CHAPTER 6 Diffusion

6.1 Introduction

Diffusion is a macroscopic interpretation of microscopic advection. Here "microscopic" refers to scales below the resolution of a model. In general diffusion can occur in three dimensions, but often in atmospheric science only vertical diffusion, i.e. one-dimensional diffusion, need be considered. The process of one-dimensional diffusion can be represented in simplified form by

$$\frac{\partial q}{\partial t} = -\frac{\partial F_q}{\partial x} . \tag{6.1}$$

Here q is the "diffused" quantity, x is the spatial coordinate, and F_q is a flux of q due to diffusion. Although very complex parameterizations for F_q are required in many applications, a simple parameterization that is often encountered in practice is

$$F_q = -K\frac{\partial q}{\partial x} , \tag{6.2}$$

where K is a "diffusion coefficient," which must be specified somehow. Physically meaningful applications of (6.2) are possible when

$$K \geq 0 . \tag{6.3}$$

Substitution of (6.2) into (6.1) gives

$$\frac{\partial q}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial q}{\partial x}\right) . \tag{6.4}$$

Because (6.4) involves second derivatives in space, it requires two boundary conditions. Here we simply assume periodicity of both q and $\frac{\partial q}{\partial x}$. It then follows immediately from (6.1) that the spatially averaged value of q does not change with time:

$$\frac{\partial}{\partial t} \int_{\text{spatial domain}} q \; dx = 0 . \tag{6.5}$$

When (6.3) is satisfied, (6.4) describes “downgradient” transport, in which the flux of q is from larger values of q towards smaller values of q. Such a process tends to reduce large values of q, and to decrease small values, so that the spatial variability of q decreases with time. In particular, we can show that

$$\frac{\partial}{\partial t} \int_{\text{spatial domain}} q^2 \; dx \le 0 . \tag{6.6}$$

To prove this, multiply both sides of (6.4) by q:

$$\begin{aligned} \frac{\partial}{\partial t}\left(\frac{q^2}{2}\right) &= q\frac{\partial}{\partial x}\left(K\frac{\partial q}{\partial x}\right) \\ &= \frac{\partial}{\partial x}\left(qK\frac{\partial q}{\partial x}\right) - K\left(\frac{\partial q}{\partial x}\right)^2 \quad . \end{aligned} \tag{6.7}$$

When we integrate the second line of (6.7) over a periodic domain, the first term vanishes and the second is negative (or possibly zero). The result (6.6) follows immediately.

With the assumed periodic boundary conditions, we can expand q in a Fourier series:

$$q(x, t) = \sum \hat{q}_k(t) e^{ikx} . \tag{6.8}$$

Substituting into (6.1), and assuming spatially constant K, we find that the amplitude of a particular Fourier mode satisfies

$$\frac{d\hat{q}_k}{dt} = -k^2 K \hat{q}_k , \tag{6.9}$$

which is the decay equation. This shows that there is a close connection between the diffusion equation and the decay equation. The solution of (6.9) is

$$\hat{q}_k(t) = \hat{q}_k(0) e^{-k^2 K t} \tag{6.10}$$

Note that higher wave numbers decay more rapidly, for a given value of K. Since

$$\hat{q}_k(t + \Delta t) = \hat{q}_k(0) e^{-k^2 K (t + \Delta t)} = \hat{q}_k(t) e^{-k^2 K \Delta t} . \tag{6.11}$$

This shows that, for the exact solution,

$$\lambda = e^{-k^2 K \Delta t} . \tag{6.12}$$

6.2 A simple explicit scheme

A finite-difference analog of (6.1) is

$$q_j^{n+1} - q_j^n = \kappa_{j+\frac{1}{2}}(q_{j+1}^n - q_j^n) - \kappa_{j-\frac{1}{2}}(q_j^n - q_{j-1}^n) , \tag{6.13}$$

where for convenience we define the nondimensional combination

$$\kappa_{j+\frac{1}{2}} \equiv \frac{K_{j+\frac{1}{2}} \Delta t}{(\Delta x)^2} \tag{6.14}$$

Here we have assumed for simplicity that Δx is a constant. The scheme given by (6.13) combines forward time differencing with centered space differencing. Recall that this combination is unconditionally unstable for the advection problem, but we will show that it is conditionally stable for diffusion. It should be obvious that, with periodic boundary conditions, (6.13) guarantees conservation of q in the sense that

$$\sum_j q_j^{n+1} \Delta x = \sum_j q_j^{n} \Delta x . \tag{6.15}$$

To analyze the stability of (6.13) using von Neumann's method, we assume that κ is a constant. Then (6.13) yields

$$(\lambda - 1) = \kappa[(e^{ik\Delta x} - 1) - (1 - e^{-ik\Delta x})] , \tag{6.16}$$

which is equivalent to

$$\lambda = 1 - 4\kappa \sin^2\left(\frac{k\Delta x}{2}\right) \le 1 . \tag{6.17}$$

Note that λ is real.

