alpha+\beta)[2\sin^2(\eta/2)(1+(1/3)\sin^2(\eta/2))+2\sin^2(\phi/2)(1+(1/3)\sin^2(\phi/2))]$$

$$\pm (\alpha-\beta)\{4[\sin^2(\eta/2)(1+(1/3)\sin^2(\eta/2))-\sin^2(\phi/2)(1+(1/3)\sin^2(\phi/2))]^2$$

$$+\sin^2\eta\sin^2\phi[1 +(2/3)\sin^2(\eta/2) + (2/3)\sin^2(\phi/2)]^{1/2}\} . \quad (24)$$

(The plus-sign gives the dispersion relation for p-waves; the minus-sign is for s-waves.) Using the definition given above for the phase error, two equations result for each approximation: one for compressional waves and one for shear waves. The phase errors depend on η and ϕ, and also on the ratio of the p-wave to s-wave velocities, α/β. Figures 2 through 5 show the relative phase error contour plots for the second and fourth order elastic wave approximations for $\alpha/\beta = 3^{1/2}$ and $\alpha/\beta = 3$. The plots indicate that, in general, the approximations are better for shear-waves than for compressional waves, and that they are better for α/β near unity than for α/β large. Again, from the plots, it can be seen that for 1% error, the fourth-order schemes require far fewer sample points per wavelength than do the second-order schemes.

For the elastic equations with constant coefficents, the necessary conditions for stability of the differencing schemes can be derived in the same way as was done above for the acoustic equations. The results are:

$$[(\alpha^2+\beta^2)^{1/2}\Delta t/h] \leq 1 \quad (25)$$

for the second order scheme, and

$$[(\alpha^2+\beta^2)^{1/2}\Delta t/h] \leq 3^{1/2}/2 \cong .866 \quad (26)$$

for the fourth order scheme. When going from the constant coefficient case to the variable-coefficient case, the resulting extra terms in the differencing schemes contain only first differences of U, and hence the stability limits for the constant coefficient equations apply to the variable coefficient equations as well. (Gustafsson, Kreiss and Sundström, 1972, theorem 4.3)

IV. Dissipative Terms

As mentioned earlier, dissipative terms can be added to the difference approximations to attenuate the higher wavenumbers which are calculated incorrectly. In this section, the appropriate terms are derived.

In order to simplify the discussion, consider the acoustic wave equation in one space variable:

$$P_{tt} = c^2 P_{zz} \, . \qquad (27)$$

The solution looks like $P = e^{\pm ick_z t}$. The idea behind dissipation is to attenuate the high spatial wavenumbers so that the solution is modified to look something like

$$P = \exp(\pm ick_z t - \varepsilon k_z^2 t) \qquad (28a)$$

or possibly

$$P = \exp(\pm ick_z t - \varepsilon k_z^4 t) . \qquad (28b)$$

This can be accomplished by adding a term of the form $2\varepsilon P_{zzt}$ or of the form $-2\varepsilon P_{zzzzt}$ to the right-hand side of equation (27). To show that the solution to the resulting equation does, in fact, attenuate in this manner, Fourier transform equation (27) in z, including the first extra term suggested above. The result is:

$$(\partial_t + 2\varepsilon k_z^2)\partial_t \hat{P} = -c^2 k_z^2 \hat{P} \, . \qquad (29)$$

Assuming that the solution to this equation is of the form $\hat{P} = \exp(i\theta t)$, the following polynomial equation for θ results:

$$\theta^2 - 2i\varepsilon k_z^2 \theta - c^2 k_z^2 = 0.$$

The solution will be

$$\theta = i\varepsilon k_z^2 \pm (-\varepsilon^2 k_z^4 + c^2 k_z^2)^{1/2}$$

$$\cong i\varepsilon k_z^2 \pm c k_z \ .$$

It is obvious that the solution will be equation (28a). The same procedure may be followed with the second term suggested, giving (28b) as the solution.

