Actin Modeling

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This is a dynamical graph grammar (DGG) model of the morphodynamics of the synaptic spine head built for actin network remodeling and biomechanics.

Loading Plenum

In[∘]:=
```
<< Plenum.m
```

Defining The Problem

User Defined Variables

In[∘]:=
```
nCG = 50.;
biomechanicalRate = 175.;
membraneRate = 175.;
```

Variable Rules

In[∘]:=
```
boundarySpineRate = 10^24;
eps = 10^-10;
rateVars = {spineFactor → membraneRate , membraneFactor → membraneRate,
    boundarySpineFactor → boundarySpineRate, networkFactor → biomechanicalRate};
potentialVars =
  {l0 → 1., ϵ → 0.9, hessianScaling → 1./Sqrt[biomechanicalRate], overgrowthL → 1.5};
```

Basic Definitions

There are four types of ends which we use to apply specific rules to only actins of those types:

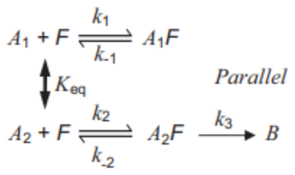
```
INT = 0.; (* internal monomer *)
POI = 1.; (* monomer at the pointed end *)
BAR = 2.; (* monomer at the barbed end *)
CAP = 3.; (* capping agent *)
POIMEM = 4.;
BARMEM = 5.;
CAPMEM = 6.;
```

Codes for specific IDs for no connection - basically null pointers

```
aIDFreeP = -10 000.;
(* constant for the empty space at the pointed end of a monomer *)
aIDFreeB = -20 000.;
(* constant for the empty space at the barbed end of a monomer *)
arpIDFree = -30 000.; (* arp free *)
membraneIDFree = -1.; (*ID for actins not attached to the membrane*)
```

We allow actins to be attached to either ATP or ADP, both when they exist in free globular form (G-Actin) and when they are attached to filaments (F-Actin).

We also model the parallel mechanism of activation of Arp2/3:



In order to accomplish this, we have IDs for Arp2/3 whether it is activated (A_2) or deactivated (A_1).

```
ARPACTID = -1.;
ARPDEACTID = -2.;
```

The following is the initial condition input into Plenum software to test grammars following the grammar definition in each section.

```
In[ ]:= myicReduced = ({
        actin[1, { 0, 0}, aIDFreeP, 2, 0.0, 0, arpIDFree, POI,
         membraneIDFree, nCG, 0, 0, 0], (* new node at the pointed end *)
        actin[2, {1, 0.05}, 1, 3, 0, 0, 4, INT,
         membraneIDFree, 0, nCG - 1, 0, 1.], (* new internal node *)
        actin[3, {2, 0.}, 2, 6, 0.0, 0, arpIDFree, INT,
         membraneIDFree, nCG, 0, 0, 0], (* new node at the pointed end *)
        actin[6, {3, 0.}, 3, aIDFreeB,
         0.0, 0, arpIDFree, BAR, membraneIDFree, nCG, 0, 0, 0],
        (* place a branch to begin with and see how it works *)
        actin[4, {1 + Cos[70 Degree], Sin[70 Degree]}, 2,
         5, 0., 0.0, arpIDFree, INT, membraneIDFree, nCG, 0, 0, 0],
        actin[5, {1 + 2 Cos[70 Degree], 2 Sin[70 Degree]}, 4, aIDFreeB,
         0.0, 0.0, arpIDFree, BAR, membraneIDFree, nCG, 0, 0, 0],

        newID[11], (* counter for new ids to be generated *)
        arpCount[initArpNum], (* counter for the amount of
         ARP floating in the system at any given point in the sim *)
        actinATPCount[initActinATPNum - 5 * nCG],
        actinADPCount[initActinADPNum],
        cofilinCount[initCofilinNum],
        spineHeadArea[area],
        cappingCount[initCappingNum],
        camCount[initCamNum]
      } /. {area → π (spineHeadRadius / actinObjectRise)^2 / 5}) // N;
```

Here are IDs representing what type of information is stored at each position of an actin object.

```
In[ ]:= ID = 1;
POS = 2;
PREV = 3;
NEXT = 4;
ANGLE = 5;
CROSSLINKING = 6;
BRANCH = 7;
TYPE = 8;
MEMBRANEBOUNDID = 9;
ATPCount = 10;(*ID for actin-ATP*)
ADPCount = 11;(*ID for actin-ADP*)
ADPPiCount = 12;(*ID for actin-ADP-Pi*)
(*IDs for Cofilin bindings*)
ADPCofCount = 13;
```

Constants

```
In[ ]:= (**CONSTANTS**)

(*Dominguez R,Holmes KC.Actin structure and function.Annu Rev Biophys.2011;*)
  40:169-86. doi:10.1146/annurev-biophys-042910-155359. PMID:21314430;
  PMCID:PMC3130349.
actinMonomerRise = 2.76 × 10^-9 (*m*) ;
actinObjectRise = actinMonomerRise nCG;

avogadros = 6.022 * 10^23;
T = 310;

θArp = 70 (*degrees*) * π/180 ;

kB = 1.38 * 10^-23 (*J/K*) / actinObjectRise^2;
kBT = kB * T;

μCam = 1/(1/(12*72) + 1/42) (*kg/mol*) / avogadros;
ωCam = Sqrt[(κS / 4) / μCam];
(*Khan S,Conte I,Carter T,Bayer KU,                              *)
  Molloy JE.Multiple CaMKII Binding Modes to the Actin
    Cytoskeleton Revealed by Single-Molecule Imaging.Biophys J.2016;
  111(2):395-408. doi:10.1016/j.bpj.2016.06.007
koffDCam = 0.23(*1/s*);

ϵUnitCam = -kBT Log[koffDCam / ωCam];
(*Dissocation energy for a coarse-grained chain*)
ρCam = Sqrt[(κS / 4) / (2 ϵUnitCam)];
camRule = {De → ϵUnitCam, ρMorse → ρCam};

(*Zero-mode waveguides visualize the first steps during gelsolin-*)
   mediated actin filament formation
ϵUnit = 6.93(*kcal/mol*) * 4184 / avogadros(*J*) / actinObjectRise^2;
(*Dissociation energy for a coarse-grained chain*)

κS = (0.1 * 10^-12/10^-9 (*N/m*)) ((200 * 10^-9) / actinObjectRise);
```

```
σA = 8.0 * 10^-9 (*m*) / actinObjectRise; (*diameter of actin molecule*)
ρ = Sqrt[(ϰS) / (2 ϵUnit)];
actinRule = {De → ϵUnit, ρMorse → ρ};

(*Measuring the flexural rigidity of actin filaments and                *)
   microtubules from their thermal fluctuating shapes:A new perspective;
  PMCID:PMC24024.
```

$$\varkappa B = \left(\left(7.51 * 10^{-26}\right)(*Nm^2*) \big/ \text{actinObjectRise}^3\right)\left(\frac{1}{1.5}\ (*\text{Tropomyosin correction}*)\right);$$

```
(*Myosin-I Synergizes with Arp2/3 Complex to Enhance Pushing Forces*)
  of Branched Actin Networks
ϰBArpFactor = 2.;

(*Hunt AJ,Gittes F,Howard J.The force exerted by a single       *)
   kinesin molecule against a viscous load.Biophys J.1994 Aug;
  67(2):766-81. doi:10.1016/S0006-3495(94)80537-5. PMID:7948690;
  PMCID:PMC1225420.
```

$$\xi A[L\_] := \text{Re}\left[\frac{4\,\pi\,\eta\,L}{\text{Log}\left[\frac{L}{\sigma A}\right] + 0.886}\right];(*\text{friction coefficient for actin}*)$$

$$\xi APar[L\_] := \text{Re}\left[\frac{2\,\pi\,\eta\,L}{\text{Log}\left[\frac{L}{\sigma A}\right] - 0.114}\right];(*\text{friction coefficient for actin}*)$$

$$\xi Cam[L\_] := \text{Re}\left[\frac{4\,\pi\,\eta\,L}{\text{Log}\left[\frac{L}{\sigma Cam}\right] + 0.886}\right];(*\text{friction coefficient for cam}*)$$

$$\text{step}[L\_] := \frac{1}{\xi A[L] * \text{biomechanicalRate}}$$

$$\text{stepCam}[L\_] := \frac{1}{\xi Cam[L] * \text{biomechanicalRate}}$$

$$\text{stepPar}[L\_] := \frac{1}{\xi APar[L] * \text{biomechanicalRate}}$$

```
(*Gittes F,Mickey B,Nettleton J,                                  *)
  Howard J.Flexural rigidity of microtubules and actin filaments
   measured from thermal fluctuations in shape.J Cell Biol.1993 Feb;
  120(4):923-34. doi:10.1083/jcb.120.4.923.PMID:8432732;
  PMCID:PMC2200075.
```

$$Lp = 17.7 * 10^{-6} (*m*) \big/ \text{actinObjectRise};$$

```
(*persistence length of actin filament*)
```

```
θp = Sqrt[2/Lp];


(*S

 mith BA,Roy H,De Koninck P,Grütter P,
 De Koninck Y.Dendritic spine viscoelasticity and soft-
  glassy nature:balancing dynamic remodeling
     with structural stability.Biophys J.2007 Feb 15;
 92(4):1419-30. doi:10.1529/biophysj.106.092361.Epub 2006 Nov 17. PMID:17114228;
 PMCID:PMC1783894.

 )
η = 19.9 / (2 Pi) (*kg / (m s)*) * actinObjectRise;
(*Newtonian viscosity of medium*)

(*Sanabria H,Swulius MT,Kolodziej SJ,Liu J,Waxham MN.{beta}CaMKII
 regulates actin assembly and structure.J Biol Chem.2009 Apr 10;
284(15):9770-80. doi:10.1074/jbc.M809518200.Epub 2009 Feb 10. PMID:19208632;
PMCID:PMC2665098. *)
```

$$\sigma\text{Arp} = \frac{(140 + 109 + 130)}{3} * 10^{-10} \text{(*m*);(*diameter of Arp2/3 Complex*)}$$

$$\text{speciesToMol} = \frac{1}{\left(10^3 \times 4/3\,\pi\,\left(\left(\text{area} * \text{actinObjectRise}^2\,1/\pi\right)^{3/2}\right)\right)\text{avogadros}};$$

```
(**KINETICS OF POLYMERIZATION**)


(*Selden LA,Kinosian HJ,Estes JE,                                      *)
  Gershman LC.Impact of profilin on actin-bound nucleotide
    exchange and actin polymerization dynamics.Biochemistry.1999 Mar 2;
  38(9):2769-78. doi:10.1021/bi981543c.PMID:10052948.

actinATPDissociation = 0.08(*1/s*);
actinNucPhos = 1.4(*1/s*);


(*Pollard TD.Rate constants for the reactions of ATP-and ADP-  *)
   actin with the ends of actin filaments.J Cell Biol.1986 Dec;
  103(6 Pt 2):2747-54. doi:10.1083/jcb.103.6.2747.PMID:3793756;
  PMCID:PMC2114620.


kPlusBarbedT = 11.6 × 10^6 (*1/(M s)*) * speciesToMol;
kMinusBarbedT = 1.4 (*1/(s)*);
```

```
kPlusPointedT = 1.3 × 10^6 (*1/(M s)*) * speciesToMol;
kMinusPointedT = 0.81 (*1/(s)*);
kPlusBarbedD = 3.8 × 10^6 (*1/(M s)*) * speciesToMol;
kMinusBarbedD = 7.2 (*1/(s)*);
kPlusPointedD = 0.16 × 10^6 (*1/(M s)*) * speciesToMol;
kMinusPointedD = 0.27 (*1/(s)*);

fActinATPHydrolysis = 0.3 (*1/s*);
gActinATPHydolysis = 7 * 10^-6 (*1/s*);

(**KINETICS OF ACTIN NETWORKS**)

θThreshArp = 25 Degree;


(*Smith BA,Daugherty-Clarke K,Goode BL,
  Gelles J.Pathway of actin filament branch formation by Arp2/3 complex revealed
    by single-molecule imaging.Proc Natl Acad Sci U S A.2013 Jan 22;
  110(4):1285-90. doi:10.1073/pnas.1211164110.Epub 2013 Jan 4. PMID:23292935;
  PMCID:PMC3557048.

 )

keqk2 = 3200 * speciesToMol;
k1 = 19 * speciesToMol;
kminus1 = 0.07;
kminus2 = 0.47;


(*Hayakawa K,Sekiguchi C,Sokabe M,Ono S,
  Tatsumi H.Real-Time Single-Molecule Kinetic Analyses of AIP1-Enhanced Actin
    Filament Severing in the Presence of Cofilin.J Mol Biol.2019 Jan 18;
  431(2):308-322. doi:10.1016/j.jmb.2018.11.010.Epub 2018 Nov 12. PMID:30439520;
  PMCID:PMC6507414.

 )

kcapon = 2.3 * 10^6 (*1/(M s)*) * speciesToMol;
kcapoff = 9.5 * 10^-4 (*1/s*);
```

```
(*Wioland H,Guichard B,Senju Y,Myram S,Lappalainen P,Jégou A,                    *
  Romet-Lemonne G.ADF/Cofilin Accelerates Actin Dynamics by Severing Filaments
    and Promoting Their Depolymerization at Both Ends.Curr Biol.2017 Jul 10;
  27(13):1956-1967.e7.doi:10.1016/j.cub.2017.05
    .048.Epub 2017 Jun 15. PMID:28625781;
  PMCID:PMC5505867.

 )
kcofcapoff = 3 * 10^-3 (*1/s*);
kcofcapon = 0.3 * 10^6 (*1/(M s)*) * speciesToMol;



(*Khan S,Conte I,Carter T,Bayer KU,                                        *)
  Molloy JE.Multiple CaMKII Binding Modes to the Actin Cytoskeleton
    Revealed by Single-Molecule Imaging.Biophys J.2016 Jul 26;
  111(2):395-408. doi:10.1016/j.bpj.2016.06.007.PMID:27463141;
  PMCID:PMC4968397.


koffcamKIIβ = 0.23 (*1/s*);
koncamKIIβ = 0.5 * 10^6 (*1 / (M s)*) * speciesToMol;

(*Estimated using HullRad on AlphaFold PDB*)
camKIIβrad = 26 * 10^-9 (*nm*) / actinObjectRise;
σCam = (camKIIβrad * 2 * 6) / (2 π) 2;

(*BROWNIAN RATCHET*)

δ = 2.7 * 10^-7 * 10^-2 (*m*) / actinObjectRise;
ωoverf = δ / kBT;

(**SYNTHESIS AND DEGRADATION OF MOLECULES**)


(*Sialana FJ,Wang AL,Fazari B,Kristofova M,Smidak R,                    ,
  Trossbach SV,Korth C,Huston JP,de Souza Silva MA,
  Lubec G.Quantitative Proteomics of Synaptosomal Fractions in a
   Rat Overexpressing Human DISC1 Gene Indicates Profound Synaptic
   Dysregulation in the Dorsal Striatum.Front Mol Neurosci.2018 Feb 6;
  11:26. doi:10.3389/fnmol.2018.00026.PMID:29467617;
  PMCID:PMC5808171.
Bonilla-Quintana M, Rangamani P. Biophysical modeling of actin-   *)
 mediated structural plasticity reveals mechanical adaptation in
  dendritic spines. 2022 Nov 15. doi: 10.1101/2022.11.06.515372.

bactSS = E^14.95951281;
actinDegRate = 0.0081(*1/s*);
actinSynthRate = 24.4428 * 10^-6(*M/s*) / speciesToMol;

arpcSS = E^5.596538302;
arpSynthRate = 0.0255 * 10^-6(*M/s*) / speciesToMol;
arpDegRate = 0.0013 (*1/s*);

cfl1SS = E^9.218833479;
cofilinSynthRate = 0.0237 * 10^-6(*M/s*) / speciesToMol;
cofilinDegRate = 0.0006(*1/s*);

camk2bSS = E^12.55662979;
camk2bSSnum = (actinSynthRate/actinDegRate) (camk2bSS/bactSS);
camSynthRate = 0.00020944238775871162` / 60 / speciesToMol(*species/s*);
camDegRate = 0.7677386644519346` / 60(*1/s*);

capzSS = E^6.697041512;
capzSSnum = (arpSynthRate/arpDegRate) (capzSS/arpcSS);
cappingSynthRate = 0.000014271505531589093` / 60 / speciesToMol(*species/s*);
cappingDegRate = 0.240757 / 60(*1/s*);


(*Roland J,Berro J,Michelot A,Blanchoin L,
  Martiel JL.Stochastic severing of actin filaments
   by actin depolymerizing factor/cofilin controls the
   emergence of a steady dynamical regime.Biophys J.2008 Mar 15;
  94(6):2082-94. doi:10.1529/biophysj.107.121988.Epub 2007 Dec 7. PMID:18065447;
  PMCID:PMC2257902.

 )
kATPHydrolysis = 0.35 (*1/s*);
ksev = 0.012(*1/s*);
kCofPiRelease = 0.035 (*1/s*);
```

```
(*Carlier MF.Measurement of Pi dissociation from               *)
    actin filaments following ATP hydrolysis using a linked
    enzyme assay.Biochem Biophys Res Commun.1987 Mar 30 143(3):
   1069-75. doi:10.1016/0006-291x(87)90361-5. PMID:3566755.

kPiRelease = 0.006(*1/s*);



(*McCullough BR,Grintsevich EE,Chen CK,et al.Cofilin-
   linked changes in actin filament flexibility promote severing.Biophys J.2011;
  101(1):151-159. doi:10.1016/j.bpj.2011.05.049

 )
bareAngle = 57 Degree;
cofAngle = 73 Degree;
boundaryAngle = 31 Degree;



(*Wioland H,Guichard B,Senju Y,Myram S,Lappalainen P,Jégou A,                  *
  Romet-Lemonne G.ADF/Cofilin Accelerates Actin Dynamics by Severing Filaments
    and Promoting Their Depolymerization at Both Ends.Curr Biol.2017 Jul 10;
  27(13):1956-1967.e7.doi:10.1016/j.cub.2017.05
    .048.Epub 2017 Jun 15. PMID:28625781;
  PMCID:PMC5505867.

 )
kOnCofEdge = 17 * 10^6 (*1/(M s)*) * speciesToMol ;
kOffCof = 0.7(*1/s*);
kMinusBarbedCof = 4.0(*1/s*);
kMinusPointedCof = 3.3(*1/s*);


(* Pandit NG,Cao W,Bibeau J,et al.Force and phosphate release from Arp2/3 comple
    promote dissociation of actin filament branches.Proc Natl Acad Sci U S A.202
   117(24):13519-13528. doi:10.1073/pnas.1911183117



(*De La Cruz EM.How cofilin severs an actin filament.Biophys Rev.2009 May 15;*
  1(2):51-59. doi:10.1007/s12551-009-0008-5. PMID:20700473;
  PMCID:PMC2917815.

 )
kOnSingleCof = 10^4 (*1/(M s*) * speciesToMol ;

(**FACTORS**)
```

```
initActinNum = actinSynthRate / actinDegRate;
initActinATPNum = initActinNum;
initActinADPNum = initActinATPNum * actinATPDissociation / actinNucPhos;
initArpNum = arpSynthRate / arpDegRate;
initCofilinNum = (cofilinSynthRate / cofilinDegRate);
initCappingNum = (cappingSynthRate / cappingDegRate);
initCamNum = (camSynthRate / camDegRate);
```

