Introduction to Finite Difference Methods

April 22, 2007

1 The One Dimensional Heat Equation

One of the simplest parabolic (or heat) equaions is the one dimensional problem

$$\begin{aligned} u_t(x,t) &= \nu u_{xx}(x,t),\ t \in (0,T],\ x \in (0,a), \\ u(t,0) &= h_1(t), u(t,a) = h_2(t), \\ u(0,x) &= f(x). \end{aligned} \tag{1}$$

Because values of the function u are specified at the endpoints $x = 0$ and $x = a$ of the space intervale, we call this problem a Dirichlet problem. If values of the derivative u_x are specified at the boundaries $x = 0$ and $x = a$, the problem is called a Neumann problem.

To approximate the solution of this equation, we construct a space-time grid. That is, we divide the rectangle

$$R = \{(x,t) : 0 \le x \le a, 0 \le t \le T\}$$

into a grid of $n-1$ by $m-1$ rectangles with sieds $\triangle x = a/n$ and $\triangle t = T/m$. Starting from the bottom row $t = t_1 = 0$, the solution is

$$u(x_i, t_1) = f(x_i),\ i = 1, 2, \ldots, n.$$

To approximate the solution at the next grid line, the differential equation is approximated by a difference equation as follows. The time derivatvie u_t is approximated by the difference formula

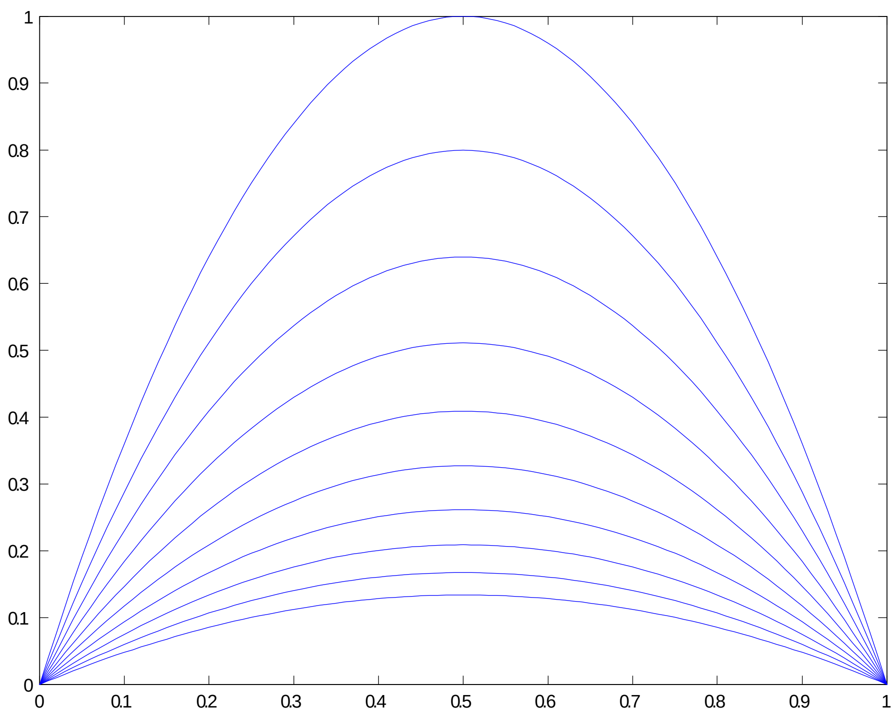
$$u_t(x,t) \approx \frac{u(x, t+\triangle t) - u(x,t)}{\triangle t}$$

and the space derivative is approximated by

$$u_{xx}(x,t) \approx \frac{u(x+\triangle x, t) - 2u(x,t) + u(x-\triangle x, t)}{\triangle x^2}$$

We can show using Taylor series expansions that these approximations are of order $\triangle t$ in time and $\triangle x^2$ in space. Denoting by u_{ij} the approximate value of $u(x_i, y_j)$ the differential equation (1) is approximated by the difference equation

$$\frac{u_{i,j+1} - u_{i,j}}{\triangle t} = \nu \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\triangle x^2}.$$



Substituting $r = \nu \triangle t / \triangle x^2$ (for conventience) and solving for $u_{i,j+1}$, we obtain

$$u_{i,j+1} = r u_{i+1,j} - (1 - 2r)\, u_{i,j} + r u_{i-1,j}. \tag{2}$$

Example For the heat equation with $f(x) = 4x - x^2, h_1(x) = h_2(x) = 0, a = 1, r = .45$, the figure below shows 10 timesteps of the evolution of the solution.

