DTU Compute

02425 Diffusions and SDEs
October 6, 2021
UHT/uht

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 $z = H$.

Solution: The following function will be our main workhorse for simulating. It has been prepared so it can be used to answer all simulation-related questions in the exercise.

```
## Main simulation loop of Np particles, simulation time Tstop,
## time step dt,
## with floating velocity v and diffusivity D
EulerSim <- function(v=0,D=1,H=1,Tstop=10,dt=1e-3,Np=1,Z0=H/2,u=function(z)0)
{
  ## Simulation duration and time step
  Nt <- ceiling(Tstop/dt)+1

  ## Initialize horiz. and vert. position
  Z <- X <- array(NA,c(Nt,Np))
  X[1,] <- 0
  Z[1,] <- Z0

  ## Useful shorthands
  s <- sqrt(2*D*dt)
  vdt <- v*dt

  ## Main time loop
  for(i in 2:Nt)
    {
      ## Update vertical position; reflect at bottom
      Z[i,] <- abs(Z[i-1,] + vdt + rnorm(Np,sd=s))
      ## Reflect at surface
      Z[i,] <- H - abs(H-Z[i,])

      ## Update horizontal position
      X[i,] <- X[i-1,] + u(Z[i,])*dt
    }
  return(list(Z=Z,X=X))
}
```

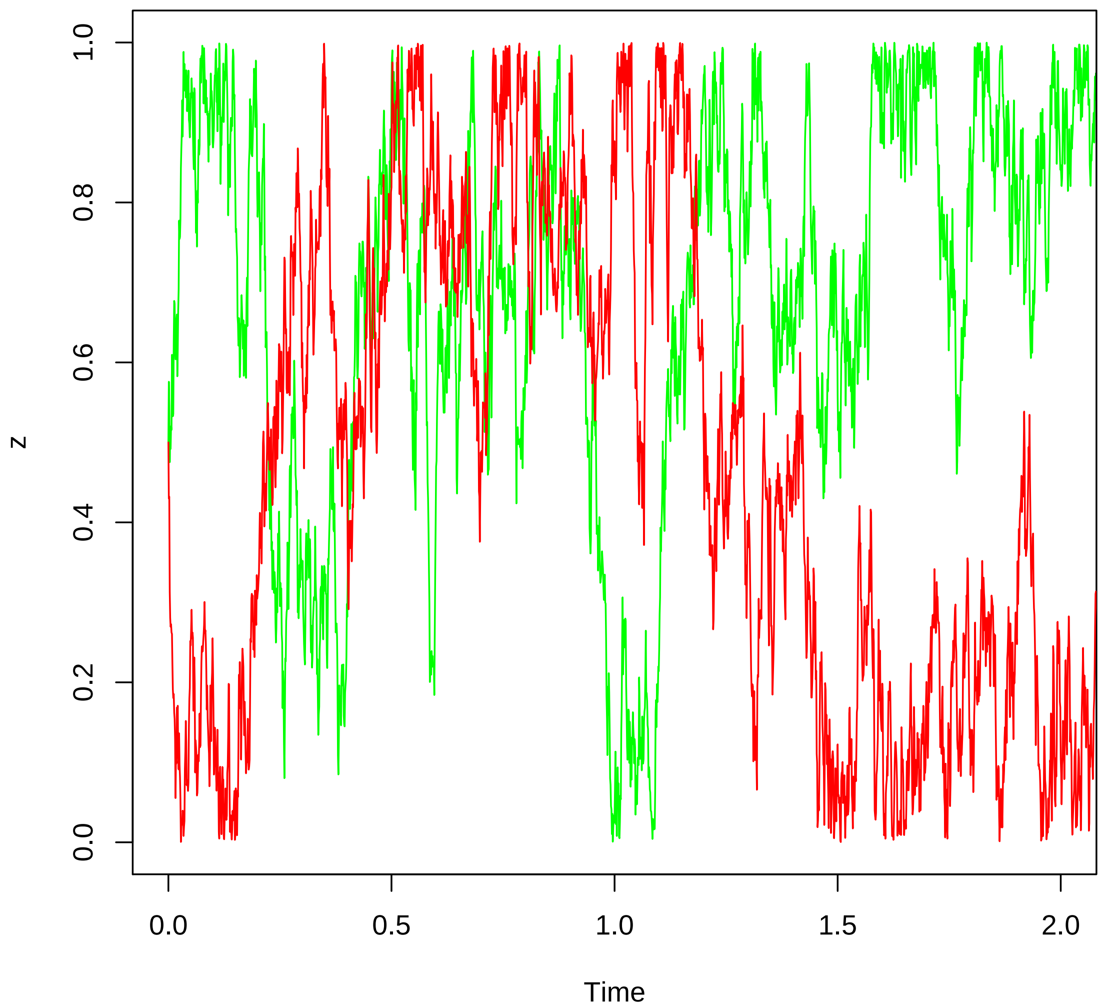
Solution of Question 1a: One very long simulation

