Finite Differences

At first glance, finite difference modeling is by far the simplest method to grasp. All that is necessary is to replace the continuous partial derivatives by discrete approximations. The main difficulty arises in producing an accurate approximation to the various derivatives. There are two generally accepted approaches to finding approximations. The first is based purely on some form of fitting algorithm, frequently using polynomials, wherein a set of basis functions with known derivatives approximate the function whose derivative is required. Once the fit is obtained the derivative is defined in terms of the approximating functions.

In the finite element method, the region of interest is divided up into numerous connected subregions or elements within which approximate functions (usually polynomials) are used to represent the unknown quantity.

The difference between the values of a function at two discrete points, used to approximate the derivative of the function.

Polynomial Differences

The easiest approach to finite difference approximation is to simply use a difference quotient in Equation 2-59 like we did when we derived the full two-way equation.

(2-59)
$$\frac{du}{dx} = \frac{u(x+\Delta x) - u(x)}{\Delta x}$$

This is what is called a first order forward difference approximation. Similarly, we have the backward difference in the form Equation 2-60.

(2-60)
$$\frac{du}{dx} = \frac{u(x) - u(x-\Delta x)}{\Delta x}$$

What may not be so clear is that these formulas are the result of approximating u by a straight line between $x+\Delta x$ and x and between $x-\Delta x$ and x.

One of the more popular methods for polynomial approximation is based on the Lagrange polynomial in Equation 2-61 defined for a sequence of points $[x_0, x_1, x_2, \ldots x_n]$.

(2-61)
$$L_{n,k}(x) = \prod_{\substack{i=0 \\ i\neq k}}^{i=n} \frac{(x-x_i)}{(x_k-x_i)}$$

Any function $f(x)$ defined that the point sequence can then be approximated by the formula of Equation 2-62.

(2-62)
$$P(x) = \sum_{k=0}^{k=n} f(x_k) L_{n,k}(x)$$

Approximations to the derivatives of $f(x)$ can then be approximated through derivatives of the polynomial P. Since P will always be of the form in Equation 2-63, the approximate derivative will always be a weighted sum of the values of $f(x)$ at the sequence $[x_0, x_1, x_2, \ldots x_n]$.

(2-63) $$P(x) = a_0 + a_1 x + a_2 x^2 + \ldots a_n x^n$$

More accurate approximations can be obtained through the use of other polynomial bases, including the Hermite and Chebychev polynomials.

Taylor Series Differences

The Taylor series for $u(x \pm \Delta x)$ in terms of $u(x)$ is given in Equation 2-64.

(2-64) $$u(x \pm \Delta x) = u(x) \pm \frac{\partial u}{\partial x}\Delta x + \frac{\partial^2 u}{\partial x^2}\frac{\Delta x^2}{2!} \pm \frac{\partial^3 u}{\partial x^3}\frac{\Delta x^3}{3!} + \ldots$$

If we rearrange this series in the form Equation 2-65, we immediately recognize that the forward and backward differences are accurate to Δx. Mathematically, we say that the forward and backward differences are $O(\Delta x)$.

(2-65) $$\frac{u(x \pm \Delta x) - u(x)}{\Delta x} = \pm\frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2}\frac{\Delta x}{2!} \pm \frac{\partial^3 u}{\partial x^3}\frac{\Delta x^2}{3!} + \ldots$$

The Taylor series in Equation 2-64 can easily form the basis for other more accurate formulas. The most obvious formula arises from the sum of the Taylor series expansions for $u(x + \Delta x) - u(x)$ and $u(x) - u(x - \Delta x)$. This immediately yields the central difference formula in Equation 2-66 which is $O(\Delta x^2)$.

(2-66) $$\frac{u(x + \Delta x) - u(x - \Delta x)}{2\Delta x} = \frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3}\frac{\Delta x^2}{3!} + \frac{\partial^5 u}{\partial x^5}\frac{\Delta x^4}{5!} + \ldots$$

Since we generally think of Δx as being much less than 1 in magnitude, this central difference formula is clearly an improvement over a first-order forward or backward difference.

Second Order Differences

When we summed the formulas for $u(x + \Delta x) - u(x)$ and $u(x) - u(x - \Delta x)$, we obtained a series that contained odd order derivatives. Accordingly, if we subtract the two formulas, we obtain a series that contains only even order derivatives. This immediately produces $O(\Delta x^2)$ formula for the second derivative with respect to x.

