Numerical Solution of Convection-Diffusion Problems

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A gentle introduction

Mathematical models that involve a combination of *convective* and *diffusive* processes are common in science and engineering. In this presentation,

- We see examples of typical problems
- We choose a model problem
- We demonstrate some numerical difficulties encountered in solving the problem

- Diffusion: A physical process that occurs in a flow of fluid in which some property is transported by the random motion of the molecules of the fluid.
- Convection: A physical process that occurs in a flow of fluid in which some property is transported by the ordered motion of the flow.

Two dimensionless parameters are used frequently:

- *Reynolds number* measures the ratio of the inertial and the viscous term.

$$Re = \frac{|\mathbf{v}| \cdot L}{\nu},$$

  where $\mathbf{v}$ (m/s) is the velocity vector, L (m) is the length scale of the problem area and ν is the kinematic viscosity (m^2/s).

- *Peclét number* measures the relative importance of convection compared to diffusion.

$$Pe = \frac{|\mathbf{v}| \cdot L}{D},$$

  where $\mathbf{v}$ (m/s) is the velocity vector, L (m) is the length scale of the problem area and D (m^2/s) is the diffusion coefficient.

Example 1. Pollutant dispersal in a river estuary

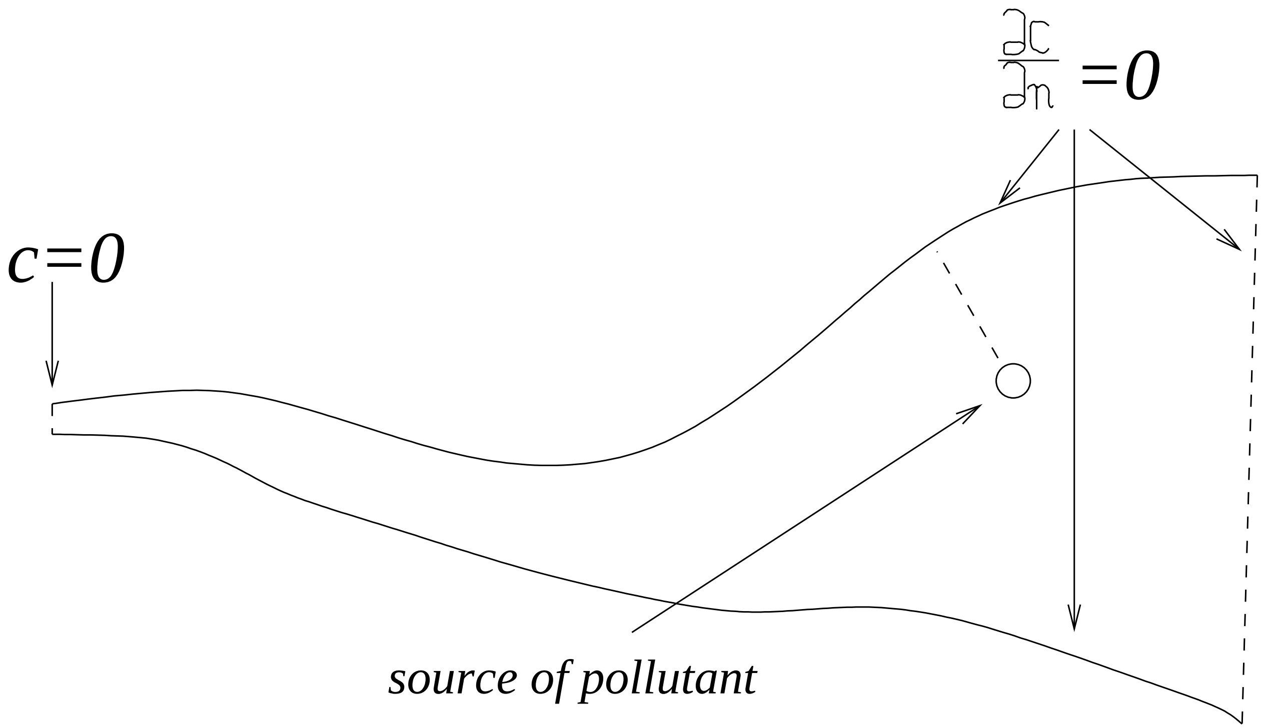

Figure 1: river estuary

Definition of the variables:

a) $c = c(x, y, t)$, concentration of a pollutant (depth-averaged),

b) $\mathbf{v} = \mathbf{v}(x, y, t)$, horizontal velocity field,

d) $S = S(x, y, t)$ is the source of pollutant,

e) D is the diffusion coefficient.

