

Tethered Cargo Motion (TCM) Monte Carlo simulation software in
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Probing Mitotic CENP-E Kinesin with the Tethered Cargo Motion Assay and Laser Tweezers

Nikita Gudimchuk,^{1,2,3} Ekaterina V. Tarasovets,¹ Vadim Mustyatsa,⁴ Alexei L. Drobyshev,³ Benjamin Vitre,⁵ Don W. Cleveland,⁵ Fazly I. Ataullakhanov,^{2,3,4,*} and Ekaterina L. Grishchuk^{1,*}

¹Department of Physiology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania; ²Department of Physics, Moscow State University, Moscow, Russia; ³Center for Theoretical Problems of Physicochemical Pharmacology, Russian Academy of Sciences, Moscow, Russia; ⁴Dmitry Rogachev National Research Centre of Pediatric Hematology, Oncology and Immunology, Moscow, Russia; and ⁵Ludwig Institute for Cancer Research and Department of Cellular and Molecular Medicine, University of California, San Diego, La Jolla, California

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1. Introduction.

The downloaded folder contains 4 MATLAB (The MathWorks, Inc., Natick, MA, USA) files. They carry out two independent functions:

- *TCM_initialization.m*
- *sigma_2_PL.m*

The remaining two functions - *TCM_sampler.m* and *chain_generator_TCM.m* - are sub-functions of *TCM_initialization.m* and are not configured to be used independently.

TCM_initialization.m is the main initialization script for the TCM modeling. It contains a list of all model parameters with their values and brief explanations. Values can be modified directly to simulate different tethers.

Running *TCM_initialization.m* will cause MATLAB to perform TCM modeling specified by the parameters values and save the results. Further explanation of the inputs and outputs can be found below and within the *TCM_initialization.m* script itself. Note that *sigma_2_PL.m* function is used in conjunction with *TCM_initialization.m*. It is required to calculate the value of sigma that should be used in *TCM_initialization.m* for a desired value of PL.

2. Input parameters used in *TCM_initialization.m*

results_folder — is used to save outputs. Default value (pwd) uses your CURRENT MatLab working folder. If you keep re-using the same folder for multiple simulations with the same parameters, new results will be ADDED to your pre-existing files and will not OVERWRITE them.

L — Length of tether you will simulate in nm.

Rbead — Radius of bead at the end of the tether in nm.

sigma — Value that dictates persistence length (PL) of your tether.

Default values:

0.115 for PL of 150

0.205 for PL of 46

0.28 for PL of 26

If you want to simulate a different PL, use *sigma_2_PL(sigma)* function to evaluate what PL will your chosen sigma correspond to (PL will be given in nm when this function is used).

sigma1 — parameter of the flexibility for the chain-MT linkage, default is 0.0

sigma2 — parameter of the flexibility for the chain-bead linkage, default is 0.3

K — total number of different chains configurations to create for EACH angle.

tether_thickness — This value is used to simulate chain self-avoidance. Default is 0 nm. Individual segments are prohibited to approach each other closer than this value in nm (excluding consecutive segments, which are by necessity always 2 nm apart).

A set of alpha angles (IN DEGREES) for each of which K different chains configurations will be created.

Dcoat — This value used for simplified DNA coat thickness modeling. Default is 0 nm.

During execution of this program, MatLab will display total number of different chains configurations already successfully created. Program will end once $K*5$ configurations (K configurations for each of 5 angles) are created. Even if your set of parameters generates few (or even no) acceptable chain configuration for a given angle, the program will keep trying to find the desired number of acceptable configuration. If this takes excessively long time, the program can be manually terminated.

3. Output files used in *TCM_initialization.m* :

After the program has finished executing (manually or automatically), the following files will be in the appropriate directory:

chain_coords.txt is a 2D array containing ALL coordinates of ALL individual segments of ALL individual chains created. Every line is X Y Z coordinates of one segment. After all segments of one configuration are listed, next line will be a first segment of the next configuration.

bead_coords.txt is a 2D array containing coordinates of the center of the bead for each configuration. Every line is X Y Z coordinates of one segment. After each K configurations, next K configurations correspond to the next angle of attachment.

angle_sampling_eff.txt contains probabilities of attachment (sampling efficiency, ratio of accepted configuration to total sampled configurations) for each angle. After program has completed all 5 angle, the last line (line #15) contains 5 values of normalized (sum = 1) probabilities of attachment for the 5 angles sampled. Line #14 contains 5 values of raw (sum \neq 1) probabilities of attachment for the 5 angles sampled. Line # 13 contains absolute number of configurations sampled before K values was accepted for all 5 angles sampled. Line 1-3, 4-6, 7-9 and 10-12 contain similar preliminary values recorded after sampling of one of the angles has been finished.

Important: all coordinates are given in coordinate system associated with the motor, with X=0, Y=0, Z=0 being the point on the coverslip right under the motor head (start of the first segment of the chain). X is direction along microtubule, Y is direction perpendicular to MT along coverslip, Z is direction perpendicular to both MT and coverslip.

4. Contact and Support

We aim to make this set of TCM modeling functions convenient and easy to use for all your TCM modeling needs. If there are any questions, comments or suggestions, you can contact us directly via email vadimmustyatsa@gmail.com.