

Example Guide for M3SYM v1.0

Papoian Lab, University of Maryland

Contents

1	Introduction	2
2	A basic cytoskeletal network	2
2.1	Initial system configuration	2
2.2	Chemistry involved	2
2.3	Mechanics involved	3
2.4	Sample visual output	3

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

2.1 Initial system configuration

This example is set up with the following initial configuration:

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

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 10uM, 50nM, and 200nM respectively.
- Actin polymerization and depolymerization
- Alpha-actinin binding and unbinding
- Arp2/3 branching and unbranching

For more information on the reaction constants and concentrations chosen, see (*paper*).

2.3 Mechanics involved

This example is set up with the following mechanical configuration:

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

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

For more information on the force field parameters chosen, please see (*paper*).

2.4 Sample visual output

Coming soon!