In[∘]:=

Curve-Fitting CamKIIβ and Aip1 (capping) Degradation Rates

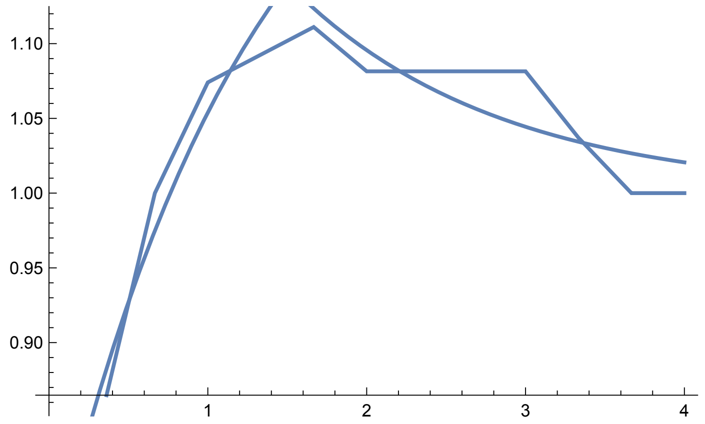
```
(*Bosch M,Castro J,Saneyoshi T,Matsuno H,Sur M,
Hayashi Y.Structural and molecular remodeling of dendritic spine
  substructures during long-term potentiation.Neuron.2014 Apr 16;
82(2):444-59. doi:10.1016/j.neuron.2014.03.021.PMID:24 742 465;
PMCID:PMC4281348.*)
```

```
In[∘]:= Export["~/Documents/aip1Data.csv", aip1Data]
Out[∘]=
        ~/Documents/aip1Data.csv

In[∘]:= Export["~/Documents/camEstimatedData.csv", Table[
          {t, eq /. Join[nlm["BestFitParameters"], {mstar → camk2bSSnum * speciesToMol}]},
          {t, 0, 4, 0.07}]]
Out[∘]=
        ~/Documents/camEstimatedData.csv

In[∘]:= Export["~/Documents/aip1EstimatedData.csv", Table[
          {t, eq /. Join[nlm["BestFitParameters"], {mstar → camk2bSSnum * speciesToMol}]},
          {t, 0, 4, 0.07}]]
Out[∘]=
        ~/Documents/aip1EstimatedData.csv

In[∘]:= Export["~/Documents/aip1Data.csv", aip1Data]
Out[∘]=
        ~/Documents/aip1Data.csv
```

```
In[ ]:= camData = {{0, 1}, {1 / 3, 1.15}, {2 / 3, 1.35},
           {1, 1.45}, {4 / 3, 1.475}, {5 / 3, 1.5}, {2, 1.46}, {7 / 3, 1.46},
           {8 / 3, 1.46}, {3, 1.46}, {10 / 3, 1.4}, {11 / 3, 1.35}, {4, 1.35}};
        camData⟦;; , 2⟧ /= 1.35;
        eq = (m[t] /.
             DSolve[{m'[t] == influx (HeavisideTheta[t] - HeavisideTheta[t - 1.5]) / mstar +
                  km (1 - m[t]), m[0] == camData⟦1, 2⟧}, m, {t, 0, 4}])⟦1⟧;

        nlm = NonlinearModelFit[camData,
           eq /. {mstar → camk2bSSnum * speciesToMol}, {influx, km}, t, Method → {NMinimize}];
        Show[{ListLinePlot[camData],
          Plot[eq /. Join[nlm["BestFitParameters"], {mstar → camk2bSSnum * speciesToMol}],
           {t, 0, 4}]}]
        Print[Join[nlm["BestFitParameters"],
           {basal → km * camk2bSSnum * speciesToMol} /. nlm["BestFitParameters"]]];
        Export["~/Documents/camEstimatedData.csv", Table[
          {t, eq /. Join[nlm["BestFitParameters"], {mstar → camk2bSSnum * speciesToMol}]},
          {t, 0, 4, 0.07}]]

        aip1Data = {{0, 1}, {1 / 3, 1.75}, {2 / 3, 2.65}, {1, 4.0}, {4 / 3, 4.25}, {5 / 3, 4.4},
           {2, 4.8}, {7 / 3, 4.7}, {8 / 3, 4.5}, {3, 4.25}, {10 / 3, 4}, {11 / 3, 3}, {4, 2.75}};
        aip1Data⟦;; , 2⟧ /= 1.5;
        eq = (m[t] /.
             DSolve[{m'[t] == influx (HeavisideTheta[t] - HeavisideTheta[t - 1.5]) / mstar +
                  km (1 - m[t]), m[0] == aip1Data⟦1, 2⟧}, m, {t, 0, 4}])⟦1⟧;

        nlm = NonlinearModelFit[aip1Data,
           eq /. {mstar → capzSSnum * speciesToMol}, {influx, km}, t, Method → {NMinimize}];
        Show[{ListLinePlot[aip1Data], Plot[eq /.
            Join[nlm["BestFitParameters"], {mstar → capzSSnum * speciesToMol}], {t, 0, 4}]}]
        Print[Join[nlm["BestFitParameters"],
           {basal → km * capzSSnum * speciesToMol} /. nlm["BestFitParameters"]]];
        Export["~/Documents/aip1EstimatedData.csv",
         Table[{t, eq /. Join[nlm["BestFitParameters"], {mstar → capzSSnum * speciesToMol}]},
          {t, 0, 4, 0.07}]]
```

```
Reduce : Reduce was unable to solve the system with inexact coefficients. The answer was obtained by solving a
    corresponding exact system and numericizing the result.

Reduce : Reduce was unable to solve the system with inexact coefficients. The answer was obtained by solving a
    corresponding exact system and numericizing the result.
```

Out[ ]=



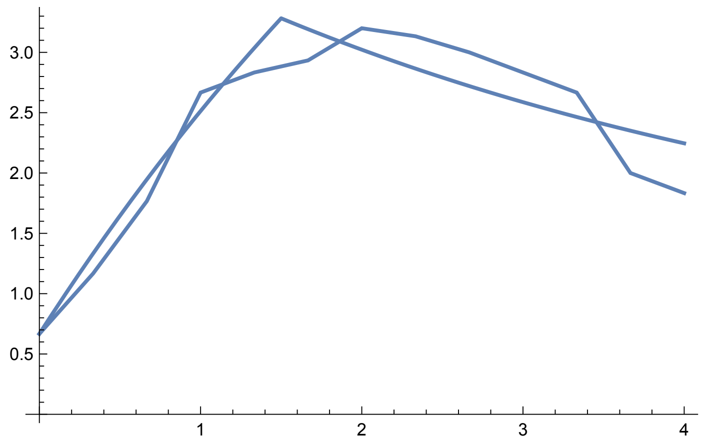
```
{influx → 0.0000680964, km → 0.767739, basal → 0.000209442}
```

Out[ ]=

```
~/Documents/camEstimatedData.csv
```

```
Reduce : Reduce was unable to solve the system with inexact coefficients. The answer was obtained by solving a
    corresponding exact system and numericizing the result.
Reduce : Reduce was unable to solve the system with inexact coefficients. The answer was obtained by solving a
    corresponding exact system and numericizing the result.
```

Out[ ]=



```
{influx → 0.000117842, km → 0.242064, basal → 0.0000142715}
```

Out[ ]=

```
~/Documents/aip1EstimatedData.csv
```

Definition of Rules

```
In[]:= (* define rates for all of the reactions,
       change them here instead of hunting through all the rules *)
       myRates = {arpRate → arpSynthRate,
          cofilinRate → cofilinSynthRate, cofilinDeg → cofilinDegRate,
          barbGrowthT → kPlusBarbedT / nCG, barbGrowthD → kPlusBarbedD / nCG,
          barbRetr → 1 / (1 / (kMinusBarbedT / (ATPCountCG+10^-8)) + 1 / (kMinusBarbedD / (ADPCountCG+ADPPiCountCG+10^-8)) + 1 / (kMinusBarbedCof / (ADPCofCountCG+10^-8))),
          pointGrowthT → kPlusPointedT / nCG, pointGrowthD → kPlusBarbedD / nCG,
          pointRetr → 1 / (1 / (kMinusPointedT / (ATPCountCG+10^-8)) + 1 / (kMinusPointedD / (ADPCountCG+ADPPiCountCG+10^-8)) + 1 / (kMinusPointedCof / (ADPCofCountCG+10^-8))), cap → kcapon,
          capoff → kcapoff, sever → ksev, branchAng → θArp, sdGrowth → θp,
          arpDeg → arpDegRate , actinRate → actinSynthRate , actinDeg → actinDegRate ,
          bundle → koncamKIIβ / nCG, unbundle → koffcamKIIβ / nCG,
          actinPhos → actinNucPhos, actinATPDc → actinATPDissociation,
          cofBindEdge → kOnCofEdge, cofBindPiEdge → kOnCofEdgeADPPi,
          cofUnbind → kOffCof, cofBindSingle → kOnSingleCof,
          branchGrowthAct → keqk2 * nCG, branchRetrAct → kminus2,
          branchGrowthDeact → k1 / nCG, branchRetrDeact → kminus1 / nCG,
          capRate → cappingSynthRate, capDeg → cappingDegRate, camRate → camSynthRate,
          camDeg → camDegRate, capoffcof → kcofcapoff, caponcof → kcofcapon};
```

```
In[]:= (*Bonilla-Quintana M,Wörgötter F,Tetzlaff C,                    *)
         Fauth M.Modeling the Shape of Synaptic Spines by
          Their Actin Dynamics.Front Synaptic Neurosci.2020 Mar 10;
         12:9. doi:10.3389/fnsyn.2020.00009.PMID:32218728;
         PMCID:PMC7078677.

       Pvar = 85.7143 (*pN μm^-2*) * actinObjectRise;
       tauvar = 15 (*pN μm^-1*) * 10^-6;

       kappavar = 0.18 (*pN μm*) * 10^-12 * 10^-6 / actinObjectRise^2;
       ξ = 0.002 / actinObjectRise (* m^2/(s N) *);
       membraneRules =
          {P → Pvar, tau → tauvar, kappa → kappavar, zeta → ξ / membraneFactor} /.
           {membraneFactor → membraneRate};
```

We also define a function for getting the relative position after rotation which works with vectorized coordinates.

```
In[ ]:= newPos[oldPos_, angIn_] := RotationTransform[angIn][oldPos];
```

Visualizing The Actin Network

Visualizer

This is the legend for visualizing actin networks:
- Circles: Actin objects
- Squares: Arp objects
- Triangles: Capping objects
- Hexagons: CamKIIβ objects
- Edge medium thickness indicates Actin-ATP and edge no thickness indicates Actin-ADP
- Opacity indicates degree of cofilin binding
- Color indicates bending angle

```
In[ ]:= VisualizeActinSnapshot[initMoleculeList_, verbose_, energyMap_] :=
          Module[{ml = initMoleculeList, viz, stack, pointCells, curCell,
            prevCell, color, prevPos, maxEnergy, minEnergy, energyFunc,
            vizLines, vizSpine, prevSpine, moleculeList, partnerCoords,
            shapeRadius = 0.15, camObjects, curCam, spineCells, i},
           (* initialize the stack and viz lists -
            using DFS to traverse the list of nodes *)
           stack = {};
           viz = {};
           vizLines = {};
           vizSpine = {Black};
           camObjects = Cases[ml, cam[__]];
           spineCells = Cases[ml, spine[_, _, _, _]];
           moleculeList = DeleteCases[initMoleculeList, spine[__]];

           For[i = 1, i ≤ Length[spineCells], i++,
            prevSpine = Cases[spineCells, spine[spineCells[[i, PREV]], __]][[1]];
            AppendTo[vizSpine, Line[{spineCells[[i, POS]], prevSpine[[POS]]}]];
           ];
           energyFunc[e_] := ColorData["TemperatureMap"][e^2/(π/4)];


           For[i = 1, i ≤ Length@camObjects, i++,
            curCam = camObjects[[i]];
```

```
 AppendTo[viz, {If[energyMap, energyFunc[curCam⟦ANGLE⟧ / Sqrt[60.]], Black],
   RegularPolygon[curCam⟦POS⟧, shapeRadius, 6], Black}];
];

(* make an array of all the pointed ends *)
pointCells = Join[Cases[moleculeList,
   actin[_, _, aIDFreeP, _, _, _, _, POI, _, _, _, _, _]], Cases[
   moleculeList, actin[_, _, aIDFreeP, _, _, _, _, POIMEM, _, _, _, _, _]]];

(* Iterate through all of the pointed ends *)
While[Length[pointCells] ≠ 0,
 curCell = pointCells⟦1⟧;
 pointCells = Drop[pointCells, 1];

 (* draw circle for the first monomer - the pointed end *)

 AppendTo[viz, {If[energyMap,
    energyFunc[curCell⟦ANGLE⟧ Boole[curCell⟦NEXT⟧ ≠ aIDFreeB &&
         curCell⟦PREV⟧ ≠ aIDFreeP]] Boole[curCell⟦ADPCofCount⟧ < nCG / 2] +
     energyFunc[curCell⟦ANGLE⟧ / Sqrt[5] Boole[curCell⟦NEXT⟧ ≠ aIDFreeB &&
         curCell⟦PREV⟧ ≠ aIDFreeP]] Boole[curCell⟦ADPCofCount⟧ ≥ nCG / 2],
    Red], Disk[curCell⟦POS⟧, shapeRadius]}];
 If[verbose, AppendTo[viz,
   {Black, Text[ToString[Round[curCell⟦ID⟧]], curCell⟦POS⟧]}]];

 If[curCell⟦CROSSLINKING⟧ ≠ 0,
  AppendTo[viz, {Black, Line[{Select[camObjects,
         #⟦ID⟧ == curCell⟦CROSSLINKING⟧ &]⟦1⟧⟦POS⟧, curCell⟦POS⟧}]}];
 ];
 (* if there is a branch,
 draw the arp-actin and add the actin to the stack*)
 If[curCell⟦BRANCH⟧ ≥ 0., Block[{curArp},
   (* grab the arp-actin that is connected to this actin *)
   curArp =
    Select[moleculeList, Head[#] === actin && #⟦1⟧ == curCell⟦BRANCH⟧ &]⟦1⟧;
   PrependTo[stack, {curCell, curArp, Black, curCell⟦POS⟧}];
  ]]; (* end if for checking the branch *)
 If[curCell⟦NEXT⟧ ≠ aIDFreeB, PrependTo[stack, {curCell, Cases[
      moleculeList, actin[curCell⟦NEXT⟧, __]]⟦1⟧, Black, curCell⟦POS⟧}]];
 (* Loop while the stack has elements in it *)
 While[Length[stack] ≠ 0,
(* grab the color, curCell,
and prevCell from the top of the stack then delete the elem *)
prevCell = stack⟦1, 1⟧;
curCell = stack⟦1, 2⟧;
color = stack⟦1, 3⟧;
prevPos = stack⟦1, 4⟧;
(* draw the arrow from the current node to the previous node *)
PrependTo[vizLines, {Black, Line[{curCell⟦POS⟧, prevPos}]}];
(** draw a triangle if it is a capping monomer, circle otherwise **)
If[curCell⟦TYPE⟧ == CAP,
 (* draw the triangle to represent the capping monomer *)
 AppendTo[viz,
  {Black, Triangle[{{curCell⟦POS⟧⟦1⟧, curCell⟦POS⟧⟦2⟧ - shapeRadius},
     curCell⟦POS⟧ + {-newPos[{0, shapeRadius}, Pi / 3]⟦1⟧,
       newPos[{0, shapeRadius}, Pi / 3]⟦2⟧},
     curCell⟦POS⟧ + { newPos[{0, shapeRadius}, Pi / 3]⟦1⟧,
       newPos[{0, shapeRadius}, Pi / 3]⟦2⟧}}]}],
 (* draw the circle to represent the monomer *)
 AppendTo[viz, {If[energyMap && curCell⟦NEXT⟧ == aIDFreeB, Green,
    energyFunc[curCell⟦ANGLE⟧] Boole[curCell⟦ADPCofCount⟧ < nCG / 2] +
     energyFunc[curCell⟦ANGLE⟧ / Sqrt[5]] Boole[curCell⟦ADPCofCount⟧ ≥ nCG / 2]],
   If[curCell⟦BRANCH⟧ ≥ 0., Triangle[{{curCell⟦POS⟧⟦1⟧, curCell⟦POS⟧⟦2⟧ +
        shapeRadius}, curCell⟦POS⟧ + {-shapeRadius, -shapeRadius},
      curCell⟦POS⟧ + { shapeRadius, -shapeRadius}}],
    Disk[curCell⟦POS⟧, shapeRadius]]}];
 (* draw the cellID *)
 If[verbose, AppendTo[viz,
   {Black, Text[ToString[Round[curCell⟦ID⟧]], curCell⟦POS⟧]}]];
];

stack = Drop[stack, 1];

If[curCell⟦CROSSLINKING⟧ ≠ 0,
 AppendTo[viz, {Black, Line[{Select[camObjects,
        #⟦ID⟧ == curCell⟦CROSSLINKING⟧ &]⟦1⟧⟦POS⟧, curCell⟦POS⟧}]}];
];
If[curCell⟦BRANCH⟧ ≥ 0., Module[{curArp},
  (* grab the arp that is connected to this actin *)
  curArp =
   Select[moleculeList, Head[#] === actin && #⟦1⟧ == curCell⟦BRANCH⟧ &]⟦1⟧;
```

```
        AppendTo[viz, {Black, Line[{curArp⟦POS⟧, curCell⟦POS⟧}],
          energyFunc[curArp⟦ANGLE⟧] Boole[curArp⟦ADPCofCount⟧ < nCG / 2] +
           energyFunc[curArp⟦ANGLE⟧ / Sqrt[5]] Boole[curArp⟦ADPCofCount⟧ ≥ nCG / 2],
          If[curArp⟦TYPE⟧ == CAP, AppendTo[viz, {Black, Triangle[
              {{curArp⟦POS⟧⟦1⟧, curArp⟦POS⟧⟦2⟧ - shapeRadius}, curArp⟦POS⟧ +
                {-newPos[{0, shapeRadius}, Pi / 3]⟦1⟧, newPos[{0, shapeRadius},
                   Pi / 3]⟦2⟧}, curArp⟦POS⟧ + { newPos[{0, shapeRadius}, Pi / 3]⟦
                  1⟧, newPos[{0, shapeRadius}, Pi / 3]⟦2⟧}}]}],
           Rectangle[curArp⟦POS⟧ - {shapeRadius, shapeRadius},
            curArp⟦POS⟧ + {shapeRadius, shapeRadius}]]}];
        If[curArp⟦NEXT⟧ ≠ aIDFreeB,
         (*add the branch's first actin to the stack*)
         PrependTo[stack, {curArp, Select[moleculeList, Head[#] ===
                actin && #⟦1⟧ == curArp⟦NEXT⟧ &]⟦1⟧, Black, curArp⟦POS⟧}];
        ];
       ]];
      If[curCell⟦NEXT⟧ ≠ aIDFreeB, PrependTo[stack, {curCell, Cases[
           moleculeList, actin[curCell⟦NEXT⟧, __]]⟦1⟧, Black, curCell⟦POS⟧}]];
     ];
    ];
    {Length[moleculeList], Flatten[Prepend[Prepend[viz, vizLines], vizSpine]],
     BarLegend[{"TemperatureMap", {0, 2}}]}];
```

In[∘]:=
```
(* function to grab a list of all the actin types from full simulation *)
makeMoleculeLists[simulationArray_] :=
 Join[Cases[simulationArray, actin[__]],
  Cases[simulationArray, spine[ __]], Cases[simulationArray, cam[ __]]]
```

