CellDynaMo

User Manual

(draft)

Version 1.0.0

Contributions from

Artem Zhmurov, Kenneth A. Marx, Alex Mogilner

Evgenii Kliuchnikov, Valeri Barsegov

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Download **master-CellDynaMo** from

https://github.com/eukliuchnikov/CellDynaMo/tree/main/v1.6.23

By default **master-CellDynaMo** is configured for simulations with a single KT pair. Before compiling the code open **Makefile** file with any text editor (manually or from terminal). Change the path to your *Cuda* directory if necessary. From the main directory (**master-CellDynaMo** by default) run

```
$ make
```

and the executable file **cell** will be created in the **master-CellDynaMo** directory.

1.3 Working directory

For a single run a directory should be prepared. This directory must contain **config** and **output** folders. In turn, **output** directory must contatin **dat** and **dcd** folders. **config** should contain configuration-files with simulation parameter.

1.3.1 Parameters

The examples of configurations-files are given. One could use them and change the values of parameters.

conf.conf - is the configuration-file responsible for the essential parameters of the simulation, such as the shape of the cell and the number of chromosomes, or technical parameters, such as GPU id, random seed, etc.

- **device** - parameter that indicates GPU id (depends on the number of GPUs available). *Example: 0*
- **rseed** - any integer number, should be different for different trajectories. *Example: 21587*
- **traj_name** - name that all output files will contain. *Example: cell*
- **total_t** - total biological time (s). *Example: 3600*
- **dt_accuracy** - kinetic time step is calculated as the time of the fastest event (reaction or diffusion). This parameter is the number the kinetic time step is devided by. *Example: 10.0*

- **kin_count** - amount of kinetochores in the model (double the amount of chromosomes). *Example: 2*
- **chrom_arms** - condition of chromosome arms presence or absence. Values: yes/no. *Example: yes*
- **armor** - condition of armor around KT pairs presence or absence. Values: yes/no. *Example: no*
- **contour_length** - contour length of a single chromatid (nm): *Example: 6000*

  If initial positions and orientations are given manually, then
- **kinetochore1_move_x** - x-coordinate of CoM of chromosome (nm). *Example: -200.0*
- **kinetochore1_move_y** - y-coordinate of CoM of chromosome (nm). *Example: -1500.0*
- **kinetochore1_move_z** - z-coordinate of CoM of chromosome (nm). *Example: 0.0*
- **x1_angle** - angle of rotation around the x-axis (radian). *Example: 0.0*
- **y1_angle** - angle of rotation around the x-axis (radian). *Example: -0.7*
- **z1_angle** - angle of rotation around the x-axis (radian). *Example: 1.57*

  If there are more then one chromosomes, then extra parameters should be given, such as **kinetochore2_move_x**, ..., **x2_angle**, ..., **kinetochore3_move_x**, ..., **x3_angle**, ...
- **outputpsf** - path and the name of the output topology (psf) file. *Recommended - output/dcd/<traj_name>.psf*
- **outputdcd** - path and the name of the output trajectory (dcd) file. *Recommended - output/dcd/<traj_name>.dcd*
- **output_membrane_psf** - path and the name of the membrane topology file. *Recommended - output/dcd/<traj_name>_membrane.psf*
- **output_membrane_xyz** - path and the name of the membrane coordinates file (static). *Recommended - output/dcd/<traj_name>_membrane.xyz*
- **dcd_freq** - period of saving coordinates in trajectory file (s). File will be updated every *<value>* s of biological time. *Example: 1.0*
- **membrane_shape** - parameter that determines the shape of the cell membrane. Values: sphere/ellipsoid/cube/cuboid. *Example: elipsoid*
- **auroraA** - condition of Aurora A presence or absence. Values: yes/no. *Example: yes*

  Some other parameters, such as **random_place**, **chrom_territory**, **ring** and **ring_radius** are not available in this version.

param.conf - is the configuration-file that includes topology parameters

- **sv_size** - parameter that determines the size of sub-cells. *Example: 250.0*
- **ellipse_a** - parameter that determines semi-major axis of ellipsoid. *Example: 8000.0*
- **ellipse_b** - parameter that determines the first semi-minor axis of ellipsoid. *Example: 5000.0*
- **ellipse_c** - parameter that determines the second semi-minor axis of ellipsoid. *Example: 5000.0*
- **pole_distance** - parameter that determines the distance between centrosomes. *Example: 5000.0*
- **pole_radius** - parameter that determines the radius of centrosomes. *Example: 400.0*
- **pole_count** - parameter that determines the number of centrosomes. *Example: 2* - DO NOT CHANGE (only works with 2)
- **mt_num** - parameter that determines the number of microtubules per centrosome. *Example: 750*
- **max_mt_length** - parameter that determines the number of beads in microtubule. *Example: 3 - the only option in this version*
- **start_length** - parameter that determines the highest initial microtubule's length (in nm). *Example: 180*
- **mt_radius** - parameter that determines the radius of microtubule cylinder. *Example: 750*
- **kin_shape** - parameter that determines the shape of outer kinetochore surface. *Example: rect = reactangular (the only option)*
- **kin_radius** - parameter that determines the radius of kinetochores and chromosome arms (in nm). *Example: 362.5*
- **beta** - parameter that determines the curvature of the outer kinetochore surface (from 0 (cover the KT surface) to 1 (flat)). *Example: 0.5*
- **corona_S** - parameter that determines the surface area of the outer kinetochore (in nm^2).*Example: 500000*
- **corona_X_N** - parameter that determines the number of beads in rectangular kinetochore surface (X-direction). *Example: 32*
- **corona_XY_ratio** - parameter that determines the ratio: number of beads in rectangular kinetochore surface (X-direction to Y-direction). *Example: 1.3*
- **distance_ndc** - parameter that determines the dencity of Ndc80 on the surface of th kinetochore (in nm). *Example: 8.0*
- **maxHarmonicKinPerMonomer** - change only if **distance_ndc** was changed). *Example: 1000*
- **ndc_length** - parameter that determines the length of the Ndc80 (harmonic string; in nm). *Example: 65.0*
- **ndc_per_mt** - parameter that determines the number of Ndc80 capable to attach to a single microtubule. *Example: 1 - the only option in this version*