(2-67) $$\frac{u(x + \Delta x) - 2u(x) + u(x - \Delta x)}{\Delta x^2} = \frac{\partial u^2}{\partial x^2} + \frac{\partial^4 u}{\partial x^4}\frac{\Delta x^2}{4!} + \frac{\partial^6 u}{\partial x^6}\frac{\Delta x^4}{6!} + \ldots$$

High Order Differences

Extension of the second order central difference formula to higher orders is tedious, but straight forward. For any given k (real or integer), there is Equation 2-68.

$$\frac{u(x+k\Delta x)+u(x-k\Delta x)}{2} = u(x)+k^2\frac{\partial u^2}{\partial x^2}\frac{\Delta x^2}{2!}+k^4\frac{\partial^4 u}{\partial x^4}\frac{\Delta x^4}{4!} + k^6\frac{\partial^6 u}{\partial x^6}\frac{\Delta x^6}{6!}+k^8\frac{\partial^8 u}{\partial x^8}\frac{\Delta x^8}{8!}\dots \tag{2-68}$$

Thus, if we want a fourth order scheme, we take the two terms in Equation 2-69 and Equation 2-70, solve the second term for the fourth order partial derivative and substitute the result into the first term to obtain Equation 2-71.

$$\frac{u(x+\Delta x)+u(x-\Delta x)}{2} = u(x)+\frac{\partial u^2}{\partial x^2}\frac{\Delta x^2}{2!}+\frac{\partial^4 u}{\partial x^4}\frac{\Delta x^4}{4!} \tag{2-69}$$

$$\frac{u(x+2\Delta x)+u(x-2\Delta x)}{2} = u(x)+4\frac{\partial u^2}{\partial x^2}\frac{\Delta x^2}{2!}+16\frac{\partial^4 u}{\partial x^4}\frac{\Delta x^4}{4!} \tag{2-70}$$

$$\frac{u(x+2\Delta x+16u(x+\Delta x)-34u(x)+16u(x-\Delta x)+u(x-2\Delta x)}{12\Delta x^2} \approx \frac{\partial u^2}{\partial x^2} \tag{2-71}$$

Higher order central difference approximations are obtained by simply adding additional terms to the mix. For example, a 10th order accurate term is obtained by back-substitution in the five equations when $k = 1,2,3,4,5$. The result is a scheme of the form in Equation 2-72, where the terms are given in Table 2.1.

$$\frac{\partial u^2}{\partial x^2} \approx \sum_{-5}^{5} w_k u(x-k\Delta x) \tag{2-72}$$

Table 2.1. Spatial Difference Terms

|k|	w
0	-5.8544444444
1	3.3333333333
2	-0.4761904762
3	0.0793650794
4	-0.0099206349
5	0.0006349206

Finite Differences for the Pressure Formulation

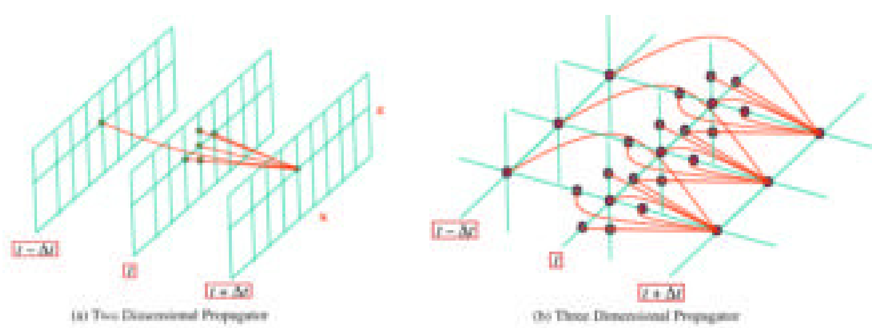
We can now formulate a finite difference propagation equation of just about any order we would like. However, it is of interest to reconsider the graphic in Figure 2-16(b). This figure, based on a simple second-order space-time difference equation shows that to compute any given fixed time stamp, the maximum extent of the stencil is exactly equal to three in each spatial direction and two in time. Thus, to make this process computationally efficient, it is prudent to keep the three $t - \Delta t$, t and $t + \Delta t$ volumes in memory at all times.

It is clear from Equation 2-72 that higher order differences will produce stencils with maximum extent determined by the maximum value of k. Thus, if we chose to use a 10th order scheme for each both space and time, our propagator will be 11 grid nodes wide in each spatial direction and 10 volumes in memory for each of the time stamps $t - k\Delta t$ for $k = -5, 5$. Even with current computational capabilities, holding this many volumes in memory is somewhat impractical. It is natural to try and find a procedure that avoids this memory explosion problem.

Graphical Descriptions

Figure 2-16(a) demonstrates two-dimensional propagation and Figure 2-16(b) demonstrates three-dimensional propagation in what is generally called acoustic Earth models. Note that the central difference stencil extends from time $t - \Delta t$ to time t to compute an output point at $t + \Delta t$.

Figure 2-16. Graphical interpretation of (a) 2-D and (b) 3-D propagators.