The following code performs two simulations; one with positive velocity, and one with negative.

```
Tlong <- 100
dt <- 1e-3
v <- 2
H <- 1
D <- 1
VeryLongSimUp <- EulerSim(v=v,D=D,Tstop=Tlong,dt=dt,Np=1)
VeryLongSimDown <- EulerSim(v=-v,D=D,Tstop=Tlong,dt=dt,Np=1)
```

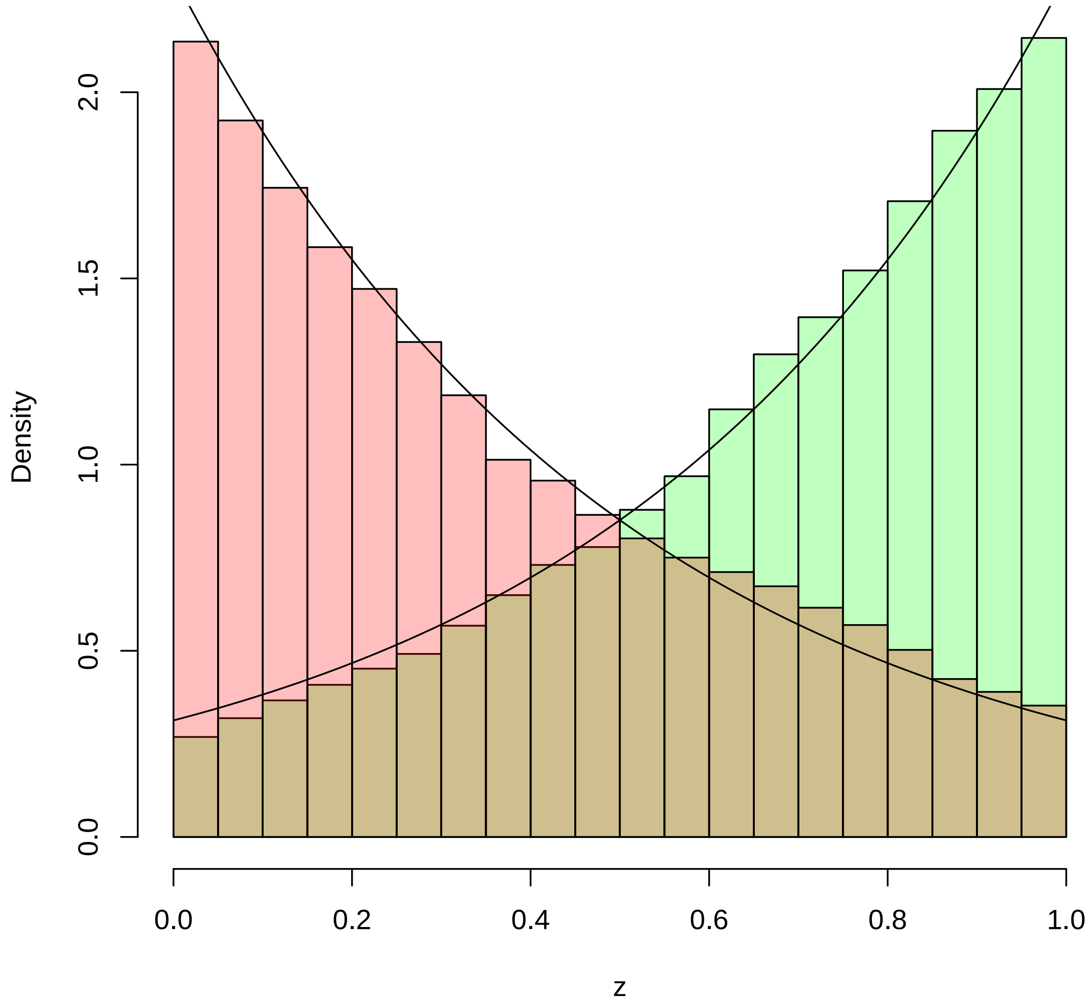
We first display a part of the trajectories.

```
tv <- seq(0,Tlong,dt)
plot(tv,VeryLongSimUp$Z,type="l",col="green",xlab="Time",ylab="z",
     xlim=c(0,2))
lines(tv,VeryLongSimDown$Z,type="l",col="red")
```



