Example Guide for M3SYM v1.1

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1 Introduction

Examples can be found in `InstallDirectory/examples`. Each example includes a `SystemFile` as well as chemical input file. To run a given example once the M3SYM executable is created, go to the `InstallDirectory` and run the following:

```
> ./M3SYM -s ./examples/<ExampleFolder>/system.txt
   -i ./examples/<ExampleFolder>/ -o <OutputDirectory>
```

where `<ExampleFolder>` is the specific example folder desired, and `<OutputDirectory>` is the directory of the desired output. See the usage guide for more details on these files and directories.

2 A basic cytoskeletal network

This example, a basic cytoskeletal network with α-actinin cross-linkers and Arp2/3 branching complexes, can be found in `InstallDirectory/examples/actinnetwork`. This is set up to be a 30 s simulation.

2.1 Initial system configuration

This example is set up with the following initial configuration:

- Compartment size of 500 nm, in a 2x2x2 grid
- 1 μm^3 cubic boundary
- 50 randomly placed filaments, all initially 0.02 μm

2.2 Chemistry involved

This example is set up with the following chemical configuration:

- Diffusing actin, Arp2/3, and alpha-actinin species
- Initial concentrations of 10 μM, 50 nM, and 200 nM respectively.
- Actin polymerization and depolymerization
- α-actinin binding and unbinding
- Arp2/3 branching and debranching

For more information on the reaction constants and concentrations chosen, see [1].

2.3 Mechanics involved

This example is set up with the following mechanical configuration:

- Harmonic actin filament stretching force field
- Cosine actin filament bending force field
- Harmonic α-actinin cross-linker stretching force field
- Harmonic branch stretching and cosine angle force field
- Exponential boundary force field
- Repulsive cylindrical excluded volume force field

Dynamic reaction rate changes involving these force fields, including α-actinin unbinding and actin polymerization, were tuned to fit single molecule experiments.

For more information on the force field parameters chosen, please see [1].

2.4 Sample visual output

Coming soon!

3 References

[1] Popov K, Komianos J, and GA Papoian. "MEDYAN: Mechanochemical Simulations of Actomyosin Networks and Other Active Matter." PLoS Computational Biology (in review), 2015.