Dissipative terms are formally not added to the differential equation itself, but to the difference approximation. Also, they must be added in such a way that they disappear in the limit. This is done to assure that the equation being approximated is the real differential equation, and not some other equation. For the second-order scheme for the acoustic equation (9), this means that the dissipative terms must be $O(h^2P_{zz} + h^2P_{xx})$ or higher, and for the fourth-order scheme (14), they should be at least $O(h^4P_{xxxx} + h^4P_{zzzz})$.

The appropriate dissipative terms to be added to equation (9) will be

$$2\varepsilon h^2 \Delta t D_-^t (D_+^z D_-^z + D_+^x D_-^x) P_{j,k}^n \qquad (30)$$

which are added to the right-hand side of the equation. For equation (14), the appropriate terms are

$$-2\varepsilon h^4 \Delta t D_-^t \ [(D_+^z D_-^z)^2 + (D_+^x D_-^x)^2] \qquad (31)$$

which are added to the right-hand side also. These additional terms operate only on the j'th and j-1'th levels, so the resulting scheme is still explicit. The choice for ε will depend on how much dissipation is desired, and can be determined by practical experimentation.

One disadvantage of the fourth-order dissipative terms (31) is that the resulting algorithm will require a large number of grid points at the j-1'th level as well as the j'th level of calculation. In actual practice, the second-order terms (30) can be used with the fourth-order differencing scheme with reasonable results. (This could probably be justified theoretically if one chose ε so that

$$|\varepsilon h^2(P_{xx} + P_{zz})| \le |\delta h^4(P_{xxxx} + P_{zzzz})|$$

for some reasonable choice of δ.)

V. Examples

We illustrate the 2^{nd} and 4^{th} order difference schemes discussed in this paper with the scalar wave equation. For both schemes we also show the effect of adding dissipative terms to the approximations. Elastic wave equation examples will be the subject of a future report.

The examples were all run on a 128 X 128 grid with a grid spacing of 50 m. Free surface boundary conditions were applied along the top edge of the grid, and simple first order absorbing boundary conditions (Clayton and Engquist, SEP-11) were used on the other three sides. The velocity model and one of the initial conditions are shown in the upper part of Figure 6. The initial conditions were taken as the far-field approximation of a 2-D point source, sampled at two successive times. The source waveform is the derivative of a Gaussian function. The examples were all run with a time interval of 0.005 seconds.

The two panels at the bottom of Figure 6 are time slices of the wavefield at 100 and 200 time steps. These are shown to aid in the interpretation of the wavefields in the next few figures.

In Figure 7, the solution of the wavefield at 300 time steps by four difference schemes is shown. The two top panels show that by increasing the order of the difference approximation a significant improvement in grid dispersion is achieved. This is particularly noticeable on the free surface reflection (the major white event in the center of the wavefield). A comparison of the two 2^{nd} order solutions shows that a similar improvement can be achieved by dissipating the higher wavenumbers. The penalty for this improvement is that the source waveform is slightly broadened. The 4^{th} order scheme shows only slight improvement with dissipation. Dissipation in these examples is measured by the percentage ratio of $\varepsilon/(v\Delta t/h)^2$.

In the next two figures the surface seismograms for the four approximations are shown. It is evident that both increasing the order of the differencing scheme and adding dissipative terms decreases the grid dispersion.

References

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Kelly, K. R., R. W. Ward, Sven Treitel, and R. M. Alford (1976), "Synthetic Seismograms: A Finite Difference Approach", Geophysics, 41, p. 2.

Mitchell, A.R. (1969), Computational Methods in Partial Differential Equations, New York: John Wiley and Sons, 255 pp.

