corticalSim user manual

This document describes the input commands and data formats produced by *corticalSim*, the plant microtubule cortical array simulation tool created by Simon Tindemans and Eva Deinum.

If you use CorticalSim in publications, please include a citation to:
[for general use] http://dx.doi.org/10.3389/fphy.2014.00019
[for microtubule dependent nucleation] http://dx.doi.org/10.1088/1478-3975/8/5/056002
[for microtubule severing] http://dx.doi.org/10.1073/pnas.1702650114

Document revision history

1 June 2017	Initial public release

Running the program

The program should be executed with a single command line parameter that specifies the location of a text file with simulation parameters.

On Linux and OS X / macOS:

```
corticalSim.release [parameter file]
```

On windows:

```
corticalSim [parameter file]
```

Simulation parameters

The parameter file is a text file with single-line command-value pairs. See `exampleParameterFile.txt` for an example. The commands are separated from the values by white space. Comments can be inserted on lines starting with #. Also, additional input at the end of a line (after the value) is disregarded and can be used for comments. All lengths are expressed in micrometers and times in seconds.

Immutable parameters

The following parameters can only be set at the start of the simulation. This is in contrast with the other parameters that can be adjusted on the fly using the 'newParameterFile' command.

geometry	[type] [options] default: "periodic 80 80"	Specifies the system geometry. Possible types are discussed below.
geometry periodic	[width] [height] Note: 3 parameters are required but the 3rd is disregarded.	Simple rectangular system with periodic boundary conditions.
geometry grid	[width] [height] [x-number]	Rectangular system with periodic boundary conditions. For computational efficiency, the field is divided into a number of approximately square sub-fields. The x-number specifies the number of patches along the x-direction (width). For maximum performance, make the sub-fields of the order l_0 (see theory).
geometry wormhole	[width] [height] Note: a 3rd parameter is required, but disregarded	2D rectangular system that approximates a cylinder. Periodic boundary conditions are used on the top and bottom, and a 'spherocylindrical tunnel' (see also Eren et al., 2010) is used on the left and right boundaries.
geometry pancake	[radius] Note: 2nd and 3rd parameters are required, but disregarded	2D disc system. If a microtubule reaches the edge, it continues growing in the same direction on a diametrically opposite position.
geometry cylinder	[length] [radius] Note: a 3rd parameter is required, but disregarded	Basic cylinder with flat end caps. Oriented in the x-direction. Microtubule behaviour on the end caps is modified by the 'forbiddenZones' or 'catastropheMultiplier' commands.
geometry gridcylinder	[length] [radius] [l-number]	Cylinder with flat end caps. For computational efficiency, the main body of the cylinder is divided into a number of approximately square (when unrolled) sub-fields. The l-number specifies the number of patches along the lengh direction.

		Microtubule behaviour on the end caps is modified by the 'forbiddenZones' or 'catastropheMultiplier' commands.
geometry box	[x-size] [y-size] [z-size]	3D box. Microtubule behaviour on the end caps is modified by the 'forbiddenZones' or 'catastropheMultiplier' commands.
geometry spherocylinder	NOT IMPLEMENTED	
geometry sphere	NOT IMPLEMENTED	
random_seed	long integer	By default, the random seed is initialized with the current time. Initializing it to a specific value is useful for 'replaying' simulations or ensuring variability in parallel computations.
discreteAngleNumber	>= 0 (int)	If non-zero, this is the number of absolute orientations that microtubules are nucleated in (discrete angle simulations). Take note of interactions with boundary conditions potentially introducing new angles.