Now the typical equation governing the pollutants dispersal is:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \nabla \cdot (D \nabla c) + S.$$

Assuming $\mathbf{v}$ incompressible i.e. : $\nabla \cdot \mathbf{v} = \frac{\partial \mathbf{v}_1}{\partial x} + \frac{\partial \mathbf{v}_2}{\partial y} = 0$, we get

$$\begin{aligned}
\mathbf{v} \cdot \nabla c &= \mathbf{v}_1 \cdot \frac{\partial c}{\partial x_1} + \mathbf{v}_2 \cdot \frac{\partial c}{\partial x_2} \\
&= \mathbf{v}_1 \cdot \frac{\partial c}{\partial x_1} + \mathbf{v}_2 \cdot \frac{\partial c}{\partial x_2} + c \cdot \underbrace{\left(\frac{\partial \mathbf{v}_1}{\partial x_1} + \frac{\partial \mathbf{v}_2}{\partial x_2} \right)}_{=0} \\
&= \nabla \cdot (\mathbf{v} c).
\end{aligned}$$

So the equation for the previous pollution dispersal example becomes

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{v} c) = \nabla \cdot (D \nabla c) + S.$$

Typical scales in the case of river estuary:

- velocity: $0.5 - 3m/s$
- diffusivity: $0.05 - 5m^2/s$
- length scale: $100 - 1000m$

So we have the Péclet number $Pe = |\mathbf{v}|L/D = 10 - 6 \times 10^3$.

Example 2. The incompressible Navier-Stokes equations

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p = \nu \nabla^2 \mathbf{v} \tag{1}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{2}$$

Here the expression $\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla := \frac{D}{Dt}$ is the convective (or the Lagrangian) derivative and is given by

$$\frac{D\mathbf{v}}{Dt} = \frac{\partial \mathbf{v}}{\partial t} + (\nabla \times \mathbf{v}) \times \mathbf{v} + \nabla(\frac{1}{2}\mathbf{v}^2).$$

To satisfy (2) we consider the vector potential for $\mathbf{v}$, $\mathbf{v} = \nabla \times \mathbf{g}$. If we take

$$\mathbf{g} = \begin{pmatrix} 0 \\ 0 \\ -\psi(x, y, t) \end{pmatrix} := -\psi(x, y, t)\mathbf{k},$$

then

$$\mathbf{v} = \nabla \times (-\psi \mathbf{k}) = -\psi \underbrace{\nabla \times \mathbf{k}}_{=0} + \mathbf{k} \times (\nabla \psi) \equiv \mathbf{k} \times (\nabla \psi)$$

$$= \begin{pmatrix} -\psi_y \\ \psi_x \\ 0 \end{pmatrix}$$

$$\equiv \begin{pmatrix} -\psi_y \\ \psi_x \end{pmatrix}.$$

Let $\mathbf{v} = (u, v)^T$. In two dimensions the vorticity is the scalar ζ: $\zeta = v_x - u_y$,and the equations (1),(2) become

$$\frac{\partial \zeta}{\partial t} + \mathbf{v} \cdot \nabla \zeta = \nu \nabla^2 \zeta, \tag{3}$$

where we can obtain $\mathbf{v}$ by solving the compatibility relation

$$\nabla^2 \psi + \zeta = 0.$$

Knowing $\mathbf{v}$ in terms of ζ, (3) becomes a linear convection-diffusion equation for the scalar vorticity.

Typical scales in the river estuary again,

- velocity: $0.5 - 3m/s$
- length scale: $100m$
- kinematic viscosity: $10^{-6}m^2/s$

So the Reynolds number in a problem like this is around 10^4.

