

Supporting Information for
**MEDYAN: Mechanochemical Simulations of
Contraction and Polarity Alignment in
Actomyosin Networks**

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A comparison of MEDYAN to other agent-based cytoskeletal models.

This table is shown on the next page, with comparison categories as discussed in the Introduction section. Those categories are organized as follows:

- **Chemistry** - The implementation of cytoskeletal chemistries within the model, which could include (but not limited to) filament, cross-linker, and molecular motor chemical dynamics.
- **Mechanics** - The force-field description of semi-flexible filaments in the model, as well as other mechanical elements, including cross-linkers and molecular motors.
- **Diffusion and active transport** - The capability of the model to include diffusion and active transport of some or all of its cytoskeletal species.
- **Mechanochemical feedback** - The model's capability to include force-dependent reaction rates for some or all of its cytoskeletal species, which are updated dynamically during runtime.
- **Dimensionality, time and length scales** - The previous time and length scales achieved by the model in its publications.
- **Public code availability** - The access of source code and/or example applications for the model in a public repository.

Model	Chemistry	Mechanics	Diffusion and active transport	Mechanochemical feedback	Dimensionality, time and length scales	Public code availability	Refs
SCPR, Bidone et al. 2014, Tang et al. 2014, Laporte et al. 2012, Wang et al. 2008	<ul style="list-style-type: none"> Stochastic growth of actin filaments Binding of cross-linkers and motors from bulk reservoir No filament branching reported 	<ul style="list-style-type: none"> Langevin dynamics with a coarse-grained point-like representation for filaments Actin filament bending and stretching, motor and cross-linker interaction potentials No inter-filament excluded volume effects reported 	<ul style="list-style-type: none"> Filaments diffuse via Brownian motion 	None reported	<ul style="list-style-type: none"> 2D, 3D 1000 <i>s</i> timescales 5-15 μm length scales 	None reported	[1–4]
Cytosim, Nédélec and Foethke 2002-2007	<ul style="list-style-type: none"> Stochastic growth of filaments Binding of cross-linkers and motors from bulk reservoir Filament branching 	<ul style="list-style-type: none"> Langevin dynamics with a coarse-grained point-like representation for filaments Interaction potentials for filaments, cross-linkers, motors, branching molecules, in various versions. Repulsion or attraction between filament points for excluded volume effects 	<ul style="list-style-type: none"> Filaments diffuse via Brownian motion 	<ul style="list-style-type: none"> Mechanochemical models for filaments, cross-linkers, motors 	<ul style="list-style-type: none"> 2D, 3D Time and length scales vary greatly depending on simulated system 	<ul style="list-style-type: none"> Example applications available for download at www.cytosim.org 	[5, 6]
Jung et al 2015, Kim et al. 2009-2014	<ul style="list-style-type: none"> Stochastic growth of actin filaments Binding of cross-linkers from bulk reservoir Stochastic myosin II filament binding and walking 	<ul style="list-style-type: none"> Langevin dynamics with a coarse-grained cylindrical segmentation for actin filaments Cross-linker interaction potentials and very detailed myosin II potentials Nearest-distance repulsion for cylinder excluded volume 	<ul style="list-style-type: none"> Filaments diffuse via Brownian motion Myosin II filaments diffuse via Brownian motion Actin monomers and cross-linkers do not diffuse 	<ul style="list-style-type: none"> Detailed mechanochemical models for cross-linker unbinding, and myosin II filament walking and unbinding 	<ul style="list-style-type: none"> 3D 200 <i>s</i> timescales 2-5 μm length scales 	None reported	[7–9]
Muller et al. 2015, Cyron et al. 2009-2013	<ul style="list-style-type: none"> Cross-linker spatially resolved binding onto filaments No growth or nucleation of filaments Does not implement filament branching 	<ul style="list-style-type: none"> Finite-element Brownian dynamics of semi-flexible filament bending and stretching Cross-linker interaction potentials Inter-filament excluded volume not reported in detail 	<ul style="list-style-type: none"> Filaments and cross-linkers diffuse via Brownian motion Actin monomers do not diffuse 	None reported	<ul style="list-style-type: none"> 3D 1000 <i>s</i> timescales 1-10 μm length scales 	None reported	[10–13]
Odell et al. 2008	<ul style="list-style-type: none"> Spatially resolved, stochastic chemical reactions via cytoplasmic domains Mass-action kinetic equations for chemical reactions within cytoplasmic domains Stochastic nucleation and growth of microtubules 	<ul style="list-style-type: none"> Coarse-grained microtubules by spring segments, with bending and stretching potentials No inter-filament excluded volume reported 	<ul style="list-style-type: none"> Continuum diffusive flux between cytoplasmic domains Convective transport modeled by viscous drag force on cytoplasmic domains 	<ul style="list-style-type: none"> Mechanochemical model for microtubules 	<ul style="list-style-type: none"> 3D 500 <i>s</i> timescales 80 μm length scales 	<ul style="list-style-type: none"> Example application available for download at www.celldynamics.org 	[14]
Rafelski et al. 2008, Alberts et al. 2004	<ul style="list-style-type: none"> Spatially resolved, stochastic chemical reactions via partial differential equation reaction-diffusion scheme Stochastic branching, nucleation and growth of actin filaments Stochastically varying biochemical states of filament 	<ul style="list-style-type: none"> Brownian dynamics of branched, rigid actin filaments and collision interactions with surfaces No inter-filament excluded volume reported 	<ul style="list-style-type: none"> Partial differential equation reaction-diffusion scheme for actin monomers and branching molecules 	None reported	<ul style="list-style-type: none"> 3D 100 <i>s</i> timescales 10 μm length scales 	<ul style="list-style-type: none"> Source code and example application available for download at www.celldynamics.org 	[15, 16]
MEDYAN	<ul style="list-style-type: none"> Stochastic reaction-diffusion master equation Stochastic, spatially resolved filament nucleation and branching, growth, and state transitions Cross-linker and motor dynamics 	<ul style="list-style-type: none"> Conjugate gradient energy minimization Interaction potentials for cross-linkers, motors, branching molecules, and filaments Novel cylindrical rigid body repulsion 	<ul style="list-style-type: none"> Stochastic, compartment based reaction-diffusion scheme for general transport of any unbound cytosolic species No Brownian motion of filaments 	<ul style="list-style-type: none"> Detailed mechanochemical models for filaments, cross-linkers, and motors 	<ul style="list-style-type: none"> 3D 2000 <i>s</i> timescales 1-3 μm length scales 	<ul style="list-style-type: none"> Source code and example applications available for download at www.medyan.org 	-

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