VI. Appendix

A. Summary of Difference Notation

$$D^x_+ P_k = (P_{k+1} - P_k)/\Delta x$$

$$D^x_- P_k = (P_k - P_{k-1})/\Delta x$$

$$D^x_o P_k = (P_{k+1} - P_{k-1})/2\Delta x$$

$$D^x_{1/2} A_k = (A_{k+1/2} - A_{k-1/2})/\Delta x$$

$$D^x_{+1/2} A_k = 2(A_{k+1/2} - A_k)/\Delta x$$

$$D^x_{-1/2} A_k = 2(A_k - A_{k-1/2})/\Delta x$$

$$P^n_{j,k} = P(k\Delta x, n\Delta z, j\Delta t)$$

$$A^n_k = A(k\Delta x, n\Delta z)$$

$${}^{x}\bar{A}^n_k = (A^n_{k+1/2} + A^n_{k-1/2})/2$$

$${}^{xo}\bar{A}^n_k = (A^n_{k+1} + A^n_{k-1})/2$$

B. Schematics

(for these operators it is assumed that $\Delta x = \Delta z = h$)

1. $h^2(D^x_+ D^x_- + D^z_+ D^z_-) = h^2[\partial_{xx} + \partial_{zz} + O(h^2)]$

$$\begin{array}{ccc} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{array}$$

2. $h^2(D_+^x D_-^x[1 - (h^2/12)D_+^x D_-^x] \;+\; D_+^z D_-^z[1 - (h^2/12)D_+^z D_-^z])$
$= \;\; h^2[\partial_{xx} + \partial_{zz} + O(h^4)]$

		-1/12		
		4/3		
-1/12	4/3	-5	4/3	-1/12
		4/3		
		-1/12		

3. $h^2 D_o^x D_o^z \;=\; h^2[\partial_x \partial_z \;+\; O(h^2)]$

1/4	0	-1/4
0	0	0
-1/4	0	1/4

4. $h^2 D_o^x D_o^z[1 - (1/6)(D_+^x D_-^x + D_+^z D_-^z)]$
$= \;\; h^2[\partial_x \partial_z + O(h^4)]$

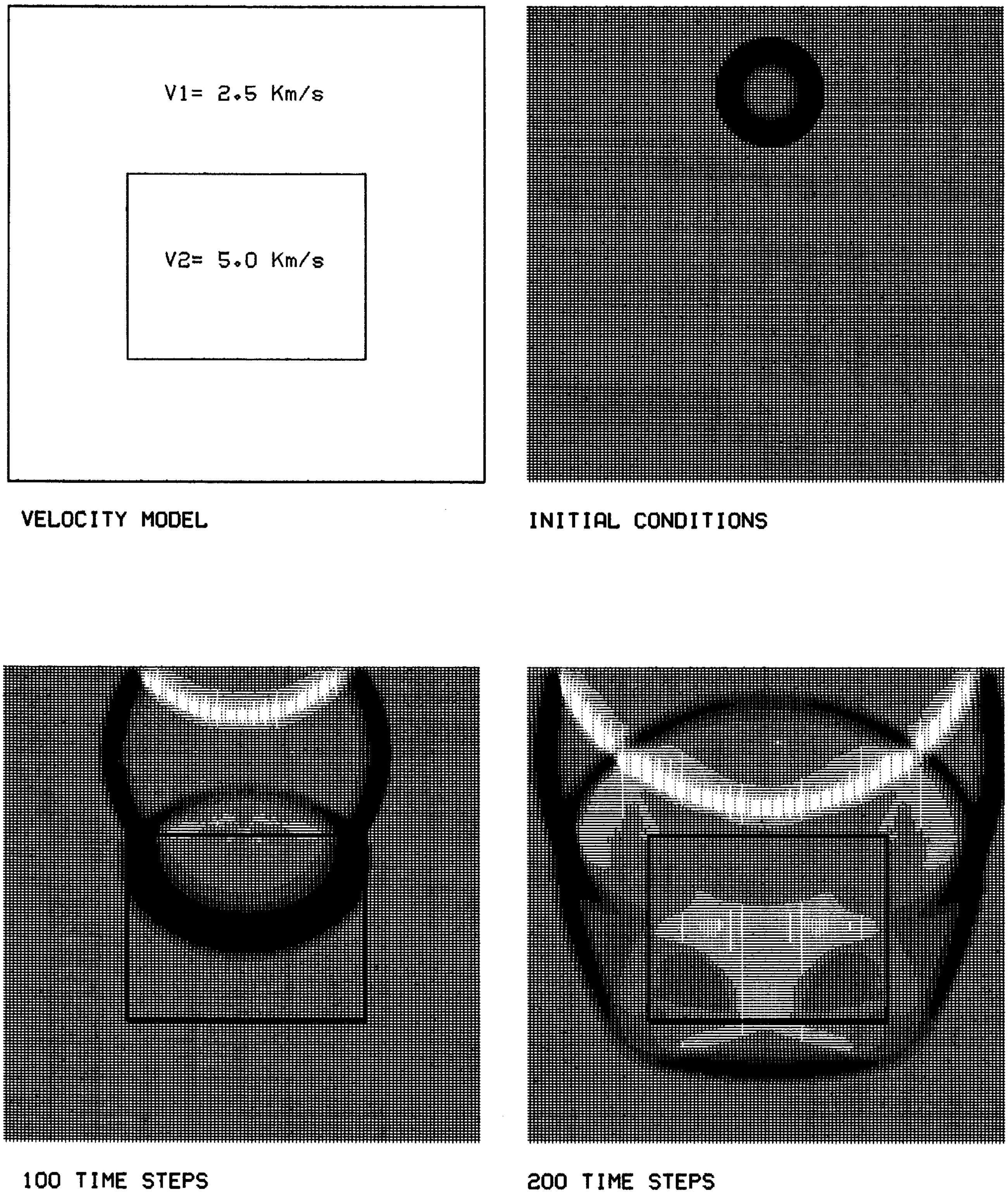
	-1/24		1/24	
-1/24	5/12	0	-5/12	1/24
	0	0	0	
1/24	-5/12	0	5/12	-1/24
	1/24		-1/24	

