User Guide

1. Bin the experimental *P(r)*. The number of displacements in individual bins is saved as a column named "exp_pr_n". The experimental *P(r)* should not be normalized. The sum of experimental *P(r)* will provide us the total number of displacements in the experimental *P(r)*. The corresponding x_axis (minimum displacement: bin size: maximum displacement) is saved as "x_ax".

2. Generate trajectories of desired length for a range of slow Diffusion coefficients using 'generate_trajectories.m'. The generated mat files are saved in a folder of your choice. Let's call it "Slow_D".

3. Similarly, generate trajectories of desired length for a range of fast Diffusion coefficients using 'generate_trajectories.m'. The generated mat files are saved in a folder of your choice. Let's call it "Fast_D"

4. Add *P(r)* to the above generated mat files using 'addprtofile.m'. The minimum and maximum displacement along with the binnings has to be equal to that chosen in Step 1. This is done to ensure that both experimental and simulated *P(r)* have same number of bins. The P(r) added to the mat files are normalized so that the area under the curve is 1.

5. Upload "exp_pr_n" and "x_ax" from Step 1 in the Workspace.

6. Run 'fit_pr.m', upon which you will be prompted to select the mat files containing slow trajectories in the folder named "Slow_D" and fast trajectories in the folder named "Fast_D" respectively. Please make sure that the slow mat files are selected first followed by the fast mat files.

7. The number of bins used for fitting by 'fit_pr.m' has to be chosen carefully so that no empty bins in experimental *P(r)* are included. To be safe, do not include bins with counts <5.

Test Run:

The zipped file "Test Run" contains "exp_pr_n.mat", "x_axis.mat", and folders : Slow_D and Fast_D. Unzip the file and load "exp_pr_n.mat" and "x_axis.mat" into the Workspace. Run 'fit_pr.m' and choose mat files containing slow trajectories in the folder named "Slow_D" and fast trajectories in the folder named "Fast_D" respectively.

Notes:

For a smooth simulated *P(r)*, number of simulated trajectories must be significantly higher than acquired experimental trajectories. The length of individual simulated trajectories must be same as experimental trajectories.