The initial solution decays towards zero with time as expected. Repeating the calculation with $r = .6$ produces the results shown below

In this case the initial solution builds up twards infinity. This is a typical case of the instability of the numerical scheme used to approximate the solution. We can show that the solution is stable if and only if $r \leq .5$.

The instability in the previous example can be predicted from mathematical analysis by a method called Neumann stability method. The idea is to consider the solution of the difference equation as a superposition of Fourier basic functions (modes) and require that none of the basic functions should blow up as time increases. In effect, what this means is that we substitute

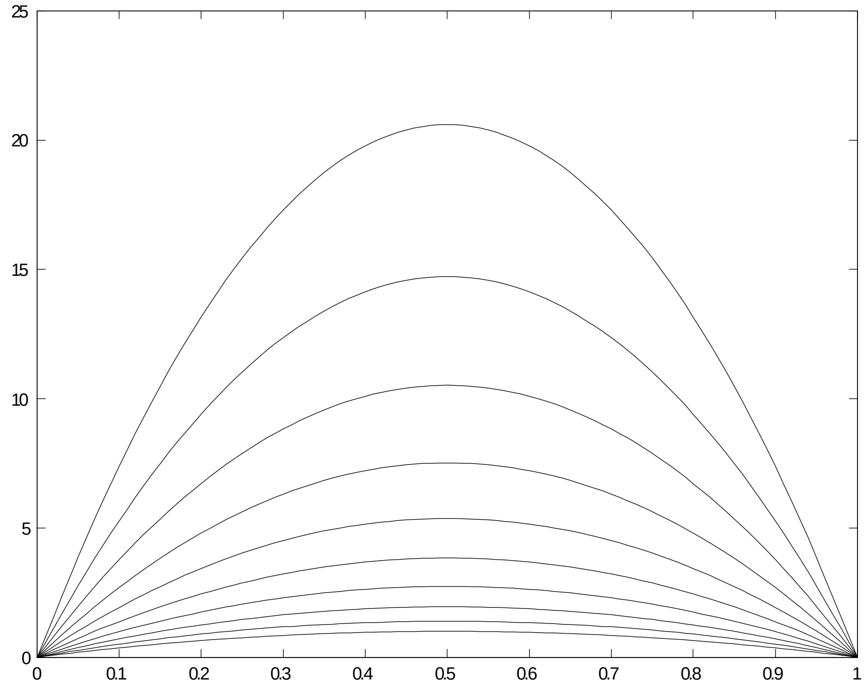
$$u_{k,j} = \xi^j e^{i\omega k \triangle x}$$

in the difference equation (2) and require that $|\xi| \leq 1$. When we carry out this idea, we obtain

$$\xi^{j+1} e^{i\omega k \triangle x} = r \xi^j e^{i\omega (k+1) \triangle x} + (1 - 2r)\, \xi^j e^{i\omega k \triangle x} + r \xi^j e^{i\omega (k-1) \triangle x},$$

which simplifies to

$$\xi = 2r \cos \omega \triangle x + (1 - 2r)\,.$$



The requirement $|\xi| \leq 1$ gives

$$\begin{aligned} -1 &\leq 2r\cos\omega\triangle x + (1-2r) \leq 1 \\ -1 &\leq r(-1+\cos\omega\triangle x) \leq 0. \end{aligned}$$

The right half of this inequality is always satisfied. The left half gives

$$r \leq \frac{1}{1-\cos\omega\triangle x}.$$

Since this inequality must hold for all values of $\omega\triangle x$, we must have

$$r \leq \min\left(\frac{1}{1-\cos\omega\triangle x}\right) = \frac{1}{2}.$$

2 The Two Dimensional Heat Equation

The heat equation in a rectangle (two dimensional) has the form

$$\begin{aligned} u_t(x,y,t) &= \nu\left(u_{xx}(x,y,t) + u_{yy}(x,y,t)\right), \\ &= \nu\triangle u(x,y,t) \;\; t \in (0,T], \;\; x \in (0,a), y \in (0,b) \\ u(0,y,t) &= h_1(y,t), u(a,y,t) = h_2(y,t), \\ u(x,0,t) &= g_1(x,t), u(x,b,t) = g_2(x,t), \\ u(0,x,y) &= f(x,y). \end{aligned}$$

Here, we assumed Dirichlet boundary conditions, but Neumann boundary conditions are also possible (the Neumann boundary conditions are specified in terms of the normal derivative of u on the boundary of the rectangle).