In[∘]:=
```
(* function to return graphics list for all snapshots in a sim *)
vizSim[simulationArray_, verbose_, energyMap_, n_ : 10, tmax_ : 0.] :=
  Module[{vizList, dt, mLists, bbox, timePos, t, start, simList = {}},
   mLists = makeMoleculeLists[#] & /@ simulationArray⟦ ;; , 2⟧;
   bbox = {White, Rectangle[{Min[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]] - 2,
       Min[Map[#⟦POS, 2⟧ &, Flatten[mLists]]] - 2},
      {Max[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]] + 2,
       Max[Map[#⟦POS, 2⟧ &, Flatten[mLists]]] + 2}]};
   timePos = {(Max[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]] +
        Min[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]]) / 2,
     Max[Flatten[Map[#⟦POS, 2⟧ &, #] & /@ mLists]] + 1};
   simList = Transpose[{simulationArray⟦ ;; , 1⟧, mLists}];
```

```
    vizList = Map[
      Graphics[Join[bbox, Append[VisualizeActinSnapshot[#[[2]], verbose, True][[2]],
           {Black, Text[Style["Time: " <> ToString[Round[(#[[1]] * 1000)] / 1000.] <>
               " secs.", Bold, FontSize → 14, FontColor → Darker[LightBlue]],
             timePos]}], {Line[{{0, Min[Map[#[[POS, 2]] &, Flatten[mLists]]] - 1},
             {2, Min[Map[#[[POS, 2]] &, Flatten[mLists]]] - 1}}],
           Text[ToString[N@Round[actinObjectRise * 10^6 * 2 * 100] / 100] <> "μm",
            {1, Min[Map[#[[POS, 2]] &, Flatten[mLists]]] -
              1.75}]}] // Flatten] &, simList]
   ];
sampleSim[directory_, dt_ : 0.005] :=
 Module[{files, simList, maxTime, simNumbers, fgi, filegroups,
    simulationArray, t, sim, i, j, globString = "simSpine*.wls"},
  simList = {};
  files = directory <> "/" <> # <> ".wls" & /@ SortBy[FileBaseName[#] & /@
      FileNames[directory <> "/" <> globString], processFileNames];

  simNumbers = Range[Length@filegroups];
  simulationArray = {};
  t = 0;
  For[i = 1, i ≤ Length@files, i += 1,
   sim = Import[files[[i]]][[2]];
   For[j = 1, j ≤ Length@sim, j++,
    If[sim[[j, 1]] ≥ t,
     AppendTo[simulationArray, sim[[j]]];
     t += dt;
    ]
   ]
  ];
  simulationArray
 ]
```

```
In[◦]:= animateGrowth[simulationArray_, verbose_ : False] :=
  Module[{mLists, bbox, timePos},
   mLists = makeMoleculeLists /@ simulationArray[[ ;; , 2]];
   bbox = {White, Rectangle[{Min[Flatten[Map[#[[POS, 1]] &, #] & /@ mLists]] - 2,
       Min[Map[#[[POS, 2]] &, Flatten[mLists]]] - 2},
      {Max[Flatten[Map[#[[POS, 1]] &, #] & /@ mLists]] + 2,
       Max[Map[#[[POS, 2]] &, Flatten[mLists]]] + 2}]};
   timePos = {(Max[Flatten[Map[#[[POS, 1]] &, #] & /@ mLists]] +
        Min[Flatten[Map[#[[POS, 1]] &, #] & /@ mLists]]) / 2,
     Max[Flatten[Map[#[[POS, 2]] &, #] & /@ mLists]] + 1};
   frames =
    Map[Show[{Graphics[Join[bbox, Append[VisualizeActinSnapshot[#⟦2⟧, verbose,
              True]⟦2⟧, {Black, Text[Style["Time: " <> ToString[#⟦1⟧] <>
                ", Frame: " <> ToString[#⟦3⟧], Bold, FontSize → 14, FontColor →
                Darker[LightBlue]], timePos]}] // Flatten]]}] &, Transpose[
      {#⟦1⟧ & /@ simulationArray, mLists, Range[Length@simulationArray]}]];
   ListAnimate[frames]
  ];

processFileNames[name_] :=
 ToExpression@StringDelete[name, LetterCharacter]

animateGrowthDirectory[directory_, globString_, outDir_, dt_ : 0.001] :=
  Module[{start, simList, t, mLists, bbox, timePos,
    files, lastFrame, i, j, frameNumber, frames},
   files = SortBy[
     FileBaseName[#] & /@ FileNames[directory <> globString], processFileNames];
   files = directory <> # <> ".wls" & /@ files;
   simList = sampleSim[directory, dt];

   mLists = makeMoleculeLists[#⟦2⟧] & /@ simList;
   bbox = {White, Rectangle[{Min[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]] - 2,
       Min[Map[#⟦POS, 2⟧ &, Flatten[mLists]]] - 2},
      {Max[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]] + 2,
       Max[Map[#⟦POS, 2⟧ &, Flatten[mLists]]] + 2}]};
   timePos = {(Max[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]] +
        Min[Flatten[Map[#⟦POS, 1⟧ &, #] & /@ mLists]]) / 2,
     Max[Flatten[Map[#⟦POS, 2⟧ &, #] & /@ mLists]] + 1};
   simList = Transpose[{Range[0, Length@mLists - 1] * dt, mLists}];
   CreateDirectory[outDir];
   frameNumber = 0;
   frames =
    Map[Graphics[Join[bbox, Append[VisualizeActinSnapshot[#⟦2⟧, False, True]⟦2⟧,
          {Black, Text[Style["Time: " <> ToString[#⟦1⟧] <> " s.",
             Bold, FontSize → 14, FontColor → Darker[LightBlue]],
            timePos]}]] // Flatten] &, simList];
   For[j = 1, j ≤ Length@frames, j++,
    frameNumber++;
    Export[
     outDir <> "frame_" <> IntegerString[frameNumber, 10, 8] <> ".png", frames⟦j⟧];
   ];
  ];

animateGrowthDirectorySet[directory_, globString_, outDir_, dt_ : 0.001] :=
Module[{simList, start, t, mLists, bbox, timePos, files, end, lastFrame,
    frames, simulationArray, frame, groupfiles, filegroups, fgi,
    maxTime, simSubList, xs, ys, maxis, simNumbers, i, j, sim, dim},
  simList = {};
  groupfiles = FileNames[directory];
  groupfiles =
    DeleteCases[groupfiles, DirectoryName[directory] <> ".DS_Store"];
  filegroups = {};
  For[i = 1, i ≤ Length@groupfiles, i++,
    AppendTo[filegroups,
      (groupfiles⟦i⟧ <> "/" <> # <> ".wls" & /@ SortBy[FileBaseName[#] & /@
          FileNames[groupfiles⟦i⟧ <> "/" <> globString], processFileNames])];
  ];

  maxTime = Max[Import[#⟦-1⟧]⟦2, -1, 1⟧ & /@ filegroups];
  simList = {};
  progressbar =
    StringRepeat["|", 1] <> StringRepeat[" ", Length@filegroups - 1] <> "|";
  Print[Dynamic[progressbar]];
  simNumbers = Range[Length@filegroups];
  For[fgi = 1, fgi ≤ Length@filegroups, fgi++,
    files = filegroups⟦fgi⟧;
    simulationArray = {};
    t = 0;
    For[i = 1, i ≤ Length@files, i += 1,
      sim = Import[files⟦i⟧]⟦2⟧;
      For[j = 1, j ≤ Length@sim, j++,
        If[sim⟦j, 1⟧ ≥ t,
          AppendTo[simulationArray, sim⟦j, 2⟧];
          t += dt;
        ]
      ]
    ];
    AppendTo[simList, simulationArray];
    progressbar =
      StringRepeat["|", fgi] <> StringRepeat[" ", Length@filegroups - fgi] <> "|";
  ];
  mLists = makeMoleculeLists /@ # & /@ simList;
  xs = #⟦1⟧ & /@ Select[#⟦POS⟧ & /@ Flatten[mLists], ListQ];
  ys = #⟦2⟧ & /@ Select[#⟦POS⟧ & /@ Flatten[mLists], ListQ];
  bbox =
    {White, Rectangle[{Min[xs] - 2, Min[ys] - 2}, {Max[xs] + 2, Max[ys] + 2}]};
  timePos = {(Max[xs] + Min[xs]) / 2, Max[ys] + 1};
```

```
    simList = Transpose@{Range[0, Length@#] & /@ mLists, mLists};
    maxis = Length@# & /@ mLists;
    CreateDirectory[outDir];
    dim = QuotientRemainder[Length@filegroups, Floor[Sqrt@Length@filegroups]];
    If[dim⟦2⟧ ≠ 0, dim = dim⟦1⟧ - 1;, dim = dim⟦1⟧;];
    Do[frame = GraphicsRow[
       {GraphicsGrid[Partition[(Graphics[Join[bbox, (VisualizeActinSnapshot[
                    simList⟦#⟧⟦2⟧⟦Min[{maxis⟦#⟧, frameN + 1}]⟧, False, True]⟦2⟧),
                 {Black, Text[Style["Time: " <> ToString[NumberForm[
                       simList⟦#⟧⟦1⟧⟦Min[{maxis⟦#⟧, frameN + 1}]⟧ * dt, {5, 4}]] <>
                     " s.", Bold, FontSize → 14, FontColor → Darker[LightBlue]],
                   timePos]}, {Line[{{0, Min[Map[#⟦POS, 2⟧ &, Flatten[mLists]]] -
                      1}, {2, Min[Map[#⟦POS, 2⟧ &, Flatten[mLists]]] - 1}}],
                  Text[ToString[N@Round[actinObjectRise * 10^6 * 2 * 1000] / 1000] <>
                    " μm", {1, Min[Map[#⟦POS, 2⟧ &, Flatten[mLists]]] -
                      1.75}]}]] & /@ Range[1, Length@filegroups]),
             (dim Boole[dim ≠ 0] + Boole[dim == 0]) // UpTo] // Transpose,
          Frame → All], BarLegend[{"TemperatureMap",
           {0, κB * actinObjectRise^2 π / 4}},
          LegendFunction → "Frame", LegendLabel →
           "Bending Energy in Joules"]}, Frame → True];
      Export[outDir <> "frame_" <> IntegerString[frameN, 10, 8] <> ".png", frame];,
      {frameN, 0, Max@maxis}];
  ];
```

Plotting

```
In[ ]:= plotSim[simulationArray_, slices_ : 1] :=
         Module[{totalActin = Map[{#[[1]], Length[Select[#[[2]], Head[#] === actin &]] * nCG +
                Cases[#[[2]], actinATPCount[_]][[1, 1]] +
                Cases[#[[2]], actinADPCount[_]][[1, 1]]} &,
             simulationArray[[1 ;; Length@simulationArray ;; slices]]],
           SA = simulationArray[[1 ;; Length@simulationArray ;; slices]], data},
          data = {
            Map[{#[[1]], Length[Select[#[[2]], Head[#] === actin &]] * nCG} &, SA],
            Map[{#[[1]], Total[If[Head[#] === actin, #[[ATPCount]], 0] & /@ #[[2]]]} &, SA],
            Map[{#[[1]], Total[If[Head[#] === actin, #[[ADPCount]], 0] & /@ #[[2]]] +
                Total[If[Head[#] === actin, #[[ADPCofCount]], 0] & /@ #[[2]]] +
                Total[If[Head[#] === actin, #[[ADPPiCount]], 0] & /@ #[[2]]]} &, SA],
            Map[{#[[1]], Total[If[Head[#] === actin, #[[ADPCofCount]], 0] & /@ #[[2]]]} &, SA],
            Map[{#[[1]], Cases[#[[2]], actinATPCount[_]][[1, 1]] +
                Cases[#[[2]], actinADPCount[_]][[1, 1]]} &, SA],
            totalActin,
            Map[{#[[1]], Cases[#[[2]], actinATPCount[_]][[1, 1]]} &, SA],
            Map[{#[[1]], Cases[#[[2]], actinADPCount[_]][[1, 1]]} &, SA]};
          ListLinePlot[data,
           PlotLegends → {"Polymerized Actin", "Polymerized Actin-ATP",
             "Polymerized Actin-ADP", "Bound Cofilin", "Free Actin",
             "Total Actin", "G-Actin-ATP", "G-Actin-ADP"}, PlotRange →
            {{simulationArray[[1, 1]], simulationArray[[-1, 1]]}, {0, Max[totalActin]}},
           Frame → True, FrameLabel → {"Time (s)", "Actin Molecule Number"},
           PlotLabel → "Plot of Number of Molecules"]
         ]
```

Molecule Rules

Here we define the rules that govern the changes in the number of free molecules without a change in the actin network structure. There is one rule that changes the type of bound nucleotide to actins in filaments. We have ARP synthesis and degradation, actin synthesis and degradation, actin-ADP and actin-ATP dissociation, F-Actin hydrolysis (conversion of F-actin-ATP to F-actin-ADP).

```
In[ ]:= (* rules for ARP synthesizing and degrading *)
        rulesMolVanilla = {
           (* ARP synthesis *)
           {arpCount[numArp], spineHeadArea[area]} →
            {arpCount[numArp], spineHeadArea[area]},
           solving[numArp' == arpRate Boole[numArp > 0]],

           (* ARP degradation *)
```

```
  (arpCount[numArp] → arpCount[numArp]),
  solving[numArp' == -arpDeg * numArp Boole[numArp > 0]],

  (* Cap synthesis *)
  {cappingCount[numCap], spineHeadArea[area]} →
   {cappingCount[numCap], spineHeadArea[area]},
  solving[numCap' == capRate],

  (* Cap degradation *)
  (cappingCount[numCap] → cappingCount[numCap ]),
  solving[numCap' == -capDeg * numCap Boole[numCap > 0]],

  (* Cam synthesis *)
  {camCount[numCam], spineHeadArea[area]} →
   {camCount[numCam], spineHeadArea[area]},
  solving[numCam' == camRate],

  (* Cam degradation *)
  (camCount[numCam] → camCount[numCam]),
  solving[numCam' == -camDeg * numCam Boole[numCam > 0]],

  (* Cofilin synthesis *)
  {cofilinCount[numCofilin], spineHeadArea[area]} →
   {cofilinCount[numCofilin], spineHeadArea[area]},
  solving[numCofilin' == cofilinRate],

  (* Cofilin degradation *)
  (cofilinCount[numCofilin] → cofilinCount[numCofilin]),
  solving[numCofilin' == -cofilinDeg * numCofilin Boole[numCofilin > 0]],

  (* Actin synthesis *)
  {actinATPCount[numActin], spineHeadArea[area]} →
   {actinATPCount[numActin], spineHeadArea[area]},
  solving[numActin' == actinRate],

  (* Actin degradation *)
  ({actinATPCount[numActin] , spineHeadArea[area]} →
    { actinATPCount[numActin], spineHeadArea[area]}),
  solving[numActin' == -actinDeg * numActin Boole[numActin > 0]],

  {actinADPCount[numActin] , spineHeadArea[area]} →
   {actinADPCount[numActin], spineHeadArea[area]},
  solving[numActin' == -actinDeg * numActin Boole[numActin > 0]]
 };
```

```
rulesNuc = {
   (*Hydrolysis of F-Actin-Nucleotides*)
   {actin[aID, coords, aIDP, NID, randAng, clID, arpID, type,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     spineHeadArea[area]} → {actin[aID, coords, aIDP, NID, randAng,
      clID, arpID, type, membraneID, ATPCountCG - 1, ADPCountCG,
      ADPPiCountCG + 1, ADPCofCountCG], spineHeadArea[area]},
   with[kATPHydrolysis Boole[ATPCountCG ≥ 1] ATPCountCG],
   {actin[aID, coords, aIDP, NID, randAng, clID, arpID, type,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     spineHeadArea[area]} → {actin[aID, coords, aIDP, NID, randAng,
      clID, arpID, type, membraneID, ATPCountCG, ADPCountCG + 1,
      ADPPiCountCG - 1, ADPCofCountCG], spineHeadArea[area]},
   with[kPiRelease Boole[ADPPiCountCG ≥ 1] ADPPiCountCG],

   {a1 == actin[aID, coords, aIDP, aIDNext, angle, clID, arpID, end,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     actin[aIDNext, coordsN, aID, aIDNN, angleN, clIDN, arpIDN, endN,
      membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
     spineHeadArea[area]} → {a1, actin[aIDNext, coordsN, aID, aIDNN,
      angleN, clIDN, arpIDN, endN, membraneIDN, ATPCountCGN, ADPCountCGN + 1,
      ADPPiCountCGN - 1, ADPCofCountCGN], spineHeadArea[area]},
   with[Boole[ADPCofCountCG > 0] kCofPiRelease ADPPiCountCGN],
   {actin[aID, coords, aIDP, aIDNext, angle, clID, arpID, end,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     aN == actin[aIDNext, coordsN, aID, aIDNN, angleN, clIDN, arpIDN, endN,
       membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
     spineHeadArea[area]} → {aN, actin[aID, coords, aIDP, aIDNext,
      angle, clID, arpID, end, membraneID, ATPCountCG, ADPCountCG + 1,
      ADPPiCountCG - 1, ADPCofCountCG], spineHeadArea[area]},
   with[Boole[ADPCofCountCGN > 0] kCofPiRelease ADPPiCountCG],

   {actin[aID, coords, aIDP, NID, randAng, clID, arpID, type,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     spineHeadArea[area]} → {actin[aID, coords, aIDP, NID, randAng,
      clID, arpID, type, membraneID, ATPCountCG, ADPCountCG + 1,
      ADPPiCountCG - 1, ADPCofCountCG], spineHeadArea[area]},
   with[kCofPiRelease Boole[ADPPiCountCG > 0 && ADPCofCountCG > 0] ADPPiCountCG],


   (*Break filaments*)
   {aP == actin[aIDP, coordsP, aIDPP, aID, angleP, clIDP, arpIDP, endP,
       distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, aIDP, aIDNext, angle, clID, aIDN, end, dist,
     ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[aIDN, coordsN, aID, aIDNN, angleN, clIDN, arpIDN, INT, distN,
     ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} → {
    aP, actin[aID, coords, aIDP, aIDNext, angle, clID, arpIDFree,
     end, dist, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[aIDN, coordsN, aIDFreeP, aIDNN, 0., clIDN, arpIDN, POI, distN,
     ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]},
  with[boundarySpineFactor Boole[
     Abs@(ArcCos[(coords - coordsP).(coordsN - coords) /
        (Norm[(coords - coordsP)] Norm[(coordsN - coords)])] - θArp) >
       25 Degree || Norm[coords - coordsN] > overgrowthL]],
  {actin[aIDP, coordsP, aIDPP, aID, angleP, clIDP, arpIDP, INT,
     distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, aIDP, aIDN, angle, clID, arpID, INT, dist,
     ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG]} → {
    actin[aIDP, coordsP, aIDPP, aIDFreeB, 0., clIDP, arpIDP, BAR,
     distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, aIDFreeP, aIDN, 0., clID, arpID, POI, dist,
     ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG]},
  with[boundarySpineFactor Boole[Norm[coords - coordsP] > overgrowthL ||
      ((Abs@angle > bareAngle && ADPCofCountCG == 0.) ||
        (Abs@angleP > bareAngle && ADPCofCountCGP == 0.)) ||
      ((Abs@angle > cofAngle && ADPCofCountCG ≥ nCG / 2) ||
        (Abs@angleP > cofAngle && ADPCofCountCGP ≥ nCG / 2)) ||
      ((Abs@angle > boundaryAngle && ADPCofCountCG ≠ ADPCofCountCGP) ||
        (Abs@angleP > boundaryAngle && ADPCofCountCGP ≠ ADPCofCountCG))]]
 };
```

Barbed End Rules

In[ ]:=
```
rulesBarb = {

   (**** elongation at the barbed end ****)
   (* Will destroy the current end and make two new nodes,
   one to recreate the current end and one to add a new node *)
   (** growing in a straight line with the previous being an actin **)
   (* X → actinP → actinEnd → newActinEnd *)
   (*Rule for elongating in the presence of free actin-ATP*)

   {aP == actin[aIDP, coordsP, aIDPP, aIDPN, angleP, clIDP, arpIDP, endP,
      membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, aIDP,  aIDFreeB, angle, clID, arpID, BAR,
     membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    newID[NID],
    actinATPCount[numActin],
    spineHeadArea[area]
   } → {
    actinATPCount[numActin - nCG],
    newID[NID + 1], aP,
    spineHeadArea[area],
    (* make the replacement node for the new INT *)
    actin[aID, coords, aIDP, NID, randAng, clID, arpID, INT,
     membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    (* make the newly created end node *)
    actin[NID,
     coords + newPos[coords - coordsP, randAng] / Norm[coords - coordsP], aID,
     aIDFreeB, angle, 0.0, arpIDFree, BAR, membraneIDFree, nCG, 0.0, 0.0, 0.0]
   },
  with[barbGrowthT numActin *
    grammarPDF[NormalDistribution[0.0, sdGrowth], randAng]],

  (*Rule for elongating when
    previous actin in the presence of free actin-ADP*)
  {aP == actin[aIDP, coordsP, aIDPP, aIDPN, angleP, clIDP, arpIDP, endP,
      membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, aIDP,  aIDFreeB, angle, clID, arpID, BAR,
     membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    newID[NID],
    actinADPCount[numActin],
    spineHeadArea[area]} → {
    actinADPCount[numActin - nCG],
    newID[NID + 1], aP,
    spineHeadArea[area],
    (* make the replacement node for the new INT *)
    actin[aID, coords, aIDP, NID, randAng, clID, arpID, INT,
     membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    (* make the newly created end node *)
    actin[NID,
     coords + newPos[coords - coordsP, randAng] / Norm[coords - coordsP], aID,
     aIDFreeB, 0.0, 0.0, arpIDFree, BAR, membraneIDFree, 0.0, nCG, 0.0, 0.0]
   },
  with[barbGrowthD numActin *
    grammarPDF[NormalDistribution[0.0, sdGrowth], randAng]],
(**** retraction at the barbed end ****)
(** remove one actin when the previous is an actin,
removal of an actin  **)
(* X → newActinEnd → oldActinEnd *)

{actin[aID, coords, aIDP, aIDFreeB, angle, 0.0, arpID, BAR, membraneIDFree,
   ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
  actin[aIDP, coordsP, aIDPP, aID, angleP, 0.0, arpIDP, INT, membraneIDP,
   ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP], actinATPCount[
   numActinATP], cofilinCount[numCofilin], actinADPCount[numActinADP],
  spineHeadArea[area]
 } →
 {
  actinATPCount[numActinATP + ATPCountCG],
  actinADPCount[numActinADP + ADPCountCG + ADPPiCountCG + ADPCofCountCG],
  cofilinCount[numCofilin + ADPCofCountCG],
  spineHeadArea[area],
  actin[aIDP, coordsP, aIDPP, aIDFreeB, 0.0, 0.0, arpIDP, BAR, membraneIDP,
   ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP]
 },
with[barbRetr Boole[arpID == arpIDFree] Boole[aIDPP ≠ aIDFreeP]],
{actin[aID, coords, aIDP, aIDFreeB, angle, 0.0, arpID, BARMEM,
   membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
  actin[aIDP, coordsP, aIDPP, aID, angleP, 0.0, arpIDP, INT, membraneIDP,
   ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP], actinATPCount[
   numActinATP], actinADPCount[numActinADP], cofilinCount[numCofilin],
  spineHeadArea[area], spineAtt[aID, sp0, sp1]
 } →
 {
  actinATPCount[numActinATP + ATPCountCG],
  actinADPCount[numActinADP + ADPCountCG + ADPPiCountCG + ADPCofCountCG],
  cofilinCount[numCofilin + ADPCofCountCG],
  spineHeadArea[area],
  actin[aIDP, coordsP, aIDPP, aIDFreeB, 0.0, 0.0, arpIDP, BAR, membraneIDP,
   ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP]
 },
with[barbRetr Boole[arpID == arpIDFree] Boole[aIDPP ≠ aIDFreeP]],

(* allow actin monomers to bind and unbind with new arp complexes *)
(* actin bind to arp *)
{aP == actin[aIDP, coordsP,
    aIDPP, aID, angleP, clIDP, arpID, INT, membraneIDFree,
    ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
  actin[aID, coords, aIDP, aIDNN, angle, clID, ARPACTID, type,
     membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    newID[NID], actinATPCount[numActin], spineHeadArea[area]} → {
    actinATPCount[numActin - nCG],
    newID[NID + 1], aP,
    spineHeadArea[area],
    (* make the replacement node for the new arp *)
    actin[aID, coords, aIDP, aIDNN, angle, clID, NID, type,
     membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    (* make the newly created end node *)
    actin[NID, coords + newPos[coords - coordsP,
        θArp (1 - 2 Boole[branchSide > 0.5])] / Norm[coords - coordsP], aID,
     aIDFreeB, 0.0, 0.0, arpIDFree, BAR, membraneIDFree, nCG, 0.0, 0.0, 0.0]
   },
  with[Boole[numActin > nCG] barbGrowthT * numActin *
    grammarPDF[UniformDistribution[{0, 1}], branchSide] Boole[type ≠ CAP]],

  (* actin unbinding from the arp complex
   if it is the last monomer and has no branches from it *)
  {actin[arpPrev, coordsP, aIDP, aIDN, angleP, clIDP, aID, type, membraneIDP,
     ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, arpPrev, aIDFreeB, angle, 0.0, arpID, BAR,
     membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actinATPCount[numActinATP], actinADPCount[numActinADP],
    cofilinCount[numCofilin],
    spineHeadArea[area], arpCount[numArp]} → {
    arpCount[numArp + Boole[arpID ≠ arpIDFree]],
    actinATPCount[numActinATP + ATPCountCG],
    actinADPCount[numActinADP + ADPCountCG + ADPPiCountCG + ADPCofCountCG],
    cofilinCount[numCofilin + ADPCofCountCG],
    (* recreate the arp complex and have it point to empty space *)
    actin[arpPrev, coordsP, aIDP, aIDN, angleP, clIDP, ARPACTID, type,
     membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    spineHeadArea[area]
   },
  with[barbRetr Boole[arpID < 0]],
  {actin[arpPrev, coordsP, aIDP, aIDN, angleP, clIDP, aID, type, membraneIDP,
     ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, arpPrev, aIDFreeB, angle, 0.0, arpID, BARMEM,
     membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actinATPCount[numActinATP], actinADPCount[numActinADP],
    spineHeadArea[area], spineAtt[aID, sp0, sp1],
    arpCount[numArp], cofilinCount[numCofilin]} → {
    arpCount[numArp + Boole[arpID ≠ arpIDFree]],
    spine[membraneID, sCoords,
       sIDP, sIDN, membraneIDFree, centralID1, centralID3],
      actinATPCount[numActinATP + ATPCountCG],
      actinADPCount[numActinADP + ADPCountCG + ADPPiCountCG + ADPCofCountCG],
      cofilinCount[numCofilin + ADPCofCountCG],
      (* recreate the arp complex and have it point to empty space *)
      actin[arpPrev, coordsP, aIDP, aIDN, angleP, clIDP, ARPACTID, type,
       membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      spineHeadArea[area]
     },
    with[barbRetr Boole[arpID < 0]]
   };
```