Simulation control

stopTime	>0 default: 36000	Simulation time after which the simulation ends.
outputDir	[valid directory name] default: "." (current directory)	Specifies the location of the output files. Can be a relative or absolute path. The directory should exist. NOTE: paths should NOT contain spaces.
createSubdir	0,1 default: 1	Specifies whether the files should be stored in an automatically created subdirectory with the timestamp name: YYMMDD-HHMMSS
newParameterReadFile	[filename]	Specifies a parameter file to be loaded after 'newParameterReadInterval'
newParameterReadInterval	>0 default: VERY_LARGE (no reload)	The simulation interval after which the parameter file from 'newParameterReadInterval' should be loaded.
densityLimit	>0 [/μm] default: VERY_LARGE	Density limit that triggers an immediate stop of the simulation. This is useful to prevent runaway simulation times due to diverging densities.
wallClockLimit	>0 [seconds] default: VERY_LARGE	Wall clock time after which the simulation should be aborted. This allows you to save the data before the process gets killed in a cluster environment.

memoryLimit	>0 [MB] default: VERY_LARGE	An APPROXIMATE limit on the memory that may be used by the program, in Megabytes. Useful in a cluster environment, to avoid excessive swapping. Set the threshold conservatively, as the measured values are underestimating actual memory usage.

Dynamic instability parameters

vPlus	>0 default: 0.08	plus end growth speed
vMin	<0 default: -0.16	plus end shrinkage speed: should be negative
vTM	>0 default: 0.01	minus end speed
treadmillingEnabled	0,1 default: 1	switch to enable/disable treadmilling (overrides vTM=0)
kCat	>=0 default: 0.005	spontaneous catastrophe rate
forbiddenZones	0,1 default: 0	If enabled, microtubules are not allowed on the end caps of cylinders or the top and bottom of box geometries. **Note**: these surfaces are still used for density calculations. Nucleation events on these surfaces are discarded.
catastropheMultiplier	>=1 default: 1	The spontaneous catastrophe rate on cylinder end caps and the top/bottom of box geometries is multiplied by this factor.
edgeCatastropheEnabled	0,1 default: 0	If enabled, there is a probability for a catastrophe associated to crossing edges. Edges that do not affect orientation at all (such as internal edges in gridcylinder systems) are excluded.
edgeCatastropheSmooth	0,1 default: 0	If enabled, the edge catastrophe probability is a smooth function of the 3D bending angle: pCat*sin(angle)^2
pCatRegularEdge	[0,1]	Edge catastrophe probability for a 90-degree turn between two regions of the same type (body, endcap)
pCatSpecialEdge	[0,1]	Edge catastrophe probability for a 90-degree turn between body and endcap regions
kRes	>=0 default: 0.007	rescue rate
kSev	>=0 default: 0.001	uniform severing rate
severingEnabled	0,1	switch to enable/disable uniform severing

	default: 0	

Nucleation parameters

kNuc	>0 default: 0.001	Nucleation rate per square micrometer per second
nucleationType	"isotropic", "biased", "discreteAngles", "chanLloyd", "chanLloydRandomPosition", "chanLloydIsotropic", "ellipse" default: isotropic	*isotropic* nucleates at random locations in random directions. *biased* nucleates preferentially in the diagonal direction, tuned by 'nucleationAlpha'. On special surfaces (cylinder caps and top/bottom of box geometry), nucleation remains isotropic. *discreteAngles* nucleates in discrete directions only. *chanLloyd* uses CL nucleation for a density-dependent fraction of events. DEPRECATED from v1.18 *chanLloydRandomPosition* randomizes the location of these nucleation events. DEPRECATED from v1.18 *chanLloydIsotropic* randomizes the orientation of the CL nucleation events. DEPRECATED from v1.18 *ellipse* uses CL nucleation as described in Deinum et al 2011 (submitted to physical biology)
nucleationAlpha	>0 default: 0	For the *biased* nucleation mode, provides an increasingly peaked distribution [see Bela's notes] Also works for the fraction of free nucleations of the *ellipse* nucleation mode
nucleationAngles	>0 (int) default: 0	For the *discreteAngles* nucleation mode, the number of discrete angles to use.
nucleationHalfIsotropicDensity	>0 default: 1	For *ellipse* nucleation, the density at which half the nucleation events is MT-related.
chanLloydForwardFraction	[0,1] default: 0.4	DEPRECATED (*chanLloyd* etc)
chanLloydBackwardFraction	[0,1] default: 0.05	DEPRECATED (*chanLloyd* etc)
chanLloydSidewaysAngle	[0,90] default: 35	DEPRECATED (*chanLloyd* etc)
chanLloydWidthToAverageAngle	default: 30	DEPRECATED (*chanLloyd* etc)

