This document contains information on files that are needed to run simulations. This document describes the role of each file and how to use and modify each file to run simulations under specific conditions.

1. main

This is a main executable file that can be obtained by compiling codes via any MPI compiler. A command for compiling the codes varies depending on environments of computing devices. An example of the command is "mpicc –lm –O3 main.c –o main". Use of the flag "-O3" is highly recommended for faster performance.

2. parallel

For parallel processing via the spatial domain decomposition, a computational domain is divided into several subdomains. Each core in CPUs is responsible for calculation of information in one subdomain. A "parallel" file has information about how the computational domain is divided in x, y, and z directions. The first column is the total number of subdomains. The second, third, and fourth columns represent the number of subdomains in x, y, and z directions, respectively. In each row, the value in the first column is equal to the product of values in other columns. If a simulation is run with a certain number of cores, the code searches for the number in the first column of the parallel file. If there is a match, the code uses values in other columns to determine how to divide a domain into subdomains. If there is no match, the code terminates the simulations with an error message.

3. condition

This file specifies conditions for each simulation. For example, parameter values related to mechanics and dynamics of elements can be specified in the condition file. In addition, it can be specified which data file is recorded during a simulation. Brief explanations for each line in condition file are provided below:

L1: Name of folder where data files generated from a simulation will be saved.

L3: A value specified in this line determines the length of one cylindrical actin segment. The actual length corresponds to this value multiplied to 7 nm.

L4: Values specified in this line determine the number of binding sites on each actin segment where motors and ACPs can bind to. The first and second values indicate the number of binding sites on an actin cylindrical segment in longitudinal and transverse directions, respectively.

L6: The size of a computational domain in micron needs to be specified in this line.

L7: A periodic boundary condition should be specified in x, y, and z direction in this line.

L8: If it is intended to simulate a thin network, the normal direction of the network can be specified here. For example, if "z" is the normal direction, the orientation of a new actin segment appearing from an actin nucleation event does not have any z component.

L9: This line specifies the duration of a network formation phase during which actins are assembled into filaments, and motors and ACPs bind to actin filaments.

L10: This line specifies the concentration of actins in uM.

L11: It is possible to include two different types of ACPs: ACPB and ACPC. A value specified in this line is the ratio of concentration of ACPCs to concentration of actins.

L12: Same as L11 except that this line is for concentration of ACPB.

L13: Same as L11 except that this line is for concentration of motor

L15: Duration of measurement. A measurement phase is a main phase where data are recorded. It starts after the network formation phase.

L17: If yes, actin filaments experience the thermal fluctuation during a simulation.

L18: Nucleation (de novo appearance of an actin segment), assembly (addition of a segment to an existing filament), and disassembly (removal of a segment from a filament) of actins during the network formation phase can be turned on or off, depending on specification in this line.

L19: If yes in this line, the nucleation of actins is allowed.

L20: If yes, the assembly of actins is allowed.

L21: If yes, the disassembly of actins is allowed.

L23: If yes, ACPs experience the thermal fluctuation.

L24: Unbinding and rebinding of ACPs during the network formation phase can be turned on or off, depending on specification in this line.

L25: If yes, unbinding of inactive ACPs is allowed. Inactive ACPs indicate ACPs forming a link to only one actin filament.

L26: If yes, binding of monomeric ACPs is allowed. Monomeric ACPs indicate ACPs that are not bound to any actin filament.

L27: If yes, unbinding of active ACPs is allowed. Active ACPs indicate ACPs forming links to two actin filaments.

L28: If yes, rebinding of inactive ACPs is allowed. Rebinding is an event where the inactive ACPs form one more link to an actin filament.

L29: If yes, ACPs in a monomer state are treated implicitly using concentration without any explicit element.

L31 If yes, motors experience the thermal fluctuation.

L32: Unbinding and rebinding of motors during the network formation phase can be turned on or off, depending on specification in this line.

L33: Motor walking during the network formation phase can be turned on or off, depending on specification in this line.

L34: If yes, motor walking is allowed. Motor walking is implemented by moving a motor from a current binding site to a next binding site toward the barbed end of the actin filament. Slide-off of motors at barbed ends is allowed.

L35: If yes, several motors are self-assembled into one motor thick filament. A motor thick filament is composed of a backbone with several motor arms attached to the backbone. Each motor thick filament will have the same size. If no, motors become simple dimers that have only two motor arms.

(L37-L41: For motors without self-assembly)

L37: If yes, unbinding of inactive motors is allowed.

L38: If yes, binding of monomeric motors is allowed.

L39: If yes, unbinding of active motors is allowed.

L40: If yes, rebinding of inactive motors is allowed.

L41: If yes, motors in a monomer state are treated implicitly using concentration without any explicit element.

(L43-L47: For motors with self-assembly)

L43: If yes, unbinding of each motor arm from an actin filament is allowed.

L44: If yes, binding of each motor arm on an actin filament is allowed.

L45: If yes, binding of motors occur only when actin filaments are favorably aligned with motor thick filaments.

L46: If 1, motors which are not bound to any actin filament are disassembled and then assembled somewhere else.

L48: A value in this line is an actin nucleation rate. The actin nucleation event occurs at a probability that is calculated from the actin nucleation rate.

L49: Values in this line indicate actin assembly rates at barbed and pointed ends of actin filaments. The actin assembly event occurs at a probability that is calculated from the actin assembly rates.