Example 3. Atmospheric pollution

A simplified form for a set of radioactive tracers of specific activity A^i can be written as

$$\frac{\partial A^i}{\partial t} + \mathbf{v}_H \cdot \nabla_H A^i + \frac{\partial}{\partial \sigma}(v_\sigma^i A^i) = \frac{\partial}{\partial \sigma}\left(K_z \frac{\partial}{\partial \sigma} A^i\right) + S^i.$$

- σ a terrain following vertical coordinate,
- $\mathbf{v}_H$ average horizontal wind vector in the σ system,
- ∇_H corresponding gradient operator
- S^i contains various sources and sinks with a matrix of coefficients describing the radioactive decay and transformation of the isotopes in the model,
- K_z is a vertical diffusion coefficient,
- v_σ^i is composed from the vertical motion in the σ system and the gravitational settling velocity.

Typical dimensions in horizontal direction:

- velocity:$10 m/s$
- length scale $1000 km$
- kinematic viscosity $1.5 \times 10^{-5} m^2/s$

So the Reynolds number $|\mathbf{v}| \cdot L/\nu$ is around $10^{11} - 10^{12}$.

In the vertical direction the length scale and velocity are smaller and the turbulent diffusion coefficient $10 - 10^3 m^2/s$, giving a Peclét number $10^{-2} - 10$.

Model problems

One of the main model problems will be the steady linear problem on a bounded domain $\Omega \subset \mathbb{R}^2$:

$$Lu := -\epsilon \nabla \cdot (a \nabla u) + \nabla \cdot (\mathbf{b} u) + cu = S,$$

with boundary conditions:

$$u = u_B \text{ on } \partial\Omega_D, \qquad \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega_N,$$

where $\partial\Omega_D, \partial\Omega_N$ form a partition of the boundary $\partial\Omega$ and $\partial\Omega_D$ is non-empty.

$$Lu := -\epsilon\nabla \cdot (a\nabla u) + \nabla \cdot (\mathbf{b}u) + cu = S,$$

Usually the following assumptions are expected to hold:

1. $\nabla \cdot \mathbf{b} = 0 \implies \qquad \nabla \cdot (\mathbf{b}u) = \mathbf{b} \cdot \nabla u,$
2. $a(\mathbf{x}) \geq 1,$
3. $c(\mathbf{x}) \geq 0,$
4. $\epsilon > 0.$

Some of the difficulties of modelling convection-diffusion can be shown in one dimensional version of this problem:

$$Lu := -\epsilon(au')' + bu' + cu = S \qquad \text{on } (0,1) \tag{4}$$

$$u(0) = u_L, \qquad u(1) = u_R. \tag{5}$$

And even in a simpler version of this:

$$-\epsilon u'' + bu' = S \tag{6}$$

$$u(0) = 0, \qquad u(1) = 1, \tag{7}$$

where $b > 0$

Numerical difficulties with simple difference schemes

Reynolds number low (<30 ?) $\rightarrow$ central difference scheme successful

Reynolds number high $\rightarrow$

- the relaxation techniques may fail to converge,
- if a solution is obtained for the steady problem it may exhibit physically unrealistic oscillations,
- if an explicit time-stepping procedure is used, it may become unstable for unexpectedly small time steps.

Central difference scheme

Assumptioms and notation:

- uniform mesh, spacing h,
- mesh points $x_j = jh, \qquad j = 0, 1, \cdots, J$ with $Jh = 1$
- approximation for the exact solution $u(x_j)$ is notated as U_j

So the central differential approximation to

$$-\epsilon u'' + bu' = S \tag{8}$$

becomes

$$L_h^{cd} U_j := -\epsilon \frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + b \frac{U_{j+1} - U_{j-1}}{2h} = S_j \tag{9}$$

or equivalently

$$-\epsilon D_h^2 U_j + b D_0 U_j = S_j, \qquad j = 1, 2, \ldots, J-1,$$

where $D_h^2 U_j := (U_{j+1} - 2U_j + U_{j-1})/h^2$, and
$D_0 U_j := \frac{1}{2}(U_{j+1} - U_{j-1})/h$.

$$L_h^{cd}U_j := -\epsilon\frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + b\frac{U_{j+1} - U_{j-1}}{2h} = S_j \qquad (10)$$