force.conf - is the configuration-file that includes parameters for Langevin Dynamics.

- **lang_ts** - parameter that determines the timestep in Langevin Dynamics. *Example: 50.0*
- **mt_persist_length** - parameter that determines the persistence length of the microtubule (in nm). *Example: 1.5e6*
- **k_spring_mt** - parameter that determines the stretching stiffness between two microtubule beads (in kJ/mol nm^2).*Example: 10*
- **k_spring_kt** - parameter that determines the stretching stiffness between kinetochore and chromosome beads (in kJ/mol nm^2).*Example: 10*
- **k_stiff_mem** - parameter that determines the strength of repulsion from membrane (in kJ/mol nm^2).*Example: 1000*
- **f_pish** - parameter that determines the average pushing force (in pN). *Example: 10.0*
- **f_pill** - parameter that determines the average pulling force (in pN). *Example: 10.0*
- **temp** - parameter that determines the temperature of the system (in K). *Example: 300*
- **viscosity** - parameter that determines the viscosity of solution inside the cell (in g/mol nm ps). *Example: 600 - default water viscosity*

chemistry.conf - is the configuration-file that includes parameters for reaction-diffusion module.

- **aurora_diff** - parameter that determines the diffusion constant for Aurora A and B (in $nm\hat{2}/s$). *Example: 7.3e7*
- **k_phos** - parameter that determines the dephosphorylation rate constant (in 1/s). *Example: 3.0*
- **k_attach** - parameter that determines the MT-Ndc80 attachment rate constant (in $1/\mu Ms$).*Example: 38000.0*
- **k_detach_0** - parameter that determines the detachment rate constant of Ndc80 with 0 phosphorylated sites from microtubule (in 1/s). *Example: 0.29*
- **k_detach_1** - parameter that determines the detachment rate constant of Ndc80 with 1 phosphorylated site from microtubule (in 1/s). *Example: 0.25*
- **k_detach_2** - parameter that determines the detachment rate constant of Ndc80 with 2 phosphorylated sites from microtubule (in 1/s). *Example: 0.21*
- **k_detach_3** - parameter that determines the detachment rate constant of Ndc80 with 3 phosphorylated sites from microtubule (in 1/s). *Example: 0.17*
- **k_detach_4** - parameter that determines the detachment rate constant of Ndc80 with 4 phosphorylated sites from microtubule (in 1/s). *Example: 0.13*
- **k_detach_5** - parameter that determines the detachment rate constant of Ndc80 with 5 phosphorylated sites from microtubule (in 1/s). *Example: 0.09*

- **k_detach_6** - parameter that determines the detachment rate constant of Ndc80 with 6 phosphorylated sites from microtubule (in 1/s). *Example: 0.05*
- **k_detach_7** - parameter that determines the detachment rate constant of Ndc80 with 7 phosphorylated sites from microtubule (in 1/s). *Example: 0.01*
- **k_growth** - parameter that determines the rate constant for microtubules growth by 24 nm (in 1/s). *Example: 8.9*
- **k_growth** - parameter that determines the rate constant for microtubules shrink by 24 nm (in 1/s). *Example: 9.8*
- **k_catastrophe** - parameter that determines the frequency of catastrophes (in 1/s). *Example: 0.116*
- **k_rescue** - parameter that determines the frequency of rescues (in 1/s). *Example: 0.045*

  Parameters **aurora_concentration**, **phosphatase_concentration**, **tubulin_concentration** do not work in this version.

1.3.2 Executable file

Place compiled **cell** file in your working directory, or specify the path to it in the command line

2 Production

2.0.1 Run the code

From your working directory:

```
$ ./cell > log &
```

The output will be saved in the **log** file, as well as coordinates will be saved in the /output/dcd/ folder, and data with implicit components will be placed in the /output/dat/ folder.

2.0.2 Visualization

Visualize your trajectory using any suitable softaware: (**VMD**, **PyMOL**, etc.).