Project #6: Symmetric Molecule - Radiation Conditions

1 Radiation Boundary

Because the solutions of the wave equation now depend on β one has to modify the equations for the radiation boundary conditions. We want only right moving waves to work on the right. So there we use

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

which is satisfied by $Af(x-(1-\beta)t)$, while on the left we use

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

which is satisfied by the left moving $Bg(x+(1+\beta)t$. So on the boundaries we get the following equations, which are second order in their discretizations.

$$(1-\beta)\rho(Q^{n+1}_{Nx-2} - 4Q^{n+1}_{Nx-1}) + 3((1-\beta)\rho+1)Q^{n+1}_{Nx} = 4Q^{n}_{Nx} - Q^{n-1}_{Nx} \tag{3}$$

$$(1+\beta)\rho(Q^{n+1}_{-Nx+2} - 4Q^{n+1}_{-Nx+1}) + 3((1+\beta)\rho+1)Q^{n+1}_{-Nx} = 4Q^{n}_{-Nx} - Q^{n-1}_{-Nx} \tag{4}$$

These equations work for $\beta \in [-1,1]$. But when $\beta > 1$, BOTH waves are left moving. So one has to modify the left boundary condition to let both solutions pass through. Futher, solutions of the form $Af(x-(1-\beta)t)$ now could come inside from the right. So we apply Equation 2 to the right side as well as Equation 1, yielding the equation.

$$(1+\beta)\rho(Q^{n+1}_{Nx-2} - 4Q^{n+1}_{Nx-1}) + 3((1+\beta)\rho-1)Q^{n+1}_{Nx} = Q^{n-1}_{Nx} - 4Q^{n}_{Nx} \tag{5}$$

We replace Equation 4 with this equation. The matrix will still have $2Nx+1$ rows and columns. But the left boundary will have no boundary conditions, and so Q^n_{-Nx} will be determined entirely by the expansion of the wave equation. This ensures that all left-moving pulses already within the grid can leave through the left side.

For $\beta <$ -1, both solutions are right moving. So one applies both Equation 1 and 2 to the left side. Equation 1 yields:

$$(1-\beta)\rho(Q^{n+1}_{-Nx+2} - 4Q^{n+1}_{-Nx+1}) + 3((1-\beta)\rho-1)Q^{n+1}_{-Nx} = Q^{n-1}_{-Nx} - 4Q^{n}_{-Nx} \tag{6}$$

while Equation 2 yields Equation 4 again. Together Equations 4 and 6 cancel out both solutions on the left side, while the right side has no boundary conditions at all.

2 Results

Mpegs 1 and 2 and 3 show the results for radiation conditions for β = -0.5, -1.0, and -1.3 respectively. As expected, these negative β's make the pulses travel faster than at β = 0.0. These pulse also experience the same oscillating errors on the left sides as the pulses with $\rho > 1$, which increase with increasing magnitude of β. Another error is a small pulse corresponding to the solution $Bg(x + (1 + \beta)t$, possibly arising from the innaccuracy of the initial conditions.

3 Convergence

The Convergence Factor section also includes graphs for the radiation conditions, with Figures 5 through 7 corresponding to the above mentioned mpegs. The graphs behave in pretty much the same was as in Project 4, but they don't break from the periodic graphs at time $t = 1$ as before, because the pulses reach the ends of the grids at different times depending on β.