Note that in both cases, the stencil surrounds the ultimate output point to compute the new value. In the 2-D case, the stencil nodes are planar, while the 3-D nodes are volumetric. Thus, the wavefields are allowed to propagate upward, downward, and laterally in all directions as the propagation continues. It also means that we must compute all nodes at step t before we can compute any of the nodes at $t + \Delta t$. The examples in the last three figures produce what is called two-way propagation. All waveform styles (for example, refractions, free-surface, and peg-leg multiples) are possible in this setting since these propagators synthesize full waveform data.

Lax-Wendroff Method

Probably the best known "trick", initially published by Peter Lax and Burton Wendroff (see also M.A. Dablain), used the wave equation to find a fourth order accurate difference for $\frac{\partial^2}{\partial t^2}$ that does not increase the overall memory requirement. To understand this trick, consider the case in two dimensions when the velocity is constant and $\rho = 1$. From earlier efforts, we have Equation 2-73.

(2-73)
$$\begin{aligned}\frac{\partial^2 p}{\partial t^2} &= \frac{1}{\Delta t^2}\left(p(t+\Delta t) - 2p(t) + p(t-\Delta t) - \sum_{i=2}^{i=\infty}\frac{\partial^{2i} p}{\partial t^{2i}}\frac{\Delta t^{2i}}{2i!}\right)\\ &\approx \frac{1}{\Delta t^2}\left(p(t+\Delta t) - 2p(t) + p(t-\Delta t) - \frac{\partial^4 p}{\partial t^4}\frac{\Delta t^4}{12!}\right)\end{aligned}$$

We also know the second order derivative, $\frac{\partial^2 p}{\partial t^2}$, in Equation 2-74.

(2-74)
$$\frac{\partial^2 p}{\partial t^2} = v^2\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial z^2}\right)$$

Thus, the fourth order derivative in time is given by Equation 2-75.

(2-75)
$$\begin{aligned}\frac{\partial^4 p}{\partial t^4} &= v^2\left[\frac{\partial^2 p}{\partial x^2}\left(\frac{\partial^2 p}{\partial t^2}\right) + \frac{\partial^2 p}{\partial z^2}\left(\frac{\partial^2 p}{\partial t^2}\right)\right]\\ &= v^2\left[\frac{\partial^2 p}{\partial x^2}\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial z^2}\right) + \frac{\partial^2 p}{\partial z^2}\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial z^2}\right)\right]\\ &= v^4\left(\frac{\partial^4 p}{\partial x^4} + 2\frac{\partial^4 p}{\partial x^2 \partial z^2} + \frac{\partial^4 p}{\partial x^4}\right)\end{aligned}$$

It should be noted that the assumptions of constant density and velocity are not necessary because the Lax-Wendroff scheme generalizes our scheme for finding higher order central difference terms through the recursive formula in Equation 2-76.

(2-76)
$$\frac{\partial^{2i} p}{\partial t^{2i}} = -\left(\rho v^2 \nabla \cdot \frac{1}{\rho}\nabla p\right)\frac{\partial^{2i-2} p}{\partial t^{2i-2}}$$

What we did in this case was to recognize that higher order time derivatives can be computed from higher order spatial derivatives by applying the spatial side of the original wave equation.

If we now replace the spatial derivatives using formulas like that in Equation 2-72, we arrive at a fourth order formula for the second partial derivative in time. After calculating all the various weights, replacing partial derivatives with central differences, and solving for $p_{i,j,n+1} = p(i\Delta x, j\Delta z, n\Delta t + \Delta t)$, we arrive at a discrete central difference formula of general form shown in Equation 2-77.

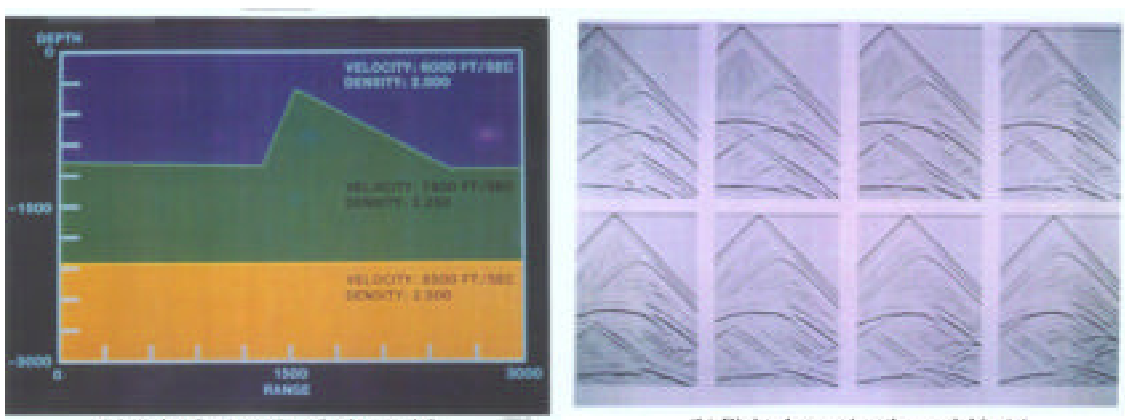
$$
\begin{aligned}
p_{i,j,n+1} &= -2p_{i,j,n} + p_{i,j,n-1} \\
&+ \Delta t^2 \left[v^4 \sum_k \sum_m a_{k,m} p_{i-k,j-m,n} + v^2 \left(\sum_k b_k p_{i-k,j,n} + \sum_m c_m p_{i,j-m,n} \right) \right] \\
&+ s_{i_0,j_0,n}
\end{aligned}
\tag{2-77}
$$