We display the histogram of the vertical positions and compare with the analytical solutions, which we find in question 2 below.

```
breaks <- seq(0,H,length=21)
hist(VeryLongSimUp$Z,breaks=breaks,freq=FALSE,col=rgb(0,1,0,0.25),
     main="",xlab="z")
hist(VeryLongSimDown$Z,breaks=breaks,freq=FALSE,col=rgb(1,0,0,0.25),add=TRUE)
plot(function(z)exp(z*v/D)*v/D/(exp(v*H/D)-1),from=0,to=1,add=TRUE)
plot(function(z)-exp(z*-v/D)*v/D/(exp(-v*H/D)-1),from=0,to=1,add=TRUE)
```



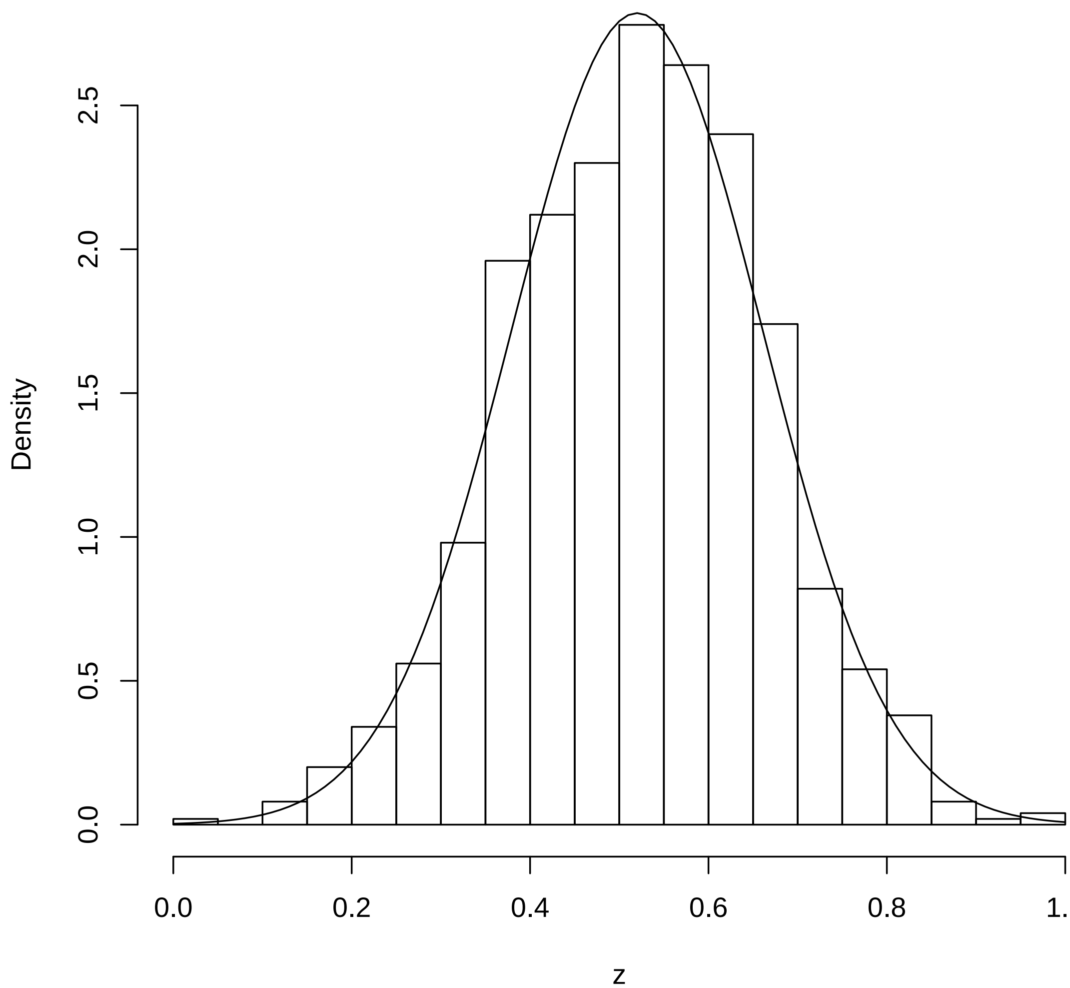
Notice that - as expected - when the velocity is positive, the histogram is biased towards large values of Z. Correspondingly, when the velocity is negative, we see more small values of Z.