5. $hD_o^x \;=\; h[\partial_x \;+\; O(h^2)]$

-1/2	0	1/2

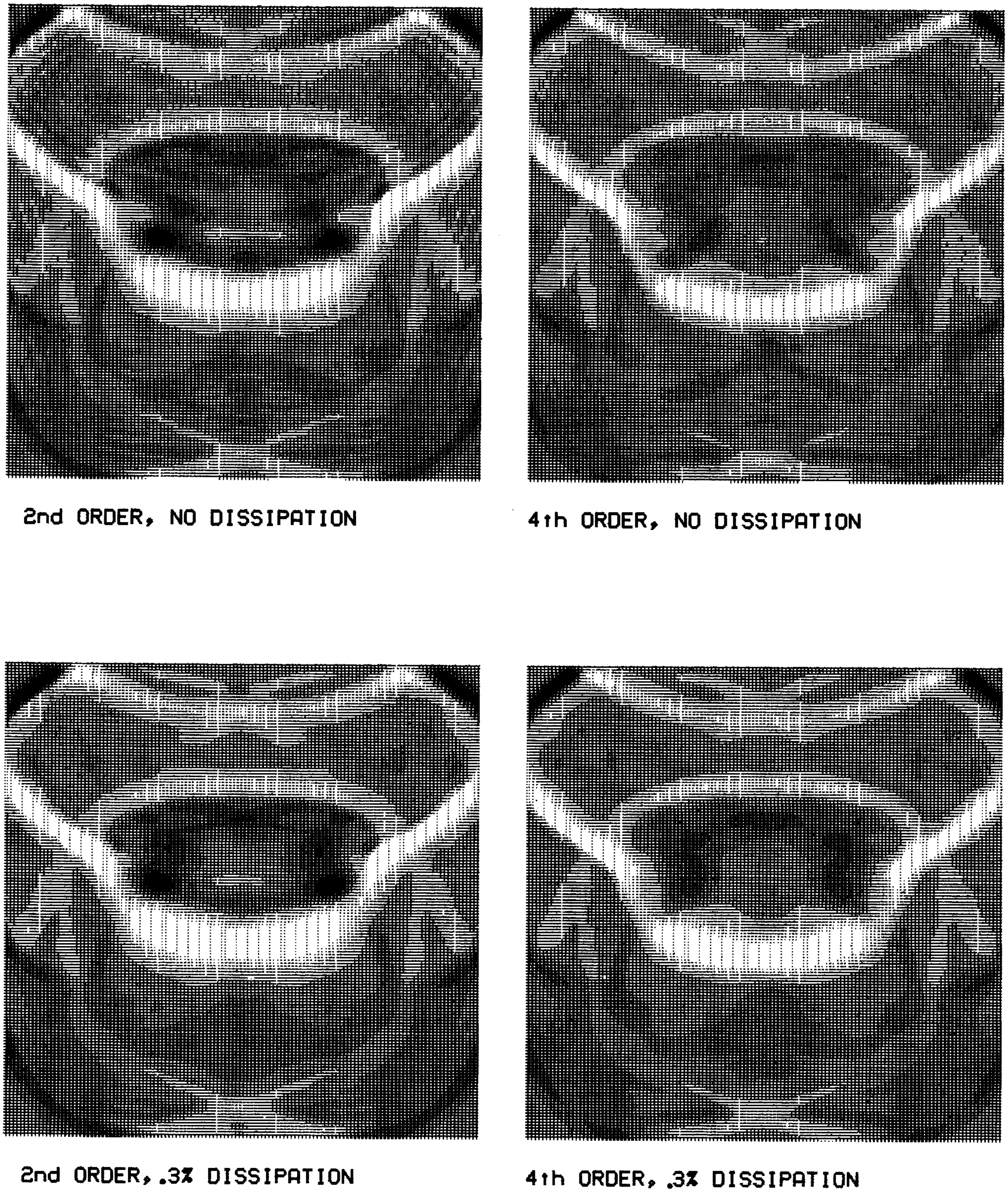
6. $$hD_0^x[1 - (h^2/6)D_+^xD_-^x] = h[\partial_x + O(h^4)]$$

