A nonlinear heat/diffusion equation in 1 D

Consider the following nonlinear diffusion equation

$$\begin{aligned}&\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x}\right), \qquad x\in(0,\,1), \quad t>0,\\ &u(0,t)=d_0(t),\; u(1,t)=d_1(t),\\ &u(x,0)=u_0(x),\end{aligned} \tag{1}$$

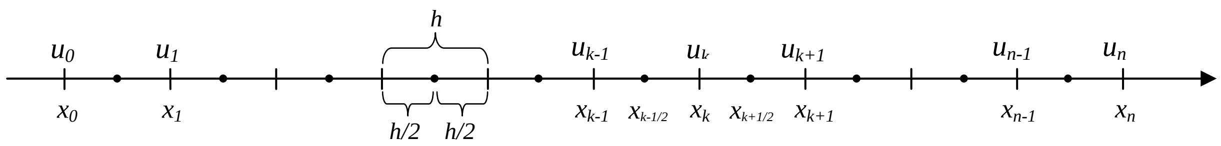
where the diffusion coefficient $D(u)$ is dependent on the concentration u. In general we could also assume the it depends on the position x, that is $D=D(u,x)$, but for the sake of simplicity we restrict analysis to the former case. The function $D(u)$ is strictly positive.

We can view the equation (1) as the balance of mass law

$$\frac{\partial u}{\partial t}=-\frac{\partial J}{\partial x}, \tag{2}$$

where the flux is given by $J=-D(u)\frac{\partial u}{\partial x}$.

The space grid is presented on the picture below.



For time discretization we use standard forward difference

$$\frac{\partial u}{\partial t}(x_i,t_m)\approx\frac{u(x_i,t_m+k)-u(x_i,k)}{k}\rightarrow\frac{u_i^{m+1}-u_i^m}{k}.$$

To obtain discretization of the term $\frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x}\right)$ we make two steps:

$$-\frac{\partial J}{\partial x}(x_i,t_m)\approx-\frac{J_{i+1/2}^m-J_{i-1/2}^m}{h},$$

and we try to deal with $J_{i\pm1/2}^m$. Observe that

$$\begin{aligned}J_{i+1/2}^m&=D(u_{i+1/2}^m)\frac{\partial u}{\partial x}(x_{i+1/2},t_m)\approx D(u_{i+1/2}^m)\frac{u_{i+1}^m-u_i^m}{h},\\ J_{i-1/2}^m&=D(u_{i-1/2}^m)\frac{\partial u}{\partial x}(x_{i-1/2},t_m)\approx D(u_{i-1/2}^m)\frac{u_i^m-u_{i-1}^m}{h}.\end{aligned} \tag{3}$$

Now the problem with the above expressions is that the values of the approximate solution are defined only in the main points of the mesh, namely only $\ldots u_{i-1}^m, u_i^m, u_{i+1}^m \ldots$ are part of the discrete solution, but discretized fluxes (3) contain terms $D(u_{i+1/2}^m)$, $D(u_{i-1/2}^m)$. One of the way to get rid of these expression is the following approximation

$$
\begin{aligned}
D(u_{i+1/2}^m) &\approx \frac{D(u_i^m) + D(u_{i+1}^m)}{2}, \\
D(u_{i-1/2}^m) &\approx \frac{D(u_i^m) + D(u_{i-1}^m)}{2}.
\end{aligned}
\tag{4}
$$

It is rather obvious that these types of approximation is correct because the mesh points are equidistant. If non-uniform mesh is used we should apply weighted average instead of the simple arithmetic average as in (4).