Instability can occur if $\lambda < -1$, or

$$\kappa \sin^2\left(\frac{k\Delta x}{2}\right) > \frac{1}{2} . \tag{6.18}$$

The worst case is $\sin^2\left(\frac{k\Delta x}{2}\right) = 1$, which occurs for $\frac{k\Delta x}{2} = \frac{\pi}{2}$, or $k\Delta x = \pi$. This is the

$2\Delta x$ wave. We conclude that with (6.13)

$$\kappa \le \frac{1}{2} \text{ is required for stability.} \tag{6.19}$$

When the stability criterion derived above is satisfied, we can be sure that

$$\sum_i (q_j^{n+1})^2 - \sum_i (q_j^n)^2 < 0 \ ; \tag{6.20}$$

this is the condition for stability according to the energy method discussed in Chapter 2.

6.3 An implicit scheme

We can obtain unconditional stability through the use of an implicit scheme, but at the cost of some additional complexity. Replace (6.13) by

$$q_j^{n+1} - q_j^n = \left[\kappa_{j+\frac{1}{2}}(q_{j+1}^{n+1} - q_j^{n+1}) - \kappa_{j-\frac{1}{2}}(q_j^{n+1} - q_{j-1}^{n+1})\right]. \tag{6.21}$$

We analyze the stability of (6.21), for the case of spatially variable but non-negative κ, using the energy method.

Multiplying (6.21) by q_j^{n+1}, we obtain:

$$\begin{gathered}(q_j^{n+1})^2 - q_j^{n+1}q_j^n = \\ \kappa_{j+\frac{1}{2}}q_{j+1}^{n+1}q_j^{n+1} - \kappa_{j+\frac{1}{2}}(q_j^{n+1})^2 - \kappa_{j-\frac{1}{2}}(q_j^{n+1})^2 + \kappa_{j-\frac{1}{2}}q_{j-1}^{n+1}q_j^{n+1} \quad .\end{gathered} \tag{6.22}$$

Sum over the domain:

$$\begin{gathered}\sum_j (q_j^{n+1})^2 - \sum_j q_j^{n+1}q_j^n = \\ \sum_j \kappa_{j+\frac{1}{2}}q_{j+1}^{n+1}q_j^{n+1} - \sum_j \kappa_{j+\frac{1}{2}}(q_j^{n+1})^2 - \sum_j \kappa_{j-\frac{1}{2}}(q_j^{n+1})^2 + \sum_j \kappa_{j-\frac{1}{2}}q_{j-1}^{n+1}q_j^{n+1} = \\ \sum_j \kappa_{j+\frac{1}{2}}q_{j+1}^{n+1}q_j^{n+1} - \sum_j \kappa_{j+\frac{1}{2}}(q_j^{n+1})^2 - \sum_j \kappa_{j+\frac{1}{2}}(q_{j+1}^{n+1})^2 + \sum_j \kappa_{j+\frac{1}{2}}q_j^{n+1}q_{j+1}^{n+1} = \\ -\sum_j \kappa_{j+\frac{1}{2}}(q_{j+1}^{n+1} - q_j^{n+1})^2 \quad .\end{gathered}$$

Rearranging, we find that

$$\sum_j q_j^{n+1} q_j^n = \sum_j \left[(q_j^{n+1})^2 + \kappa_{j+\frac{1}{2}} (q_{j+1}^{n+1} - q_j^{n+1})^2 \right]. \tag{6.23}$$

Next, note that

$$\sum_j (q_j^{n+1} - q_j^n)^2 = \sum_j [(q_j^{n+1})^2 + (q_j^n)^2 - 2q_j^{n+1} q_j^n] \geq 0 . \tag{6.24}$$

Substitute (6.23) into (6.24), to obtain

$$\sum_j \left\{ (q_j^{n+1})^2 + (q_j^n)^2 - 2\left[(q_j^{n+1})^2 + \kappa_{j+\frac{1}{2}} (q_{j+1}^{n+1} - q_j^{n+1})^2 \right] \right\} \geq 0 . \tag{6.25}$$

This can be simplified and rearranged to

$$\sum_j [(q_j^{n+1})^2 - (q_j^n)^2] \geq -2 \sum_j \left\{ \left[\kappa_{j+\frac{1}{2}} (q_{j+1}^{n+1} - q_j^{n+1})^2 \right] \right\}. \tag{6.26}$$

This shows that $\sum_j [(q_j^{n+1})^2 - (q_j^n)^2]$ is less than a negative number. Therefore

$$\sum_j [(q_j^{n+1})^2 - (q_j^n)^2] < 0 \tag{6.27}$$

This is the desired result.