The agreement with the analytical stationary distribution is reassuring. Notice that that it is actually a bold claim that the empirical histogram should match the analytical steady-state: The process is not strictly in steady state, since it starts at a fixed position (in the center), and not according to the stationary distribution. However, the simulation time is very long, so that the process approaches steady state, and the process *mixes*, so we effectively see a large number of (almost) independent samples from the stationary distribution. This probably matches your intuition, but is actually a quite advanved mathematical result.

Solution of Question 1b: Many short simulations

The following code simulates 1000 particles over a short period of time and plots a histogram of the 1000 end points. Then it compares with the analytical solution (the Gaussian bell).

```
## Simulate a short run; compare with Gaussian
Tshort <- 0.01
Np <- 1000
ShortSim <- EulerSim(v=v,D=D,H=H,Tstop=Tshort,dt=1e-4,Np=Np)
hist(tail(ShortSim$Z,1),freq=FALSE,breaks=21,xlab="z",main="")
plot(function(z)dnorm(z,mean=H/2+v*Tshort,sd=sqrt(2*D*Tshort)),
     from=0,to=1,add=TRUE)
```



The agreement is quite good.

If the simulation time had been a little longer, then a significant fraction of the particles would interact with the boundary, and the histogram would disagree with the Gaussian bell, which neglects the boundary and assumes that the particles spread in infinite space. If the simulation time had been a lot longer, we would see the stationary distribution from question 1a. The transition from Gaussian to exponential can be elucidated with a more detailed (analytical or numerical) analysis of the advection-diffusion equation with the no-flux boundary conditions.

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.

Solution: We aim to solve the steady-state equation

$$-(vC - DC')' = 0$$

for $C = C(z)$ with no-flux conditions: $vC - DC' = 0$ at $z \in \{0, H\}$.

The easy solution is to recognize that the flux $vC - DC'$ must be constant on the interval, and due to the boundary conditions, the constant value of the flux must be 0. Hence

$$vC - DC' = 0$$

which has the solution

$$C = \frac{1}{Z}\exp(vz/D)$$

The normalization constant Z is found by the requirement that C integrates to 1, i.e.

$$Z = \int_0^H \exp(vz/D)\ dz = \frac{D}{v}(\exp(vH/D) - 1)$$

Here we assume $v \neq 0$ - I leave the case $v = 0$ to you.