Pointed End Rules

```
In[ ]:= (* rules for model b *)
rulesPoint := {
   (* elongation at the pointed end *)
   (* identical in many ways to the barbed end elongation*)
   {aP == actin[aIDN, coordsN, aID, aIDNN, angleN, clIDP, arpIDN, typeN,
        membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
     actin[aID, coords, aIDFreeP, aIDN, angle, clID, arpID, POI,
      membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     newID[NID], actinATPCount[numActin],
     spineHeadArea[area]} → {
     actinATPCount[numActin - nCG],
     spineHeadArea[area],
     (* update the newID object so it can create unique object ids *)
     newID[NID + 1],
     aP,
     (* recreate the current node as a INT *)
     actin[aID, coords, NID, aIDN, -randAng, clID, arpID, INT,
      membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (* make the new node at the pointed end *)
     actin[NID,
      coords + newPos[coords - coordsN, randAng] / Norm[coords - coordsN],
      aIDFreeP, aID, 0.0, 0.0, arpIDFree, POI, membraneIDN,
      nCG, 0.0, 0.0, 0.0] (* same as with barbed,
     for the sake of simplicity it will grow in a simple line *)
    },
    with[Boole[numActin > nCG] pointGrowthT numActin *
      grammarPDF[NormalDistribution[0.0, sdGrowth], randAng]],
   (*Rule for elongating in the presence of free actin-ADP*)
```

```
{aP == actin[aIDN, coordsN, aID, aIDNN, angleN, clIDP, arpIDN, typeN,
     membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
   actin[aID, coords, aIDFreeP, aIDN, angle, clID, arpID, POI,
    membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   newID[NID], actinADPCount[numActin],
   spineHeadArea[area]} → {
   actinADPCount[numActin - nCG],
   spineHeadArea[area],
   (* update the newID object so it can create unique object ids *)
   newID[NID + 1],
   aP,
   (* recreate the current node as a INT *)
   actin[aID, coords, NID, aIDN, -randAng, clID, arpID, INT,
    membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   (* make the new node at the pointed end *)
   actin[NID,
    coords + newPos[coords - coordsN, randAng] / Norm[coords - coordsN],
    aIDFreeP, aID, 0.0, 0.0, arpIDFree, POI, membraneIDN,
    0.0, nCG, 0.0, 0.0] (* same as with barbed,
   for the sake of simplicity it will grow in a simple line *)
  },
with[Boole[numActin > nCG] pointGrowthD numActin
   grammarPDF[NormalDistribution[0.0, sdGrowth], randAng]],
(* retraction at the pointed end *)

{actin[aID, coords, aIDFreeP, aIDN, angle, 0.0, arpID, POIMEM,
    membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   actin[aIDN, coordsN, aID, aIDNN, angleN, 0.0, arpIDN, INT, membraneIDN,
    ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
   actinATPCount[numATPActin], cofilinCount[numCofilin],
   actinADPCount[numADPActin],
   spineHeadArea[area], spineAtt[aID, sp0, sp1]} → {
   spineHeadArea[area],
   actinATPCount[numATPActin + ATPCountCG],
   actinADPCount[numADPActin + ADPCountCG + ADPPiCountCG + ADPCofCountCG],
   cofilinCount[numCofilin + ADPCofCountCG],
   (* change the next node so that the current POI is dropped *)
   actin[aIDN, coordsN, aIDFreeP, aIDNN, 0.0, 0.0, arpIDN, POI, membraneIDN,
    ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
  },
with[pointRetr Boole[arpID == arpIDFree] Boole[aIDNN ≠ aIDFreeB]],
{actin[aID, coords, aIDFreeP, aIDN, angle, 0.0, arpID, POI,
    membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   actin[aIDN, coordsN, aID, aIDNN, angleN, 0.0, arpIDN, INT, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
      actinATPCount[numATPActin], cofilinCount[numCofilin],
      actinADPCount[numADPActin],
      spineHeadArea[area]} → {
      spineHeadArea[area],
      actinATPCount[numATPActin + ATPCountCG],
      actinADPCount[numADPActin + ADPCountCG + ADPPiCountCG + ADPCofCountCG],
      cofilinCount[numCofilin + ADPCofCountCG],
      (* change the next node so that the current POI is dropped *)
      actin[aIDN, coordsN, aIDFreeP, aIDNN, 0.0, 0.0, arpIDN, POI, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
     },
    with[pointRetr Boole[arpID == arpIDFree] Boole[aIDNN ≠ aIDFreeB]]
   };
```

Branching Rules

In[ ]:=
```
(* rules for model D *)
rulesBranch = {
    (* arp binding to open actin monomer *)
    {actin[aID, coords, aIDP, aIDN, angle, clID, arpIDFree, type,
       membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      arpCount[numArp], actinATPCount[numActin],
      spineHeadArea[area]} → {
      (* update the arpcount variable *)
      arpCount[numArp - 1],
      actinATPCount[numActin - 1],
      (* re-create the current actin
        monomer and have it point to the new arp protein *)
      actin[aID, coords, aIDP, aIDN, angle, clID, ARPACTID, type,
       membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      spineHeadArea[area]
     },
    with[Boole[numArp > 1] Boole[numActin > 1] numArp * branchGrowthAct],

    (* arp unbinding from an actin monomer -
     only if it does not have actin attached to it *)
    {actin[aID, coords, aIDP, aIDN, angle, clID, ARPACTID, type, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG], arpCount[numArp],
      spineHeadArea[area]} → {
      (* increase the floating arp counter *)
      arpCount[numArp + 1],
      (* recreate the actin on the parent strand *)
      actin[aID, coords, aIDP, aIDN, angle, clID, arpIDFree, type,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      spineHeadArea[area]
     },
    with[branchRetrAct],
    {actin[aID, coords, aIDP, aIDN,
       angle, clID, arpIDFree, type, membraneIDFree, ATPCountCG,
       ADPCountCG, ADPPiCountCG, ADPCofCountCG], arpCount[numArp],
      spineHeadArea[area]} → {
      (* update the arpcount variable *)
      arpCount[numArp - nCG],
      (* re-create the current actin
        monomer and have it point to the new arp protein *)
      actin[aID, coords, aIDP, aIDN, angle, clID, ARPDEACTID, type,
       membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      spineHeadArea[area]
     },
    with[Boole[numArp > nCG] numArp * branchGrowthDeact],

    (* arp unbinding from an actin monomer -
     only if it does not have actin attached to it *)
    {actin[aID, coords, aIDP, aIDN, angle, clID, ARPDEACTID, type, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG], arpCount[numArp],
      spineHeadArea[area]} → {
      (* increase the floating arp counter *)
      arpCount[numArp + nCG],
      (* recreate the actin on the parent strand *)
      actin[aID, coords, aIDP, aIDN, angle, clID, arpIDFree, type,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      spineHeadArea[area]
     },
    with[branchRetrDeact]
   };
```

Capping Rules

```
In[•]:= rulesCap := {
    (* add a capping node to the end of a filament *)
    {aP == actin[aIDP, coordsP, aIDPP, aID, angleP, clIDP, arpIDP, typeP,
        distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDFreeB, angle, clID, arpIDFree, BAR,
       membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      cappingCount[capNum], spineHeadArea[area]} → {
      (* add back the current end node
       pointing to the cap node as an internal monomer *)
      aP,
      actin[aID, coords, aIDP, aIDFreeB, angle, clID, arpIDFree, CAP,
       membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      spineHeadArea[area],
      cappingCount[capNum - 1]
     },
    with[If[ADPCofCountCG < nCG/2, cap, caponcof] * capNum],
    {actin[aID, coords, aIDP, aIDFreeB,
       angle, clID, arpID, end, membraneID, ATPCountCG, ADPCountCG,
       ADPPiCountCG, ADPCofCountCG], cappingCount[capNum]} → {
      actin[aID, coords, aIDP, aIDFreeB, angle, clID, arpID,
       Boole[end == CAP] BAR + Boole[end == CAPMEM] BARMEM, membraneID, ATPCountCG,
       ADPCountCG, ADPPiCountCG, ADPCofCountCG], cappingCount[capNum + 1]
     },
    with[
     If[ADPCofCountCG < nCG/2, capoff, capoffcof] Boole[end == CAP || end == CAPMEM]]
  };
```

Cofilin Rules

```
In[•]:= rulesCof := {
    (*Bind and unbind Cofilin to actin-ADP*)
    {
      actin[aID, coords, aIDP, aIDN, angle, clID, arpID,
       end, membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, 0.],
      cofilinCount[numCofilin],
      spineHeadArea[area]
     } → {
      actin[aID, coords, aIDP, aIDN, angle, clID, arpID,
    end, membraneID, ATPCountCG, ADPCountCG - 1, ADPPiCountCG, 1.],
   cofilinCount[numCofilin - 1], spineHeadArea[area]
  },
 with[cofBindSingle * ADPCountCG * numCofilin ],

 {
   actin[aID, coords, aIDP, aIDN, angle, clID, arpID, end,
    membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   cofilinCount[numCofilin],
   spineHeadArea[area]
  } → {
   actin[aID, coords, aIDP, aIDN, angle, clID, arpID, end, membraneID,
    ATPCountCG, ADPCountCG - 1, ADPPiCountCG, ADPCofCountCG + 1],
   cofilinCount[numCofilin - 1], spineHeadArea[area]
  },
 with[cofBindEdge ADPCountCG * numCofilin Boole[ADPCofCountCG > 0.]],
 {
   actin[aID, coords, aIDP, aIDN, angle, clID, arpID, end,
    membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   cofilinCount[numCofilin],
   spineHeadArea[area]
  } → {
   actin[aID, coords, aIDP, aIDN, angle, clID, arpID, end, membraneID,
    ATPCountCG, ADPCountCG, ADPPiCountCG - 1, ADPCofCountCG + 1],
   cofilinCount[numCofilin - 1], spineHeadArea[area]
  },
 with[cofBindPiEdge ADPPiCountCG * numCofilin Boole[ADPCofCountCG > 0.]],


 {
   actin[aID, coords, aIDP, aIDN, angle, clID, arpID, end,
    membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   cofilinCount[numCofilin],
   spineHeadArea[area]
  } → {
   actin[aID, coords, aIDP, aIDN, angle, clID, arpID, end, membraneID,
    ATPCountCG, ADPCountCG + 1, ADPPiCountCG, ADPCofCountCG - 1],
   cofilinCount[numCofilin + 1], spineHeadArea[area]
  },
 with[(ADPCofCountCG) cofUnbind ],

 (*Accelerated bind cofilin*)
 {
   a1 == actin[aID, coords, aIDP, aIDN, angle, clID, arpID,
      end, membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, nCG],
    actin[aIDN, coordsN, aID, aIDNN, angleN, clIDN, arpIDN, endN,
     membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, 0.],
    cofilinCount[numCofilin],
    spineHeadArea[area]
   } → {
    actin[aIDN, coordsN, aID, aIDNN, angleN, clIDN, arpIDN, endN,
     membraneIDN, ATPCountCGN, ADPCountCGN - 1, ADPPiCountCGN, 1.],
    cofilinCount[numCofilin - 1], a1, spineHeadArea[area]
   },
  with[cofBindEdge ADPCountCGN * numCofilin],
  {
    actin[aIDP, coordsP, aIDPP, aID, angleP, clIDP, arpIDP, endP,
     membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, 0.],
    a1 == actin[aID, coords, aIDP, aIDN, angle, clID, arpID,
      end, membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, nCG],
    cofilinCount[numCofilin],
    spineHeadArea[area]
   } → {
    actin[aIDP, coordsP, aIDPP, aID, angleP, clIDP, arpIDP, endP,
     membraneIDP, ATPCountCGP, ADPCountCGP - 1, ADPPiCountCGP, 1.],
    cofilinCount[numCofilin - 1], a1, spineHeadArea[area]
   },
  with[cofBindEdge ADPCountCGP * numCofilin],
  {
    a1 == actin[aID, coords, aIDP, aIDN, angle, clID, arpID,
      end, membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, nCG],
    actin[aIDN, coordsN, aID, aIDNN, angleN, clIDN, arpIDN, endN,
     membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, 0.],
    cofilinCount[numCofilin],
    spineHeadArea[area]
   } → {
    actin[aIDN, coordsN, aID, aIDNN, angleN, clIDN, arpIDN, endN,
     membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN - 1, 1.],
    cofilinCount[numCofilin - 1], a1, spineHeadArea[area]
   },
  with[cofBindPiEdge ADPPiCountCGN * numCofilin],
  {
    actin[aIDP, coordsP, aIDPP, aID, angleP, clIDP, arpIDP, endP,
     membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, 0.],
    a1 == actin[aID, coords, aIDP, aIDN, angle, clID, arpID,
      end, membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, nCG],
    cofilinCount[numCofilin],
    spineHeadArea[area]
    } → {
     actin[aIDP, coordsP, aIDPP, aID, angleP, clIDP, arpIDP, endP,
      membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP - 1, 1.],
     cofilinCount[numCofilin - 1], a1, spineHeadArea[area]
    },
   with[cofBindPiEdge ADPPiCountCGP * numCofilin]
  };
```

Network Remodeling Test

This section tests the actin remodeling rules defined so far.

Function for Getting Filament Lengths

In[ ]:=

```
getFActinDistribution[initMoleculeList_] :=
 Module[{pointCells, arpIDs, arps, curCell, branchLengths, moleculeList =
    initMoleculeList, branchLength, branchLengthArp = {}, branchLengthPOI = {}},
  branchLengths = {};

  (* make an array of all the pointed ends *)
  pointCells = Select[moleculeList, Head[#] === actin && #[[TYPE]] == POI & ];
  (* make an array of all the arps *)
  arpIDs = #[[BRANCH]] & /@
    Select[moleculeList, Head[#] === actin && #[[BRANCH]] ≠ arpIDFree &];
  arps = Select[moleculeList, Head[#] === actin && MemberQ[arpIDs, #[[ID]]] &];
  For[i = 1, i ≤ Length@pointCells, i ++,
   curCell = pointCells[[i]];
   branchLength = 1;
   While[curCell[[NEXT]] ≠ aIDFreeB,
    curCell =
     Select[moleculeList, Head[#] === actin && #[[ID]] == curCell[[NEXT]] &][[1]];
    branchLength ++;
    If[curCell[[TYPE]] == CAP, Break;]
   ];
   AppendTo[branchLengthPOI, branchLength * nCG];
  ];
  For[i = 1, i ≤ Length@arps, i ++,
   curCell = arps[[i]];
   branchLength = 1;
   While[curCell[[NEXT]] ≠ aIDFreeB,
    curCell =
     Select[moleculeList, Head[#] === actin && #[[ID]] == curCell[[NEXT]] &][[1]];
    branchLength ++;
   ];
   AppendTo[branchLengthArp, branchLength * nCG];
  ];

  Join[branchLengthPOI, branchLengthArp]
 ]
```