To approximate the solution we divide the box

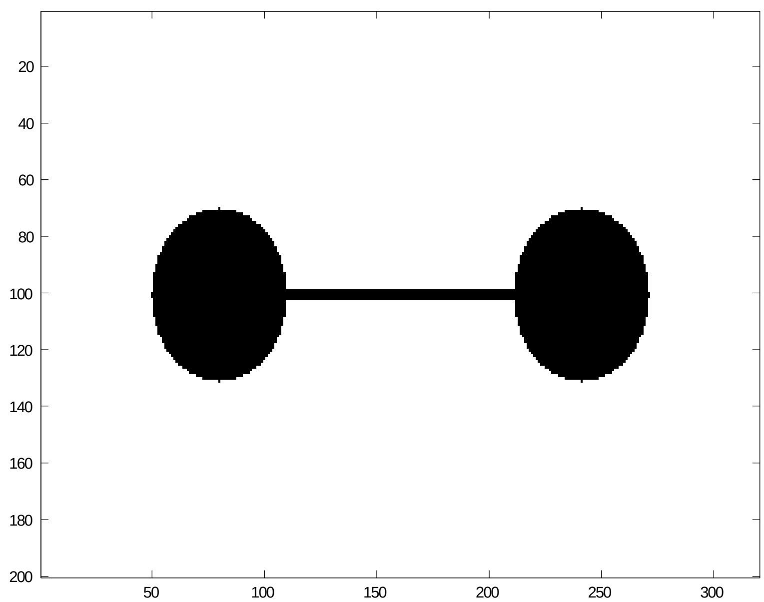
$$B = \{(x, y, t) : 0 \leq x \leq a, 0 \leq y \leq b, 0 \leq t \leq T\}$$

into $n-1 \times m-1 \times p-1$ cells of sides $\triangle x = \triangle y = a/n = b/m$ (for convenience, we assume that $am = bn$) and $\triangle t = T/p$. Following the same method of dicritization as for the heat equation in one space dimension we arrive at the difference equations

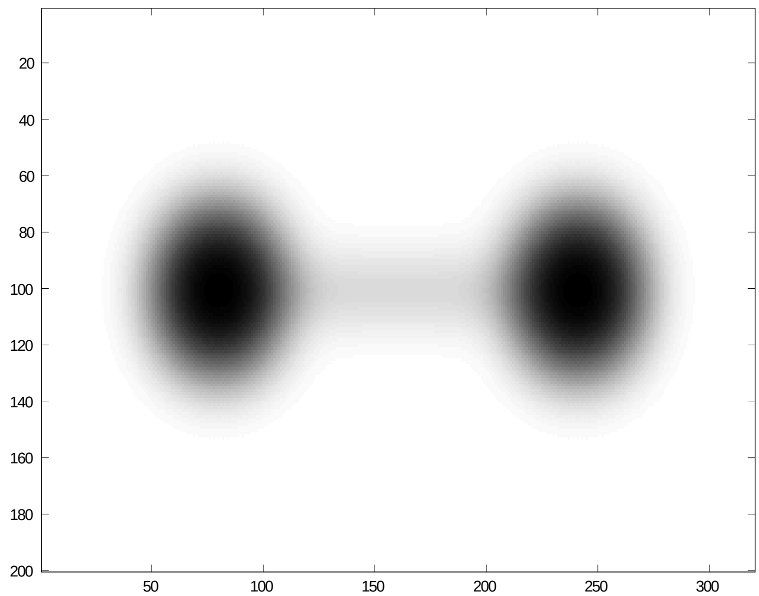
$$u_{j,k,i+1} = r\left(u_{j+1,k,i} + u_{j-1,k,i} + u_{j,k+1,i} + u_{j,k-1,i}\right) + (1-4r)\, u_{j,k,i},$$

where $u_{j,k,i} \approx u\left(x_j, y_k, t_i\right), r = \nu \triangle t / \triangle x^2$.

