8.3 Random walk

As already emphasized by the phrase "random walk" the motion (in space) does not have a certain preferential direction, e.g. it is not driven into a "downhill" direction. Random walk thus directly implies that no change in energy is related with any parameter value (i.e. position) change. Thus according to the Metropolis algorithm any random position change will be accepted with the probability 1. In addition random walk is typically applied for simulating classical particles which of course do not interact (since this would imply energy contribution related to the motion). Thus the order for testing value changes of all parameter can be chosen arbitrarily; typically just a simple "for"-loop is used to change randomly all positions of the particles. Step size Δs and time step Δt in each iteration loop can be translated by some renormalization. Most often a diffusion constant $D = g\ a^2\ r$ (g lattice dependent geometry factor, a lattice constant, r jump rate) is used to translate the simulation into a real world scenario which is described by the standard (1D)-diffusion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + sources - drains \tag{8.2}$$

We will see that boundary condition, sources, and drains can often be included into the Mont-Carlo-simulation much more conveniently as into the mathematical solution of the above differential equation.
Often at least parts or special cases of the solution of the diffusion equation can be compared to some simple standard solutions. E.g. the solution for the finite source is

$$c(x,t) = \frac{c_0}{2\sqrt{Dt}} \exp\left(-\frac{(x-x_0)^2}{4\,D\,t}\right) \quad , \tag{8.3}$$

and the solution for the infinite source is

$$c(x,t) = c_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{D\,t}}\right) \quad ; \tag{8.4}$$

here erfc is the complement of the error function, i.e

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) \quad . \tag{8.5}$$