Bundling Rules

Rules

This set of rules implements bundling by CamKIIβ which has the effect of strengthening filaments.

```
In[ ]:= (*These rules bundle actin nodes that exist close to each other*)
rulesBundling =
  {
   {
     a1P == actin[aID1P, coords1P, aIDP1P, aID1,
       angle1P, CL1P, arpID1P, INT, membraneIDFree, ATPCountCG1P,
       ADPCountCG1P, ADPPiCountCG1P, ADPCofCountCG1P],
     actin[aID1, coords1, aID1P, aIDN1, angle1, 0.0, arpID1, INT,
      membraneIDFree, ATPCountCG1, ADPCountCG1, ADPPiCountCG1, ADPCofCountCG1],
     a1N == actin[aIDN1, coords1N, aID1,
       aIDN1N, angle1N, CL1N, arpID1N, INT, membraneIDFree,
       ATPCountCG1N, ADPCountCG1N, ADPPiCountCG1N, ADPCofCountCG1N],
     a2P == actin[aID2P, coords2P, aIDP2P, aID2,
       angle2P, CL2P, arpID2P, INT, membraneIDFree, ATPCountCG2P,
       ADPCountCG2P, ADPPiCountCG2P, ADPCofCountCG2P],
     actin[aID2, coords2, aID2P, aIDN2, angle2, 0.0, arpID2, INT,
      membraneIDFree, ATPCountCG2, ADPCountCG2, ADPPiCountCG2, ADPCofCountCG2],
     a2N == actin[aIDN2, coords2N, aID2,
       aIDN2N, angle2N, CL2N, arpID2N, INT, membraneIDFree,
       ATPCountCG2N, ADPCountCG2N, ADPPiCountCG2N, ADPCofCountCG2N],
     newID[IDCounter], spineHeadArea[area], camCount[numCam]
    } →
    {
     a1P, a2P, a2N, a1N,
     actin[aID1, coords1, aID1P, aIDN1, angle1, IDCounter, arpID1, INT,
      membraneIDFree, ATPCountCG1, ADPCountCG1, ADPPiCountCG1, ADPCofCountCG1],
     actin[aID2, coords2, aID2P, aIDN2, angle2, IDCounter, arpID2, INT,
      membraneIDFree, ATPCountCG2, ADPCountCG2, ADPPiCountCG2, ADPCofCountCG2],
     cam[IDCounter, (coords1 + coords2) / 2,
      aID1, aID2, 0.0, Norm[coords1 - coords2]],
     newID[IDCounter + 1], spineHeadArea[area], camCount[numCam - 12]
    },
   with[Boole[Abs[ArcCos[(coords1 - coords1P).(coords2 - coords2P) / (Norm[coords1 - coords1P] Norm[coords2 - coords2P])]] <
       15 Degree] Boole[aID1 ≠ aIDP2P && aID2 ≠ aIDP1P] Boole[aID1P ≠ aID2] *
     Boole[aIDN1 ≠ aID2] * Boole[aID2P ≠ aID1] * Boole[aIDN2 ≠ aID1] *
```

```
      Boole[aID1 ≠ aID2] * Boole[arpID1 ≠ aID2 && arpID2 ≠ aID1] Boole[
        0.3 < pointLineDistance[coords2P, coords2, coords1] < 1] bundle * numCam],
    {
      actin[aID1, coords1, aIDP1, aIDN1, angle1, camID, arpID1, end1,
        membraneID1, ATPCountCG1, ADPCountCG1, ADPPiCountCG1, ADPCofCountCG1],
      actin[aID2, coords2, aIDP2, aIDN2, angle2, camID, arpID2, end2,
        membraneID2, ATPCountCG2, ADPCountCG2, ADPPiCountCG2, ADPCofCountCG2],
      cam[camID, camCoords, aID1, aID2, camAngle, camLength],
      spineHeadArea[area], camCount[numCam]
     } →
     {
      camCount[numCam + 12],
      actin[aID1, coords1, aIDP1, aIDN1, angle1, 0.0, arpID1, end1,
        membraneID1, ATPCountCG1, ADPCountCG1, ADPPiCountCG1, ADPCofCountCG1],
      actin[aID2, coords2, aIDP2, aIDN2, angle2,
        0.0, arpID2, end2, membraneID2, ATPCountCG2, ADPCountCG2,
        ADPPiCountCG2, ADPCofCountCG2], spineHeadArea[area]
     },
    with[unbundle]};

rulesBundlingMovement = {
    (*Movement of junctions of actin with a CamKIIβ protein*)
    {
      a1 == actin[aID, coordsA, aIDP, aIDN, angleA, camID, arpID, endA,
         membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      cam[camID, camCoords, aID, aIDBund, camAngle, camLength],
      aBund == actin[aIDBund, coordsABund, aIDPBund, aIDNBund, angleABund,
         camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
         ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund]
     } → With[{camDelta = 1 / 60 deltaFuncPairwiseP2Angular[
           coordsA, camCoords, coordsABund, 0 Degree, stepCam[
            Norm[coordsA - camCoords] + Norm[coordsABund - camCoords]], 0.]}, {
        (*Re-create actin object across the bundle*)
        aBund,
        (*Update position and angle of middle actin*)
        a1,
        (*Update position and angle of cam*)
        cam[camID, camCoords + camDelta, aID, aIDBund, middleThetaMovement[
          coordsA, camCoords + camDelta, coordsABund], camLength]
      }],
    with[networkFactor],
    {
      actin[aIDP, coordsAP, aIDPP, aID, angleAP, camIDP, arpIDP, endAP,
      membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coordsA, aIDP, aIDN, angleA, camID, arpID, endA,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     actin[aIDN, coordsAN, aID, aIDNN, angleAN, camIDN, arpIDN, endAN,
      membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
     cam[camID, camCoords, aID, aIDBund, camAngle, camLength],
     actin[aIDBundP, coordsABundP, aIDPBundP, aIDBund, angleABundP,
      camIDP, arpIDBundP, endABundP, membraneIDBundP, ATPCountCGBundP,
      ADPCountCGBundP, ADPPiCountCGBundP, ADPCofCountCGBundP],
     actin[aIDBund, coordsABund, aIDBundP, aIDNBund, angleABund,
      camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
      ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund],
     actin[aIDNBund, coordsABundN, aIDBund, aIDNBundN, angleABundN,
      camIDN, arpIDBundN, endABundN, membraneIDBundN, ATPCountCGBundN,
      ADPCountCGBundN, ADPPiCountCGBundN, ADPCofCountCGBundN]
    } → With[
     {pDelta = 1 / 60 deltaFuncPairwiseP1Angular[coordsA, camCoords, coordsABund,
         0 Degree, step[Norm[coordsA - camCoords] + Norm[coordsABund - camCoords]],
         ADPCofCountCGP], nDelta = 1 / 60 deltaFuncPairwiseP3Angular[coordsA,
         camCoords, coordsABund, 0 Degree, step[Norm[coordsA - camCoords] +
           Norm[coordsABund - camCoords]], ADPCofCountCGN]}, {
      (*Update position and angle of middle actin*)
      actin[aID, coordsA + pDelta, aIDP, aIDN,
       middleThetaMovement[coordsAP, coordsA + pDelta, coordsAN], camID, arpID,
       endA, membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      (*Update angles of adjacent actins*)
      actin[aIDP, coordsAP, aIDPP, aID, If[endAP ≠ INT, 0,
         angleAP + startActinDeltaTheta[coordsAP, coordsA, coordsA + pDelta]],
       camIDP, arpIDP, endAP, membraneIDP, ATPCountCGP,
       ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aIDN, coordsAN, aID, aIDNN, If[endAN ≠ INT, 0,
         angleAN + endActinDeltaTheta[coordsA, coordsAN, coordsA + pDelta]],
       camIDN, arpIDN, endAN, membraneIDN, ATPCountCGN,
       ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
      (*Update position and angle of cam*)
      cam[camID, camCoords, aID, aIDBund, middleThetaMovement[
         coordsA + pDelta, camCoords, coordsABund + nDelta], camLength],

      actin[aIDBundP, coordsABundP,
       aIDPBundP, aIDBund, If[endABundP ≠ INT, 0, angleABundP +
          startActinDeltaTheta[coordsABundP, coordsABund, coordsABund + nDelta]],
       camIDP, arpIDBundP, endABundP, membraneIDBundP, ATPCountCGBundP,
       ADPCountCGBundP, ADPPiCountCGBundP, ADPCofCountCGBundP],
      actin[aIDBund, coordsABund + nDelta, aIDBundP, aIDNBund,
      middleThetaMovement[coordsABundP, coordsABund + nDelta, coordsABundN],
      camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
      ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund],
     actin[aIDNBund, coordsABundN,
      aIDBund, aIDNBundN, If[endABundN ≠ INT, 0, angleABundN +
        endActinDeltaTheta[coordsABund, coordsABundN, coordsABund + nDelta]],
      camIDN, arpIDBundN, endABundN, membraneIDBundN, ATPCountCGBundN,
      ADPCountCGBundN, ADPPiCountCGBundN, ADPCofCountCGBundN]
    }],
  with[networkFactor],
  {
    a1 == actin[aID, coordsA, aIDP, aIDN, angleA, camID, arpID, endA,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    cam[camID, camCoords, aID, aIDBund, camAngle, camLength],
    aBund == actin[aIDBund, coordsABund, aIDPBund, aIDNBund, angleABund,
      camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
      ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund]
   } → With[
    {camDelta = deltaFuncPairwiseP2[coordsA, camCoords, camRule, camLength / 2,
        stepCam[Norm[coordsA - camCoords] + Norm[coordsABund - camCoords]], ϵ] +
       deltaFuncPairwiseP1[camCoords, coordsABund,
        camRule, camLength / 2, stepCam[
         Norm[coordsA - camCoords] + Norm[coordsABund - camCoords]], ϵ]}, {
     (*Re-create actin object across the bundle*)
     aBund,
     (*Update position and angle of middle actin*)
     a1,
     (*Update position and angle of cam*)
     cam[camID, camCoords + camDelta, aID, aIDBund, middleThetaMovement[
       coordsA, camCoords + camDelta, coordsABund], camLength]
    }],
  with[networkFactor],
  {
    actin[aIDP, coordsAP, aIDPP, aID, angleAP, camIDP, arpIDP, endAP,
     membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coordsA, aIDP, aIDN, angleA, camID, arpID, endA,
     membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[aIDN, coordsAN, aID, aIDNN, angleAN, camIDN, arpIDN, endAN,
     membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
    cam[camID, camCoords, aID, aIDBund, camAngle, camLength],
    actin[aIDBundP, coordsABundP, aIDPBundP, aIDBund, angleABundP,
     camIDP, arpIDBundP, endABundP, membraneIDBundP, ATPCountCGBundP,
     ADPCountCGBundP, ADPPiCountCGBundP, ADPCofCountCGBundP],
    actin[aIDBund, coordsABund, aIDBundP, aIDNBund, angleABund,
     camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
     ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund],
    actin[aIDNBund, coordsABundN, aIDBund, aIDNBundN, angleABundN,
     camIDN, arpIDBundN, endABundN, membraneIDBundN, ATPCountCGBundN,
     ADPCountCGBundN, ADPPiCountCGBundN, ADPCofCountCGBundN]
   } →
   With[{pDelta = deltaFuncPairwiseP1[coordsA, camCoords, camRule, camLength / 2,
       step[Norm[coordsA - camCoords] + Norm[coordsABund - camCoords]], ϵ],
     nDelta = deltaFuncPairwiseP2[camCoords, coordsABund, camRule, camLength / 2,
       step[Norm[coordsA - camCoords] + Norm[coordsABund - camCoords]], ϵ]}, {
     (*Update position and angle of middle actin*)
     actin[aID, coordsA + pDelta, aIDP, aIDN,
      middleThetaMovement[coordsAP, coordsA + pDelta, coordsAN], camID, arpID,
      endA, membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (*Update angles of adjacent actins*)
     actin[aIDP, coordsAP, aIDPP, aID, If[endAP ≠ INT, 0,
       angleAP + startActinDeltaTheta[coordsAP, coordsA, coordsA + pDelta]],
      camIDP, arpIDP, endAP, membraneIDP, ATPCountCGP,
      ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aIDN, coordsAN, aID, aIDNN, If[endAN ≠ INT, 0,
       angleAN + endActinDeltaTheta[coordsA, coordsAN, coordsA + pDelta]],
      camIDN, arpIDN, endAN, membraneIDN, ATPCountCGN,
      ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
     (*Update position and angle of cam*)
     cam[camID, camCoords, aID, aIDBund, middleThetaMovement[
       coordsA + pDelta, camCoords, coordsABund + nDelta], camLength],

     actin[aIDBundP, coordsABundP,
      aIDPBundP, aIDBund, If[endABundP ≠ INT, 0, angleABundP +
        startActinDeltaTheta[coordsABundP, coordsABund, coordsABund + nDelta]],
      camIDP, arpIDBundP, endABundP, membraneIDBundP, ATPCountCGBundP,
      ADPCountCGBundP, ADPPiCountCGBundP, ADPCofCountCGBundP],
     actin[aIDBund, coordsABund + nDelta, aIDBundP, aIDNBund,
      middleThetaMovement[coordsABundP, coordsABund + nDelta, coordsABundN],
      camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
      ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund],
     actin[aIDNBund, coordsABundN,
      aIDBund, aIDNBundN, If[endABundN ≠ INT, 0, angleABundN +
        endActinDeltaTheta[coordsABund, coordsABundN, coordsABund + nDelta]],
      camIDN, arpIDBundN, endABundN, membraneIDBundN, ATPCountCGBundN,
      ADPCountCGBundN, ADPPiCountCGBundN, ADPCofCountCGBundN]
    }],
  with[networkFactor]};
```

```
rulesBundlingMovementHessian = {
   {

     a1 == actin[aID, coordsA, aIDP, aIDN, angleA, camID, arpID, endA,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     cam[camID, camCoords, aID, aIDBund, camAngle, camLength],
     aBund == actin[aIDBund, coordsABund, aIDPBund, aIDNBund, angleABund,
       camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
       ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund]
    } → {
     (*Re-create actin object across the bundle*)
     aBund,
     (*Update position and angle of middle actin*)
     a1,
     (*Update position and angle of cam*)
     cam[camID, addVectors[dcoords, camCoords],
      aID, aIDBund, middleThetaMovement[coordsA,
       addVectors[dcoords, camCoords], coordsABund], camLength]
    },
   with[networkFactor heatBathHessianAcceptance[coordsA, camCoords,
      coordsABund, camRule, camLength / 2, camLength / 2, dcoords] ×
     grammarPDF[MultinormalDistribution[{0, 0}, hessianScaling
        Symmetrize[Abs[kBT safeInverse@HessianFuncPot[coordsA, camCoords,
             coordsABund, camRule, camLength / 2, camLength / 2]]]], dcoords]],
   {
     actin[aIDP, coordsAP, aIDPP, aID, angleAP, camIDP, arpIDP, endAP,
      membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coordsA, aIDP, aIDN, angleA, camID, arpID, endA,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     actin[aIDN, coordsAN, aID, aIDNN, angleAN, camIDN, arpIDN, endAN,
      membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
     a1 == actin[aIDBund, coordsABund, aIDBundP, aIDNBund, angleABund,
       camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
       ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund],
     cam[camID, camCoords, aID, aIDBund, camAngle, camLength]
    } → {
     (*Update position and angle of middle actin*)
     actin[aID, addVectors[dcoords, coordsA], aIDP, aIDN, middleThetaMovement[
       coordsAP, addVectors[dcoords, coordsA], coordsAN], camID, arpID, endA,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (*Update angles of adjacent actins*)
     actin[aIDP, coordsAP, aIDPP, aID, If[endAP ≠ INT, 0, angleAP +
        startActinDeltaTheta[coordsAP, coordsA, addVectors[dcoords, coordsA]]],
      camIDP, arpIDP, endAP, membraneIDP, ATPCountCGP, ADPCountCGP,
       ADPPiCountCGP, ADPCofCountCGP],
      actin[aIDN, coordsAN, aID, aIDNN, If[endAN ≠ INT, 0, angleAN +
          endActinDeltaTheta[coordsA, coordsAN, addVectors[dcoords, coordsA]]],
       camIDN, arpIDN, endAN, membraneIDN, ATPCountCGN, ADPCountCGN,
       ADPPiCountCGN, ADPCofCountCGN],
      (*Update position and angle of cam*)
      cam[camID, camCoords, aID, aIDBund, middleThetaMovement[
        addVectors[dcoords, coordsA], camCoords, coordsABund], camLength],
      a1
     },
    with[networkFactor heatBathEndHessianAcceptance[
       coordsA, camCoords, camRule, camLength / 2, dcoords] ×
      grammarPDF[MultinormalDistribution[{0, 0}, hessianScaling
          Symmetrize[Abs[kBT safeInverse@HessianFuncPotEnd[coordsA, camCoords,
               camRule, camLength / 2]]]], dcoords]],
    {
      a1 == actin[aID, coordsA, aIDP, aIDN, angleA, camID, arpID, endA,
        membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      cam[camID, camCoords, aID, aIDBund, camAngle, camLength],
      actin[aIDBundP, coordsABundP, aIDPBundP, aIDBund, angleABundP,
       camIDP, arpIDBundP, endABundP, membraneIDBundP, ATPCountCGBundP,
       ADPCountCGBundP, ADPPiCountCGBundP, ADPCofCountCGBundP],
      actin[aIDBund, coordsABund, aIDBundP, aIDNBund, angleABund,
       camID, arpIDBund, endABund, membraneIDBund, ATPCountCGBund,
       ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund],
      actin[aIDNBund, coordsABundN, aIDBund, aIDNBundN, angleABundN,
       camIDN, arpIDBundN, endABundN, membraneIDBundN, ATPCountCGBundN,
       ADPCountCGBundN, ADPPiCountCGBundN, ADPCofCountCGBundN]
     } → {
      actin[aIDBundP, coordsABundP, aIDPBundP, aIDBund,
       If[endABundP ≠ INT, 0, angleABundP + startActinDeltaTheta[
          coordsABundP, coordsABund, addVectors[dcoords, coordsABund]]],
       camIDP, arpIDBundP, endABundP, membraneIDBundP, ATPCountCGBundP,
       ADPCountCGBundP, ADPPiCountCGBundP, ADPCofCountCGBundP],
      actin[aIDBund, addVectors[dcoords, coordsABund], aIDBundP, aIDNBund,
       middleThetaMovement[coordsABundP, addVectors[dcoords, coordsABund],
        coordsABundN], camID, arpIDBund, endABund, membraneIDBund,
       ATPCountCGBund, ADPCountCGBund, ADPPiCountCGBund, ADPCofCountCGBund],
      actin[aIDNBund, coordsABundN, aIDBund, aIDNBundN,
       If[endABundN ≠ INT, 0, angleABundN + endActinDeltaTheta[
          coordsABund, coordsABundN, addVectors[dcoords, coordsABund]]],
       camIDN, arpIDBundN, endABundN, membraneIDBundN, ATPCountCGBundN,
       ADPCountCGBundN, ADPPiCountCGBundN, ADPCofCountCGBundN],
      (*Update position and angle of cam*)
      cam[camID, camCoords, aID, aIDBund, middleThetaMovement[coordsA,
        camCoords, addVectors[coordsABund, dcoords]], camLength],
      a1
     },
    with[networkFactor heatBathEndHessianAcceptance[
       coordsABund, camCoords, camRule, camLength / 2, dcoords] ×
      grammarPDF[MultinormalDistribution[{0, 0}, hessianScaling
         Symmetrize[Abs[kBT safeInverse@HessianFuncPotEnd[coordsABund,
              camCoords, camRule, camLength / 2]]]], dcoords]]
   };
```

The cell below shows the Lennard-Jones potential as a function of a distance d, size of the well ϵ and ratio constant σLJ where the minimum occurs at σLJ .

In[∘]:=
```
potentialElectro[d_, rules_] :=
 With[{eps = 0}, De (1 - E^(ρMorse (d0-d)))^2 /. Join[potentialVars, rules]]
clipFunction[func_, var_, ϵ_] :=
 func Boole[d ≥ ϵ] +
  ((func /. var → ϵ) + (d - ϵ) (D[func, var] /. var → ϵ)) Boole[d < ϵ]

clipped = clipFunction[potentialElectro[d, {}], d, clipFactor d0];

potential[dIn_, rules_, clipFactorIn_, optimal_ : 1.] :=
  clipped /. Join[{d → dIn, clipFactor → clipFactorIn, d0 → optimal}, rules];
```

The total energy in this section is a combination of anistropic buckling, angular bending energy, membrane areal energy, membrane line tension energy, and membrane mean Helfrich energy.

Tri-nodal Anisotropic Force

Rules

To create anisotropic movement, buckling occurs in a series of three actin beads with only the center one moving. The total potential equals the sum of potentials of the two rods such that main movement occurs perpendicular to the axis connecting the first and third actins.

The negative gradient of the Lennard - Jones potential with respect the coordinates of each point is the restoring force acting on each point .

In[ ]:=
```
Norm'[d_] := d/Norm[d]
Unprotect[Power];
Clear[Power]; (*Removes any previous custom definitions of Power.*)

Power[Abs[x_], 2] := x^2

Protect[Power];
dij = Norm[x1 - x2];
gradP1[{x1x_, x1y_}, {x2x_, x2y_}, rules_, l_, clipFactor_] :=
  Re[D[potential[dij, rules, clipFactor, l], x1] /.
    {x1 → {x1x, x1y}, x2 → {x2x, x2y}}];
gradP2[{x1x_, x1y_}, {x2x_, x2y_}, rules_, l_, clipFactor_] :=
  Re[D[potential[dij, rules, clipFactor, l], x2] /.
    {x1 → {x1x, x1y}, x2 → {x2x, x2y}}];
```

In[ ]:=
```
getNetworkDeltaAniso[{x1o_, y1o_},
  {x2o_, y2o_}, {x3o_, y3o_}, rules_, l0In1_, l0In2_, step_] :=
 Block[{forceFunc1 = -gradP2[{x1o, y1o}, {x2o, y2o}, rules, l0In1, ϵ],
   forceFunc2 = -gradP1[{x2o, y2o}, {x3o, y3o}, rules, l0In2, ϵ], p2Delta},
  p2Delta = ((step forceFunc1 + step forceFunc2) // Flatten) /.
    {Infinity → 0., Indeterminate → 0., ComplexInfinity → 0.}
 ]
```

In[ ]:=
```
deltaFuncPairwiseP1[{x1o_, y1o_},
  {x2o_, y2o_}, rules_, l0In_, step_, clipFactor_] :=
 Block[{p1Delta},
  p1Delta = Re[(- step gradP1[{x1o, y1o}, {x2o, y2o}, rules, l0In, clipFactor] /.
       {Infinity → 0., ComplexInfinity → 0.}) /. Indeterminate → 0.]
 ]

deltaFuncPairwiseP2[{x1o_, y1o_},
  {x2o_, y2o_}, rules_, l0In_, step_, clipFactor_] :=
 Block[{p2Delta},
  p2Delta = Re[(-step gradP2[{x1o, y1o}, {x2o, y2o}, rules, l0In, clipFactor] /.
       {Infinity → 0., ComplexInfinity → 0.}) /. Indeterminate → 0.]
 ]

potentialFunc[{x1o_, y1o_}, {x2o_, y2o_}, rules_, l0In_] :=
 potential[dij, rules, ϵ, l0In] /. {x1 → {x1o, y1o}, x2 → {x2o, y2o}}
```

In[ ]:=
```
(*Change angle range*)
transformAngle[ang_] :=
 If[Mod[ang, 2 Pi] ≤ Pi,
  Mod[ang, Pi],
  Mod[ang, 2 Pi] - 2 Pi
 ]

(*Functions for determining the change to the angle of the first actin*)

getStartActinDeltaTheta[{p1x_, p1y_}, {p2x_, p2y_}, {pnewx_, pnewy_}] :=
 transformAngle[Block[{angNext = ArcTan @@ ({pnewx, pnewy} - {p1x, p1y}),
    angPrev = ArcTan @@ ({p2x, p2y} - {p1x, p1y})},
   If[Abs[angNext] > Pi / 2 && Sign[angNext] ≠ Sign[angPrev],
    Evaluate@(Mod[angNext, 2 Pi] - Mod[angPrev, 2 Pi]),
    Evaluate@(angNext - angPrev)
   ]
  ]]

With[{tmp = getStartActinDeltaTheta[{p1x, p1y}, {p2x, p2y}, {pnewx, pnewy}]},
 startActinDeltaTheta[{p1xIn_, p1yIn_},
   {p2xIn_, p2yIn_}, {pnewxIn_, pnewyIn_}] :=
  tmp /. {p2x → p2xIn, p2y → p2yIn,
    p1x → p1xIn, p1y → p1yIn, pnewx → pnewxIn, pnewy → pnewyIn}
]

(*Functions for determining the change to the angle of the third actin*)

getEndActinDeltaTheta[{p2x_, p2y_}, {p3x_, p3y_}, {pnewx_, pnewy_}] :=
 transformAngle[Block[{angNext = ArcTan @@ ({p3x, p3y} - {pnewx, pnewy}),
    angPrev = ArcTan @@ ({p3x, p3y} - {p2x, p2y})},
   If[Abs[angNext] > Pi / 2 && Sign[angNext] ≠ Sign[angPrev],
    Evaluate@(-(Mod[angNext, 2 Pi] - Mod[angPrev, 2 Pi])),
    Evaluate@(-(angNext - angPrev))
   ]
  ]]


With[{tmp = getEndActinDeltaTheta[{p2x, p2y}, {p3x, p3y}, {pnewx, pnewy}]},
 endActinDeltaTheta[{p2xIn_, p2yIn_}, {p3xIn_, p3yIn_}, {pnewxIn_, pnewyIn_}] :=
  tmp /. {p2x → p2xIn, p2y → p2yIn,
    p3x → p3xIn, p3y → p3yIn, pnewx → pnewxIn, pnewy → pnewyIn}
]

(*Function for determining the angle of the middle actin*)
middleThetaMovement[{p1x_, p1y_}, {p2newx_, p2newy_}, {p3x_, p3y_}] :=
 transformAngle[Block[{angNext = ArcTan @@ ({p3x, p3y} - {p2newx, p2newy}),
    angPrev = ArcTan @@ ({p2newx, p2newy} - {p1x, p1y})},
   If[Abs[angNext] > Pi / 2 && Sign[angNext] ≠ Sign[angPrev],
    Evaluate@ (Mod[angNext, 2 Pi] - Mod[angPrev, 2 Pi]),
    Evaluate@ (angNext - angPrev)
   ]
  ]]
```