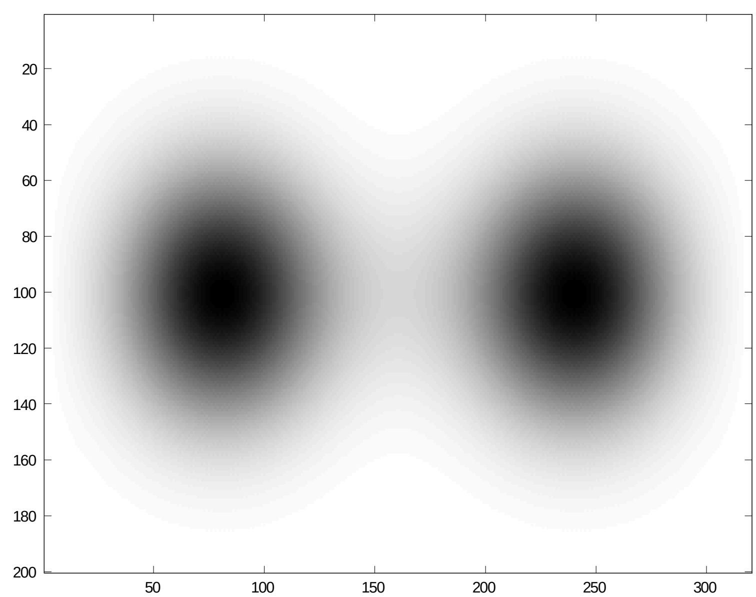
Example We apply the heat equation in two space dimensions to evolve the image



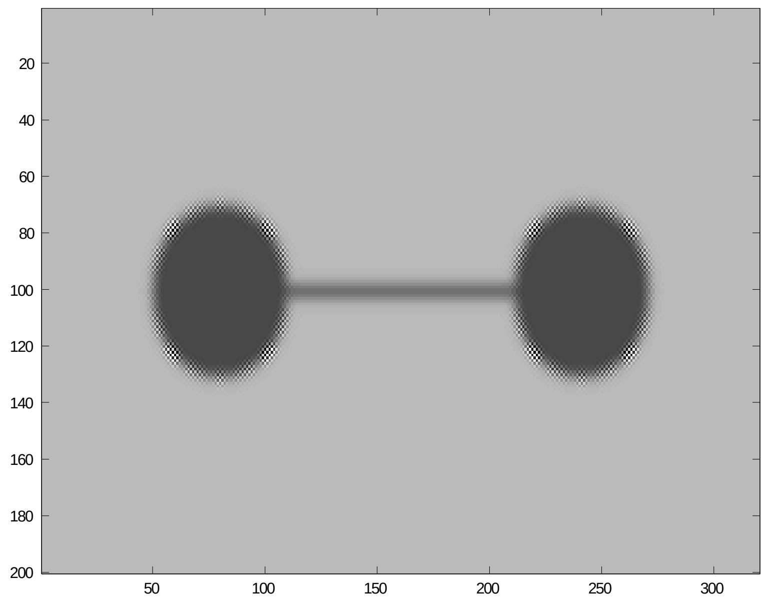
The image dimensions are 200 by 320. We then can take $\triangle x = \triangle y = 1$, $\nu = 1$, $r = .25$, so that $\triangle t = .25$. The boundary conditions are taken as 1 (white color) on the boundary of the image. After 240 time steps the image evolves into the shape shown below.



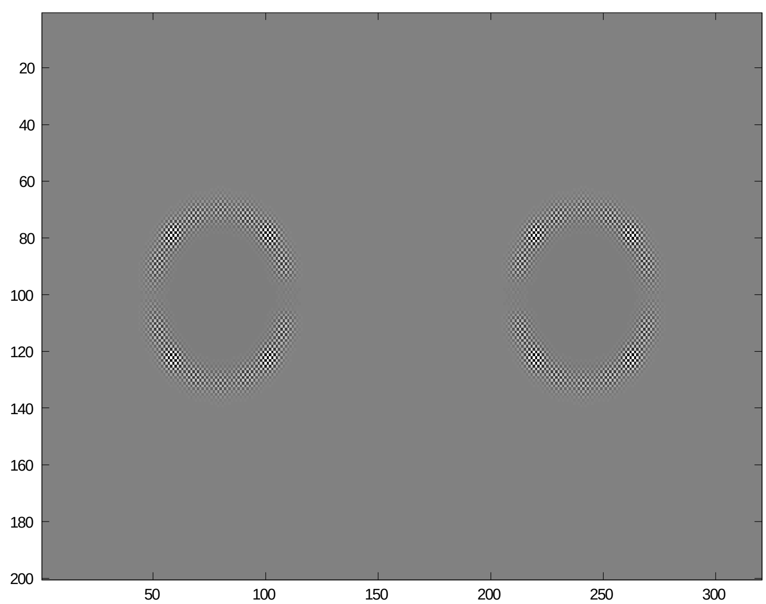
After 1280 time steps, the image takes the form shown below.



