Project #4: The T-Molecule

1 The Five-Point Implicit Scheme

For this project, we change strategies and expand around point (j, $n+1$), leading to the following equations. ($\rho = \frac{\Delta t}{\Delta x}$):

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

The left hand side can be rewritten as a matrix multiplying the vector $\vec{Q}^{n+1}$. One then has to multiply both sides by the inverse of this matrix to calculate $\vec{Q}^{n+1}$. Setting $Q_j^n = \xi e^{ik(j\Delta x)}$ yields

$$|\xi|^2 = \frac{1}{1 + 4\rho^2 sin^2(\frac{k\Delta x}{2})}$$

So, unlike in the explicit schemes, Q should remain stable for any values of ρ. But the time expansion in this scheme has only a first order

The size of the matrix depends on the boundary conditions. The periodic boundary has $Q_J^n = Q_{-J}^n$. Therefore the matrix will have only $2J$ rows and columns, and the coefficients that would be for Q_J^n are assigned to Q_{-J}^n instead. Fixed conditions have Q_{-J}^n and $Q_J^n = 0$ for all time. So one needs only $2J-1$ rows and columns corresponding to the internal points. For the outgoing radiation condition, one uses a $2J+1$ matrix, using the recursion formula for the internal points and the radiation formula from the previous projects for the boundaries.

The program for this project is split into two parts. I've written a main body titled ProjImp.f which can serve as the main body for any implicit scheme. The main body calls the subroutines Initial to initialize data, Matrix to create and invert the matrix, and Evol to create the right hand side and solve the equation. The specific versions of these three subroutines determine the particular scheme being used. The T-Molecule scheme is worked out in the subroutine collection Subs04.f.

2 Results

Mpegs 1, 2, and 3 show the solutions for a right-moving wave, corresponding to $\rho = 0.5$, 1.0, and 1.5 respectively. In all cases $\Delta x = 0.005$ and periodic conditions are used. All three values of ρ have stable solutions as expected. But the wave tends to dissipate over time, and does so more severely with increasing ρ. This dissipation could result from the first order accuracy.

The pulse also tends to spread out. For many rows j the right hand side of the matrix equation will equal zero. The correct answer should be for Q_{j+1}^{n+1}, Q_j^{n+1}, and Q_{j-1}^{n+1} to all equal 0.0, but the program finds a non-zero solution instead. So the program tends to smooth out the edges where the pulse jumps to zero and allow for it to spread out.

3 Convergence

Figures 1, 2, and 3 show the convergence factors corresponding to each mpeg, but also include the factors for fixed boundaries and outgoing radiation. Comparisons between grids with $\Delta x = 0.0025$, 0.005, and 0.01 were used to calculate the factors. In all cases the factors start out around two, but the graphs then smoothly decrease to around one. By then, the amplitudes of each solution differ by a considerable amount. One other cause for the graphs' behavior could be that the scheme is first order accurate in time but second order accurate in space.

The periodic solutions have the best behaved factors, as the grid along the x-axis loops into itself. The fixed solutions have some deviation at time $t = 1.0$ when the pulse is reflecting back. For radiation conditions, the pulse leaves the grid altogether at $t = 1.0$, leaving only a flat line with inaccuracies. These inaccuracies make the graphs jump to about 1.3.