

Code description:

The `computeDiffusionCurrent` program defines a 2D periodic cylindrical system of size L connected to two reservoirs with densities equal to $\lambda_l = \lambda$ and $\lambda_r = \lambda + \varepsilon$. The particle density of the system is set at $\rho(\lambda)$ (which is determined by the `getParticleDensity` function) and the diffusion current N is initialized at 0.

While the macroscopic time t is lower than the final time t_{max} , the system undergoes particle jumps. If a particle jumps from a site at section $x = L/2 - 1$ to its right neighbor, then N increases. If a particle jumps from a site at section $x = L/2$ to its left neighbor, then N decreases.

The results are saved in the `diffusion_current_lambda0xx.txt` file ('xx' corresponding to the reservoir density λ). The user-defined parameter `n_points` determines the number of data points recorded.

Input parameters:

Parameter	Variable name	Data type
Save folder	<code>save_folder</code>	string
System size L	<code>L</code>	integer
Reservoir density λ	<code>lambda</code>	double
Reservoir density increment ε	<code>epsilon</code>	double
Final time t_{max}	<code>t_max</code>	double
Number of data points	<code>n_points</code>	integer

Post process:

The `post_process.py` script retrieves all the values from the files `diffusion_current_lambda0xx.txt`. It then plots the diffusion current N as a function of the macroscopic time t .