Chapter 7: Diffusion

7.1 Introduction

Diffusion is a macroscopic statistical description 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, has to be considered. The process of one-dimensional diffusion can be represented in simplified form by

\[
\frac{\partial q}{\partial t} = -\frac{\partial F_q}{\partial x}.
\]

(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

\[
F_q = -K \frac{\partial q}{\partial x},
\]

(2)

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

\[
K \geq 0.
\]

(3)

Substitution of (2) into (1) gives

\[
\frac{\partial q}{\partial t} = \frac{\partial}{\partial x} \left( K \frac{\partial q}{\partial x} \right).
\]

(4)
Because (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 (1) that the spatially averaged value of $q$ does not change with time:

$$\frac{d}{dt} \left( \int_{\text{spatial domain}} q \, dx \right) = 0.$$  \hfill (5)

When (3) is satisfied, (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 increase small values, so that the spatial variability of $q$ decreases with time. In particular, we can show that

$$\frac{d}{dt} \left( \int_{\text{spatial domain}} q^2 \, dx \right) \leq 0.$$  \hfill (6)

To prove this, multiply both sides of (4) by $q$:

$$\frac{\partial}{\partial t} \left( \frac{q^2}{2} \right) = q \frac{\partial}{\partial x} \left( K \frac{\partial q}{\partial x} \right)$$

$$= \frac{\partial}{\partial x} \left( qK \frac{\partial q}{\partial x} \right) - K \left( \frac{\partial q}{\partial x} \right)^2$$  \hfill (7)

When we integrate the second line of (7) over a periodic domain, the first term vanishes and the second is negative (or possibly zero). The result (6) follows immediately.

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

$$q(x,t) = \sum_k \hat{q}_k(t) e^{ikx}.$$  \hfill (8)

Substituting into (1), and (temporarily) assuming spatially constant $K$, we find that the amplitude of a particular Fourier mode satisfies

$$\frac{d\hat{q}_k}{dt} = -k^2 K \hat{q}_k,$$  \hfill (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 (9) is

\[ \hat{q}_k(t) = \hat{q}_k(0) e^{-k^2Kt}. \]  

(10)

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

\[ \hat{q}_k(t + \Delta t) = \hat{q}_k(0) e^{-k^2K(t + \Delta t)} = \hat{q}_k(t) e^{-k^2K\Delta t}, \]

(11)

we see that, for the exact solution, the amplification factor is given by

\[ \lambda = e^{-k^2K\Delta t} < 1. \]

(12)

### 7.2 A simple explicit scheme

A finite-difference analog of (1) is

\[ q_{j}^{n+1} - q_{j}^{n} = \kappa_{j+\frac{1}{2}} \left( q_{j+1}^{n} - q_{j}^{n} \right) - \kappa_{j-\frac{1}{2}} \left( q_{j}^{n} - q_{j-1}^{n} \right), \]

(13)

where for convenience we define the nondimensional combination

\[ \kappa_{j+\frac{1}{2}} \equiv \frac{K}{(\Delta x)^2}. \]

(14)

Here we have assumed for simplicity that \( \Delta x \) is a constant. It should be obvious that, with periodic boundary conditions, (13) guarantees conservation of \( q \) in the sense that

\[ \sum_{j} q_{j}^{n+1} \Delta x = \sum_{j} q_{j}^{n} \Delta x. \]

(15)

The scheme given by (13) combines forward time differencing with centered space differencing. Recall that this combination is unconditionally unstable for the advection problem, but it turns out to be conditionally stable for diffusion. To analyze the stability of (13) using von Neumann’s method, we assume that \( \kappa \) is a constant. Then (13) yields

\[ (\lambda - 1) = \kappa \left[ \left( e^{ik\Delta x} - 1 \right) - \left( 1 - e^{-ik\Delta x} \right) \right], \]

(16)
which is equivalent to

\[ \lambda = 1 - 4\kappa \sin^2 \left( \frac{k\Delta x}{2} \right) \leq 1. \]  

(17)

Note that \( \lambda \) is real.

Instability occurs for \( \lambda < -1 \), which is equivalent to

\[ \kappa \sin^2 \left( \frac{k\Delta x}{2} \right) > \frac{1}{2}. \]  

(18)

The worst case is \( \sin^2 \left( \frac{k\Delta x}{2} \right) = 1 \), which occurs for \( \left( \frac{k\Delta x}{2} \right) = \frac{\pi}{2} \), or \( k\Delta x = \pi \). This is the \( 2\Delta x \) wave. We conclude that with (13)

\[ \kappa \leq \frac{1}{2} \]  

is required for stability.

(19)

When the scheme is unstable, it blows up in an oscillatory fashion.

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

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

(20)

this is the condition for stability according to the energy method discussed in Chapter 2. Eq. (20) is analogous to (6).