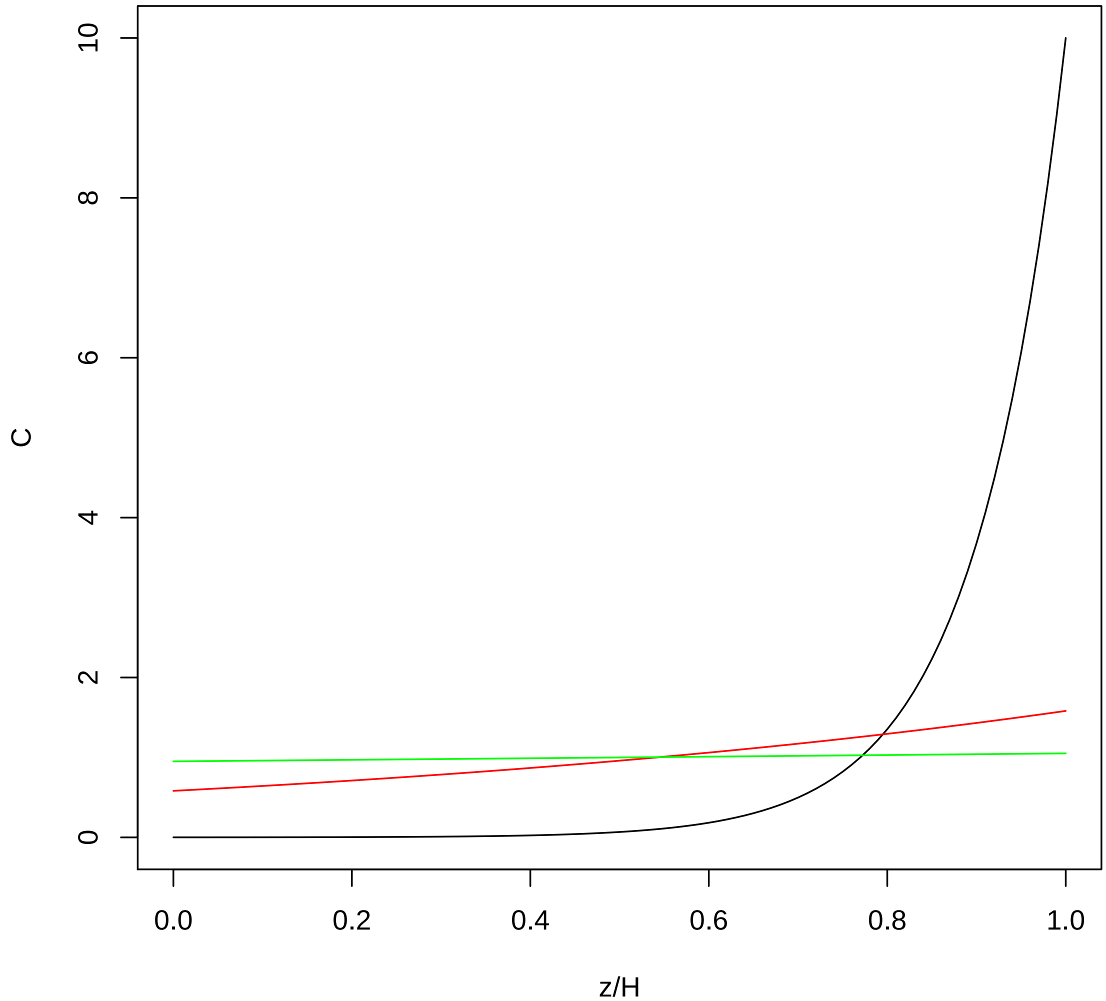
The more brute-force approach recognizes that the steady-state equation is a second order linear homogenous ordinary differential equation. Writing up the characteristic equation, we find roots 0 and v/D. We then seek linear combinations of the two solutions $C = \exp(0z)$ and $C = \exp(vz/D)$ that match the boundary conditions and the normalization. This can be written as an algebraic linear system in the two coefficients and solved. So it is possible to solve the question "mechanically", but much more elegant and brief if we use our insight into the system.

Question 3: From the parameters in the model, one may form the non-dimensional Peclét number as $\text{Pe} = |v|H/D$. 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.

Solution: The following code plots the steady-state solution for three values of the Peclét number. On the abscissa we plot the non-dimensional vertical position z/H.

```
Cs <- function(Pe)function(zp)exp(Pe*zp)*Pe/(exp(Pe)-1)

plot(Cs(10),from=0,to=1,ylim=c(0,10),xlab="z/H",ylab="C")
plot(Cs(1),from=0,to=1,add=TRUE,col="red")
plot(Cs(0.1),from=0,to=1,add=TRUE,col="green")
```



We see that the larger the Peclét number, the more the steady-state distribution is concentrated at the upper boundary. Notice that the shape depends only on the Peclét number, and not the individual parameters v, D, H. Non-dimensional quantities such as the Peclét number are useful for determining the relative importance of different phenomena (here, advection and diffusion). We shall see during the course that high Peclét numbers correspond to large signal-to-noise ratios.

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. 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?*