In[ ]:=
```
rulesAnisotropic := {
   {actin[aIDP, coordsP, aIDPP, aID, angleP, CLP, arpIDP, endP, membraneIDFree,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coords, aIDP, aIDN, angle, CL, arpIDFree, INT,
      membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     actin[aIDN, coordsN, aID, aIDNNN,
      angleN, CLN, arpIDN, endN, membraneIDFree, ATPCountCGN,
      ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
    With[{delta = deltaFuncPairwiseP2[ coordsP, coords, actinRule, l0,
         step[(Norm[ coords - coordsP])], ϵ] + deltaFuncPairwiseP1[coords,
         coordsN, actinRule, l0, step[Norm[ coordsN - coords]], ϵ]}, {
      (*Move position of middle actin and update angle*)
      actin[aID, addVectors[coords, delta], aIDP, aIDN,
       middleThetaMovement[coordsP, addVectors[coords, delta], coordsN], CL
       , arpIDFree, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      (*Update angle of first actin*)
      actin[aIDP, coordsP, aIDPP, aID, If[endP == INT, angleP +
         startActinDeltaTheta[ coordsP, coords, addVectors[coords, delta]],
        angleP], CLP, arpIDP, endP, membraneIDFree, ATPCountCGP,
       ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      (*Update angle of last actin*)
      actin[aIDN, coordsN, aID, aIDNNN, If[endN == INT,
        angleN + endActinDeltaTheta[coords, coordsN, addVectors[coords, delta]],
        angleN], CLN, arpIDN, endN, membraneIDFree,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
     }],
   with[networkFactor],
   {actin[aIDP, coordsP, aIDPP, aID, angleP, CLP, arpIDP, endP,
      distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     arpObject == actin[arpID, arpCoords, aID, aIDArpN, angleArp,
       CLArp, arp2ID, endArp, distArp, ATPCountCGArp,
       ADPCountCGArp, ADPPiCountCGArp, ADPCofCountCGArp],
     actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, distN,
      ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
    With[{delta = deltaFuncPairwiseP2[coordsP, coords, actinRule,
          l0 Boole[distP == membraneIDFree] + distP Boole[distP ≠ membraneIDFree],
          step[(Norm[coords - coordsP])], ϵ] +
         deltaFuncPairwiseP1[coords, coordsN, actinRule,
          l0 Boole[distN == membraneIDFree] + distN Boole[distN ≠ membraneIDFree],
          step[Norm[coordsN - coords]], ϵ] + deltaFuncPairwiseP1[coords,
          arpCoords, actinRule, l0 Boole[distArp == membraneIDFree] + distArp Boole[
             distArp ≠ membraneIDFree], step[Norm[arpCoords - coords]], ϵ]}, {
      (*Move position of middle actin and update angle*)
      actin[aID, coords + delta, aIDP, aIDN,
       middleThetaMovement[coordsP, coords + delta, coordsN], CL
       , arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      (*Update angle of first actin*)
      actin[aIDP, coordsP, aIDPP, aID, If[endP == INT,
         angleP + startActinDeltaTheta[coordsP, coords, coords + delta], angleP],
       CLP, arpIDP, endP, distP, ATPCountCGP, ADPCountCGP,
       ADPPiCountCGP, ADPCofCountCGP],
      (*Update angle of last actin*)
      actin[aIDN, coordsN, aID, aIDNN,
       If[endN == INT, angleN + endActinDeltaTheta[coords, coordsN, coords + delta],
         angleN], CLN, arpIDN, endN, distN, ATPCountCGN,
       ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN], arpObject
     }], with[networkFactor],
   (*When there's a boundary condition attached to the spine head membrane*)
   {spineAtt[aIDP, s0, s1],
     actin[aIDP, coordsP, aIDPP, aID, angleP, CLP, arpIDP, endP,
      dist, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     actin[aIDN, coordsN, aID, aIDNNN,
      angleN, CLN, arpIDN, endN, membraneIDFree, ATPCountCGN,
      ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
    With[{delta = deltaFuncPairwiseP2[coordsP, coords, actinRule, dist,
          step[(Norm[coordsN - coords] + Norm[coords - coordsP])], ϵ] +
         deltaFuncPairwiseP1[coords, coordsN, actinRule, l0,
          step[(Norm[coordsN - coords] + Norm[coords - coordsP])], ϵ]}, {
      (*Move position of middle actin and update angle*)
      spineAtt[aIDP, s0, s1],
      actin[aID, coords + delta, aIDP, aIDN,
       middleThetaMovement[coordsP, coords + delta, coordsN], CL
       , arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
       (*Update angle of first actin*)
       actin[aIDP, coordsP, aIDPP, aID, If[endP == INT,
         angleP + startActinDeltaTheta[coordsP, coords, coords + delta], angleP],
        CLP, arpIDP, endP, dist, ATPCountCGP, ADPCountCGP,
        ADPPiCountCGP, ADPCofCountCGP],
       (*Update angle of last actin*)
       actin[aIDN, coordsN, aID, aIDNNN,
        If[endN == INT, angleN + endActinDeltaTheta[coords, coordsN, coords + delta],
         angleN], CLN, arpIDN, endN, membraneIDFree,
        ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
      }],
    with[networkFactor],
    {spineAtt[aIDN, s0, s1],
      actin[aIDP, coordsP, aIDPP, aID, angleP, CLP, arpIDP, endP,
       membraneIDFree, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[aIDN, coordsN, aID, aIDNNN, angleN, CLN, arpIDN, endN, dist,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
     With[{delta = deltaFuncPairwiseP2[coordsP, coords, actinRule, l0,
          step[(Norm[coordsN - coords] + Norm[coords - coordsP])], ϵ] +
         deltaFuncPairwiseP1[coords, coordsN, actinRule, dist,
          step[(Norm[coordsN - coords] + Norm[coords - coordsP])], ϵ]}, {
       (*Move position of middle actin and update angle*)
       spineAtt[aIDN, s0, s1],
       actin[aID, coords + delta, aIDP, aIDN,
        middleThetaMovement[coordsP, coords + delta, coordsN], CL
        , arpID, INT, membraneID,
        ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
       (*Update angle of first actin*)
       actin[aIDP, coordsP, aIDPP, aID, If[endP == INT,
         angleP + startActinDeltaTheta[coordsP, coords, coords + delta], angleP],
        CLP, arpIDP, endP, membraneIDFree, ATPCountCGP,
        ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
       (*Update angle of last actin*)
       actin[aIDN, coordsN, aID, aIDNNN,
        If[endN == INT, angleN + endActinDeltaTheta[coords, coordsN, coords + delta],
         angleN], CLN, arpIDN, endN, dist, ATPCountCGN,
        ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
      }],
    with[networkFactor]
   };

rulesEndPairwiseAnisotropic := {
    {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, POI, membraneIDFree,
       ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDNN, angle, CL, arpID, end, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG]} →
     With[{deltaP = deltaFuncPairwiseP1[coordsP, coords,
         actinRule, l0, stepPar[Norm[coords - coordsP]], ϵ]}, {
       (*Move position of middle actin and update angle*)
       actin[aID, coords, aIDP, aIDNN,
        angle, CL
        , arpID, end, membraneID,
        ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
       (*Update angle of first actin*)
       actin[aIDP, coordsP + deltaP, aIDPP, aIDPN, angleP, CLP, arpIDP, POI,
        membraneIDFree, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP]
      }],
    with[networkFactor],
    {actin[aID, coords, aIDP, aIDNN, angle, CL, arpID, endP,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[aIDN, coordsN, aID, aIDNNN,
       angleN, CLN, arpIDN, endN, membraneIDFree, ATPCountCGN,
       ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
     With[{deltaN = deltaFuncPairwiseP1[coordsN,
         coords, actinRule, l0, stepPar[Norm[coordsN - coords]], ϵ]}, {
       (*Move position of middle actin and update angle*)
       actin[aID, coords, aIDP, aIDNN,
        angle, CL
        , arpID, endP, membraneID,
        ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
       (*Update angle of last actin*)
       actin[aIDN, coordsN + deltaN, aID, aIDNNN, angleN, CLN, arpIDN, endN,
        membraneIDFree, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
      }],
    with[networkFactor Boole[endN == BAR || endN == CAP]]
   };
```

Angle Bending

In[◦]:=
```
getPotentialBending[a_, b_, c_, ang_] :=
```
$$\left(\text{Boole}[\text{ADPCofCountCG} \geq \text{nCG}/2]\,\frac{1}{5} + \text{Boole}[\text{ADPCofCountCG} < \text{nCG}/2]\right)$$
$$\frac{\kappa B}{2} * \left(\left(\text{ArcCos}\left[\frac{(c-b).(b-a)}{(\text{Norm}[(c-b)]\ \text{Norm}[(b-a)] + \text{eps})}\right] - \text{ang}\right)^2\right)$$

```
Norm'[vec_] := vec / Norm[vec]


K[x1_, x2_, x3_] := (x2 - x3) - a[x1, x2, x3] × b[x1, x2, x3] (x1 - x2);

a[x1_, x2_, x3_] := ((x2 - x1).(x3 - x2)) / (Norm[x2 - x1] Norm[x3 - x2]);
b[x1_, x2_, x3_] := Norm[x3 - x2] / Norm[x2 - x1];
c[x1_, x2_, x3_] := Norm[x2 - x1] Norm[x3 - x2];

DbendInt = Re[With[{asub = a[x1, x2, x3]},
    (Boole[ADPCofCountCG ≥ nCG / 2] 1/5 + Boole[ADPCofCountCG < nCG / 2])
    κB (ArcCos[asub] - ang) / (c[x1, x2, x3] Sqrt[Clip[1 - asub^2, {0, ∞}]] + eps)
    (K[x1, x2, x3] + K[x3, x2, x1])]];
DbendEnd1 = Re[With[{asub = a[x1, x2, x3]},
    -(Boole[ADPCofCountCG ≥ nCG / 2] 1/5 + Boole[ADPCofCountCG < nCG / 2]) κB
    (ArcCos[asub] - ang) / (c[x1, x2, x3] Sqrt[Clip[1 - asub^2, {0, ∞}]] + eps) (K[x1, x2, x3])]];
DbendEnd3 = Re[With[{asub = a[x1, x2, x3]},
    -(Boole[ADPCofCountCG ≥ nCG / 2] 1/5 + Boole[ADPCofCountCG < nCG / 2]) κB
    (ArcCos[asub] - ang) / (c[x1, x2, x3] Sqrt[Clip[1 - asub^2, {0, ∞}]] + eps) (K[x3, x2, x1])]];

deltaFuncPairwiseP1Angular[{x1o_, y1o_}, {x2o_, y2o_},
  {x3o_, y3o_}, θtarget_, step_, ADPCofCountCGIn_] :=
 -(step DbendEnd1 /. {x1 → {x1o, y1o}, x2 → {x2o, y2o},
      x3 → {x3o, y3o}, ang → θtarget, ADPCofCountCG → ADPCofCountCGIn}) /.
  {Indeterminate → 0., ComplexInfinity → 0.}
deltaFuncPairwiseP2Angular[{x1o_, y1o_}, {x2o_, y2o_},
  {x3o_, y3o_}, θtarget_, step_, ADPCofCountCGIn_] :=
 -(step DbendInt /. {x1 → {x1o, y1o}, x2 → {x2o, y2o},
      x3 → {x3o, y3o}, ang → θtarget, ADPCofCountCG → ADPCofCountCGIn}) /.
  {Indeterminate → 0., ComplexInfinity → 0.}
deltaFuncPairwiseP3Angular[{x1o_, y1o_}, {x2o_, y2o_},
  {x3o_, y3o_}, θtarget_, step_, ADPCofCountCGIn_] :=
 -(step DbendEnd3 /. {x1 → {x1o, y1o}, x2 → {x2o, y2o},
      x3 → {x3o, y3o}, ang → θtarget, ADPCofCountCG → ADPCofCountCGIn}) /.
  {Indeterminate → 0., ComplexInfinity → 0.}
```

```
In[◦]:= rulesBending := {
    {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
       ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
     With[{delta = deltaFuncPairwiseP2Angular[coordsP, coords, coordsN, 0., step[
          (Norm[coords - coordsP] + Norm[coordsN - coords])], ADPCofCountCG]}, {
       (*Move position of middle actin and update angle*)
       actin[aID, coords + delta, aIDP, aIDN,
        middleThetaMovement[coordsP, coords + delta, coordsN], CL
        , arpID, INT, membraneID,
        ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
       (*Update angle of first actin*)
       actin[aIDP, coordsP, aIDPP, aIDPN, If[endP == INT && aID == aIDPN,
          angleP + startActinDeltaTheta[coordsP, coords, coords + delta], angleP],
        CLP, arpIDP, endP, membraneIDP, ATPCountCGP,
        ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
       (*Update angle of last actin*)
       actin[aIDN, coordsN, aID, aIDNN,
        If[endN == INT, angleN + endActinDeltaTheta[coords, coordsN, coords + delta],
          angleN], CLN, arpIDN, endN, membraneIDN,
        ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
      }],
    with[networkFactor],
    (*Movement to the actin that comprises the branching junction*)
    {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
       ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[arpID, coordsAArpN, aID, aIDarpNN, angleAArpN,
       CLAArpN, arpIDAArpN, endAArpN, membraneIDArp, ATPCountCGAArpN,
       ADPCountCGAArpN, ADPPiCountCGAArpN, ADPCofCountCGAArpN],
      actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
     With[{delta = κBArpFactor deltaFuncPairwiseP2Angular[
          coordsP, coords, coordsAArpN, 70 π/180,
          step[(Norm[coords - coordsP] + Norm[coordsAArpN - coords])], 0.]}, {
      (*Move position of middle actin and update angle*)
      actin[aID, coords + delta , aIDP, aIDN,
       middleThetaMovement[coordsP, coords + delta, coordsN], CL
       , arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      (*Update angle of first actin and arp*)
      actin[aIDP, coordsP, aIDPP, aIDPN, If[endP == INT && aIDPN == aID,
        angleP + startActinDeltaTheta[coordsP, coords, coords + delta], angleP],
       CLP, arpIDP, endP, membraneIDP, ATPCountCGP,
       ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],

      actin[arpID, coordsAArpN, aID, aIDarpNN, If[endAArpN == INT, angleAArpN +
          endActinDeltaTheta[coords, coordsAArpN, coords + delta], angleAArpN],
       CLAArpN, arpIDAArpN, endAArpN, membraneIDArp, ATPCountCGAArpN,
       ADPCountCGAArpN, ADPPiCountCGAArpN, ADPCofCountCGAArpN],

      (*Update angle of last actin*)
      actin[aIDN, coordsN, aID, aIDNN,
       If[endN == INT, angleN + endActinDeltaTheta[coords, coordsN, coords + delta],
        angleN], CLN, arpIDN, endN, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
     }],
  with[networkFactor],
  (*Movement to the actin that comprises the branching junction*)
  {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT,
     membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[arpID, coordsAArpN, aID, aIDarpNN, angleAArpN,
     CLAArpN, arpIDAArpN, endAArpN, membraneIDArp, ATPCountCGAArpN,
     ADPCountCGAArpN, ADPPiCountCGAArpN, ADPCofCountCGAArpN],
    actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
     ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
   With[{delta = κBArpFactor deltaFuncPairwiseP2Angular[
          coordsN, coords, coordsAArpN, π - 70 π/180,
          step[(Norm[coords - coordsN] + Norm[coordsAArpN - coords])], 0.]}, {
      (*Move position of middle actin and update angle*)
      actin[aID, coords + delta , aIDP, aIDN,
       middleThetaMovement[coordsP, coords + delta, coordsN], CL
       , arpID, INT, membraneID,
        ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
       (*Update angle of first actin and arp*)
       actin[aIDP, coordsP, aIDPP, aIDPN, If[endP == INT && aIDPN == aID,
          angleP + startActinDeltaTheta[coordsP, coords, coords + delta], angleP],
        CLP, arpIDP, endP, membraneIDP, ATPCountCGP,
        ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],

       actin[arpID, coordsAArpN, aID, aIDarpNN, If[endAArpN == INT, angleAArpN +
           endActinDeltaTheta[coords, coordsAArpN, coords + delta], angleAArpN],
        CLAArpN, arpIDAArpN, endAArpN, membraneIDArp, ATPCountCGAArpN,
        ADPCountCGAArpN, ADPPiCountCGAArpN, ADPCofCountCGAArpN],

       (*Update angle of last actin*)
       actin[aIDN, coordsN, aID, aIDNN,
        If[endN == INT, angleN + endActinDeltaTheta[coords, coordsN, coords + delta],
          angleN], CLN, arpIDN, endN, membraneIDN,
        ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
      }],
    with[networkFactor]
   };

rulesEndPairwiseBending := {
    {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
       ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
     With[{deltaP = Boole[endP == POI] deltaFuncPairwiseP1Angular[coordsP, coords,
           coordsN, 0., step[Norm[coords - coordsP]], ADPCofCountCGP], deltaN =
         Boole[(endN == BAR || endN == CAP)] deltaFuncPairwiseP3Angular[coordsP,
           coords, coordsN, 0., step[Norm[coordsN - coords]], ADPCofCountCGN]}, {
       (*Move position of middle actin and update angle*)
       actin[aID, coords, aIDP, aIDN,
        middleThetaMovement[coordsP + deltaP, coords, coordsN + deltaN], CL
        , arpID, INT, membraneID,
        ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
       (*Update angle of first actin*)
       actin[aIDP, coordsP + deltaP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
        membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
       (*Update angle of last actin*)
       actin[aIDN, coordsN + deltaN, aID, aIDNN, angleN, CLN, arpIDN, endN,
        membraneIDN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
   }],
  with[networkFactor Boole[endP == POI || endN == BAR || endN == CAP]],
  {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
     dist, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
     ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
     ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
    spineAtt[aIDP, centralID1, centralID3],
    s0 == spine[adjID1a, coords0, adjID0a, centralID1],
    spine[centralID1, coords1, adjID1a, centralID3],
    spine[centralID3, coords3, centralID1, adjID3b],
    s4 == spine[adjID3b, coords4, centralID3, adjID4b],
    spineHeadArea[area]} →
   With[{deltaP = deltaFuncPairwiseP1Angular[
       lineIntersectionPoint[coords1, coords3, coords, coordsP],
       coords, coordsN, 0., zeta, ADPCofCountCGP]}, {
     (*Move position of middle actin and update angle*)
     actin[aID, coords, aIDP, aIDN,
      middleThetaMovement[coordsP + deltaP, coords, coordsN], CL
      , arpID, INT, membraneID,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (*Update angle of first actin*)
     actin[aIDP,
      lineIntersectionPoint[coords1 + (1 - Norm[coords - coords1]/Norm[coords1 - coords3]) deltaP,
       coords3 + (1 - Norm[coords - coords3]/Norm[coords1 - coords3]) deltaP, coords, coordsP + deltaP],
      aIDPP, aIDPN, angleP, CLP, arpIDP, endP, dist, ATPCountCGP,
      ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     (*Update angle of last actin*)
     actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
      ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
     spineAtt[aIDP, centralID1, centralID3], spineHeadArea[area], s0, s4,
     spine[centralID1,
      coords1 + (1 - Norm[coords - coords1]/Norm[coords1 - coords3]) deltaP, adjID1a, centralID3],
     spine[centralID3,
      coords3 + (1 - Norm[coords - coords3]/Norm[coords1 - coords3]) deltaP, centralID1, adjID3b]
    }],
with[membraneFactor],
{actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
   ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
  actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
   ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
  actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN,
   dist, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
  spineAtt[aIDN, centralID1, centralID3],
  s0 == spine[adjID1a, coords0, adjID0a, centralID1],
  spine[centralID1, coords1, adjID1a, centralID3],
  spine[centralID3, coords3, centralID1, adjID3b],
  s4 == spine[adjID3b, coords4, centralID3, adjID4b],
  spineHeadArea[area]} →
 With[{deltaN =
     deltaFuncPairwiseP3Angular[coordsP, coords, lineIntersectionPoint[
       coords1, coords3, coords, coordsN], 0., zeta, ADPCofCountCGN]}, {
   (*Move position of middle actin and update angle*)
   actin[aID, coords, aIDP, aIDN,
    middleThetaMovement[coordsP, coords, coordsN + deltaN], CL
    , arpID, INT, membraneID,
    ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   (*Update angle of first actin*)
   actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
    membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
   (*Update angle of last actin*)
   actin[aIDN,
```

$$\texttt{lineIntersectionPoint}\Big[\texttt{coords1} + \left(1 - \frac{\texttt{Norm[coords - coords1]}}{\texttt{Norm[coords1 - coords3]}}\right)\texttt{deltaN},$$

$$\texttt{coords3} + \left(1 - \frac{\texttt{Norm[coords - coords3]}}{\texttt{Norm[coords1 - coords3]}}\right)\texttt{deltaN, coords, coordsN + deltaN}\Big],$$

```
    aID, aIDNN, angleN, CLN, arpIDN, endN, dist, ATPCountCGN,
    ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN],
   spineAtt[aIDN, centralID1, centralID3], spineHeadArea[area], s0, s4,
   spine[centralID1,
```

$$\texttt{coords1} + \left(1 - \frac{\texttt{Norm[coords - coords1]}}{\texttt{Norm[coords1 - coords3]}}\right)\texttt{deltaN, adjID1a, centralID3}\Big],$$

```
   spine[centralID3,
```

$$\texttt{coords3} + \left(1 - \frac{\texttt{Norm[coords - coords3]}}{\texttt{Norm[coords1 - coords3]}}\right)\texttt{deltaN, centralID1, adjID3b}\Big]$$

```
  }],
    with[membraneFactor]
   };
```

Hessian Thermal Noise

Rules

In this section, another term of the Taylor expansion of the potential includes such that the force term also depends on the Hessian, a matrix of second derivatives of the potential, which adds noise to the gradient minimization.
Below, we utilize a pairwise Lennard-Jones potential between two points ri and rj. The equilibrium displacement vector between ri and rj where rj moves to the minimum coordinate denotes by u.