For clarity, Δx^2 and Δy^2 have been suppressed, and $s_{i_0,j_0,n}$ represents a source at the location specified by i_0 and j_0.

Formulas of this kind are generally called *difference equations* and provide what is usually called an *explicit* forward marching algorithm for data synthesis. Schemes of this kind are also called *quadrature methods* because they are integrating the wave equation to synthesize a response to a given stimulus.

Figure 2-17 shows a simple pyramid model and data. The finite difference data over this model was synthesized on VAX 11-780 computers in late 1981 and early 1982. At that time, the calculations necessary to compute each shot required on the order of 48 hours. Today, most laptops can compute the entire set of 24 shots in minutes.

Figure 2-17. A simple pyramid model and data.



(a) A simple acoustic velocity model (b) Eight shots using the model in (a)

Elastic Finite Differences

We now turn our attention to discrete simulation of vector elastic data. We can do this using either Equation 2-35 or Equation 2-36. Choosing the first equation leads to a method that is essentially the same as the pure explicit finite difference algorithm discussed in the previous section. To gain a slightly different perspective, we base our

Propagation Stability

Each of the various finite difference methods you might construct contains a ratio of the form $\frac{v\Delta t}{\Delta v}$, where v is one of the spatial increments Δx, Δy or Δz. It might come as somewhat of a surprise that if this ratio is too large, the propagation scheme it helps define will not be stable. An unstable scheme will eventually produce excessively large numbers and exceed the numerical accuracy of the machine it is running on.

Derivation of a formula that can provide an accurate bound for these ratios requires that we first relate frequency to wavenumber. To do this in a simple manner, we begin with the 1-D version of the Lax-Wendroff discrete pressure equation (Equation 2-17), as shown in Equation 2-95, where v is velocity.

(2-95)
$$\frac{1}{\Delta t^2}\left(p(t+\Delta t) - 2p(t) + p(t-\Delta t) - \sum_{i=2}^{i=\infty} \frac{\partial^{2i} p}{\partial t^{2i}} \frac{\Delta t^{2i}}{2i!}\right) = v^2 \frac{\partial^2 p}{\partial t^2}$$

To make our life just a bit easier, we assume a solution of the form $\exp[ik_x x - \omega \Delta t]$ and ignore the higher order terms to obtain the dispersion relation in Equation 2-96 and Equation 2-97.

(2-96)
$$\frac{1}{\Delta t^2}[2\cos(\omega \Delta t) - 2] = \frac{4}{\Delta t^2}\sin^2\left(\frac{\omega \Delta t}{2}\right) = v^2 k_x^2$$

(2-97)
$$\frac{2}{\Delta t}\sin\left(\frac{\omega \Delta t}{2}\right) = v k_x$$

Although the true dispersion relation for the 1-D equation has $c = \frac{\omega}{k_x}$, Equation 2-98 says that the discrete velocity is greater than the true velocity.

(2-98)
$$\bar{v} = \frac{v}{\frac{\sin(\pi f \Delta t)}{\pi f \Delta t}}$$

Thus, to avoid explosive growth, we must have the relation in Equation 2-99.

(2-99)
$$\Delta t \leq \frac{2}{\pi}\left(\frac{\Delta x_{min}}{v_{max}}\right)$$

A similar analysis shows that to achieve stable isotropic elastic $(P - SV)$ waves, we must have the relation in Equation 2-100.

(2-100)
$$\Delta t \leq \frac{\Delta x_{min}}{\sqrt{v_P^2 + v_{SV}^2}}$$

The important aspect of this analysis is that we cannot choose our time step size arbitrarily. We must use the appropriate version of Equation 2-99 or Equation 2-100 to assure ourselves that the calculations we perform and consequently the waveform we produce will not grow exponentially.