

Data for:

“Astonishing structural transformations of actin bundles are driven by their initial polarity, motor activity, crosslinking, and filament treadmilling”

1. Data format

Data is organized into three major compressed (zip) folders, namely **non-treadmilling**, **Unipolar_treadmilling** and **Apolar_treadmilling**. These zip files contain datafro and input files for studies on non-treadmilling (unipoalr and apolar), treadmilling unipolar and treadmilling apolar bundles respectively.

This data upload contains a set of system configurations that have been studied. The following table describes what each folder name denotes.

Folder Name	Content signifier
alpha:A values: 0.01, 0.05, 0.1, 0.4, 0.6, 0.8	Crosslinker mole ratio
M:A values: 0.0225, 0.045, 0.09, 0.18, 0.225, 0.675	Myosin mole ratio
1E-1, 3E-1, 6E-1, 1E+0, 3E+0, 6E+0, 1E+1	Treadmilling factor values
*_wdata	contains a sample trajectory inside subfolder run1

In these run folders, the following files and formats are found for each trajectory:

1. Input Files

Input files are provided for all system configurations studied. Trajectories were generated from MEDYAN 3.2 (<http://medyan.org/>) using the following syntax

```
MEDYAN -s systeminputfile -i inputfiledirectory -o outputdirectory
```

In addition, representative trajectories are provided for selected system configurations under subfolder titled “run1”. The following output files can be found in run1.

a. snapshot.traj

The snapshot file gives coordinate information of filaments, linkers and motors in addition to simulation time. The frequency of snapshot output is user defined in the system input file. snapshot file contains the following information.

```
frame_number time numfilaments numlinkers nummotors numbranchers
```

```

F filamentid filamenttype filamentcyllength deltal deltar
beadcoord1x beadcoord1y beadcoord1z beadcoord2x beadcoord2y
beadcoord2z ...
...
L linkerid linkertype
startcoordx startcooridy startcoordz endcoordx endcooridy endcoordz
...
M motorid motortype
startcoordx startcooridy startcoordz endcoordx endcooridy endcoordz
...
B brancherid branchertype
coordx cooridy coordz

```

b. forces.traj, tensions.traj, birthtimes.traj

These files give the various properties of each element in the system, in similar form to the snapshot file. It is produced with the following format:

```

frame_number time numfilaments numlinkers nummotors numbranchers
F filamentid filamenttype filamentcyllength deltal deltar
bead1property bead2property ...
...
L linkerid linkertype
linkerproperty
...
M motorid motortype
Motorproperty

```

where the properties are as follows:

01. forces.traj: the magnitude of force on each bead, as well as the magnitude of the stretching force in each cross-linker and motor (same as tension).
02. tensions.traj: the stretching tension on each cylinder, cross-linker, and motor.
03. birthtimes.traj: the birth time of each bead, cross-linker, and motor.

c. chemistry.traj

The chemistry trajectory file gives the copy numbers of all species in the system, along with the current chemical step and time. It is produced with the following form:

```

chemstepnumber time
SPECIESNAME COPYNUMBER

```

where SPECIESNAME represents the name of the system species and COPYNUMBER is the current copy number of that species at the given time step.

d. monomers.traj

Monomer file contains information on number of filament end polymerization/depolymerization reactions that were executed in the last chemical cycle. In addition, information on nucleation

reactions are also mentioned. The following is the syntax for the data in monomer file.

```
chemstepnumber time numfilaments numlinkers nummotors numbranchers
F filamentid filamenttype filamentcylength DeltaMinusEnd
DeltaPlusEnd
DeltaMinusEnd DeltaPlusEnd PolyMinusEnd PolyPlusEnd DepolyMinusEnd
DepolyPlusEnd
IfNucleation TotalNumMonomers
```

e. concentration.traj

Concentration file gives the concentration of each diffusing molecule in a compartment. The following syntax is adopted for the data in concentration file.

```
chemstepnumber time
COMPARTMENT: coordx coordy coordz
SPECIESNAME COPYNUMBER
```

For further information, please refer to the Usage Guide under docs folder of Medyan3.2 source code.