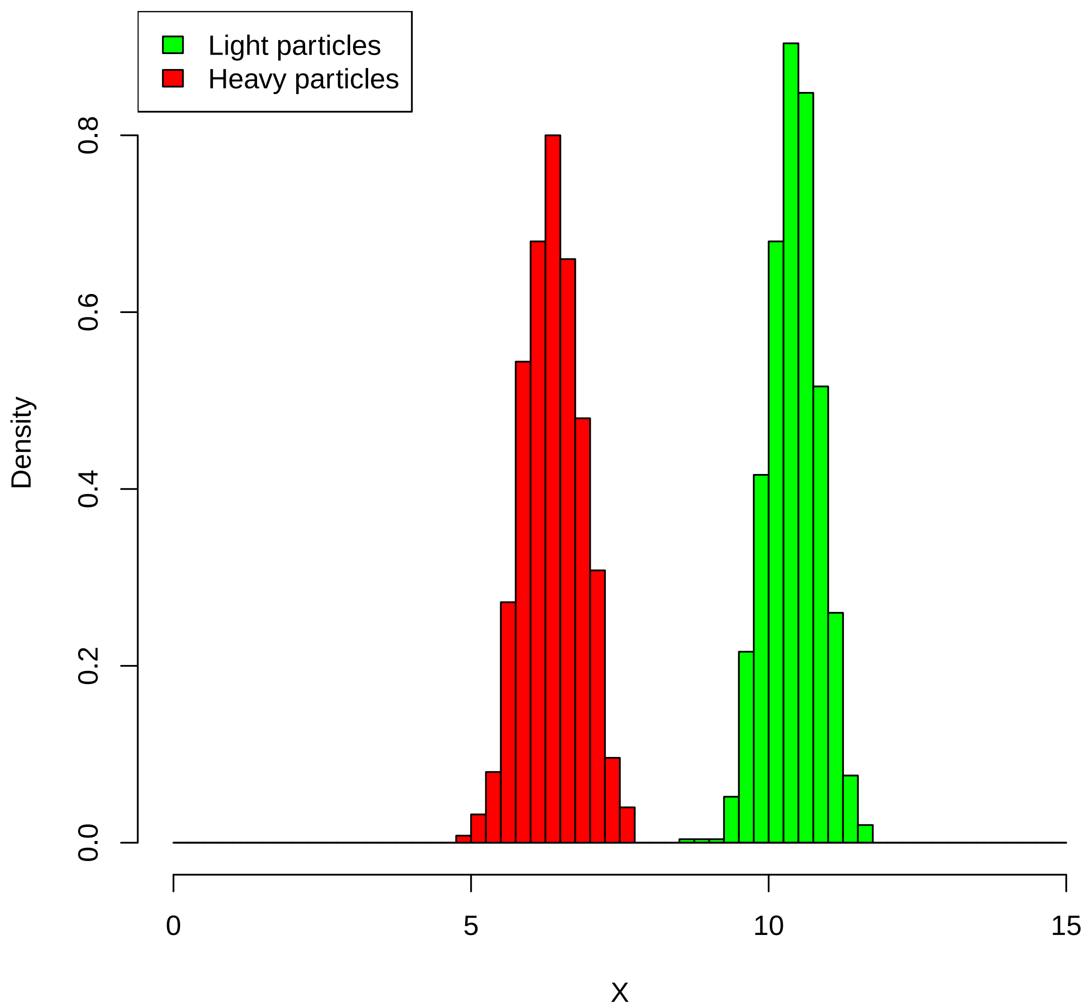
Solution: The following code does the simulation and plots the histograms.

```
Np <- 1000

## Horiztonal flow field
u <- function(z) log(1+3*z)

FloatSim <- EulerSim(v=v,D=D,Tstop=10,Np=Np,u=u)
SinkSim <- EulerSim(v=-v,D=D,Tstop=10,Np=Np,u=u)

hist(tail(FloatSim$X,1),breaks=seq(0,15,0.25),freq=FALSE,col="green",xlab="X",main="")
hist(tail(SinkSim$X,1),freq=FALSE,breaks=seq(0,15,0.25),add=TRUE,col="red")
legend(x="topleft",legend=c('Light particles','Heavy particles'),fill=c("green","red"))
```



The light particles go to the surface, where the horizontal velocities are larger, and therefore they travel further downstream.

The heavy particles go to the bottom, where the velocity *gradients* are larger (inspect the velocity profile u to check this), and therefore their horizontal transport is more sensitive to the random vertical motion. The result is that the heavy particles spread out more, horizontally.

Both of these differences would have been more pronounced at higher Peclét numbers.

We can quantify this by computing the mean and variance of the horizontal displacement in the two groups:

```
meanFloat <- mean(tail(FloatSim$X,1))
varFloat <- var(as.numeric(tail(FloatSim$X,1)))
meanSink <- mean(tail(SinkSim$X,1))
varSink <- var(as.numeric(tail(SinkSim$X,1)))

tab <- array(c(meanFloat,meanSink,varFloat,varSink),c(2,2))
colnames(tab) <- c("Mean","Var")
rownames(tab) <- c("Float","Sink")
print(tab)
```

```
##           Mean       Var
## Float 10.41379 0.1913912
## Sink   6.37758 0.2367837
```

It would be possible to compute these statistics analytically - we shall see how about half-way through the course.

Notice that the two distributions resemble Gaussian bells. If the simulation time had been longer, the resemblance would have been more pronounced: A *central limit theorem* applies. This also means that if we care only about horizontal transport over long periods of time, we can consider the horizontal motion a random walk / Brownian motion, so that the horizontal velocity can be considered ”white noise”. In this case, the details of vertical motion become irrelevant; we only care about the emergent properties of the horizontal movements. A central question for stochastic differential equations is which time scales we focus on in the modelling exercise; and thereby which processes should be approximated with white noise.