# Project #4: The Symmetric Molecule

## 1 The Nine-Point Implicit Scheme

We need to replace the five-point scheme with an implicit scheme that will have second order accuracy in both time and space. So we turn to the nine-point Symmetric Molecule. Here, one expands in the outer rows and columns around their center points, $Q_j^{n+1}, Q_{j+1}^n, Q_{j-1}^n$, and $Q_j^{n-1}$. Then one expands the derivatives in these expansions in terms of $Q_j^n$. One can bring all these expansions together to form the following equation.

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

$\theta_x$ and $\theta_t = 0.0$ correspond to the explicit scheme. We can rearrange this equation to get it in matrix form.:

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

The stability test yields the following condition.

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

So setting $\theta_x$ and $\theta_t = 0.5$ should guarentee stability for all values of $\rho$.

The subroutines that apply to this particular molecule are contained in the file Subs05.f.

## 2 Results

Mpegs 4, 5, and 6 show solutions corresponding to $\rho = 0.5$, 1.0, and 2.0 respectively, for the periodic case. Here one doesn't see the dissipation that the T-molecule produced. But for $\rho < 1.0$ the right-moving pulse develops an error on its right side. This error could come from the inaccurate solving of rows with 0.0 on the right hand side, giving non-zero solutions when they should be zero.

But this error gets smaller as $\rho \to 1$. And the solution at $\rho = 1$ has no error at all. At $\rho = 1$ the matrix becomes the identity matrix, and because of the values of the $\theta$'s the equation simplifies to

$$Q_j^{n+1} = Q_{j-1}^n + Q_{j+1}^n - Q_j^{n-1}$$

With each timestep point $j$ shifts to point $j+1$. Therefore $Q_{j+1}^{n} = Q_{j}^{n-1}$. So the program essentially shifts the pulse one spacestep at a time.

The pulse has an error on its left side when $\rho > 1$, and the error tends to be more severe than that for $\rho < 1$. The left side tends to oscillate around the zero axis and take away from the pulse's amplitude.

## 3 Convergence

Figure 4 shows the convergence factors for cases with $\rho = 0.5$. The graphs start around 4 instead of 2. But they have a negative slope due to the error that arises on the right side. By time $t$ =2.5 seconds the factors for the fixed and periodic conditions have decreased to slightly less than 3. The factor for the radiation condition drops to two once the pulse leaves the grid.

But as the error decreases the graphs become more horizontal. Figure 5 shows the graphs at $\rho = 0.99$, which are nearly level around four. The radiation condition's factor also jumps to 7 after the pulse leaves.

Complications arise when $\rho =$ exactly 1 though. Up to then, the largest absolute values of $(Q(4x) - Q(2x))$ were on the order of $10^{-8}$. But at $\rho = 1$, the values are only of the order or $10^{-16}$. So the calculation of the convergence factors become very suspect here. Figure 6 show the actual results, where the graphs form a straight line around 1 instead of 4. But if one applies the following smoothing technique:

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

to each step the factors shift to four, as shown in Figure 7.

Figure 8 shows the factors for $\rho = 1.5$. The graphs have similar behavior to those in Figure 4, but have a steeper negative slope.