The Hessian approximation to the potential where the gradient or the first derivative approaches zero follows from the Taylor expansion of a potential which, in this case, equals
$U(R+u) \approx U(R) + U`(R)^{\intercal} u + 1/2\, u^{\intercal} H\, |_{R}\, u + ...,$
where U is the potential function, R is the equilibrium displacement vector and u the displacement from equilibrium. Again, we use gradient clipping.

```
In[ ]:= addVectors[{v1_, v2_}, {dx_, dy_}] :=
         {v1, v2} + {dx, dy}
        potentialTrinodal[x1_, x2_, x3_, rules_, l01_, l02_] :=
         (potential[Norm[x2 - x1], rules, ϵ, l01] +
            potential[Norm[x3 - x2], rules, ϵ, l02]) /. potentialVars
```

```
In[ ]:= DPotInt =
          D[((potential[Norm[x2 - x1], {}, ϵ, l01]) + potential[Norm[x3 - x2], {}, ϵ, l02]),
            x2] /. potentialVars;
        HPotInt = D[DPotInt, x2];
        HessianFuncPot[{x1xIn_, x1yIn_}, {x2xIn_, x2yIn_},
          {x3xIn_, x3yIn_}, rules_, l0In1_, l0In2_, scale_ : 1.] :=
         Module[{H = HPotInt /. Join[rules, {x1 → {x1xIn, x1yIn},
                x2 → {x2xIn, x2yIn}, x3 → {x3xIn, x3yIn}, l01 → l0In1, l02 → l0In2}]},
          scale {{Total[H] /. {0. → 1 / eps}, 0.}, {0., Total[H] /. {0. → 1 / eps}}} /.
           {Indeterminate → 1 / eps, Infinity → 1 / eps, ComplexInfinity → 1 / eps}
         ]

        DPotEnd = D[potential[Norm[x2 - x1], {}, ϵ, l], x1] /. potentialVars;
        HPotEnd = (D[DPotEnd, x1]);
        HessianFuncPotEnd[{x1xIn_, x1yIn_},
          {x2xIn_, x2yIn_}, rules_, l0In_, scale_ : 1.] := Module[
          {H = HPotEnd /. Join[rules, {x1 → {x1xIn, x1yIn}, x2 → {x2xIn, x2yIn}, l → l0In}]
```

```
  }, scale {{Total[H] /. {0. → 1 / eps}, 0.}, {0., Total[H] /. {0. → 1 / eps}}} /.
    {Indeterminate → 1 / eps, Infinity → 1 / eps, ComplexInfinity → 1 / eps}
 ]



getPotentialJunc[x1_, x2_, x3_, x4_, l1_, l2_, l3_] :=
 (potential[Norm[x4 - x2], {}, ϵ, l3] + potential[Norm[x3 - x2], {}, ϵ, l2] +
    potential[Norm[x1 - x2], {}, ϵ, l1]) /. potentialVars
DPotJunc = (D[getPotentialJunc[x1, x2, x3, x4, l1, l2, l3], x2]);
HPotJunc = D[DPotJunc, x2];
HessianFuncPotJunc[{x1xIn_, x1yIn_},
  {x2xIn_, x2yIn_}, {x3xIn_, x3yIn_}, {x4xIn_, x4yIn_}, rules_,
  l0In1_, l0In2_, l0In3_, scale_ : 1.] := With[{H = ((HPotJunc /.
       Join[rules, {x1 → {x1xIn, x1yIn}, x2 → {x2xIn, x2yIn}, x3 → {x3xIn, x3yIn},
         x4 → {x4xIn, x4yIn}, l1 → l0In1, l2 → l0In2, l3 → l0In3}]))},
  scale {{Total[H] /. {0. → 1 / eps}, 0.}, {0., Total[H] /. {0. → 1 / eps}}} /.
    {Indeterminate → 1 / eps, Infinity → 1 / eps, ComplexInfinity → 1 / eps}
 ]



heatBathHessianAcceptance[{ax_, ay_}, {bx_, by_},
  {cx_, cy_}, rules_, l01_, l02_, {rdx_, rdy_}, scale_ : 1.] :=
 Block[
  {dGoverkBT = Clip[Re[scale/kBT (((potentialTrinodal[{ax, ay}, {bx, by} + {rdx, rdy},
               {cx, cy}, rules, l01, l02]) -
             potentialTrinodal[{ax, ay}, {bx, by}, {cx, cy}, rules, l01, l02]) -
           1 / 2 (({{rdx, rdy}}.HessianFuncPot[{ax, ay}, {bx, by},
                  {cx, cy}, rules, l01, l02].{{rdx}, {rdy}})[[1, 1]] -
               ({{rdx, rdy}}.HessianFuncPot[{ax, ay}, {bx, by} + {rdx, rdy},
                  {cx, cy}, rules, l01, l02].{{rdx}, {rdy}})[[1, 1]]))], {-5, 5}],
   proposalDist = √Abs[(Det[HessianFuncPot[{ax, ay}, {bx, by}, {cx, cy},
             rules, l01, l02, scale]] / (Det[HessianFuncPot[{ax, ay},
               {bx, by} + {rdx, rdy}, {cx, cy}, rules, l01, l02, scale]] + eps))]},
  Clip[Re[(E^-dGoverkBT proposalDist)/(1 + E^-dGoverkBT (proposalDist))] /.
     {Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}, {0, 1}]
 ]
heatBathEndHessianAcceptance[{ax_, ay_}, {bx_, by_},
  rules_, l01_, {rdx_, rdy_}, scale_ : 1.] := Block[{dGoverkBT =
    Clip[Re[scale/kBT ((((potential[Norm[{ax, ay} + {rdx, rdy} - {bx, by}], rules, ϵ,
                l01]) - (potential[Norm[{ax, ay} - {bx, by}], rules, ϵ, l01])) /.
            potentialVars) - 1 / 2 (({{rdx, rdy}}.HessianFuncPotEnd[
                {ax, ay}, {bx, by}, rules, l01].{{rdx}, {rdy}})[[1, 1]] -
             ({{rdx, rdy}}.HessianFuncPotEnd[{ax, ay} + {rdx, rdy}, {bx, by},
                rules, l01].{{rdx}, {rdy}})[[1, 1]]))], {-5, 5}], proposalDist =
    √Abs[(Det[HessianFuncPotEnd[{ax, ay}, {bx, by}, rules, l01, scale]] /
        (Det[HessianFuncPotEnd[{ax, ay} + {rdx, rdy},
             {bx, by}, rules, l01, scale]] + eps))]},
   Clip[Re[E^-dGoverkBT proposalDist / (1 + E^-dGoverkBT (proposalDist))] /.
     {Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}, {0, 1}]
  ]
heatBathJuncHessianAcceptance[{ax_, ay_}, {bx_, by_}, {cx_, cy_},
   {dx_, dy_}, rules_, l01_, l02_, l03_, {rdx_, rdy_}, scale_ : 1.] := Block[
   {dGoverkBT = Clip[Re[scale/kBT ((((getPotentialJunc[{ax, ay}, {bx, by} + {rdx, rdy},
                {cx, cy}, {dx, dy}, rules, l01, l02, l03]) - (getPotentialJunc[
                {ax, ay}, {bx, by}, {cx, cy}, {dx, dy}, rules, l01, l02, l03]))) -
           1 / 2 (({{rdx, rdy}}.HessianFuncPotJunc[{ax, ay}, {bx, by}, {cx, cy},
                {dx, dy}, rules, l01, l02, l03].{{rdx}, {rdy}})[[1, 1]] - ({{rdx,
                 rdy}}.HessianFuncPotJunc[{ax, ay}, {bx, by} + {rdx, rdy}, {cx,
                 cy}, {dx, dy}, rules, l01, l02, l03].{{rdx}, {rdy}})[[1, 1]]))],
      {-5, 5}], proposalDist = √Abs[(Det@HessianFuncPotJunc[{ax, ay},
           {bx, by}, {cx, cy}, {dx, dy}, rules, l01, l02, l03, scale] /
        (Det@HessianFuncPotJunc[{ax, ay}, {bx, by} + {rdx, rdy},
             {cx, cy}, {dx, dy}, rules, l01, l02, l03, scale] + eps))]},
   Clip[Re[E^-dGoverkBT proposalDist / (1 + E^-dGoverkBT (proposalDist))] /.
     {Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}, {0, 1}]
  ]
safeInverse[m_?MatrixQ] := If[m === ConstantArray[0., Dimensions[m]],
   DiagonalMatrix@Diagonal@ConstantArray[eps / kBT, Dimensions[m]],
   (*Return the 0 matrix if m is the zero matrix*)
   Inverse[m]   (*Otherwise,compute the inverse*)]
```

```
In[◦]:= rulesHessian = {
   {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
      distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, dist,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     actin[aIDN, coordsN, aID, aIDNNN, angleN, CLN, arpIDN, endN, distN,
      ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} →
    {(*Move position of middle actin and update angle*)
     actin[aID, addVectors[coords, dcoords], aIDP, aIDN,
      middleThetaMovement[coordsP, addVectors[coords, dcoords], coordsN], CL,
      arpID, INT, dist, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (*Update angle of first actin*)actin[aIDP, coordsP, aIDPP, aIDPN,
      If[endP == INT && aID == aIDPN, angleP + startActinDeltaTheta[coordsP,
         coords, addVectors[coords, dcoords]], angleP], CLP, arpIDP, endP,
      distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     (*Update angle of last actin*)actin[aIDN, coordsN, aID, aIDNNN,
      If[endN == INT, angleN + endActinDeltaTheta[coords, coordsN,
         addVectors[coords, dcoords]], angleN], CLN, arpIDN, endN, distN,
      ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]}, with[
    networkFactor heatBathHessianAcceptance[coordsP, coords, coordsN, actinRule,
      l0 Boole[distP == membraneIDFree] + distP Boole[distP ≠ membraneIDFree],
      l0 Boole[distN == membraneIDFree] + distN Boole[distN ≠ membraneIDFree],
      dcoords] × grammarPDF[MultinormalDistribution[{0, 0},
       hessianScaling Symmetrize[Abs[kBT safeInverse@HessianFuncPot[coordsP,
             coords, coordsN, actinRule, l0 Boole[distP == membraneIDFree] + distP
               Boole[distP ≠ membraneIDFree], l0 Boole[distN == membraneIDFree] +
              distN Boole[distN ≠ membraneIDFree]]]]], dcoords]]
  };


rulesHessianEnds = {
   {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
      membraneIDFree, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coords, aIDP, aIDN, angle, CL, arpID, end, membraneID,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG]} → {
     (*Move position of middle actin and update angle*)
     actin[aID, coords, aIDP, aIDN,
      endActinDeltaTheta[coordsP,
        coords, addVectors[coordsP, dcoords]] + angle, CL
      , arpID, end, membraneID,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (*Update angle of first actin*)
     actin[aIDP, addVectors[coordsP, dcoords],
      aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDFree,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP]
    },
   with[networkFactor heatBathEndHessianAcceptance[coordsP, coords,
      actinRule, l0, dcoords] × grammarPDF[MultinormalDistribution[{0, 0},
       hessianScaling Symmetrize[Abs[kBT safeInverse@HessianFuncPotEnd[coordsP,
             coords, actinRule, l0]]]], dcoords] Boole[endP == POI]],
   {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coords, aIDP, aIDN, angle, CL, arpID, end, membraneIDFree,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG]} → {
     (*Move position of middle actin and update angle*)
     actin[aID, addVectors[coords, dcoords], aIDP, aIDN, angle, CL, arpID, end,
      membraneIDFree, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (*Update angle of first actin*)
     actin[aIDP, coordsP, aIDPP, aIDPN, angleP + Boole[aIDPN == aID]
        startActinDeltaTheta[coordsP, coords, addVectors[coords, dcoords]],
      CLP, arpIDP, endP, membraneIDP, ATPCountCGP, ADPCountCGP,
      ADPPiCountCGP, ADPCofCountCGP]
    },
   with[networkFactor
     heatBathEndHessianAcceptance[coords, coordsP, actinRule, l0, dcoords] ×
     grammarPDF[MultinormalDistribution[{0, 0}, hessianScaling Symmetrize[
         Abs[kBT safeInverse@HessianFuncPotEnd[coords, coordsP, actinRule,
             l0]]]], dcoords] Boole[end == BAR || end == CAP]]
  };
```

In[•]:=
```
getPotentialBendingJunc[x1_, x2_, x3_, x4_] :=
  (getPotentialBending[x1, x2, x4, 70 π/180])
HBendInt = (Boole[ADPCofCountCG ≥ nCG/2] 1/5 + Boole[ADPCofCountCG < nCG/2])
    κB/2 1. / (c[x1, x2, x3]^2 (1 - a[x1, x2, x3]^2))
    (K[x1, x2, x3] + K[x3, x2, x1]) * (K[x1, x2, x3] + K[x3, x2, x1]);
HessianFuncBend[{x1xIn_, x1yIn_}, {x2xIn_, x2yIn_},
   {x3xIn_, x3yIn_}, ADPCofCountCGIn_, scale_ : 1.] :=
  Module[{H = Re[HBendInt /. {x1 → {x1xIn, x1yIn}, x2 → {x2xIn, x2yIn},
         x3 → {x3xIn, x3yIn}, ADPCofCountCG → ADPCofCountCGIn}]},
   scale {{2 Total[H] /. {0. → 1 / eps}, 0.}, {0., 2 Total[H] /. {0. → 1 / eps}}} /.
    {Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}
  ]

HBendEndP1 = (Boole[ADPCofCountCG ≥ nCG/2] 1/5 + Boole[ADPCofCountCG < nCG/2]) κB/2
```

```
    1./(c[x1, x2, x3]^2 (1 - a[x1, x2, x3]^2)) (K[x1, x2, x3]) * (K[x1, x2, x3]);
HessianFuncBendEndP1[{x1xIn_, x1yIn_}, {x2xIn_, x2yIn_},
  {x3xIn_, x3yIn_}, ADPCofCountCGIn_, scale_ : 1.] :=
 Module[{H = Re[HBendEndP1 /. {x1 → {x1xIn, x1yIn}, x2 → {x2xIn, x2yIn},
        x3 → {x3xIn, x3yIn}, ADPCofCountCG → ADPCofCountCGIn}]
  },
  scale {{2 Total[H] /. {0. → 1 / eps}, 0.}, {0., 2 Total[H] /. {0. → 1 / eps}}} /.
   {Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}
 ]



HBendEndP3 = (Boole[ADPCofCountCG ≥ nCG/2] 1/5 + Boole[ADPCofCountCG < nCG/2]) κB/2
    1./(c[x1, x2, x3]^2 (1 - a[x1, x2, x3]^2)) (K[x3, x2, x1]) * (K[x3, x2, x1]);
HessianFuncBendEndP3[{x1xIn_, x1yIn_}, {x2xIn_, x2yIn_},
  {x3xIn_, x3yIn_}, ADPCofCountCGIn_, scale_ : 1.] :=
 Module[{H = Re[HBendEndP3 /. {x1 → {x1xIn, x1yIn}, x2 → {x2xIn, x2yIn},
        x3 → {x3xIn, x3yIn}, ADPCofCountCG → ADPCofCountCGIn}]
  },
  scale {{2 Total[H] /. {0. → 1 / eps}, 0.}, {0., 2 Total[H] /. {0. → 1 / eps}}} /.
   {Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}
 ]



HessianFuncBendJunc[{x1xIn_, x1yIn_}, {x2xIn_, x2yIn_},
  {x3xIn_, x3yIn_}, {x4xIn_, x4yIn_}, ADPCofCountCG_, scale_ : 1.] :=
 κBArpFactor HessianFuncBend[{x1xIn, x1yIn},
   {x2xIn, x2yIn}, {x4xIn, x4yIn}, ADPCofCountCG, scale]

heatBathHessianBendAcceptance[{ax_, ay_}, {bx_, by_}, {cx_, cy_},
  {rdx_, rdy_}, angle_ : 0., ADPCofCountCGIn_, scale_ : 1.] :=
 Block[{dGoverkBT = Clip[
     Re[scale/kBT (((getPotentialBending[{ax, ay}, {bx, by} + {rdx, rdy}, {cx, cy},
             angle]) - getPotentialBending[{ax, ay}, {bx, by}, {cx, cy}, angle]) -
          1 / 2 (({{rdx, rdy}}.HessianFuncBend[{ax, ay}, {bx, by},
                 {cx, cy}, ADPCofCountCGIn].{{rdx}, {rdy}})⟦1, 1⟧ -
             ({{rdx, rdy}}.HessianFuncBend[{ax, ay}, {bx, by} + {rdx, rdy},
                 {cx, cy}, ADPCofCountCGIn].{{rdx}, {rdy}})⟦1, 1⟧))], {-5, 5}],
   proposalDist =
    √Abs[(Det@HessianFuncBend[{ax, ay}, {bx, by}, {cx, cy}, ADPCofCountCGIn,
          scale] / (Det@HessianFuncBend[{ax, ay}, {bx, by} + {rdx, rdy},
            {cx, cy}, ADPCofCountCGIn, scale] + eps))]},
  Clip[Re[(E^-dGoverkBT proposalDist)/(1 + E^-dGoverkBT (proposalDist)) /. {ADPCofCountCG → ADPCofCountCGIn,
       Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}], {0, 1}]
 ]

heatBathEndHessianBendAcceptanceP1[{ax_, ay_}, {bx_, by_},
  {cx_, cy_}, {rdx_, rdy_}, angle_, ADPCofCountCGIn_, scale_ : 1.] :=
 Block[{dGoverkBT = Clip[Re[scale/kBT
       (((getPotentialBending[{ax, ay} + {rdx, rdy}, {bx, by}, {cx, cy}, angle]) -
           (getPotentialBending[{ax, ay}, {bx, by}, {cx, cy}, angle])) -
         1 / 2 (({{rdx, rdy}}.HessianFuncBendEndP1[{ax, ay}, {bx, by},
                 {cx, cy}, ADPCofCountCGIn].{{rdx}, {rdy}})[[1, 1]] -
            ({{-rdx, -rdy}}.HessianFuncBendEndP1[{ax, ay} + {rdx, rdy}, {bx, by},
                 {cx, cy}, ADPCofCountCGIn].{{-rdx}, {-rdy}})[[1, 1]]))], {-5, 5}],
   proposalDist = √Abs[(Det@HessianFuncBendEndP1[{ax, ay} + {rdx, rdy},
           {bx, by}, {cx, cy}, ADPCofCountCGIn, scale] /
         (Det@HessianFuncBendEndP1[{ax, ay}, {bx, by}, {cx, cy},
            ADPCofCountCGIn, scale] + eps))]},
  Clip[Re[(E^-dGoverkBT proposalDist)/(1 + E^-dGoverkBT (proposalDist)) /. {ADPCofCountCG → ADPCofCountCGIn,
       Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}], {0, 1}]
 ]
heatBathEndHessianBendAcceptanceP3[{ax_, ay_}, {bx_, by_},
  {cx_, cy_}, {rdx_, rdy_}, angle_, ADPCofCountCGIn_, scale_ : 1.] :=
 Block[{dGoverkBT = Clip[Re[scale/kBT
       (((getPotentialBending[{ax, ay}, {bx, by}, {cx, cy} + {rdx, rdy}, angle]) -
           (getPotentialBending[{ax, ay}, {bx, by}, {cx, cy}, angle])) -
         1 / 2 (({{rdx, rdy}}.HessianFuncBendEndP3[{ax, ay}, {bx, by}, {cx, cy},
                ADPCofCountCGIn].{{rdx}, {rdy}})[[1, 1]] - ({{-rdx, -rdy}}.
               HessianFuncBendEndP3[{ax, ay}, {bx, by}, {cx, cy} + {rdx, rdy},
                ADPCofCountCGIn].{{-rdx}, {-rdy}})[[1, 1]]))], {-5, 5}],
   proposalDist = √Abs[(Det@HessianFuncBendEndP3[{ax, ay}, {bx, by},
           {cx, cy}, ADPCofCountCGIn, scale] / (Det@HessianFuncBendEndP3[{ax, ay},
             {bx, by}, {cx, cy} + {rdx, rdy}, ADPCofCountCGIn, scale] + eps))]},
  Clip[Re[(E^-dGoverkBT proposalDist)/(1 + E^-dGoverkBT (proposalDist)) /. {ADPCofCountCG → ADPCofCountCGIn,
      Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}], {0, 1}]
  ]



heatBathJuncHessianBendAcceptance[{ax_, ay_}, {bx_, by_},
   {cx_, cy_}, {dx_, dy_}, {rdx_, rdy_}, ADPCofCountCGIn_, scale_ : 1.] :=
 Block[{dGoverkBT = Clip[Re[scale/kBT (((getPotentialBendingJunc[
                {ax, ay}, {bx, by} + {rdx, rdy}, {cx, cy}, {dx, dy}]) -
              (getPotentialBendingJunc[{ax, ay}, {bx, by}, {cx, cy}, {dx, dy}])) -
           1 / 2 (({{rdx, rdy}}.HessianFuncBendJunc[{ax, ay}, {bx, by},
                   {cx, cy}, {dx, dy}, ADPCofCountCGIn].{{rdx}, {rdy}})[[1, 1]] -
              ({{rdx, rdy}}.HessianFuncBendJunc[{ax, ay}, {bx, by} + {rdx, rdy},
                   {cx, cy}, {dx, dy}, ADPCofCountCGIn].{{rdx}, {rdy}})[[1, 1]]))],
      {-5, 5}], proposalDist = √Abs[((Det@HessianFuncBendJunc[{ax, ay},
              {bx, by}, {cx, cy}, {dx, dy}, ADPCofCountCGIn, scale] + eps) /
          (Det@HessianFuncBendJunc[{ax, ay}, {bx, by} + {rdx, rdy},
              {cx, cy}, {dx, dy}, ADPCofCountCGIn, scale] + eps))]},
   Clip[Re[(E^-dGoverkBT proposalDist)/(1 + E^-dGoverkBT (proposalDist))] /. {ADPCofCountCG → ADPCofCountCGIn,
      Indeterminate → 0., Infinity → 0., ComplexInfinity → 0.}, {0, 1}]
  ]
```

```
In[ ]:= rulesHessianBend := {
    {
      actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
       ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDN, angle, CL, arpIDFree, INT,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
     } → {
      (*Move position of middle actin and update angle*)
      actin[aID, addVectors[coords, dcoords], aIDP, aIDN,
       middleThetaMovement[coordsP, addVectors[coords, dcoords], coordsN], CL
       , arpIDFree, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      (*Update angle of first actin*)
      actin[aIDP, coordsP, aIDPP, aIDPN,
       If[endP == INT && aID == aIDPN, angleP + startActinDeltaTheta[coordsP, coords,
         addVectors[coords, dcoords]], angleP], CLP, arpIDP, endP, membraneIDP,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     (*Update angle of last actin*)
     actin[aIDN, coordsN, aID, aIDNN, If[endN == INT,
       angleN + endActinDeltaTheta[coords, coordsN, addVectors[coords, dcoords]],
       angleN], CLN, arpIDN, endN, membraneIDN,
      ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
    },
   with[networkFactor heatBathHessianBendAcceptance[
      coordsP, coords, coordsN, dcoords, 0., ADPCofCountCG] ×
     grammarPDF[MultinormalDistribution[{0, 0}, hessianScaling
        Symmetrize[0.5 kBT Abs[ safeInverse@HessianFuncBend[coordsP,
             coords, coordsN, ADPCofCountCG]]]], dcoords]],

   {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     actin[arpID, arpCoords, aID, aIDArpN,
      angleArp, CLArp, arp2ID, endArp, membraneIDArp, ATPCountCGArp,
      ADPCountCGArp, ADPPiCountCGArp, ADPCofCountCGArp],
     actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
      ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
    } → {
     (*Move position of middle actin and update angle*)
     actin[aID, addVectors[coords, dcoords], aIDP, aIDN,
      middleThetaMovement[coordsP, addVectors[coords, dcoords], coordsN], CL
      , arpID, INT, membraneID,
      ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
     (*Update angle of first actin*)
     actin[aIDP, coordsP, aIDPP, aIDPN,
      If[endP == INT && aID == aIDPN, angleP + startActinDeltaTheta[coordsP, coords,
         addVectors[coords, dcoords]], angleP], CLP, arpIDP, endP, membraneIDP,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],

     actin[arpID, arpCoords, aID, aIDArpN, If[aIDArpN ≠ aIDFreeB, angleArp +
        endActinDeltaTheta[coords, arpCoords, addVectors[coords, dcoords]],
       angleArp], CLArp, arp2ID, endArp, membraneIDArp, ATPCountCGArp,
      ADPCountCGArp, ADPPiCountCGArp, ADPCofCountCGArp],

     (*Update angle of last actin*)
     actin[aIDN, coordsN, aID, aIDNN, If[endN == INT,
       angleN + endActinDeltaTheta[coords, coordsN, addVectors[coords, dcoords]],
       angleN], CLN, arpIDN, endN, membraneIDN,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
     },
    with[networkFactor heatBathJuncHessianBendAcceptance[coordsP,
       coords, coordsN, arpCoords, dcoords, ADPCofCountCG, ϰBArpFactor] ×
      grammarPDF[MultinormalDistribution[{0, 0}, hessianScaling
         Symmetrize[0.5 kBT Abs[safeInverse@HessianFuncBendJunc[coordsP, coords,
              coordsN, arpCoords, ADPCofCountCG, ϰBArpFactor]]]], dcoords]]
   };


rulesHessianEndsBend = {
    {actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
       membraneIDFree, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      aN ==
       actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDN,
        ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} → {
      (*Move position of middle actin and update angle*)
      actin[aID, coords, aIDP, aIDN,
       endActinDeltaTheta[coordsP,
         coords, addVectors[coordsP, dcoords]] + angle, CL
       , arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      (*Update angle of first actin*)
      actin[aIDP, addVectors[coordsP, dcoords],
       aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDFree,
       ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP], aN
     },
    with[networkFactor heatBathEndHessianBendAcceptanceP1[
       coordsP, coords, coordsN, dcoords, 0 Degree, ADPCofCountCGP] ×
      grammarPDF[MultinormalDistribution[{0, 0}, hessianScaling
         Symmetrize[0.5 kBT Abs[safeInverse@HessianFuncBendEndP1[coordsP,
              coords, coordsN, ADPCofCountCGP]]]], dcoords] Boole[endP == POI]],
    {aP == actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
        membraneIDP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
      actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, membraneID,
       ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[aIDN, coordsN, aID, aIDNN,
       angleN, CLN, arpIDN, endN, membraneIDFree, ATPCountCGN,
       ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]} → {
      aP, actin[aID, coords, aIDP, aIDN, startActinDeltaTheta[coords,
         coordsN, addVectors[coordsN, dcoords]] + angle, CL, arpID, INT,
       membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
      actin[aIDN, addVectors[coordsN, dcoords],
       aID, aIDNN, angleN, CLN, arpIDN, endN, membraneIDFree,
       ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
     },
    with[
     networkFactor heatBathEndHessianBendAcceptanceP3[coordsP, coords, coordsN,
       dcoords, 0 Degree, ADPCofCountCGN] × grammarPDF[MultinormalDistribution[
        {0, 0}, hessianScaling Symmetrize[0.5 kBT Abs[ safeInverse@
              HessianFuncBendEndP3[coordsP, coords, coordsN, ADPCofCountCGN]]]],
       dcoords] Boole[endN == BAR || endN == CAP]]
  };
```