Combining all these approximations we have

$$
\frac{u_i^{m+1} - u_i^m}{k} = -\frac{-D(u_{i+1/2}^m)\dfrac{u_{i+1}^m - u_i^m}{h} + D(u_{i-1/2}^m)\dfrac{u_i^m - u_{i-1}^m}{h}}{h}, \tag{5}
$$

and

$$
\frac{u_i^{m+1} - u_i^m}{k} = \frac{(D(u_i^m) + D(u_{i+1}^m))(u_{i+1}^m - u_i^m) - (D(u_{i-1}^m) + D(u_i^m))(u_i^m - u_{i-1}^m)}{2h^2}, \tag{6}
$$

what finally gives the following discrete explicit scheme

$$
\begin{aligned}
&u_i^{m+1} = \\
&\tfrac{1}{2} r((D(u_i^m) + D(u_{i+1}^m))u_{i+1}^m + (1 - \tfrac{1}{2} r(D(u_{i-1}^m) + 2D(u_i^m) + D(u_{i+1}^m)))u_i^m + \tfrac{1}{2} r(D(u_{i-1}^m) + D(u_i^m))u_{i-1}^m.
\end{aligned}
\tag{7}
$$

In short, we can write the above formula as

$$
\begin{aligned}
&u_i^{m+1} = \tfrac{1}{2} r((D_i^m + D_{i+1}^m)u_{i+1}^m + (1 - \tfrac{1}{2} r(D_{i-1}^m + 2D_i^m + D_{i+1}^m))u_i^m + \tfrac{1}{2} r(D_{i-1}^m + D_i^m)u_{i-1}^m, \\
&i = 1, \ldots, n, \\
&u_0^m = d_0(t_m), \quad u_1^m = d_1(t_m), \\
&t_m = m \cdot k.
\end{aligned}
\tag{8}
$$

where $D_i^m = D\left(u_i^m\right)$. Of course, when the diffusion coefficient D does not depend on concentration we have $D_i^m \equiv D$ and the expression (8) takes the form

$$
u_i^{m+1} = rDu_{i+1}^m + (1 - 2rD)u_i^m + rDu_{i-1}^m,
$$

which is known iteration for the 1D diffusion equation derived previously. Thus the scheme (8) presents an explicit procedure for nonlinear diffusion equation.

An Introduction to Reaction-Diffusion Equations

Reaction-diffusion equations arise as mathematical models in several areas of applications, for example in models of chemical kinetics, biochemical systems, predator-prey systems in ecology. Both numerical and mathematical analysis of reaction-diffusion equations have received a great deal of attention in recent years. In the simplest models, these systems equations take the following compact form

$$\frac{\partial u}{\partial t} = D\Delta u + f(u), \qquad x \in \Omega \subset \mathbb{R}^k, \quad t > 0, \tag{9}$$

where $u : \bar{\Omega} \times [0, \infty) \to \mathbb{R}^k$, $D \in \mathbb{R}^{n \times n}$ is an $n \times n$ matrix, and $f(u)$ some differentiable function. In an expanded form we can write (9) explicitly as a system for $u(x,t) = (u_1(x,t), \dots, u_k(x,t))$

$$\begin{cases} \dfrac{\partial u_1}{\partial t} = \sum_{i=1}^{n} D_{1,j} \Delta u_j + f_1(u_1, \dots, u_n), \\ \cdots \\ \dfrac{\partial u_n}{\partial t} = \sum_{i=1}^{n} D_{n,j} \Delta u_j + f_n(u_1, \dots, u_n), \end{cases} \tag{10}$$

where $x \in \Omega \subset \mathbb{R}^k$, $D = [D_{i,j}]$.

The combination of diffusion terms together with the nonlinear interaction terms, produce the behavior that are not easily predictable from either mechanism alone. Thus, the term $D_{ij} \Delta u_j$ acts as if to dampen u, while the nonlinear function tends to drive it out of equilibrium by producing large solutions, steep gradients, etc. This leads to the possibility of threshold phenomena which is one of the interesting features of this class of equations