1/12 -2/3 0 2/3 -1/12



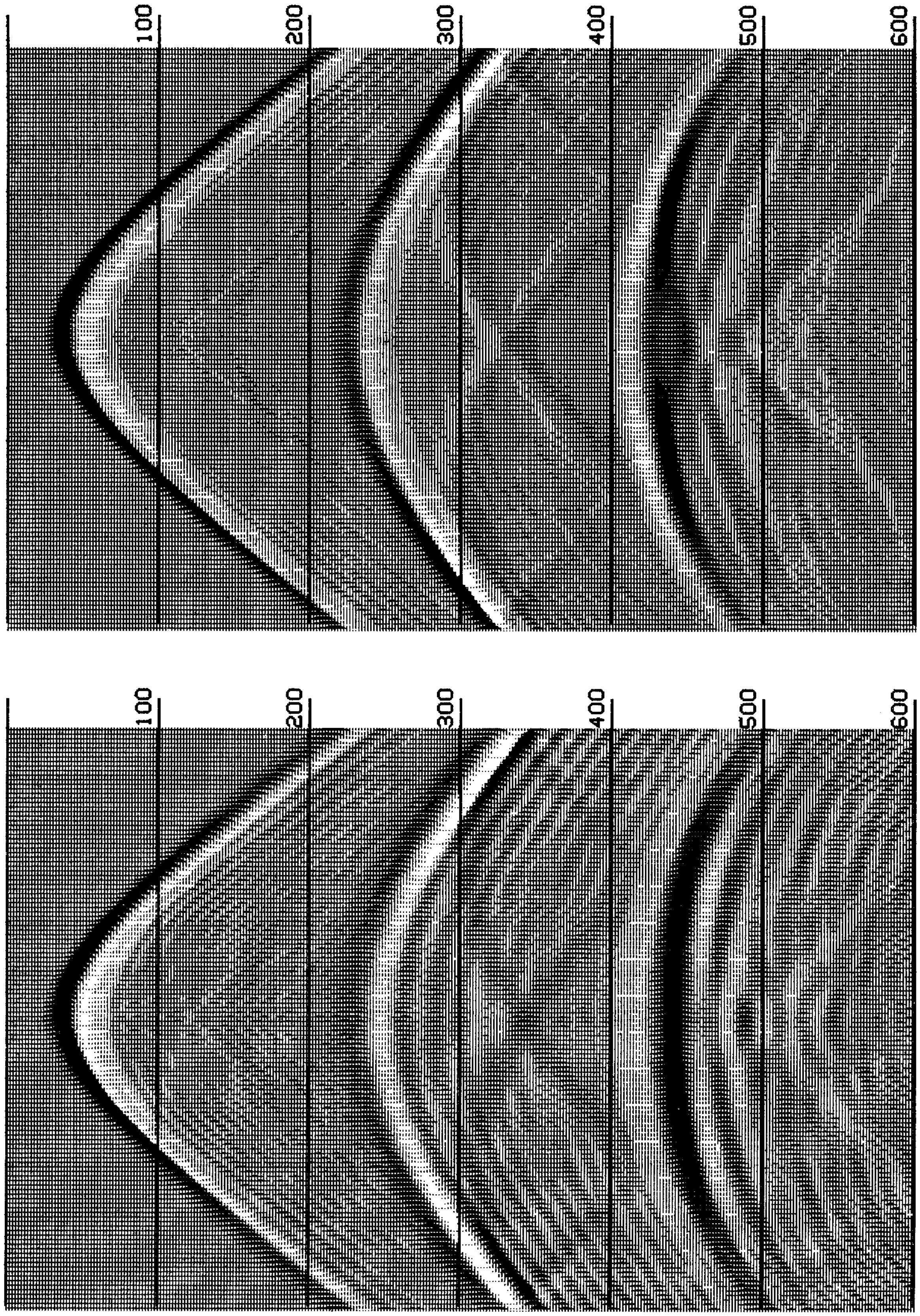
4th ORDER, 3% DISSIPATION

Figure 6



