

### 3D stochastic process simulation for better interpretation of molecular dynamics related to cell wall biogenesis observed with TIRF microscopy

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The mechanism of the construction of cell wall is an essential subject for the biologists. With the recent development of super-resolution fluorescence microscopy, we can have better inspection into the role of some key proteins and their interactions in live cells during the cell wall extension. Knowing that MreB is one of the key proteins responsible for cell wall construction, we aim to analyze the dynamics of MreB in rod-shaped bacteria *Bacillus*.

Previous work concerning the dynamics of MreB started from the classification of the trajectories<sup>[1]</sup>, constructed by single particle tracking (SPT). Trajectories are classified into three categories, directed motion, Brownian motion and confined motion. The images used are acquired by TIRFM which records only the events near the observation plan. So the images obtained are actually the projection of the dynamics on the cell membrane near the observation plan. The classification is simply done with 2D images ignoring the curvature of the rod-shaped cell wall and the thickness of TIRFM plan. To evaluate the effect of these approximations, we have developed a simulator to generate the trajectories on the surface of the cylinder. The processes for simulating the three kinds of motion mentioned above are Brownian with drift, Brownian motion and Uhlenbeck-Ornstein process<sup>[2]</sup>.

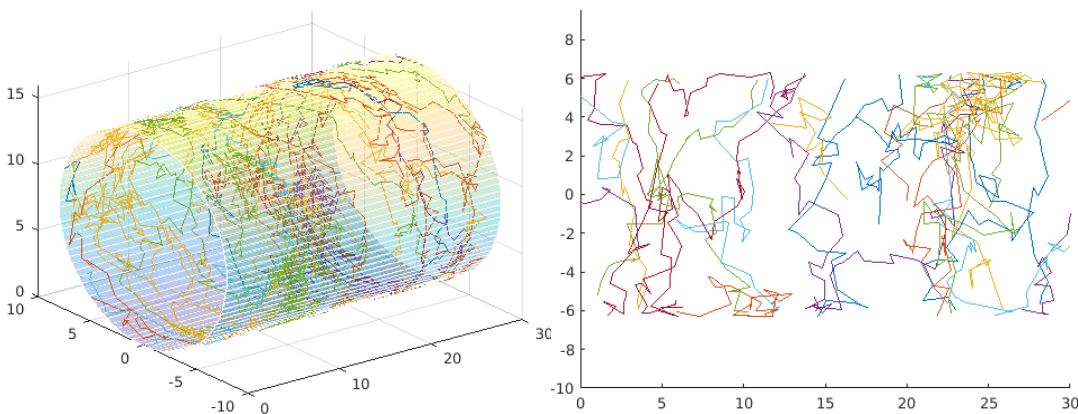


Figure 1 trajectories generated on the surface of the cylinder (left) and the view of TIRF microscope (right) which is the projection of the dynamics on the cylinder near the support surface. The unity in the two figures is in pixel and in our TIRF images 1pixel  $\approx$  64 nm. As the theoretical thickness of TIRF is 200nm, the trajectories whose z coordinate is under 3.125 pixels are projected into x-y plan. Colors for different trajectories are random.

Currently our work concerns spatial distribution exploration. For particles doing directed motion, we are interested in exploring its spatial distribution and the number of times a particle circles the cell wall before disappearing from the TIRF observation field. Furthermore, we model motions by Langevin Stochastic Equation  $\dot{\mathbf{X}} = \mathbf{b}(\mathbf{X}) + \sigma(\mathbf{X})\dot{\mathbf{w}}$ , and thereafter the velocity field and diffusion field are calculated using local information in each point. We aim to reconstruct the dynamics on the surface of the cylinder for the part that can't be seen by the microscope.

[1] Billaudeau C. et al. *Nature Communication* (2017) [2] Briane V. et al. *Phys. Rev.* (2018)