Project #5: Symmetric Molecule in Moving Frame

1 The Shift Factor

Suppose one wants to look at the wave equation in a moving frame that has a speed β. β is known as the shift factor of a frame. To make calculations in that frame, one has to modify the wave equation to:

$$0 = (1-\beta^2)\frac{\partial^2 Q}{\partial x^2} + 2\beta\frac{\partial^2 Q}{\partial x \partial t} - \frac{\partial^2 Q}{\partial t^2}$$

The solutions for these equations then become $Af(x-(1-\beta)t)$ and $Bg(x+(1+\beta)t$. A $\beta \in [-1,1]$ will make the rightward moving wave move slower, while the leftward moving wave will be faster. This observation is obvious when one thinks of the solution as the view from a moving frame.

Applying the expansion terms derived through the symmetric molecule, one can rewrite the wave equation as the following matrix equation.

$$\begin{aligned}
\frac{1}{2}(\theta_t - \rho^2(1-\beta^2)\theta_x)(Q_{j-1}^{n+1} + Q_{j+1}^{n+1}) & \\
+\beta\rho(Q_{j-1}^{n+1} - Q_{j+1}^{n+1}) & \\
+(1-\theta_t+\rho^2(1-\beta^2)\theta_x)Q_j^{n+1} &= (\rho^2(1-\theta_x)(1-\beta^2)+\theta_t)(Q_{j+1}^n + Q_{j-1}^n) \\
&\quad +2(1-\theta_t-\rho^2(1-\theta_x)(1-\beta^2))Q_j^n \\
&\quad +\frac{1}{2}(\rho^2(1-\beta^2)\theta_x - \theta_t)(Q_{j+1}^{n-1} + Q_{j-1}^{n-1}) \\
&\quad -\frac{1}{2}\beta\rho(Q_{j+1}^{n-1} - Q_{j-1}^{n-1}) \\
&\quad +(\theta_t - 1 - \rho^2\theta_x(1-\beta^2))Q_j^{n-1}
\end{aligned}$$

with the condition for stability:

$$1 \geq \rho^2(1-2\theta_x)(1-\beta^2)^2 + \beta^2(1-2\theta_t) + 2\theta_t$$

Once again, $\theta_x = 0.5$ and $\theta_t = 0.5$ will guarentee stability for all values of ρ. The results in Project 4 corresponded to the case when $\beta = 0$.

2 Results

Mpegs 1 to 4 show the results for $\beta = 0.5$, 0.99, 1.0, and 1.3 respectively. All cases are periodic, and in all cases, $\rho = 1.0$. As expected, $\beta = 0.5$ makes a right going pulse travel at half its speed in Project 4. The results are equivalent to having $\beta = 0$ but $\rho = 0.5$, as the pulse travels the same distance between timesteps in both cases. Thus it has been found that the $\beta = 0.5$ pulse develops the same error on its right side that the $\rho = 0.5$ pulse develops.

The pulse gets slower as $\beta \to 1.0$. $\beta = 0.99$ in Mpeg 2, and so the pulse looks almost like its not moving at all. But the program suddenly doesn't work at $\beta =$ exactly 1.0. At $\beta = 0.99$, the matrix had a condition number of 73.3. But at $\beta = 1.0$, the matrix becomes singular. The program calculates a finite condition number of $3 * 10^{18}$, but only because of rounding-off errors. The singular matrix yields unstable results as shown in Figure 1. The program maps out two pulses placed wide apart from each other and equally away from the x-axis, and the solution oscillating between them. The same thing happens in the case of $\beta =$ -1. But in both cases the behavior of the pulse is still correct: The $\beta = 1$ pulse doesn't move while the $\beta = -1$ pulse moves at twice the normal speed.

One possible solution to the singularity problem is to "smooth out" the solution. In Figure 1 Q alternates between 0.0075 and -0.0075 in the rows that have 0 for the right hand side. So if one recalculates Q as

$$Q_j^{n+1} = \frac{1}{4}Q_{j-1}^{n+1} + \frac{1}{2}Q_j^{n+1} + \frac{1}{4}Q_{j+1}^{n+1}$$

those rows will have $Q_j^{n+1} = 0$. The smoothing out has the effect of averaging the two pulses together, yielding the correct pulse. Mpeg 3 shows a smoothed pulse with $\beta = 1$. But one must only smooth the data, and send the unsmoothed data back into the evolution. Smoothed data would cause inaccuracies in the evolution.

Mpeg 4 shows the case of $\beta = 1.3$. Here β is large enough to make the right moving pulse travel leftward instead, yielding the same results as a left moving pulse with $\beta = -0.7$. This pulse has the same error problems as the right moving pulse with $\beta = 0.7$, only its error appears on the left side.

3 Convergence

The Convergence Factor section in the web site has several graphs of convergence factors. Figure 1 corresponds to $\beta = 0.5$ and Figure 4 corresponds to $\beta = 1.3$. Both graphs have results similar to themselves and to Project 4, starting at a factor = 4 but linearly decreasing. But the pulse in Figure 1 doesn't reach the end of the grid until time $t = 2$, and at time $t =$ 3.3 in Figure 2. So the slopes are not as steep, and stay straight for a longer amount of time than in Project 4.

As in Project 4, the slope goes to zero as $\beta \to 1$. Figure 2 shows the graph nearly horizontal at 4.2 for $\beta = 0.99$. But one has to calculate the factor for the smoothed data for $\beta = 1$. One gets the curious results shown in Figure 3 of the factor equalling about 3.99 at all times.