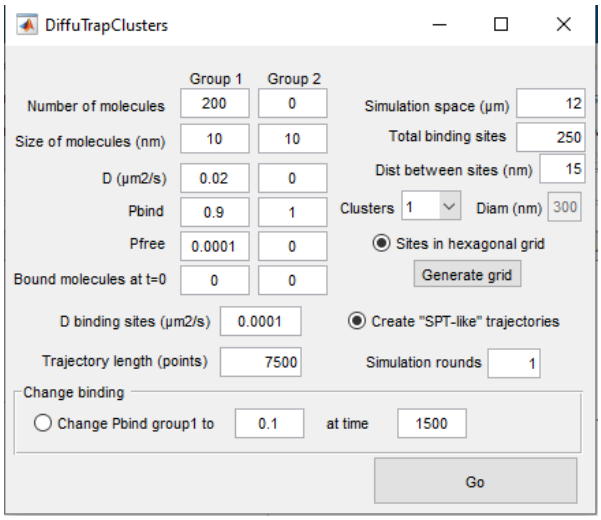
DiffuTrapClusters.m

« Graphic User Interface » (GUI) to simulate diffusion and trapping in 2D (beta version).

More information in: Kokolaki, Fauquier and Renner (2020), "The good and the bad of molecular crowding for the diffusion-capture of molecules in synapses". Manuscript under revision.

Please do not hesitate to contact marianne.renner@sorbonne-universite.fr to report bugs, for more detailed instructions or to suggest modifications. Thank you!



Basic settings

1) Simulated molecules

Group 1 and Group 2 are the types of molecules simulated. This allows for example to simulate a receptor and obstacles to diffusion. Group 2 is optional.

Number of molecules: number of simulated molecules for each group.
D (µm2/s): diffusion coefficient.
Size of molecules (nm): diameter of the simulated molecules.
Pbind: probability of to bind to a site.
Pfree: probability to unbind.
Bound molecules at t=0: number of molecules already immobilized at t=0 (for example, obstacles present at t=0).
D binding sites (µm2/s): diffusion coefficient of scaffolding sites.

2) Simulation

Trajectory length: length of trajectories in "points" (each point represents one x,y coordinate in the space).
Simulation rounds: Number of simulations made with the same parameters (repetitions).
Create "SPT-like" trajectories: Records trajectories with characteristics similar to those obtained with the SPT (single particle tracking) technique (sampling frequency, the pixel size and the localization precision of the experiment to be simulated).

3) Simulation space and binding sites

Simulation space (µm): size of the simulation space (side of the square).
Total binding sites: total number of binding sites.
Dist between sites (nm): distance between binding sites (minimum distance if the hexagonal distribution is not used).
Clusters: Number of clusters of sites (1, 2, 4 or 7). The number of binding sites is equivalently sorted between the clusters.
Diam (nm): diameter of the synapse (calculated from the number of sites chosen in case of the hexagonal grid).

Sites in hexagonal grid: the position of scaffolding sites is randomly chosen from a hexagonal grid. If this option is not chosen, the distribution of sites is randomly distributed in a circle with a diameter Diam. In this case, the distance between sites corresponds to the minimum distance between sites. The distribution on hexagonal mesh is done using a .txt file (datahexgrid...). This file can be created with **Generate grid**.

Generate grid: please set the desired diameter and distance between sites. Please note that to simulate a synapse with several clusters, the grid represents only one cluster. You must create one different grid for each configuration. Grid can be generated only once. The size of the grid must have the size taken into account by the code distributing the clusters in the same. Please check or modify this sizes in the code synnanohexamask2.m if the clusters overlap.

4) Interaction modification

This possibility makes it possible to simulate a change in affinity of the molecule-scaffold site interaction, for example, during synaptic plasticity.

Change Pbind group 1 to... at time point... : Choice to change the probability of interaction between group 1 molecules and the scaffold to the indicated value at the indicated time point.

5) Running the simulations

Go : The simulation starts. If the choice " Create " SPT-like " trajectories " is active, the program will ask for the sampling frequency, the pixel size and the localization precision of the experiment to be simulated. The standard values for our laboratory are displayed by default.

A progress bar indicates the progress of the simulation. This bar disappears once the simulation is finished. It is possible to interrupt the simulation by closing the window of this bar (no data related to the current simulation is saved).

6) Results

They are stored in a "simsyn" folder. All files are named after the order number of the simulation:

- Reportsim- # simulation.txt" file: parameters used for the simulation, recorded in a readable way.
For example, with the parameters indicated in the window shown above:

- File "sim- # simulation -sites.tif": Image of the simulation space with synapse and scaffold sites.

- File " sim- # simulation -slots.txt: number of molecules bound to the sites at each time point (“frame”). To simplify the display, not all values are recorded but only 1 /75 (this corresponds to the typical SPT sampling rate). The file contains three columns:
    - column 1: time (frames)
    - column 2: bound molecules group 1
    - column 3: bound molecules group 2

To have a more precise counting of bound molecules, you can generate trajectories with higher sampling rate (up to 1ms between trajectory points). We aware that this will slow down considerably the process and that there could be memory issues depending on the computer that you use.

If the choice " Create " SPT-like " trajectories " is active, the trajectories will be saved in the “trc” folder. The files (.trc, one per group of molecules) contain:

- column 1: trajectory number
- column 2: time (frames)
- column 3: x
- column 4: D
- column 5 and 6: localization codes (with respect to the area with binding sites)
- column 7: group (1 or 2)