If we increase r to 0.3 and run for 4 time steps, we get the image



Running further, we get the image



The entries in the pixel coloring run into the range of 10^7. So, again, this is an unstable case. The stability condition in this case is $r \leq 0.25$.

3 Hyperbolic Equations

The one dimensional advection equation (also called the transport or wave equation)

$$\begin{aligned}\frac{\partial u}{\partial t}(x,t)+a\frac{\partial u}{\partial x}(x,t) &= 0, t>0, x\in\mathbb{R},\\ u(x,0) &= u_0(x),\end{aligned}$$

where a is a constant is a standard example of hyperbolic problems. It can be easily verified that the solution is

$$u(x,t) = u_0(x - at).$$

It follows that, on the lines $x - at = c$, $u(x,t) = u_0(c)$ is constant. These lines are called characteristics. Information is propagated in the direction of the sign of a, for example, from left to right if a is positive. The discretizaion of this equation is done as follows. The time discretization is

$$u_t(x_k, t_j) \approx \frac{u_{k,j+1} - u_{k,j}}{\triangle t}.$$

For discretization in space, we have two possibilities

$$u_x(x_k, t_j) \approx \frac{u_{k+1,j} - u_{k,j}}{\triangle x} \text{ (forward difference)}$$

or

$$u_x(x_k, t_j) \approx \frac{u_{k,j} - u_{k,j-1}}{\triangle x} \text{ (backword difference).}$$

Consequently, we have one of the following difference equatoins

$$u_{k,j+1} = u_{k,j} - \rho \left\{ \begin{array}{c} u_{k+1,j} - u_{k,j} \\ u_{k,j} - u_{k,j-1} \end{array} \right. , \tag{3}$$

where

$$\rho = a\frac{\triangle t}{\triangle x}.$$

3.1 The CFL Condition

Let's apply the Von Neumann stability method for both possibilities. We substitute

$$u_{k,j} = \xi^j e^{i\omega k \triangle x}$$

in the difference scheme (3) to get

$$\xi = 1 - \rho \left\{ \begin{array}{c} e^{i\omega\triangle x} - 1 \\ 1 - e^{-i\omega\triangle x} \end{array} \right. .$$

If $a > 0$, and we use forward difference in space, then

$$\begin{aligned} \xi &= 1 - \rho\left(e^{i\omega\triangle x} - 1\right) \\ &= 1 + \rho - \rho e^{i\omega\triangle x} \\ &= 1 + \rho - \rho\cos(\omega\triangle x) - i\rho\sin(\omega\triangle x). \end{aligned}$$

Therefore,

$$\begin{aligned} |\xi|^2 &= (1 + \rho - \rho\cos(\omega\triangle x))^2 + \rho^2\sin^2(\omega\triangle x) \\ &= 1 + 2\rho - 2\rho\cos\omega\triangle x + 2\rho^2 - 2\rho^2\cos\omega\triangle x \end{aligned}$$

and the condition $|\xi|^2 \leq 1$ gives

$$(1+\rho)(1-\cos\omega\triangle x) \leq 0,$$

which cannot be satisfied for all $\omega\triangle x$. Hence, a forward difference in space produces an unstable scheme.

If $a > 0$, and we use backword difference in space, then

$$\xi = 1 - \rho + \rho\cos(\omega\triangle x) - i\rho\sin(\omega\triangle x)$$

and

$$\begin{aligned} |\xi|^2 &= (1-\rho+\rho\cos(\omega\triangle x))^2 + \rho^2\sin^2(\omega\triangle x) \\ &= 1 - 2\rho + 2\rho\cos\omega\triangle x + 2\rho^2 - 2\rho^2\cos\omega\triangle x. \end{aligned}$$