Fisher's equation

Let us denote by $u = u(x,t)$ the population density of some species. This means that the quantity should be non-negative, $u \geq 0$. If take into account the tendency of the population to spread out over the area where it is possible to live, the Fickian flux term, $D\frac{\partial^2 u}{\partial x^2}$, should be present in the model. On the other hand we have to consider that the growth of a population faces the limited resources which become more pronounced for greater densities but for small densities the population may growth exponentially. This leads to the following terms: αu and $-\alpha u^2$ so we get the source term as

$$f(u) = \alpha u(A - u) = \alpha A u - \alpha u^2.$$

Combination of these two features, diffusion spread and growth model produces the equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + \alpha u(A - u). \tag{11}$$

The source term $f(u)=\alpha u(A-u)$ acts thus as follows. For small $u>0,\ \ f(u)\approx \alpha Au,$ which gives an exponential growth. But if u approaches $A,$ so $f(u)\approx 0,$ and the growth slows down to zero. Hence, we can interpret constant $A>0$ the carrying capacity of the environment.

In mathematical ecology, this model of population growth is called *Fisher's equation*. Usually this equation is studied in conjunction with a Neumann-type boundary condition, that is

$$\frac{\partial u}{\partial x}(a,t)=0,\ \frac{\partial u}{\partial x}(b,t)=0,$$

where $\Omega=(a,\ b)$ is the domain in which the population lives. Such boundary condition can be interpreted as no flux through boundary, i.e. the system is closed.

Since we are interested in the qualitative behavior of this model we can introduce a new variables (rescaling)

$$\overline{u}(\overline{x},\overline{t})=u(x,t)/A,\ \ \overline{x}=\frac{x-a}{b-a},\ \ \overline{t}=t/t_c,$$

and re-write equation (11) as

$$\frac{\partial\overline{u}}{\partial\overline{t}}=\overline{D}\frac{\partial^2\overline{u}}{\partial\overline{x}^2}+\overline{\alpha}\overline{u}(1-\overline{u}), \tag{12}$$

where $\overline{D}=D\frac{(b-a)^2}{t_c},\ \overline{\alpha}=\frac{\alpha A}{t_c}$. In particular, if we take the time scaling factor $t_c=D\cdot(b-a)^2,$ then $\overline{D}=1$ and we can write

$$\frac{\partial\overline{u}}{\partial\overline{t}}=\frac{\partial^2\overline{u}}{\partial\overline{x}^2}+\overline{\alpha}\overline{u}(1-\overline{u}),\quad \overline{x}\in(0,\ 1),\ \ \overline{t}>0. \tag{13}$$

To ease the burden of notation we henceforth drop the overbars in the notation and consider the following model problem

$$\begin{aligned}&\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+\alpha u(1-u),\quad x\in(0,\ 1),\ t>0,\\&\frac{\partial u}{\partial x}(0,t)=0,\ \frac{\partial u}{\partial x}(1,t)=0,\\&u(x,0)=u_0(x),\end{aligned} \tag{14}$$

where $u_0:[0,\ 1]\rightarrow\mathbb{R}$ is the initial population density. We will be mainly interested in the initial density that is within the carrying capacity of the environment, that is

$$0\le u_0(x)\le 1, \tag{15}$$

for all $x\in[0,\ 1].$

A finite difference scheme for Fisher's equation

Let u_i^m denote an approximation of $u(x_i, t_m)$, where $u = u(x,t)$ is the solution to the problem (14). The explicit finite difference scheme can be written as follows

$$u_i^{m+1} = ru_{i-1}^m + (1-2r)u_i^m + ru_{i+1}^m + ku_i^m(1-u_i^m), \;\; i = 1, \ldots, n, \tag{16}$$

where $r = k/h^2$, $h -$ space step, $k -$ time step.

