Implementation of artifical boundary conditions in simulations of the 1D and 2D Fokker-Planck equations

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Theoretical background

Consider a particle that obeys the stochastic differential equation

$$\mathrm{d}x = f(x(t))\mathrm{d}t + g(x(t))\mathrm{d}W, \tag{1}$$

where $f(x(t))$ is called the *drift* term and $g(x(t))$ is called the *diffusion* term. Here we assume $g(x(t)) = g$ constant. The probability distribution $p(x,t)$ of possible particle trajectories is given by the Fokker-Planck equation,

$$\begin{aligned}
\frac{\mathrm{d}p(x,t)}{\mathrm{d}t} &= -\frac{\mathrm{d}}{\mathrm{d}x}\left[f(x)p(x,t)\right] + \frac{g^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}[p(x,t)] \\
&= -\frac{\mathrm{d}}{\mathrm{d}x}\left[f(x)p(x,t) - \frac{g^2}{2}\frac{\mathrm{d}}{\mathrm{d}x}[p(x,t)]\right] \\
&\equiv -\frac{\mathrm{d}}{\mathrm{d}x}J(x,t),
\end{aligned} \tag{2}$$

where $J(x,t)$ is the probability current.

Numerical implementation

To simulate this partial differential equation numerically we use a forward-time central-space (FTCS) method. The quantity $p^j[i]$ denotes the probability density at a point x_i at time t_j, and likewise for $f^j[i]$. The x_i range from $x_0 = 0$ to $x_N = x_{max}$, and the t_j range from $t_0 = 0$ to $t_M = t_{max}$. The spatial step is $\Delta x = x_{max}/N$, and the time step is $\Delta t = t_{max}/M$. Then, an update step for the FTCS integration scheme is given by

$$\begin{aligned}
\frac{p^{j+1}[i] - p^j[i]}{\Delta t} = &- \frac{f^j[i+1]p^j[i+1] - f^j[i-1]p^j[i-1]}{2\Delta x} \\
&+ \frac{g^2}{2}\left[\frac{p^j[i+1] - 2p^j[i] + p^j[i-1]}{\Delta x^2}\right].
\end{aligned}$$

Equivalently,

$$\begin{aligned}
p^{j+1}[i] = p^j[i-1]&\left[\frac{\Delta t}{2\Delta x}f^j[i-1] + \frac{g^2}{2}\frac{\Delta t}{\Delta x^2}\right] + p^j[i]\left[1 - g^2\frac{\Delta t}{\Delta x^2}\right] \\
&+ p^j[i+1]\left[\frac{-\Delta t}{2\Delta x}f^j[i+1] + \frac{g^2}{2}\frac{\Delta t}{\Delta x^2}\right].
\end{aligned} \tag{3}$$

This can be written as a matrix equation $\vec{p}^{j+1} = A^j \vec{p}^j$ (where the superscript once again denotes the timestep) in which

$$\vec{p}^j = \left[p^j[0],\ p^j[1],\ p^j[2],\ \ldots,\ p^j[N-1],\ p^j[N]\right]^T,$$

and

$$A^j = \begin{bmatrix} 1-g^2\frac{\Delta t}{\Delta x^2} & \frac{-\Delta t}{2\Delta x}f^j[1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 0 & 0 & 0 & \cdots \\ \frac{\Delta t}{2\Delta x}f^j[0]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 1-g^2\frac{\Delta t}{\Delta x^2} & \frac{-\Delta t}{2\Delta x}f^j[2]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 0 & 0 & \cdots \\ 0 & \frac{\Delta t}{2\Delta x}f^j[1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 1-g^2\frac{\Delta t}{\Delta x^2} & \frac{-\Delta t}{2\Delta x}f^j[3]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 0 & \cdots \\ 0 & 0 & \frac{\Delta t}{2\Delta x}f^j[2]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 1-g^2\frac{\Delta t}{\Delta x^2} & \frac{-\Delta t}{2\Delta x}f^j[4]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix}.$$

Note that except for the first and the last columns, all columns have unit sum. This implies that for $i \in 1,\ 2,\ \ldots,\ N-1$, each unit of probability $p^j[i]$ is entirely allocated between $p^{j+1}[i-1]$, $p^{j+1}[i]$, and $p^{j+1}[i+1]$ in the next timestep, and hence this unit of probability is conserved over the integration step. However, as is the first and last columns do not have unit sum, which will cause probability to leak in or out of the system. Therefore, we impose an artificial boundary condition such that

$$A^j = \begin{bmatrix} 1-g^2\frac{\Delta t}{\Delta x^2}+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}-\frac{\Delta t}{2\Delta x}f^j[0] & \frac{-\Delta t}{2\Delta x}f^j[1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 0 & 0 & \cdots \\ \frac{\Delta t}{2\Delta x}f^j[0]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 1-g^2\frac{\Delta t}{\Delta x^2} & \frac{-\Delta t}{2\Delta x}f^j[2]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 0 & \cdots \\ 0 & \frac{\Delta t}{2\Delta x}f^j[1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 1-g^2\frac{\Delta t}{\Delta x^2} & \frac{-\Delta t}{2\Delta x}f^j[3]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & \cdots \\ 0 & 0 & \frac{\Delta t}{2\Delta x}f^j[2]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2} & 1-g^2\frac{\Delta t}{\Delta x^2} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix},$$

and similarly modify the $A^j[N,N]$ entry according to $A^j[N,N] \rightarrow A^j[N,N]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}+\frac{\Delta t}{2\Delta x}f^j[N]$. All together, the modified update rules for the two endpoints are

$$p^{j+1}[0] = p^j[0]\left[1-\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}-\frac{\Delta t}{2\Delta x}f^j[0]\right]+p^j[i+1]\left[\frac{-\Delta t}{2\Delta x}f^j[i+1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}\right] \tag{4}$$

and

$$p^{j+1}[N] = p^j[N-1]\left[\frac{\Delta t}{2\Delta x}f^j[N-1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}\right]+p^j[N]\left[1-\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}+\frac{\Delta t}{2\Delta x}f^j[N]\right], \tag{5}$$

while the update rule for all other values of i, unchanged from Eq. (3), is

$$\begin{aligned} p^{j+1}[i] = p^j[i-1]\left[\frac{\Delta t}{2\Delta x}f^j[i-1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}\right]+p^j[i]\left[1-g^2\frac{\Delta t}{\Delta x^2}\right] \\ +p^j[i+1]\left[\frac{-\Delta t}{2\Delta x}f^j[i+1]+\frac{g^2}{2}\frac{\Delta t}{\Delta x^2}\right]. \end{aligned} \tag{6}$$

Generalization to 2D Fokker-Planck equations

Fokker-Planck equations in 2D may also be numerically simulated using a FTCS method, and will require similar considerations to ensure no probability leaks at the boundaries. The method outlined here may be implemented in an identical way in the 2D system once the system is written in the matrix form $\vec{p}^{j+1} = A^j \vec{p}^j$. However, in the 2D system the probability density vector $\vec{p}^j$ has N^2 values according to

$$\vec{p}^j = \Big[p^j[0,0],\ p^j[0,1],\ p^j[0,1],\ \ldots,\ p^j[1,0],\ p^j[1,1],\ p^j[1,2], \ldots,\ p^j[N,N-1],\ p^j[N,N]\Big]^T,$$

with a somewhat more complicated matrix A^j. As before, since probability is conserved when the columns of A^j all have unit sums, all edge terms in A^j should be modified as in the 1D case to ensure probability is conserved at each timestep. In the 2D case $4(N-1)$ elements of A^j must be modified, while in the 1D case only 2 modifications are required.