We set the "Mesh peclét number" as $\beta := \frac{bh}{\epsilon}$. And collect the terms of (10) together:

$$(\frac{1}{2}\beta - 1)U_{j+1} + 2U_j - (\frac{1}{2}\beta + 1) = (\frac{h^2}{\epsilon})S_j.$$

We first solve homogeneous linear difference problem

$$(\frac{1}{2}\beta - 1)U_{j+1} + 2U_j - (\frac{1}{2}\beta + 1) = 0, \qquad (11)$$

by seeking for a solutions of the form $u = \lambda^n$, and calculating the roots of the characteristic equation

$$(\frac{1}{2}\beta - 1)\lambda^2 + 2\lambda - (\frac{1}{2}\beta + 1) = 0.$$

The roots are $\lambda_0 = 1,\ \lambda_+ = \frac{1+\frac{1}{2}\beta}{1-\frac{1}{2}\beta}$.

The boundary conditions were $U_0 = 0, U_J = 1 \implies$

$$\begin{cases} 0 & = c_1 + c_2 \\ 1 & = c_1 + c_2 (\frac{1+\frac{1}{2}\beta}{1-\frac{1}{2}\beta})^J \end{cases}$$

Thus, when $\beta \neq 2$, then the solution of (11) is $U_j = \frac{\lambda_+^j - 1}{\lambda_+^J - 1}$.

The exact solution for the equation $-\epsilon u'' + bu' = 0$ is

$$u(x_j) = \frac{e^{bx_j/\epsilon} - 1}{e^{b/\epsilon} - 1} = \frac{e^{\beta j} - 1}{e^{\beta J} - 1}.$$

Now we can compare the exact solution and the numerical solution obtained by the central difference scheme, with $J = 20$, $b = 1$ and $\epsilon = .25,\ .05,\ .01$. (That is with $\beta = 0.2,\ 1.0,\ 5.0$.)

