User Guide For SPICER

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Introduction

SPICER is an algorithm to eliminate confinement error in single particle tracking (SPT). In this guide, you will learn how to apply SPICER to simulated SPT data and how to interpret the results.

Applying SPICER to Simulated Data

1. Once you have downloaded the appropriate files for SPICER, you should open up the latest version of Matlab and proceed to the directory where the SPICER files are stored. These files include a large sample dataset, 'syntheticData.mat', which we will be analyzing in this section.

The 4 parameters of this simulated data are $D_1 = 1$, $D_2 = .7$, $P_{12} = P_{21} = .0244$.

2. To begin, open up the script 'SPICER.m', this file contains lots of information in the form of comments to help you understand every function taking place. All of the values of the different parameters are set for you, except one, but it is a good idea to look through the different variables to get a sense of what's going on.

The two pieces of information that will influence the amount of time the algorithm will take to finish is the number of trajectories and the number of steps used during the MCMC phase space search. In the actual manuscript the number of steps, 'numofsteps', was 25000, which takes a considerable amount of time. (1 day)

IMPORTANT: For this run through you will set the number of steps to 5000 as this will allow you to analyze the results in a more timely fashion.

If you have multiple cores, you should modify your preferred number of workers to 3, as SPICER runs in parallel.

3. Hit Run for 'SPICER.m', you will then select the data you will be analyzing. Click on the data 'syntheticData.mat' and wait for SPICER to

get going.

SPICER will update you on its progress throughout the analysis. (As long as you have at least three cores running) If you set the number of steps to 5000 and you have at least three cores, the analysis should take no longer than 60 minutes and will save the data to 'AnalyzedDataShort.mat'.

The results of the parameter scan are stored in the variable 'scanner' with the three different conditions stored in the three different cells. The first four rows of these cells pertain to the four parameters being maximized; the fifth row is the log of the likelihood at each step of the MCMC scan.

4. To look at the results of the analysis there is a script called 'MakeFigureForGuide.m', hit run. This script will make a bar plot showing the percent error for each of the parameters with the different types of analysis.

IMPORTANT: It should be noted that the lower the number of steps the less likely you can adequately sample the phase space. To look at the results of an analysis with a larger number of steps load the data stored in 'PreAnalyzedData/Analyzeddata.mat.' Or if you want to look at the results of multiple repeats of a 5000 step scan load the data in 'AnalyzeddataShort5Repeats.mat'.

Congratulations, you have successfully applied SPICER to a data set!

Notes:

modfinaltraj.m: This function modifies the trajectories based off of the location of the molecule inside of the cell and the R-value provided. If the molecule is outside of the confinement zone defined by the R-value, it will not modify the data, if the molecule is inside of the confinement zone the function will eliminate the displacements along the short axises of the cell and only keep the displacement along the long axis of the cell.

MCMC.m: Performs the parameter scan to maximize the likelihood, see manuscript for details.