ellipseEpsilon	0 <= eE < 1 default: 0	For *ellipse* nucleation. Eccentricity of the ellipse used (0 = uniform angles, 1 = single angle (delta peak)
ellipseForwardAlongMT	[0,1] default: 0	For *ellipse* nucleation. Forward and backward nucleations will be exactly on the parent trajectory if 1 (true), otherwise an ellipse is used with eccentricity ellipseEpsilon
ellipseLeftFraction	default: 0	For *ellipse* nucleation, the fraction of MT-related sideways nucleation events with counter clockwise orientation relative to the +end of the parent
ellipseRightFraction	default: 0	For *ellipse* nucleation, the fraction of MT-related sideways nucleation events with clockwise orientation relative to the +end of the parent
ellipseBackwardFraction	default: 0	For *ellipse* nucleation, the fraction of MT-related nucleation events in the backward direction.
ellipseSidewaysAngle	[0,90] default: 40	For ellipse nucleation, the average relative angle of (left and right) sideways nucleations
ellipseReducedFreeRate	0,1 default: 0	Indicates whether the free (non-MT-bound) nucleation complexes have a lower nucleation success rate.
ellipseReducedFreeRateAcceptFraction	[0,1] default: 1	If ellipseReducedFreeRate is enabled, fraction of free nucleation attempts that is successful.
preSeededSeedDensity	>= 0 default: 0	Density per square micrometer of nucleation seeds that are present at t=0. Each seed only fires *once*. Unlike many other parameters, it is reset to zero on each parameter change, unless the new parameter file specifies a nonzero value.
preSeededRate	>0 default: 0	Nucleation rate (per second) of the *individual* nucleation seeds.
preSeededType	“isotropic”, “biased” default: “isotropic”	Nucleation type of pre-seeded nucleations. As in *nucleationType*
preSeededAlpha	>=0 default: 0	As *nucleationAlpha* for biased nucleation.

MT interaction parameters

interactionType	"zipFirst", "catFirst", "minimalFourier" default: zipFirst	For the *zipFirst* interaction type, only zippering or cross-over is permitted below the 'magicAngle'. The *catFirst* mode evaluates induced catastrophes first, and then assigns the remaining probability below 'magicAngle' to zippering. The *minimalFourier* mode uses the smooth interaction functions used in the PRE and PRL.
bundleType	"simple", "sticky", "noZip", "multiCollision", "Ncollision" default: simple	For the *simple* bundle type, bundles are treated as single microtubules for the collision process. With the *sticky* option, microtubules in a bundle do not collide at all. With the *noZip* option, they do not zipper, but can have catastrophic collisions. The *multiCollision* interaction mode approximates bundles by a dense 'net' of microtubules. The *Ncollision* interaction mode is meant for the weak interaction limit, and multiplies the zippering and catastrophe rates by the number of microtubules in the encountered bundle. When the resulting probabilities would exceed 1, they are scaled back so that P(zip)+P(cat)=1.
zipperingEnabled	0,1 default: 1	Switch to enable/disable zippering.
catastrophesEnabled	0,1 default: 1	Switch to enable/disable *induced* catastrophes. Not applicable to the *minimalFourier* mode.
proportionalCatastrophes	0,1 default: 0	For the zipFirst and *catFirst* modes. If enabled, the probability for induced catastrophes increases linearly with the angle from 'catStartAngle' to the final value (inducedCatastropheFraction) at 90 degrees.
inducedCatastropheFraction	[0,1] default: 0.5	Specifies the induced catastrophe probability for perpendicular collisions.
catStartAngle	[0,90] default: 0	For the *zipFirst* and *catFirst* modes, specifies the minimum angle for induced catastrophes.
zipFraction	0,1 default: 1	For the *zipFirst* interaction type, specifies the zippering probability below 'magicAngle'.
magicAngle	[0,90] default: 40	The maximum angle at which zippering can occur. For *zipFirst* and *catFirst*, no cross-overs occur below this angle if zippering is enabled.

