Numerical Solution of the Diffusion Equation with No-Flux Boundary Conditions

For no-flux boundary conditions, we want $\frac{\partial c}{\partial x}\Big|_{x=0} = \frac{\partial c}{\partial x}\Big|_{x=1} = 0$. Notice that

$$\frac{\partial c(x,t)}{\partial x}\Bigg|_{x=0} \approx \frac{c_{2,j} - c_{1,j}}{\delta x},$$

$$\frac{\partial c(x,t)}{\partial x}\Bigg|_{x=1} \approx \frac{c_{N_x,j} - c_{N_x-1,j}}{\delta x}.$$

Thus, the no-flux boundary conditions are enforced by explicitly requiring that $c_{1,j} = c_{2,j}$ and $c_{N_x,j} = c_{N_x-1,j}$ for all j. We'll use the same initial condition as we did for the constant concentration boundary conditions.

Note that since no flux leaves the boundaries, conservation of mass implies that

$$s(t) \equiv \int_0^1 c(x,t)dx$$

should be a constant for all time.

The following Matlab code solves the diffusion equation according to the scheme given by (5) and for no-flux boundary conditions:

```
numx = 101;   %number of grid points in x
numt = 2000;  %number of time steps to be iterated
dx = 1/(numx - 1);
dt = 0.00005;

x = 0:dx:1;   %vector of x values, to be used for plotting

C = zeros(numx,numt);   %initialize everything to zero

%specify initial conditions
t(1) = 0;      %t=0
mu = 0.5;
sigma = 0.05;
for i=1:numx
   C(i,1) = exp(-(x(i)-mu)^2/(2*sigma^2)) / sqrt(2*pi*sigma^2);
end

%iterate difference equations
for j=1:numt
   t(j+1) = t(j) + dt;
   for i=2:numx-1
      C(i,j+1) = C(i,j) + (dt/dx^2)*(C(i+1,j) - 2*C(i,j) + C(i-1,j));
   end
   C(1,j+1) = C(2,j+1);          %C(1,j+1) found from no-flux condition
   C(numx,j+1) = C(numx-1,j+1);  %C(numx,j+1) found from no-flux condition
end

figure(1);
hold on;
plot(x,C(:,1));
plot(x,C(:,11));
plot(x,C(:,101));
plot(x,C(:,1001));
plot(x,C(:,2001));
xlabel('x');
ylabel('c(x,t)');

%calculate approximation to the integral of c from x=0 to x=1
for j=1:numt+1
   s(j) = sum(C(1:numx-1,j))*dx;
end

figure(2);
plot(t,s);
xlabel('t');
ylabel('c_{total}');
axis([0 0.1 0.9 1.1]);
```

Text version of this program

This program produces the following figures:

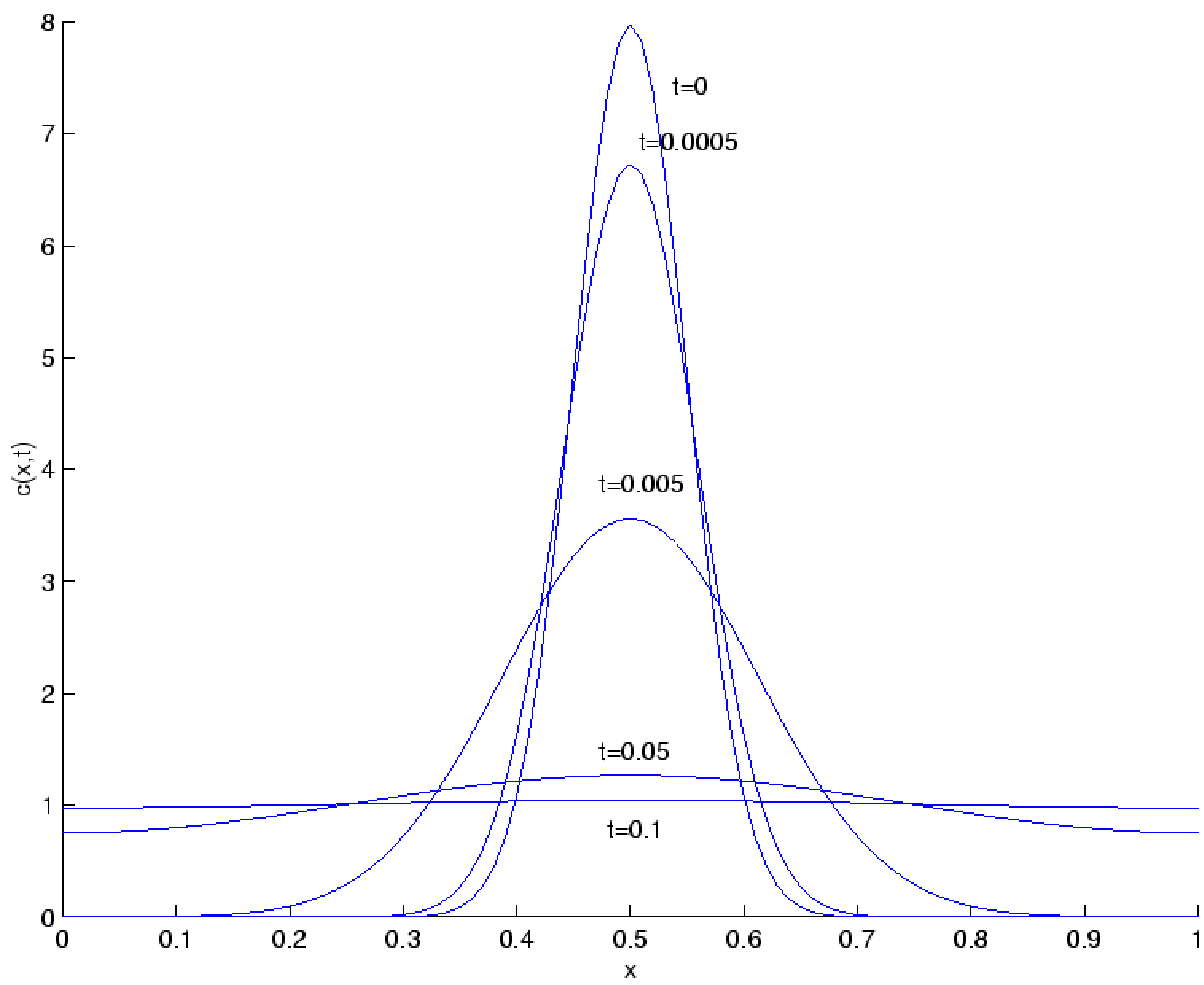

Figure 6: Numerical solution of the diffusion equation for different times with no-flux boundary conditions.

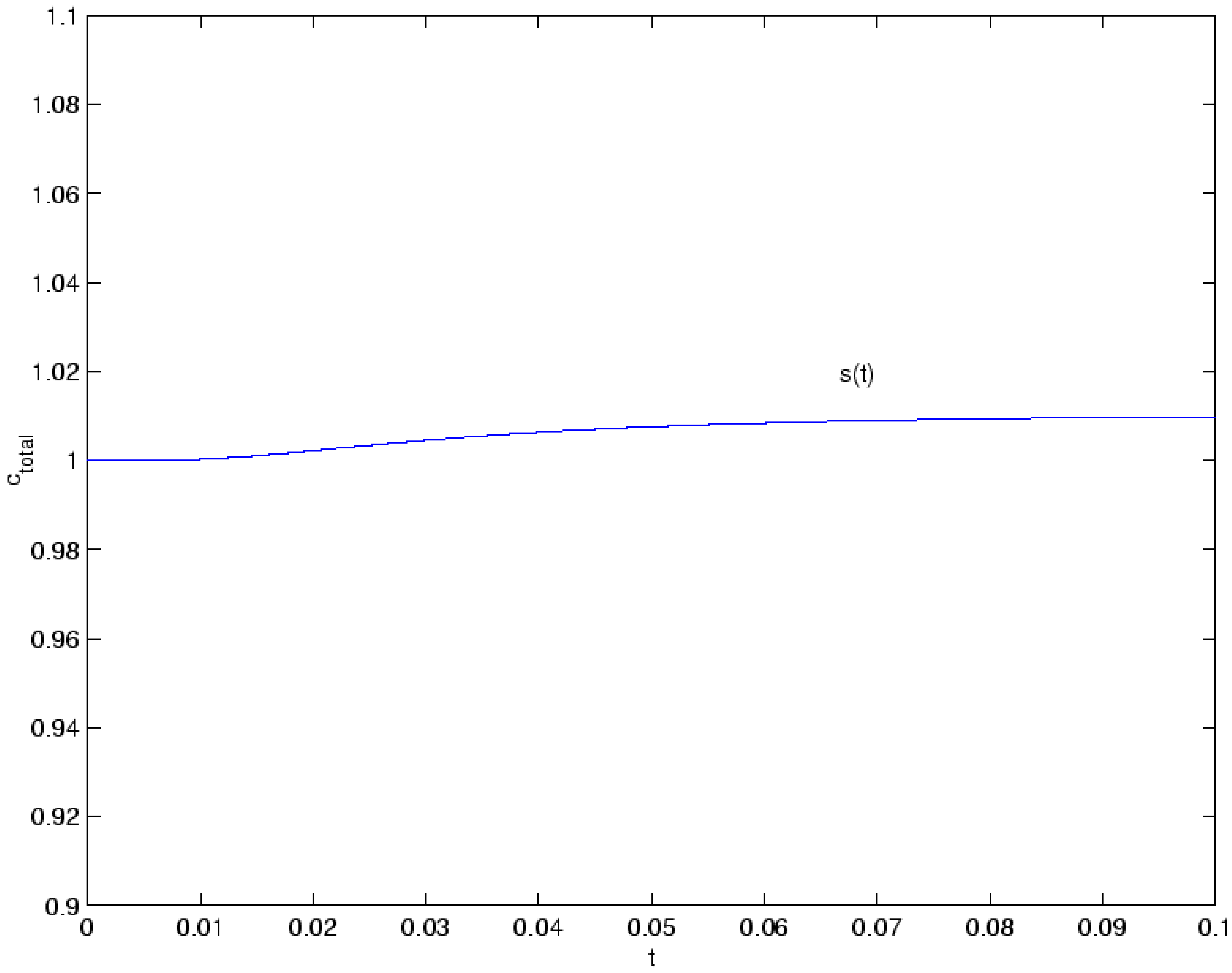

Figure 7: Verification that $s(t)$ is (approximately) constant.

We see that the solution eventually settles down to c being uniform in x. Because of the normalization of our initial condition, this uniform state is given by $c=1$. We also notice that $s(t)$ is not quite constant in time - this must be a result of numerical error (both in our finite difference scheme and our numerical calculation of integrals, etc). We could get a better result with different choices of δx and δt, or by using a more sophisticated finite difference scheme.
