Data for:
"MEDYAN: Mechanochemical Simulations of Contraction and Polarity Alignment in Actomyosin Networks"

1. **Data format**

   This folder contains a number of system configurations at the top level, all of which have run folders (in the name RunX where X is an integer trajectory ID). In these run folders, the following files and formats are found for each trajectory:

   a. **snapshot.traj**

   The snapshot file gives the basic trajectory information of the system. It includes a brief description for all filaments, cross-linkers, motors, and branching points in the system, as well as information on the current chemical step. It is produced with the following form:

   ```
   chemstepnumber time numfilaments numlinkers nummotors
   numbranchers
   F filamentid filamenttype filamentcyllength deltal deltar
   beadcoord1x beadcoord1y beadcoord1z beadcoord2x beadcoord2y
   beadcoord2z ...
   ...
   L linkerid linkertype
   startcoordx startcoordy startcoordz endcoordx endcoordy endcoordz
   ...
   M motorid motortype
   startcoordx startcoordy startcoordz endcoordx endcoordy endcoordz
   ```

   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:

   ```
   chemstepnumber 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:
- 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).
- tensions.traj: the stretching tension on each cylinder, cross-linker, and motor.
- 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.

2. System configurations

The top level of folders represents the system configuration simulated. Below is a brief outline of the abbreviations used. See the Results section of the publication for details on the meanings of these values.

M – Motor concentration ratio
 L – cross-linker concentration ratio
TR – Treadmilling (turnover) factor
BENCH – benchmarking simulations
LARGE – Larger 3x3x3 um^3 simulations
exbind – simulations with binding site exclusivity