c0Value	[0.75, 1.125] default: 0.75	For the *minimalFourier* interaction type. Shape modifier for the analytical induced catastrophe function, as introduced in the PRE theory paper.
z0Value	>0 default: 0.5	For the *minimalFourier* interaction type. Modifies the strength of the zippering interactions, as defined in the PRE theory paper.
kCross	>=0 default: 0.001	Intersection severing rate, per intersection of microtubules or bundles.
crossSeveringEnabled	0,1 default: 0	Switch to enable/disable severing at intersections
crossSeveringTop	0,1 default: 1	If enabled, an intersection severing event always cuts a microtubule from the bundle 'on top', i.e. the one that arrived later. If disabled, the top and bottom one are selected with 50% probability each. [LOOK UP: what happens when the lower bundle retreats and grows again?]
crossSeveringStartAngle	[0-90] default: 0	Intersections are only cut if the angle between the microtubules exceeds this number. Note that this is *not* taken into account in the severing rate, so the effective severing rate is decreased.

Measurement parameters

measurementInterval	>0 default: 100	The interval at which measurements of the system parameters are made.
movieEnabled	0,1 default: 0	Switch to enable/disable snapshot recording.
movieFrameInterval	>0 default: -1 (disabled)	Interval at which snapshots are saved.
angleHistogramBins	>=0 (int) default: 0	If larger than zero, the number of bins for the segment angle length histogram.
hiresLengthHistogramBins	>=0 (int) default: 0	If larger than zero, the number of bins for the microtubule length histogram. The range is automatically adjusted to fit the largest element.
hiresLifetimeHistogramBins	>=0 (int) default: 0	If larger than zero, the number of bins for the microtubule life time histogram. Life times are measured from nucleation until disappearance. The histogram range is automatically adjusted to fit the largest element.
loresAngleHistogramBins	>=0 (int) default: 0	If larger than zero, the number of angle bins for the 2D angle-length and angle-lifetime histograms.

loresLengthHistogramBins	>=0 (int) default: 0	If larger than zero, the number of length bins for the 2D angle-length histogram.
loresLifetimeHistogramBins	>=0 (int) default: 0	If larger than zero, the number of lifetime bins for the 2D angle-lifetime histogram.
histogramAverageSamples	>=1 (int) default: 1	The number of measurements that is used to construct a single histogram.

Output files

At the end of a run, a number of text files will have been created in the specified output directory. The contents of these files are described below.

parameters.txt

This file lists all (relevant) parameters given above, for a given simulation. It includes the random seed, so it can be used to re-run the exact same simulation (note that different compilers/settings can lead to different results). In addition, it lists the program code version as `corticalSim x.xx`

measurements.txt

This file contains a number of measurements of important system parameters. The first line consists of tab-delineated short names of the measured properties, and each subsequent line gives the corresponding values at a given time. The reported values are listed in order in the following table.

1	time	Measurement time
2	density	The average microtubule length density
3	<l>	The average microtubule length
4	S2	The S2 value
5	S2 angle	The associated angle in radians, in the range 0..pi
6	S4	The S4 value
7	S4 angle	The associated angle in radians, in the range 0..pi
8	#growing	Number of growing microtubules
9	#shrinking	Number of shrinking microtubules
10	#segments	Number of microtubule segments
11	#trajectories	Number of trajectories
12	zippering events	Cumulative total number of zippering events
13	crossover events	Cumulative total number of crossover events
14	induced catastrophe events	Cumulative total number of catastrophe events
15	valid deterministic events	Cumulative total number of deterministic events that were valid at the time of execution.
16	invalid deterministic events	Cumulative total number of deterministic events that were invalidated before their time of execution. If this number is large with respect to the previous number, the simulation runs inefficiently, and it may help to decrease the grid spacing.
17	stochastic events	Cumulative total number of stochastic events
18	optical density	Optical density, counting the
19	microtubules	Number of microtubules
20	segments per MT	Average number of segments per microtubules
21	random severing events	Cumulative total number of random severing events
22	intersection severing events	Cumulative total number of severing events at intersections
23	S2 opt	Optical S2 measure
24	S2 opt angle	Optical S2 angle

