DTU Compute

02425 Diffusions and SDEs
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# Diffusive transport in shear flow

We consider the vertical transport of a substance in water column, modeled by advection-diffusion equation in one dimension

$$\dot{C} = -(vC - DC')'$$

where $C = C(z,t)$, $z \in [0,H]$, $t \in \mathbf{R}$, and where $v$ and $D$ are constant. This equation governs the concentration field of a substance which is slightly denser or lighter than water (depending on the sign of $v$), and subject to molecular diffusivity $D$.

We add *no flux* boundary conditions to the equation, i.e. $vC - DC' = 0$ at $z = 0$ and $z = H$.

**Question 1:** Perform a Monte Carlo simulation of the transient vertical motion $\{Z_t : t \geq 0\}$ of a particle starting at the position $Z_0 = H/2$.

*Implementation:* Use reflection to implement the no-flux boundary condition: If a particle passes the lower boundary $z = 0$ during a time step, reflect it back into the domain by changing the sign of its position. Use the corresponding algorithm at the upper boundary. Take e.g. $H = 1$, $D = 1$, $v = 2$.

a Investigate the long-term distribution of the particle, using one simulation of a very long duration (e.g. $T = 100$) with a moderate time step (perhaps $\Delta t = 10^{-3}$). Plot a segment of the trajectory to confirm that it looks as you would expect. Then plot the histogram of the position. Change $v$ and repeat.

b Investigate the initial dispersion, using a large number of simulations of short duration (e.g. $T = 0.01$) and with short time step (e.g. $\Delta t = 10^{-4}$). Compare with the analytical solution to the advection-diffusion on the infinite domain, i.e., without boundaries at $z = 0$ and $z = H$.

**Question 2:** Find an analytical expression for steady-state concentration, normalized so that the total amount of the substance is 1. I.e., find a solution with $\dot{C} = 0$ and $\int_0^H C(z)\ dz = 1$. For the parameters in question 1, plot the analytical solution on top of the histogram and compare. *Hint:* There are two possible approaches: First, write a second order ordinary differential equation that governs the concentration field and solve using standard techniques. Alternatively and easier, show that the flux $J(x)$ must vanish at each point $x$. Then use this to write a *first order* ordinary differential equation that governs the concentration field, and solve this using standard techniques.

**Question 3:** From the parameters in the model, one may form the non-dimensional Peclét number as $\mathrm{Pe} = |v|H/D$. Plot the steady-state concentration for different values of the Peclét number (for example Pe=0.1, Pe=1, and Pe=10). Point out how this number determines the steady-state concentration.

## Add horizontal flow

We now add a horizontal dimension to the problem: Assume that there is a horizontal flow, so that the horizontal position $\{X_t : t \geq 0\}$ satisfies

$$\frac{d}{dt} X_t = u(Z_t) \text{ with } u(z) = \log(1 + 3z)$$

**Question 4:** Simulate the vertical and horizontal motion of a particle, starting at $(x, z) = (0, H/2)$ at time 0. Take $t = 10$, simulate a trajectory uo time $t$, and plot Taking $N = 1000$ replicate particles, plot a histogram of $X_t$ for time $t = 10$, and compute the mean and the variance of $X_t$. Repeat for $v = -2$ and comment: Does it appear that the mean of $X_t$ can be predicted from the vertical distribution, i.e. from the $C$ you found in the previous? Why does the variance of $X_t$ appear to depend on $v$? If $t$ is large enough, does it appear reasonable to diregard the vertical position and claim that the horizontal position is a random walk, i.e. that there is an *effective horizontal diffusivity?*