L50: Values in this line indicate actin disassembly rates at barbed and pointed ends of actin filaments. The actin disassembly event occurs at a probability that is calculated from the actin disassembly rates.

L51: It is possible to modulate the disassembly rate of actin segments if there are ABPs bound to the actin segments. A value specified here is multiplied to the disassembly rates specified in line 50.

L53: A value in this line is multiplied to a reference rate for ACP binding and rebinding (K_ACP_BIND in header.h).

L54: Zero-force unbinding rate constant (k0) and force sensitivity (x) for slip part of ACP unbinding

L55: Zero-force unbinding rate constant (k0) and force sensitivity (x) for catch part of ACP unbinding

L57: A value in this line is multiplied to a reference rate for motor binding and rebinding (K_MOT_BIND in header.h).

L58: A value in this line is multiplied to reference rates of motor unbinding and walking.

L59: A value in this line indicates the number of real myosin heads that each motor arm represents.

L60: Five values in this line are mechanochemical rates for cross-bridge cycles of each myosin head.

L62: A value in this line is the average number of motor dimers in thick filaments.

L63: Assembly rate of thick filaments.

L64: Turnover rate of free thick filaments.

L66: A value in this line will be multiplied to the rates for dynamic events of actins and dynamic events of ABPs during the network formation phase.

L68: A value in this line is multiplied to a reference value for repulsion strength between actin filaments (STF_ACT_REP in header.h).

L69: A value in this line is multiplied to a reference value for bending stiffness of actin filaments (STF_ACT_BEND in header.h).

L70: A value in this line is multiplied to a reference value for extensional stiffness of actin filaments (STF_ACT_SPR in header.h).

L72: A value in this line is multiplied to a reference value for repulsion strength between actin filaments (STF_ABP_REP in header.h).

L73: Values in this line are multiplied to reference values for bending stiffness which maintains an assigned angle between two arms of ACPC (STF_ACPC_BEND in header.h), ACPB (STF_ACPB_BEND in header.h), and motor (STF_MOT_BEND in header.h).

L74: Values in this line are multiplied to reference values for bending stiffness which maintains 90 deg between the axis of an actin filament and the arm of ACPC (STF_ACPC_90 in header.h), ACPB (STF_ACPB_90 in header.h), and motor (STF_MOT_90 in header.h) bound to the actin filament.

L75: Values in this line are multiplied to reference values for extensional stiffness of ACPC (STF_ACPC_SPR in header.h), ACPB (STF_ACPB_SPR in header.h), and motor (STF_MOT_SPR in header.h).

L77: A value in this line determines how frequently "Output" and "Progress" files are recorded. The Output file shows all output texts from a simulation. It also shows how many dynamic events of actins, ACPs, and motors (assembly, disassembly, binding, unbinding, etc.) have occurred. Also, it shows the number of actins, ACPs, and motors in each state (monomeric, active and inactive) at each time step. The Progress file also shows the accumulated number of dynamic events and the number of elements in each state as well as time and date in the real world.

L79: A value in this line determines how frequently an AccuConf file is recorded. If "-1", the AccuConf file is not generated. The file has accumulated information of Config files.

L80-L84: Parameters for generating files for visualization via VMD (PDB & PSF).

L85: A value in this line determines a period for recording an ActFilaLen file. The ActFilaLen file contains distribution of length of actin filaments at each time point. If "-1", the file is not generated.

L87: A value in this line determines a period for recording an AbpLongFor file. The AbpLogFor file contains information on forces exerted on ABPs and projection of the forces onto actin filaments where the ABPs are bound. If "-1", the file is not generated.

L88: A value in this line determines how frequently files recording mechanical energy are recorded. If "-1", those files are not saved.

L90: A value in this line determines how frequently files recording the unbinding events of ABPs are recorded. If "-1", those files are not saved.

L91: A value in this line determines how frequently files recording the binding events of ABPs are recorded. If "-1", those files are not saved.

L92: A value in this line determines how frequently files recording the turnover events of ABPs are recorded. If "-1", those files are not saved.

L94: A value in this line indicates a period for recording ElasViscIndv, ElasViscSeg, and ElasViscFila files. These files contain information recorded in the unit of individual elements, segments between adjacent cross-linking points, and filaments, respectively. If "-1", these files are not generated.

L96-L104: Parameters for rho activation and those for acceleration of actin polymerization and activation of myosin activation induced by rho.

L96: Period of rho activation. If "-1", rho is not activated.

L97: The number of regions in x, y, and z directions. The domain is divided into these regions for rho activation.

L98: The maximum number of regions where rho can be activated at once.

L99: Delay and duration of motor activation induced by rho. For example, if these are 5 s and 15 s, motors are activation 5 s after the rho activation, and then it is maintained for 15 s.

L100: Delay and duration of altered actin polymerization induced by rho.

L101: Fraction of barbed ends that are subjected to the alteration in the polymerization rate induced by rho activation. For example, if this is 0.01, 1% of the barbed ends in the region with rho activation undergo altered actin polymerization.

L102: Two factors for actin polymerization due to rho activation. The second factor is multiplied to a reference actin polymerization rate during the duration specified in L100. Then, till the end of the rho activation, the first factor is multiplied to the reference actin polymerization rate.

L103: Fraction of motors activated by rho activation.

L104: The extent of enhancement of assembly rate of activated motors. Activated motors undergo faster assembly into thick filaments at a rate enhanced by this factor.