25	S4 opt	Optical S4 measure
26	S4 opt angle	Optical S4 angle
27	occupied intersections	Total number of intersections between microtubules or bundles. Determines the total intersection severing rate.
28	R	The R2 order parameter
29	R_x	The x-component of the normalized eigenvector corresponding to the R2 order parameter.
30	R_y	As above; the y-component
31	R_z	As above; the z-component
32	G_eff_adjusted normal	G' on regular surfaces
33	G_eff_adjusted special	G' on special surfaces. This differs from the regular value if 'catastropheMultiplier' is different from 1.

snapshots.txt

This file contains a series of snapshots that can be used as single images or converted into a movie. The snapshots consist of a series of one line drawing commands that need to be interpreted. For each frame, they occur in the order specified below.

time	[time]	Start of a frame. Specifies the simulation time of the snapshot
order	[R2] [eigenvector: x y z]	The magnitude and orientation of the R2 order vector. One per frame.
canvas	*various (see below)*	The canvas command, followed by the base command, specifies how the 2D coordinates of lines and points should be converted into 3D coordinates. A frame can contain any number of canvases.
canvas rectangle	[width] [height]	A rectangular base with Cartesian coordinates and the origin at its center.
canvas disc	[radius]	A disc with Cartesian coordinates and the origin at its center.
canvas cylinder	[length] [radius]	A cylindrical domain. The 'base' is located in the middle of the cylinder body. Positions are described using a Cartesian coordinate system with its origin such that the two basis vectors are tangent vectors. The 'seam' is located on the opposite side.
base	[center: x y z] [e1: x y z] [e2: x y z]	Follows a 'canvas' command and specifies its orientation in 3D space: the base, and the 3D direction of the two tangent vectors (basis vectors) at the origin.
p	[type] [u v]	Specifies a microtubule tip. Type 2 tips are growing, type 3 tips are shrinking.
l	[type] [base: u v] [angle] [length]	Specifies a section of a microtubule as a base, angle and length. The angle (in radians) is specified from the u-axis in the direction of the v-axis. Currently, the type is always zero.

endOfFrame	Indicates the end of a frame.

angleHistogramHalf.txt

This file contains a series of tab-delineated length histograms of 'angleHistrogramBins' with a range of 0..pi. Note that this implies that the orientation of the microtubules is disregarded. The first bin is centred on zero. **Note:** For cylinders, the end caps are disregarded, and for the box geometry, only the front face is counted [this should ideally be coupled to the 'r_accounting_dontcount' flag, but it's currently hardcoded].

Other histograms

The remaining histograms are

- **mtLengthHistogram.txt**
  histogram of microtubule lengths
- **mtLifetimeHistogram.txt**
  histogram of microtubule lifetimes
- **segAngleLengthHistogram.txt**
  2D histogram of angles and lengths of **segments**. Segments in special regions (cylinder caps and top/bottom of the box geometry) are disregarded.
- **segAngleLifetimeHistogram.txt**
  2D histogram of angles and lifetimes of **segments**. Segments in special regions (cylinder caps and top/bottom of the box geometry) are disregarded.

These can all contain a number of histograms, recorded at different times, according to the following structure.

time	[time]	Time at which the histogram was recorded.
numberOfAngles	[a-bins]	Number of angle bins. Note that these cover a range 0..pi, so that microtubule orientation is disregarded. The first bin is centred on zero.
numberOfBins	[o-bins]	Number of length or lifetime bins.
[angle]	[range] [data: o-bins]	For each angle bin, *range* specifies the edge of the last length/lifetime bin. The range is extended to fit the largest item stored. At every new histogram, it attempts to decrease the range by a factor 2, to ensure a good fit between the resolution and the data. The range is followed by the counts for all bins.