The condition $|\xi|^2 \leq 1$ gives

$$\rho(1-\cos\omega\triangle x) \leq 1 - \cos\omega\triangle x,$$

or

$$\rho \leq 1.$$

Thus, the scheme will be stable if we use backword difference in space and restrict ρ such that

$$\rho = a\frac{\triangle t}{\triangle x} \leq 1.$$

Similar considerations for the case $a < 0$ reveal that we must use forward difference in space and restrict ρ such that

$$-\rho = -a\frac{\triangle t}{\triangle x} \leq 1.$$

In summary, the difference scheme takes the form

$$u_{k,j+1} = u_{k,j} - \rho\begin{cases} u_{k+1,j} - u_{k,j} & \text{if } a > 0 \\ u_{k,j} - u_{k,j-1} & \text{if } a < 0 \end{cases}$$

and the stability condition is

$$|a|\frac{\triangle t}{\triangle x} \leq 1. \tag{4}$$

These schemes are called *upwind schemes* because they conform with the slope $\frac{1}{a}$ of the characteristics. The stability condition (4) is known as the CFL condition in reference to the authors Courant-Friedrichs-Lewy. It states that the numderical velocity (or slope) $\frac{\triangle t}{\triangle x}$ must be less that or equal to the continuous velocity $\frac{dt}{dx} = \frac{1}{a}$.

3.2 Hyperbolic Equations and Shocks

Let's consider the equation

$$\begin{aligned} \frac{\partial u}{\partial t}(x,t) + a(x)\frac{\partial u}{\partial x}(x,t) &= 0, t > 0, x \in \mathbb{R}, \\ u(x,0) &= u_0(x), \end{aligned}$$

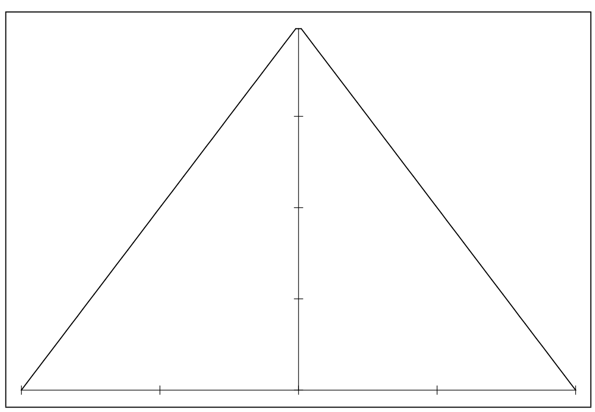
where

$$a(x) = \begin{cases} 1, & x < 0 \\ -1, & x > 0. \end{cases}$$

In this case, the solution is

$$u(x,t) = \begin{cases} u_0(x-t), & x-t < 0 \\ u_0(x+t), & x+t > 0. \end{cases}.$$

In other words the initial value $u_0(x_0)$ propagates along the characterisitics $x + t = x_0$ if $x_0 > 0$ and along the the characterisitics $x - t = x_0$ if $x_0 < 0$. The two characteristics are shown below. Now, consider what happens at the point $(0, x_0)$. The solution propagated from the point $x = x_0$ reaches $(0, x_0)$ at $t = x_0$. Thus $u(0^+, x_0) = u_0(x_0)$. On the other haned, the solution propagated from the point $x = -x_0$ reaches $(0, x_0)$ at $t = -x_0$. Thus $u(0^-, x_0) = u_0(-x_0)$. If $u_0(x_0) \neq u_0(-x_0)$ a shock develops at the point $(0, x_0)$. This means that $u(0, x_0)$



becomes undefined and it is not clear how to propagate the solution beyond this instant.

From the numerical solution point of view, the numerical scheme must be different on either side of 0. We must use both forward and backword difference schemes at the same time. This is accomplished by the difference equation

$$\begin{aligned} u_{k,j+1} &= u_{k,j} - (\min\{\rho, 0\}(u_{k+1,j} - u_{k,j}) + \max\{\rho, 0\}(u_{k,j} - u_{k,j-1})) \\ &= u_{k,j} - \left(\frac{\rho}{2}(u_{k+1,j} - u_{k,j-1}) - \frac{|\rho|}{2}(u_{k+1,j} - 2u_{k,j} + u_{k,j-1})\right). \end{aligned}$$

Observe that the last term in this equation resembles the discretization of a second derivative in space. It turns out that the above difference scheme approximates the "parapolic" equation

$$u_t = -au_x + \epsilon u_{xx},$$

where $\epsilon = \triangle x$. The effect is adding the smoothing properties of parabolic equations and, consequently, no numerical shocks develop under this scheme. Of course, the numerical soluion is meaningless as a classical solution of the hyperbolic equation beyond the shock points. This kind of solution is called a viscosity solution and will be discussed in the next section.