7.3 An implicit scheme

We can obtain unconditional stability through the use of an implicit scheme, but at the cost of some additional complexity. Replace (13) by

\[ q_j^{n+1} - q_j^n = \kappa \left[ j_{+\frac{1}{2}} (q_{j+1}^{n+1} - q_j^{n+1}) - \kappa j_{-\frac{1}{2}} (q_j^{n+1} - q_{j-1}^{n+1}) \right]. \]  

(21)

We use the energy method to analyze the stability of (21), for the case of spatially variable but non-negative \( K \). Multiplying (21) by \( q_j^{n+1} \), we obtain:
\[(q_j^{n+1}) - q_j^n = \kappa_{j+\frac{1}{2}} q_j^{n+1} - \kappa_{j-\frac{1}{2}} (q_j^{n+1})^2 - \kappa_{j-\frac{1}{2}} (q_j^n)^2 + \kappa_{j+\frac{1}{2}} q_j^{n+1} \]

(22)

Summing over the domain gives

\[\sum_j (q_j^{n+1})^2 - \sum_j q_j^n q_j = \sum_j \kappa_{j+\frac{1}{2}} q_j^{n+1} - \sum_j \kappa_{j-\frac{1}{2}} (q_j^n)^2 - \sum_j \kappa_{j-\frac{1}{2}} (q_j^{n+1})^2 + \sum_j \kappa_{j+\frac{1}{2}} q_j^{n+1} q_j^n\]

(23)

Next, note that

\[\sum_j (q_j^{n+1} - q_j^n)^2 = \sum_j \left[ (q_j^{n+1})^2 + (q_j^n)^2 - 2q_j^{n+1} q_j^n \right] \geq 0 \]

(24)

Substitute (23) into (24), to obtain

\[\sum_j \left[ (q_j^{n+1})^2 + (q_j^n)^2 - 2q_j^{n+1} q_j^n \right] \geq 0 \]

(25)

which can be simplified and rearranged to

\[\sum_j \left[ (q_j^{n+1})^2 - (q_j^n)^2 \right] \leq -2 \sum_j \left[ \kappa_{j+\frac{1}{2}} (q_j^{n+1} - q_j^n)^2 \right] \leq 0 \]

(26)

Eq. (26) demonstrates that \[\sum_j \left[ (q_j^{n+1})^2 - (q_j^n)^2 \right] \] is less than or equal to a not-positive number. In short,

\[\sum_j \left[ (q_j^{n+1})^2 - (q_j^n)^2 \right] \leq 0 \]

(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 discussed above.

Eq. (21) contains three unknowns, namely \( q_{j+1}^n \), \( q_{j+1}^{n+1} \), 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 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 not always practical.

7.4 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

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

(28)

Notice that three time levels appear, which means that we will have a computational mode in time, in addition to a physical mode. \textit{Time level \( n+1 \) appears only in connection with grid point \( j \), so the solution of (28) can be obtained without solving a system of simultaneous equations:}

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

(29)

To apply von Neumann’s method, we assume spatially constant \( \kappa \), and for convenience define

\[
\alpha \equiv 2\kappa \geq 0.
\]

(30)

The amplification factor satisfies

\[
\lambda^2 - 1 = \alpha \left( e^{i\Delta x} - \lambda^2 - 1 + e^{-i\Delta x} \right),
\]

(31)

which is equivalent to
\[ \lambda^2 (1 + \alpha) - \lambda 2\alpha \cos(k\Delta x) - (1 - \alpha) = 0. \]  
\[ (32) \]

The solutions are

\[ \lambda = \frac{\alpha \cos(k\Delta x) \pm \sqrt{\alpha^2 \cos^2(k\Delta x) + (1 - \alpha^2)}}{1 + \alpha} \]

\[ = \frac{\alpha \cos(k\Delta x) \pm \sqrt{1 - \alpha^2 \sin^2(k\Delta x)}}{1 + \alpha}. \]  
\[ (33) \]

The plus sign corresponds to the physical mode, for which \( \lambda \to 1 \) as \( \alpha \to 0 \), and the minus sign corresponds to the computational mode. This can be seen by taking the limit \( k\Delta x \to 0 \).

Consider two cases. First, if \( \alpha^2 \sin^2(k\Delta x) \leq 1 \), then \( \lambda \) is real, and by considering the two solutions separately it is easy to show that

\[ |\lambda| \leq \frac{1 + |\alpha \cos(k\Delta x)|}{1 + \alpha} \leq 1. \]  
\[ (34) \]

Second, if \( \alpha^2 \sin^2(k\Delta x) > 1 \), which implies that \( \alpha > 1 \), then \( \lambda \) is complex, and we find that

\[ |\lambda| = \frac{\sqrt{\alpha^2 \cos^2(k\Delta x) + \alpha^2 \sin^2(k\Delta x) - 1}}{1 + \alpha} = \frac{\sqrt{\alpha^2 - 1}}{1 + \alpha} = \sqrt{\frac{\alpha - 1}{\alpha + 1}} < 1. \]  
\[ (35) \]

We conclude that the scheme is unconditionally stable.

It does not follow, however, that the scheme gives a good solution for large \( \Delta t \). For \( \alpha \to \infty \) (strong diffusion and/or a long time step), (35) gives

\[ |\lambda| \to 1. \]  
\[ (36) \]

We conclude that the Dufot-Frankel scheme does not damp when the diffusion coefficient is large or the time step is large. This is very bad behavior.

7.5 Summary

Diffusion is a relatively simple process that preferentially wipes out small-scale features. The most robust schemes for the diffusion equation are fully implicit, 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 $\Delta t$. 
Problems

1. Prove that the trapezoidal implicit scheme with centered second-order space differencing is unconditionally stable for the one-dimensional diffusion equation. Do not assume that $K$ is spatially constant.

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

$$q_j = 100, \ j \in [1, \ 50], \ and \ q_j = 110 \ for \ j \in [51, \ 100].$$

(37)

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

3. Use the energy method to evaluate the stability of

$$q_j^{n+1} - q_j^n = \kappa \frac{j-\frac{1}{2}}{(j+\frac{1}{2})} (q_{j+1}^{n} - q_j^n) + \kappa \frac{j-\frac{1}{2}}{(j+\frac{1}{2})} (q_j^n - q_{j-1}^n).$$

Do not assume that $K$ is spatially constant.