Monte Carlo simulation of diffusion

We are here focusing on diffusion in one dimension, and therefore you need to keep track of the position $x(i, j)$ of particles $i = 1 \ldots N$ at time step $j = 1 \ldots n$.

1. At time $j = 0$, initialize $N = 10000$ particles at $x = 0 \mu m$. Create a loop to update the positions of the particles at each time step: the position must be updated by a normal distributed random step of mean zero and variance $\sigma = 1 \mu m$ (in matlab use the function `randn`). Produce a plot of the average position and mean square displacement as a function of time step $j = 1 \ldots n$ with $n = 1000$. On the latter plot, include a line corresponding to the theoretical expectation (which you can derive and relate to D, diffusivity).
2. What is the effect of increasing the number of particles N (try $N = 100000, 500000$).
3. Repeat 1) using 10000 particles, and $\sigma = 2 \mu m$. Plot the mean square displacement including the theoretical expectation.
4. So far, no reference has been made to the collision time or the value of the time step Δt. What value have you been using implicitly so far? Repeat 3) using instead $\Delta t = 0.5$ ms and $\Delta t = 2$ ms, and plot the mean square displacement as a function of time (not time step). How is D related to σ and Δt?
5. Restricted diffusion with reflecting boundary conditions: now we imagine placing the particles in a box of total length 100 μm. Each time a particle attempts to update its position beyond $x = \pm 50 \mu m$, nothing happens. In other words, the positions of those particles are not updated at that time step. Plot the mean square displacement as a function of time, and the apparent diffusion coefficient is a function of time. Include the theoretical expectations on both plots.

Next we use the narrow pulse approximation to compute the MR signal resulting from this simulation.

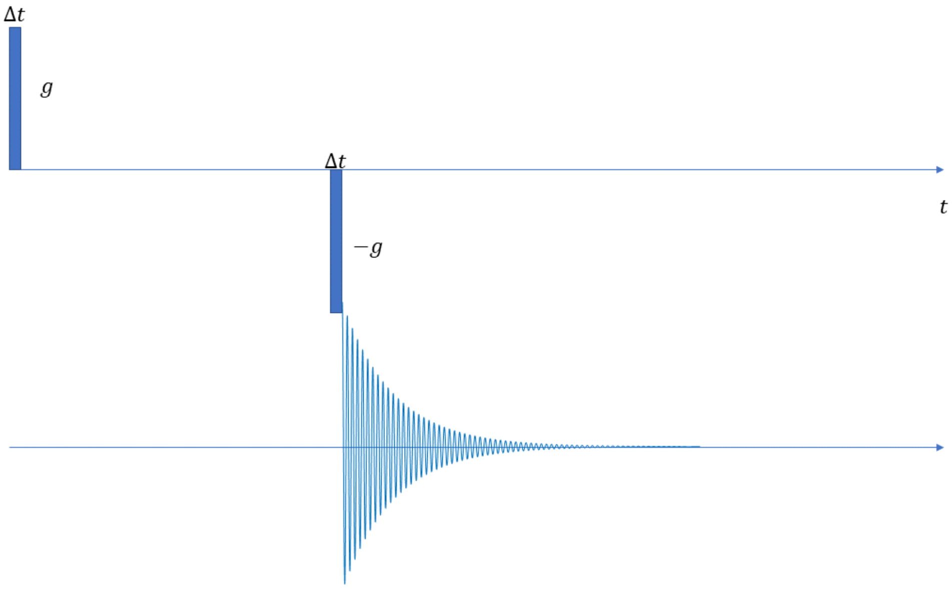

Figure 1 Narrow pulse diagram. Assume that the first gradient is applied immediately after a $\pi/2$ pulse, and gradients are applied with a time separation of Δ. They are only on for a time equal to your simulation time step, so phase increment is $\pm\gamma g \Delta t x(t)$. Hence total MR signal is $\langle \exp\left(-i\gamma g \Delta t\left(x(t) - x(0)\right)\right)\rangle$. You need to take real part because of "numerical noise".

6. Use a simulation defined by $\sigma = 0.1\mu m$ and $D = 0.5\mu m^2/ms$ using $N = 50000$ particles starting at $x = 0$. Compute the signal at $t = 10ms$ for different g given by $q = 0\ldots0.1\mu m^{-1}$, where $q \equiv \gamma g \Delta t$. Plot it as a function of b-factor, $b \equiv q^2 t$. Include the theoretical curve $S = \exp(-bD)$.
7. Now we consider diffusion in a box with reflecting walls placed at -50 μm and +50 μm, like in question 5. Compute the diffusion signal corresponding to a fixed diffusion wave vector of $q = 0.01$, and as a function of diffusion time $t = \Delta t \ldots 1000\Delta t$. Plot the results as a function of b-factor, and include the theoretical curve corresponding to free diffusion. Explain your observations.
8. Diffusion diffraction: Finally, plot the signal as a function of $q = 0\ldots0.3\,\mu m^{-1}$ and for a fixed time corresponding to $t = 10ms$. You should see zero crossings, which you may try to explain.

Please remember plot titles, legends and axis labels, and units where applicable.

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