

Example Guide for M3SYM v1.0

Papoian Lab, University of Maryland

Contents

| | | |
|----------|-------------------------------------|----------|
| 1 | Introduction | 2 |
| 2 | A basic cytoskeletal network | 2 |
| 2.1 | Chemistry involved | 2 |
| 2.2 | Mechanics involved | 2 |
| 2.3 | 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 myosin IIA motors, can be found in `InstallDirectory/examples/actinnetwork`.

2.1 Initial system configuration

This example is set up with the following initial configuration:

- Compartment size of 100nm, in a 10x10x10 grid
- 1um diameter spherical boundary
- 100 randomly placed filaments, all initially 0.2um

2.2 Chemistry involved

This example is set up with the following chemical configuration:

- Diffusing actin, myosin, and alpha-actinin species
- Initial concentrations of 10uM, 200nM, and 500nM respectively.
- Actin polymerization and depolymerization
- Alpha-actinin binding and unbinding
- Myosin IIA binding, unbinding, and walking

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 myosin IIA motor stretching force field
- Harmonic alpha actinin cross-linker stretching force field
- Exponential boundary force field
- Repulsive excluded volume force field

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

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

2.4 Sample visual output