The scheme is initialized by

$$u_i^0 = u_0(x_i), \qquad i = 0, \ldots, n+1. \tag{17}$$

The boundary conditions of (14) can be tackled in two ways (see Notes for Lab02): ghost point method or three-points one sided method. Here we adopt the ghost point method. Thus we introduce the auxiliary ("ghost") points $x_{-1} = x_0 - h = -h$ and $x_{n+2} = x_{n+1} + h = 1 + h.$ Since $\frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(1,t) = 0,$ we have discretization on boundaries

$$\frac{u_1^m - u_{-1}^m}{h} = 0 \quad \text{and} \quad \frac{u_{n+2}^m - u_n^m}{h} = 0, \tag{18}$$

what gives $u_{-1}^m = u_1^m$, $u_{n+2}^m = u_n^m$. Combining these equalities with (16) for $i = 0$ and $i = n+1,$ we get

$$\begin{aligned} &u_0^{m+1} = (1-2r)u_0^m + 2ru_1^m + ku_0^m(1-u_0^m), \\ &u_{n+1}^{m+1} = 2ru_n^m + (1-2r)u_{n+1}^m + ku_{n+1}^m(1-u_{n+1}^m), \\ &m = 0, 1, \ldots \end{aligned} \tag{19}$$

The finite difference scheme is now fully specified by (16), (17) and (19).

Some general properties of Fisher's equation

In order to test the computations based on the above explicit scheme and also to get some deeper insight into the properties of the solution of the problem (14) we will state below two important facts about the solution for any time $t > 0.$ One is *an invariance property* and second is *the convergence toward equilibrium*.

The invariance property states that if the values of the function stay in some special region (in 1D this is usually just an interval) at some point of time (usually at $t = 0$, then it will also have values in that region for any time later on. We call this region an invariant region (for the system of equations it may have much more complicated geometry than in 1D). Specifically we have the following:

> *Suppose that $u : [0,1] \times [0, \infty) \to \mathbb{R}$ is smooth solution of the problem (14). If the initial condition u_0 satisfies the condition*
>
> $$0 < \varepsilon \le u_0(x) \le 1 + \varepsilon, \tag{20}$$
>
> *then the solution u also satisfies it for any time $t > 0,$ that is the following holds*

$$0 < \varepsilon \le u(x,t) \le 1+\varepsilon, \tag{21}$$

for any $x \in [0,1],\ t > 0.$

The steady (or stationary) state solution is obtained when there is no dependency on time, hence $\frac{\partial u}{\partial t} = 0.$ This leads the problem (14) to the following equation

$$\begin{aligned} &\frac{d^2u}{dx^2} + \alpha u(1-u) = 0, \\ &\frac{du}{dx}(0) = \frac{du}{dx}(1) = 0. \end{aligned} \tag{22}$$

which have an obvious constant solution $u_s(x) \equiv 1.$ It turns out that the time dependent solution of the problem (14) tends to this stationary solution as $t \to 0.$ Formally we have

Let $u : [0,1] \times [0,\infty) \to \mathbb{R}$ *be a solution of (14) with initial data* u_0 *satisfying*

$$0 < \varepsilon \le u_0(x) \le 1+\varepsilon,$$

for all $x \in [0,1].$ *Then* u *approaches the steady state solution* $u_s(x) \equiv 1$ *in the following sense*

$$\begin{aligned} &\lim_{t\to\infty} \int_0^1 (u(x,t) - u_s(x))^2 \, dx = 0, \\ &\lim_{t\to\infty} \int_0^1 \left(\tfrac{\partial u}{\partial x}(x,t)\right)^2 dx = 0. \end{aligned} \tag{23}$$

In practice we can conclude that the time dependent solution approaches the steady state solution point-wise

$$u(x,t) \to u_s(x) = 1 \ \ as \ \ t \to \infty, \tag{24}$$

for any fixed $x \in [0,1].$

Stability condition for the explicit scheme

As we remember, the stability condition for the explicit scheme for linear diffusion equation is $r \le 1/2,$ where $r = D \cdot (k/h^2).$ It turns out that for the explicit scheme (16) for the reaction-diffusion problem (14) the similar stability condition must be met if the scheme is to produce correct results for long times. It can be proved that this condition now reads (assuming the diffusion coefficient $D = 1$)

$$k < \frac{h^2}{2+h^2}, \tag{25}$$

which is slightly more restrictive than the corresponding condition for linear diffusion, $k \le h^2/2.$