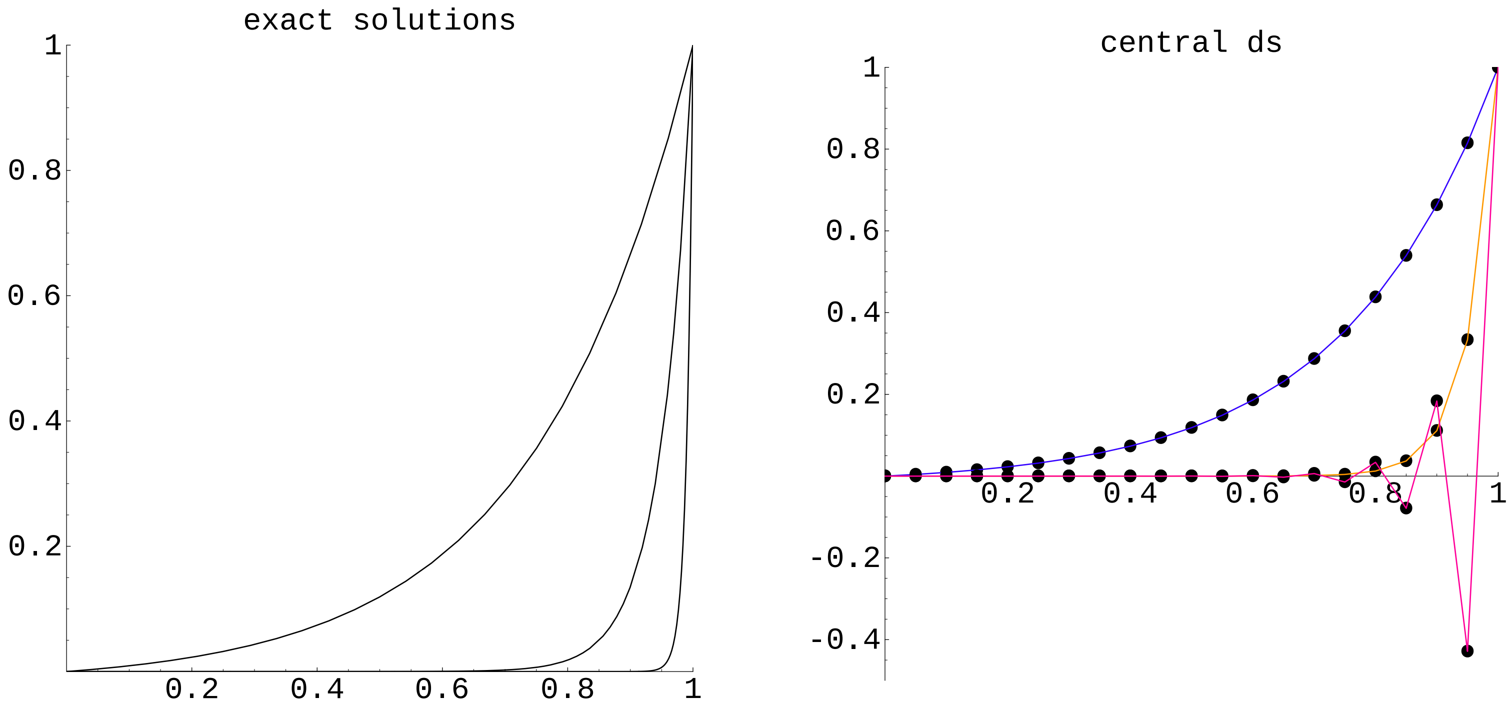

Figure 2: Solutions of the model problem with $S = 0$, $\beta = 0.2, 1.0, 5.0$.

Now the same situation applies for any source function $S(x) \neq 0$, because the solution for the equation

$$-\epsilon u'' + bu' = S, \text{ on } (0,1)$$

can be written as

$$u(x) = \int_0^1 G(x,t)S(t)dt + \frac{e^{bx/\epsilon} - 1}{e^{b/\epsilon} - 1},$$

where $G(x,t)$ is the Green's function for the problem, that is a function that solves the problem

$$-\epsilon G(x,t)'' + bG(x,t)' = \delta(x-t),$$

and it can be calculated to be

$$G(x,t) = \begin{cases} \frac{(e^{bx/\epsilon}-1)(e^{b(1-t)/\epsilon}-1)}{b(e^{b/\epsilon}-1)} & \text{for } x \leq t \\ \frac{(e^{bt/\epsilon}-1)(e^{b(1-t)/\epsilon}-e^{b(x-t)/\epsilon})}{b(e^{b/\epsilon}-1)} & \text{for } x \geq t \end{cases}$$

The solution for the difference equation

$$(\frac{1}{2}\beta - 1)U_{j+1} + 2U_j - (\frac{1}{2}\beta + 1) = (\frac{h^2}{\epsilon})S_j,$$

can be written in the same way, when $\beta \neq 2$, as

$$U_j = \sum_{k=1}^{J-1} hG_{j,k}S_k + \frac{\lambda_+^j - 1}{\lambda_+^J - 1},$$

where

$$G_{j,k} = \begin{cases} \frac{(\lambda_+^j - 1)(\lambda_+^{J-k} - 1)}{b(\lambda_+^J - 1)} & \text{for } j \leq k \\ \frac{(\lambda_+^j - 1)(\lambda_+^{J-k} - \lambda_+^{j-k})}{b(\lambda_+^J - 1)} & \text{for } j \geq k \end{cases}$$

So how well the term λ_+^j approximates the value $e^{\beta j}$ affects any solution of the model problem.

Upwind difference scheme

Replace

$$L_h^{cd}U_j := -\epsilon\frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + b\frac{U_{j+1} - U_{j-1}}{2h} = S_j,$$

with

$$L_h^{ud}U_j := -\epsilon\frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + b\frac{U_j - U_{j-1}}{2h} = S_j.$$

With mesh Peclét number β this becomes

$$-U_{j+1} + (2+\beta)U_j - (1+\beta)U_{j-1} = (h^2/\epsilon)S_j.$$

The characteristic equation

$$\lambda^2 - (2+\beta)\lambda + (1+\beta) = 0,$$

has roots $\lambda_0 = 1$, $\lambda_+ = 1+\beta$. The solution to the homogeneous problem is thus

$$U_j = \frac{\lambda_+^j - 1}{\lambda_+^J - 1}.$$

Again comparing to the exact solutions...