The trapezoidal implicit scheme is also unconditionally stable for the diffusion equation and it is more accurate than the backward implicit scheme.

Eq. (6.21) contains three unknowns, namely q_j^{n+1}, q_{j+1}, and q_{j-1}^{n+1}. We must therefore solve a system of such equations, for the whole domain at once. Assuming that K is independent of q (often not true in practice), the system of equations is linear and tridiagonal, so it is not too hard to solve. In realistic models, however, K can depend strongly on multiple dependent variables which are themselves subject to diffusion, so that multiple coupled systems of nonlinear equations must be solved simultaneously in order to obtain a fully implicit solution to the diffusion problem. For this reason, implicit methods are often avoided in practice.

6.4 The DuFort-Frankel scheme

The DuFort-Frankel scheme is partially implicit and unconditionally stable, but does not lead to a set of equations that must be solved simultaneously. The scheme is given by

$$\frac{q_j^{n+1} - q_j^{n-1}}{2\Delta t} = \frac{1}{(\Delta x)^2}\left[\kappa_{j+\frac{1}{2}}(q_{j+1}^n - q_j^{n+1}) - \kappa_{j-\frac{1}{2}}(q_j^{n-1} - q_{j-1}^n)\right] . \tag{6.28}$$

Notice that three time levels appear, which means that we will have a computational mode in time, in addition to a physical mode. Time level $n+1$ appears only in connection with grid point i, so that the solution can be obtained without solving a system of simultaneous equations:

$$q_j^{n+1} = \frac{q_j^{n-1} + 2\left[\kappa_{j+\frac{1}{2}} q_{j+1}^n - \kappa_{j-\frac{1}{2}}(q_j^{n-1} - q_{j-1}^n)\right]}{1 + 2\kappa_{j+\frac{1}{2}}} . \tag{6.29}$$

Consider spatially constant κ, and define

$$\alpha \equiv 2\kappa \tag{6.30}$$

The amplification factor satisfies

$$\lambda^2 - 1 = \alpha(\lambda e^{ik\Delta x} - \lambda^2 - 1 + \lambda e^{-ik\Delta x}) \tag{6.31}$$

which is equivalent to

$$\lambda^2(1+\alpha) - \lambda 2\alpha\cos(k\Delta x) - (1-\alpha) = 0 . \tag{6.32}$$

The solutions are

$$\begin{aligned} \lambda &= \frac{\alpha\cos(k\Delta x) \pm \sqrt{\alpha^2\cos^2(k\Delta x) - (1-\alpha^2)}}{1+\alpha} \\ &= \frac{\alpha\cos(k\Delta x) \pm \sqrt{1 - \alpha^2\sin^2(k\Delta x)}}{1+\alpha} . \end{aligned} \tag{6.33}$$

It should be clear that the plus sign corresponds to the physical mode, and the minus sign to the computational mode. Consider two cases. First, if $\alpha^2\sin^2(k\Delta x) \le 1$, then λ is real, and we find that

$$|\lambda| \le \frac{1 + |\alpha\cos(k\Delta x)|}{1+\alpha} \le 1 . \tag{6.34}$$

Second, if $\alpha^2\sin^2(k\Delta x) > 1$, which implies that $\alpha > 1$, then

$$|\lambda| = \frac{\sqrt{\alpha^2\cos^2(k\Delta x) + \alpha^2\sin^2(k\Delta x) - 1}}{1+\alpha} = \frac{\sqrt{\alpha^2 - 1}}{1+\alpha} = \sqrt{\frac{\alpha-1}{\alpha+1}} < 1 \,. \tag{6.35}$$

We conclude that the scheme is unconditionally stable.

It does not follow, however, that the scheme gives a good solution for large Δt. Consider the case of constant κ, and let $\alpha \to \infty$. Then (6.35) reduces to

$$|\lambda| \to 1 \,. \tag{6.36}$$

There is no damping, which is very wrong for the case of diffusion over a long time interval.

6.5 Summary

Diffusion is a relatively simple process which preferentially wipes out small-scale features. The most robust schemes for the diffusion equation are fully implicit schemes, but these give rise to systems of simultaneous equations. The DuFort-Frankel scheme is unconditionally stable and easy to implement, but behaves badly as the time step becomes large for fixed Δx.

Problems

1. Prove that the trapezoidal implicit scheme with centered second-order space differencing is unconditionally stable for the diffusion equation.

2. Program both the explicit and implicit versions of the diffusion equation, for a periodic domain consisting of 100 grid points, with constant $K = 1$ and $\Delta x = 1$. Also program the Dufort-Frankel scheme. Let the initial condition be

$$q_l = 100,\ j = 1, 50\text{ , and } q_j = 110 \text{ for } j = 51, 100\ . \tag{6.37}$$

   Compare the three solutions for different choices of the time step.

3. Use the energy method to evaluate the stability of (6.13).