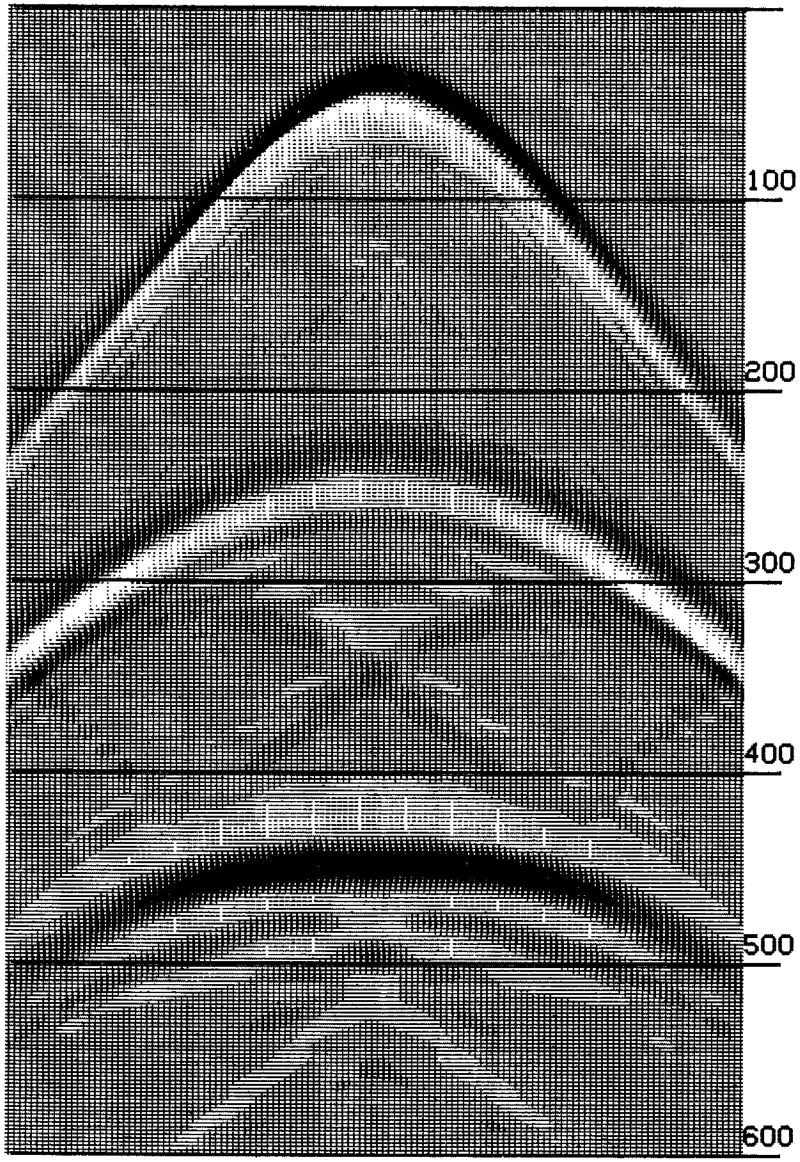
300th TIME STEP

Figure 7

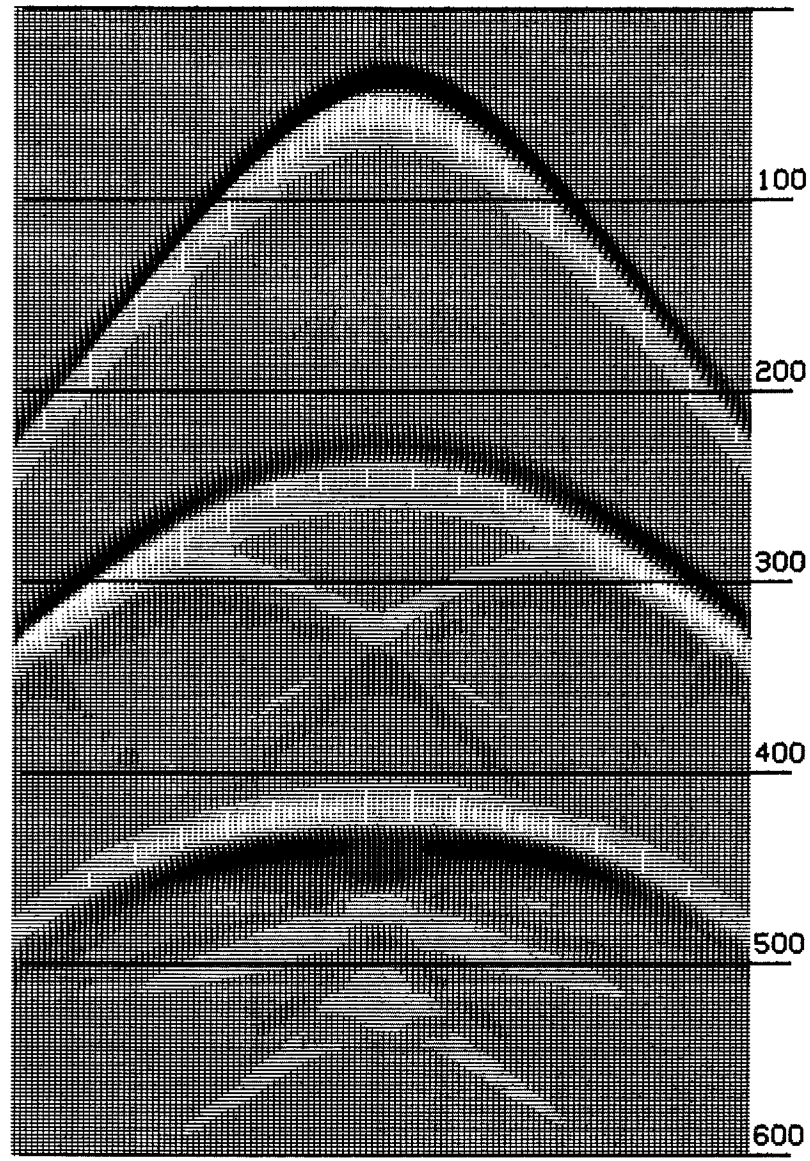


100
200
300
400
500
600
4th ORDER, NO DISSIPATION
2nd ORDER, NO DISSIPATION

Figure 8



2nd ORDER, .3% DISSIPATION



4th ORDER, .3% DISSIPATION

Figure 9