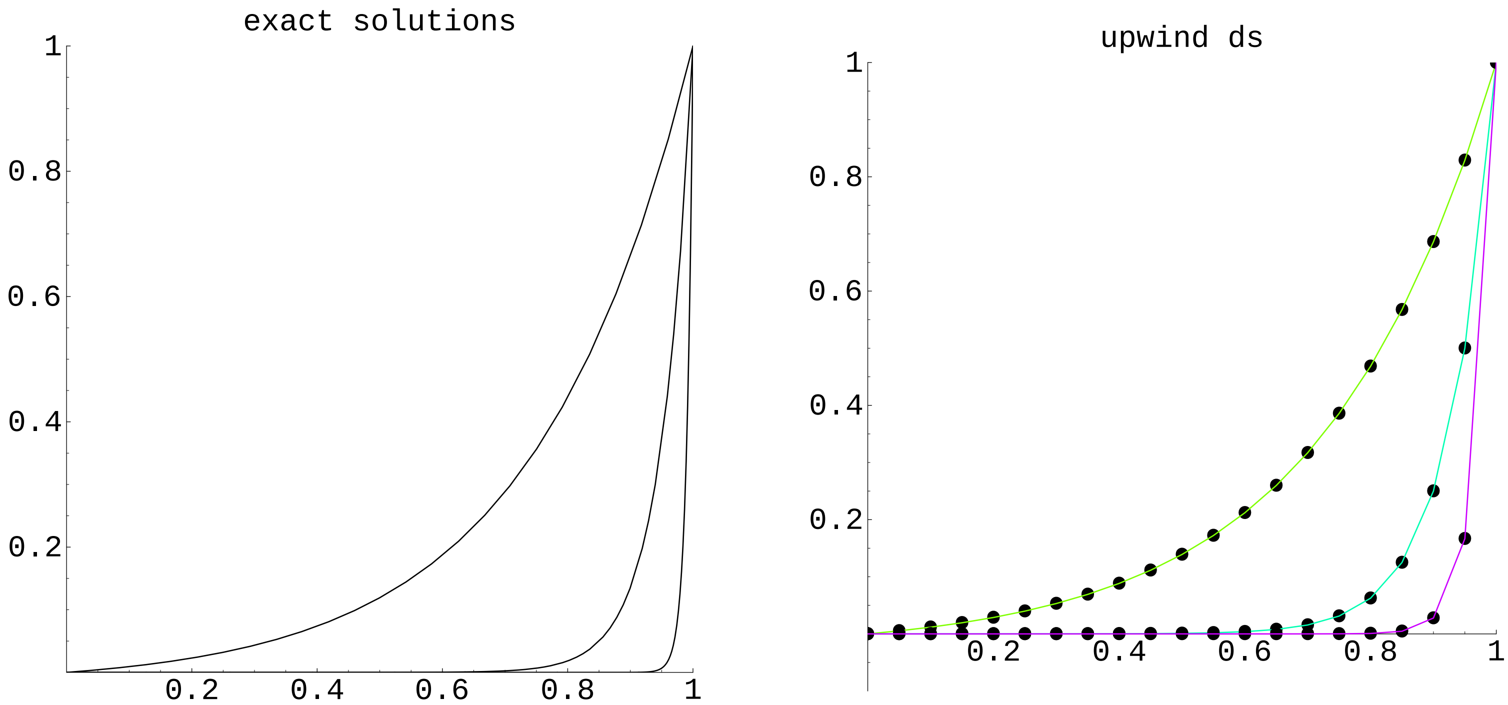

Figure 3: Solutions of the model problem with $S = 0$, $\beta = 0.2, 1.0, 5.0$.

Summary

We saw some examples of mathematical models that involve terms that come from convective-diffusive processes.

We saw that in a simple model problem, when the Mesh Peclét number exceeds certain value, the solutions by central difference scheme show oscillation. We saw that the upwind difference scheme provides a better solution in this sence, due to its positivity, although for small Mesh Peclét number it is less accurate than the central difference scheme.