Spine Head Morphodynamics

Rules

In the actin network ends' interaction with the membrane. There are rules that check for intersection and attach actin ends to the membrane. Then, the actin object can elongate to apply a force onto the membrane. Meanwhiile, there are random deviations of the actin’s angle and by chance, according to Brownian elastic ratchet theory, the random angle change brings the end off the membrane. Afterwards, another actin can polymerize onto the membrane. Also, when the membrane force opposite the direction of the actin attached to the membrane is larger than the propulsive force of actin onto membrane, the actin de-attaches.

```
In[ ]:= (*1 means clockwise and 2 means counterclockwise*)
tripletOrientation[{p1x_, p1y_}, {p2x_, p2y_}, {p3x_, p3y_}] :=
 If[(p2y - p1y) * (p3x - p2x) - (p2x - p1x) * (p3y - p2y) > 0, 1, 2]

(*Formula for checking if two line segments intersect*)
intersectingLinesQ[{p11x_, p11y_},
  {p12x_, p12y_}, {p21x_, p21y_}, {p22x_, p22y_}] :=
 ((tripletOrientation[{p11x, p11y}, {p12x, p12y}, {p21x, p21y}] ≠
     tripletOrientation[{p11x, p11y}, {p12x, p12y}, {p22x, p22y}]) &&
   (tripletOrientation[{p21x, p21y}, {p22x, p22y}, {p11x, p11y}] ≠
     tripletOrientation[{p21x, p21y}, {p22x, p22y}, {p12x, p12y}]))
```

Functions to initialize the spine membrane according to a regular polygon.

In[ ]:=
```
generateSpinePoints[numPoints_, r_] :=
 Module[{coords, theta},
  coords = {};
  For[theta = 0, theta < 2 Pi, theta += 2 Pi / numPoints,
   coords = AppendTo[coords, {r Cos[theta], r Sin[theta]}];
  ];
  coords
 ]
```

In[ ]:=
```
myic = {
   actin[1, { 0, 0} + radiusInUnitLength / Sqrt[2] 4 / 5, aIDFreeP, 2., 0.0, 0,
    arpIDFree, POI, membraneIDFree, ATPID], (* new node at the pointed end *)
   actin[2., {1, 0} + radiusInUnitLength / Sqrt[2] 4 / 5, 1, 3, 0.0,
    0, 4, INT, membraneIDFree, ATPID], (* new internal node *)
   actin[3, {2., 0} + radiusInUnitLength / Sqrt[2] 4 / 5, 2., aIDFreeB, 0.0, 0,
    arpIDFree, BAR, membraneIDFree, ATPID], (* new node at the pointed end *)

   arp[4, {1, 0} + newPos[{σArp / actinObjectRise / 2, 0}, 70 * π / 180] +
     radiusInUnitLength / Sqrt[2] 4 / 5, 2., 5, 0.0, membraneIDFree, ARPACTID],
   actin[5, {1 , 0} + newPos[{σArp / actinObjectRise / 2, 0}, 70 * π / 180] +
     newPos[{1, 0}, 70 * π / 180] + radiusInUnitLength / Sqrt[2] 4 / 5,
    4, aIDFreeB, 0.0, 0, arpIDFree, BAR, membraneIDFree, ATPID],

   actin[6, { 0, 0} +
     {-radiusInUnitLength / Sqrt[2] 4 / 5, radiusInUnitLength / Sqrt[2] 4 / 5},
    7, aIDFreeB, 0.0, 0, arpIDFree, BAR, membraneIDFree, ATPID],
   (* new node at the pointed end *)
   actin[7, {1, 0} +
     {-radiusInUnitLength / Sqrt[2] 4 / 5, radiusInUnitLength / Sqrt[2] 4 / 5}, 8,
    6, 0.0, 0, 9, INT, membraneIDFree, ATPID], (* new internal node *)
   actin[8, {2., 0} +
     {-radiusInUnitLength / Sqrt[2] 4 / 5, radiusInUnitLength / Sqrt[2] 4 / 5},
    aIDFreeP, 7, 0.0, 0, arpIDFree, POI, membraneIDFree, ATPID],
   (* new node at the pointed end *)

   arp[9, {1 , 0} + newPos[{-σArp / actinObjectRise / 2, 0}, -70 * π / 180] +
     {-radiusInUnitLength / Sqrt[2] 4 / 5, radiusInUnitLength / Sqrt[2] 4 / 5},
    7, 10, 0.0, membraneIDFree, ARPACTID],
   actin[10, {1 , 0} + newPos[{-σArp / actinObjectRise / 2, 0}, -70 * π / 180] +
     newPos[{-1, 0}, -70 * π / 180] +
     {-radiusInUnitLength / Sqrt[2] 4 / 5, radiusInUnitLength / Sqrt[2] 4 / 5},
    9, aIDFreeB, 0.0, 0, arpIDFree, BAR, membraneIDFree],
   newID[11], (* counter for new ids to be generated *)
   arpCount[Round[initArpNum]], (* counter for the amount of
    ARP floating in the system at any given point in the sim *)
   actinADPCount[Round[initActinADPNum]],
   actinATPCount[Round[initActinATPNum]],
   spineHeadArea[π (spineHeadRadius * 10)^2],
   cofilinCount[initCofilinNum],
   cappingCount[initCappingNum],
   spineHeadCentroid[{0., 0.}],
   numVertices[25]
  };
```

In[ ]:=
```
spineCoords = generateSpinePoints[25, 7.5];
spineic = myic;
For[i = 0, i ≤ Length[spineCoords] - 1, i++,
 AppendTo[spineic, spine[i, spineCoords⟦i + 1⟧, Mod[i - 1, Length[spineCoords]],
   Mod[i + 1, Length[spineCoords]], membraneIDFree]]
]
AppendTo[spineic, spineIDMax[Length@spineCoords + 1]];
```

Functions to compute the area of enclosed by the spine membrane at each time point .

In[ ]:=
```
getSpineArea[moleculeList_] :=
 Module[{spineObjects, curID, initID, coordList = {}, curSpine, area, i},
  spineObjects = Cases[moleculeList, spine[__]];
  initID = spineObjects⟦1, ID⟧;
  AppendTo[coordList, spineObjects⟦1, POS⟧];
  curID = spineObjects⟦1, NEXT⟧;
  curSpine = Cases[spineObjects, spine[curID, __]]⟦1⟧;
  While[curID ≠ initID,
   AppendTo[coordList, curSpine⟦POS⟧];
   curID = curSpine⟦NEXT⟧;
   curSpine = Cases[spineObjects, spine[curID, __]]⟦1⟧;
  ];
  area = 0;
  For[i = 1, i ≤ Length@coordList - 1, i++,
   area += Det[coordList⟦i ;; i + 1⟧];
  ];
  area += Det[{coordList⟦i⟧, coordList⟦1⟧}];
  area /= 2;
  area
 ]
getPolygonArea[coords_] :=
  Module[{area, i},
   area = 0;
   For[i = 1, i ≤ Length@coords - 1, i ++,
    area += Det[coords⟦i ;; i + 1⟧];
   ];
   area += Det[{coords⟦i⟧, coords⟦1⟧}];
   area /= 2;
   area];
membraneAreaPlotter[sim_, title_ : "Membrane Area Over Time",
  plotRange_ : Automatic, export_ : False] :=
 Block[{spineVertices = (Select[#⟦2⟧, Head[#] === spine &] & /@ sim),
   i, j, spineAreas, data, firstVert, spineCoordsSnapshot, nextVert},
  spineAreas = {};
  For[i = 1, i ≤ Length@spineVertices, i ++,
   spineCoordsSnapshot = {};
   firstVert = spineVertices⟦i, 1⟧;
   AppendTo[spineCoordsSnapshot, firstVert⟦2⟧];
   For[j = 2, j ≤ Length@spineVertices⟦i⟧, j ++,
    nextVert = Cases[spineVertices⟦i⟧, spine[firstVert⟦4⟧, _, _, _]]⟦1⟧;
    AppendTo[spineCoordsSnapshot, nextVert⟦2⟧];
    firstVert = nextVert;
   ];
   AppendTo[spineAreas, getPolygonArea[spineCoordsSnapshot]];
  ];
  data = spineAreas * (actinObjectRise / 10^-6)^2;
  ListLinePlot[Transpose[{sim⟦ ;; , 1⟧, data}],
   DataRange → {0, Max[data]}, AxesLabel → {"Time (s)", "Area (μm^2)"},
   PlotLabel → title, PlotRange → plotRange]
 ]
membraneAreaRawPlotter[sim_, title_ : "Membrane Area Over Time",
  plotRange_ : Automatic, export_ : False] :=
 Block[{spineObjects = (Select[#⟦2⟧, Head[#] === spineHeadArea &] & /@ sim),
   spineAreas, data},
  spineAreas = #⟦1, 1⟧ & /@ spineObjects;
  data = spineAreas * (actinObjectRise / 10^-6)^2;
  ListLinePlot[Transpose[{sim⟦ ;; , 1⟧, data}],
   DataRange → {0, Max[data]}, AxesLabel → {"Time (s)", "Area (μm^2)"},
   PlotLabel → title, PlotRange → plotRange]
 ]
```

Some membrane energy and force terms from Bonilla-Quintana et al. 2020:

For the area term, we have that the areal energy Ω equals

In[ ]:= $$\Omega = \frac{1}{2}\sum_{i=1}^{n} x_1^i\, x_2^{i+1} - x_2^i\, x_1^{i+1}$$

from vector cross products and find that the derivative of the areal energy equals

$$\frac{\partial \Omega}{\partial x_1^i} = \frac{1}{2}\left(x_2^{i+1} - x_2^{i-1}\right), \frac{\partial \Omega}{\partial x_2^i} = \frac{1}{2}\left(-x_1^{i+1} + x_1^{i-1}\right).$$

The surface energy term, S, derivative equals

$$\frac{\partial S}{\partial x_{1,2}} = \frac{x_{1,2}^i - x_{1,2}^{i-1}}{v^i} + \frac{x_{1,2}^i - x_{1,2}^{i+1}}{v^{i+1}},$$

where variable *v* is distance between point and next point.

```
In[∘]:= areaEnergyTerm[p1_, p2_, p3_] :=
         1 / 2 (p1⟦1⟧ × p2⟦2⟧ - p1⟦2⟧ × p2⟦1⟧ + p2⟦1⟧ × p3⟦2⟧ - p2⟦2⟧ × p3⟦1⟧)
        surfaceEnergyTerm[p1_, p2_, p3_] :=
         1 / 2 (((p1 - p2).(p1 - p2))^(1/2) + ((p3 - p2).(p3 - p2))^(1/2))
        (*Distance between two neighboring vertices*)
        v[{p1x_, p1y_}, {p2x_, p2y_}] :=
         Sqrt[(p2x - p1x) ^ 2 + (p2y - p1y) ^ 2]

        Abs'[x_] := Sign[x]
        (*Helfrich energy computed with the
         neighboring points onto the point itself*)
        (*Distance between two neighboring vertices*)
        v[{p1x_, p1y_}, {p2x_, p2y_}] :=
         Sqrt[(p2x - p1x) ^ 2 + (p2y - p1y) ^ 2]

        (*Some terms to compute Helfrich energy*)
        g[{p1x_, p1y_}, {p2x_, p2y_}, {p3x_, p3y_}] :=
         ((p3x - p2x) / v[{p2x, p2y}, {p3x, p3y}] - (p2x - p1x) / v[{p1x, p1y}, {p2x, p2y}]) ^
           2 + ((p3y - p2y) / v[{p2x, p2y}, {p3x, p3y}] -
              (p2y - p1y) / v[{p1x, p1y}, {p2x, p2y}]) ^ 2
        z[p1_, p2_, p3_] := (v[p1, p2] + v[p2, p3]) / 2

        (*Helfrich energy computed with the
         neighboring points onto the point itself*)
        HelfrichEnergyDw[{p0x_, p0y_},
          {p1x_, p1y_}, {p2x_, p2y_}, {p3x_, p3y_}, {p4x_, p4y_}] :=
         g[{p0x, p0y}, {p1x, p1y}, {p2x, p2y}] / z[{p0x, p0y}, {p1x, p1y}, {p2x, p2y}] +
          g[{p1x, p1y}, {p2x, p2y}, {p3x, p3y}] / z[{p1x, p1y}, {p2x, p2y}, {p3x, p3y}] +
          g[{p2x, p2y}, {p3x, p3y}, {p4x, p4y}] / z[{p2x, p2y}, {p3x, p3y}, {p4x, p4y}]
```

```
In[∘]:= vectorProj[{v1x_, v1y_}, {v2x_, v2y_}] :=
         ({v1x, v1y}.{v2x, v2y} / Norm[{v2x, v2y}]^2) {v2x, v2y}
        membraneEnergy[{p0x_, p0y_},
          {p1x_, p1y_}, {p2x_, p2y_}, {p3x_, p3y_}, {p4x_, p4y_}] :=
         ( 2 kappa HelfrichEnergyDw[{p0x, p0y}, {p1x, p1y}, {p2x, p2y}, {p3x, p3y},
              {p4x, p4y}] + P areaEnergyTerm[{p1x, p1y}, {p2x, p2y}, {p3x, p3y}] +
            tau surfaceEnergyTerm[{p1x, p1y}, {p2x, p2y}, {p3x, p3y}]) /. membraneRules
        membraneRawForce = Compile[{p0x, p0y, p1x, p1y, p2x, p2y, p3x, p3y, p4x, p4y},
           Evaluate[-{∂p2x membraneEnergy[{p0x, p0y}, {p1x, p1y}, {p2x, p2y},
                {p3x, p3y}, {p4x, p4y}], ∂p2y membraneEnergy[{p0x, p0y}, {p1x, p1y},
                {p2x, p2y}, {p3x, p3y}, {p4x, p4y}]}], CompilationTarget → "C"];
        membraneRawForceP1 = Compile[{p0x, p0y, p1x, p1y, p2x, p2y, p3x, p3y, p4x, p4y},
           Evaluate[-{∂p1x membraneEnergy[{p0x, p0y}, {p1x, p1y}, {p2x, p2y},
                {p3x, p3y}, {p4x, p4y}], ∂p1y membraneEnergy[{p0x, p0y}, {p1x, p1y},
                {p2x, p2y}, {p3x, p3y}, {p4x, p4y}]}], CompilationTarget → "C"];
        membraneRawForceP3 = Compile[{p0x, p0y, p1x, p1y, p2x, p2y, p3x, p3y, p4x, p4y},
           Evaluate[-{∂p3x membraneEnergy[{p0x, p0y}, {p1x, p1y}, {p2x, p2y},
                {p3x, p3y}, {p4x, p4y}], ∂p3y membraneEnergy[{p0x, p0y}, {p1x, p1y},
                {p2x, p2y}, {p3x, p3y}, {p4x, p4y}]}], CompilationTarget → "C"];
        membraneRawForceMag =
          Compile[{p0x, p0y, p1x, p1y, p2x, p2y, p3x, p3y, p4x, p4y, pax, pay},
           Evaluate[Norm[vectorProj[-{∂p2x membraneEnergy[{p0x, p0y}, {p1x, p1y},
                   {p2x, p2y}, {p3x, p3y}, {p4x, p4y}], ∂p2y membraneEnergy[{p0x, p0y},
                   {p1x, p1y}, {p2x, p2y}, {p3x, p3y}, {p4x, p4y}]}, {pax, pay}]]
             Boole[Dot[-{∂p2x membraneEnergy[{p0x, p0y}, {p1x, p1y}, {p2x, p2y},
                    {p3x, p3y}, {p4x, p4y}], ∂p2y membraneEnergy[{p0x, p0y},
                    {p1x, p1y}, {p2x, p2y}, {p3x, p3y}, {p4x, p4y}]},
                {pax, pay}] < 0.]], CompilationTarget → "C"];
        (*Compute the sum of the three force terms contributing to membrane shape*)
        membraneForce[{p0xIn_, p0yIn_}, {p1xIn_, p1yIn_}, {p2xIn_, p2yIn_},
          {p3xIn_, p3yIn_}, {p4xIn_, p4yIn_}, {paxIn_, payIn_}] :=
         Clip[membraneRawForceMag[p0xIn, p0yIn, p1xIn, p1yIn,
           p2xIn, p2yIn, p3xIn, p3yIn, p4xIn, p4yIn, paxIn, payIn], {-5, 5}]
```

```
In[∘]:= (*Compute the sum of the three force terms contributing to membrane shape*)
        membraneDelta[{p0xIn_, p0yIn_}, {p1xIn_, p1yIn_},
          {p2xIn_, p2yIn_}, {p3xIn_, p3yIn_}, {p4xIn_, p4yIn_}] :=
         (zeta /. membraneRules) * membraneRawForce[p0xIn,
           p0yIn, p1xIn, p1yIn, p2xIn, p2yIn, p3xIn, p3yIn, p4xIn, p4yIn]
```

The Helfrich energy, defined as

$\|\frac{dT}{d\overline{\omega}}\|$, where $\overline{\omega}$ is arc length,

takes all points starting from two points preceding the point of interest and ending at two points after it . The form of the energy shows below where p0 is the starting point, p4 the ending point, and p2 the point of interest .

The following two functions get the intersection point of two lines given a, b corresponding to point 1 and c, d corresponding to point 2

```
In[ ]:= lineIntersectionPoint[{l1p1x_, l1p1y_},
          {l1p2x_, l1p2y_}, {l2p1x_, l2p1y_}, {l2p2x_, l2p2y_}] :=
         ((Det[{{l1p1x, l1p1y}, {l1p2x, l1p2y}}] ({l2p1x, l2p1y} - {l2p2x, l2p2y}) -
             Det[{{l2p1x, l2p1y}, {l2p2x, l2p2y}}] ({l1p1x, l1p1y} - {l1p2x, l1p2y})) /
           Det[{{l1p1x, l1p1y} - {l1p2x, l1p2y}, {l2p1x, l2p1y} - {l2p2x, l2p2y}}])
```

Intersection functions in the cell below function to check whether a rotation of an actin attached to the membrane detaches. If it stays attached, a new intersection point calculates as a function of extending the actin rod and of membrane forces.

```
In[ ]:= projpointline =
          {sp1x, sp1y} + (Dot[{p3x, p3y} - {sp1x, sp1y}, {sp2x, sp2y} - {sp1x, sp1y}] /
              Dot[{sp2x, sp2y} - {sp1x, sp1y}, {sp2x, sp2y} - {sp1x, sp1y}])
            ({sp2x, sp2y} - {sp1x, sp1y});

        deltaFuncWF[{rix_, riy_}, {rjx_, rjy_}, rules_, l0In_, clipFactor_, step_] :=
         (-step gradP2[{rix, riy}, {rjx, rjy}, rules, l0In, clipFactor])
```

```
In[ ]:= lineIntersectionWithNeighboringSpinesQ[{s1p_, s2p_, s3p_}, {aP_, a_}, ang_] :=
          Block[{norm = Norm[a - aP]},
           (intersectingLinesQ[s1p, s2p, aP, a]) ||
            (intersectingLinesQ[s2p, s3p, aP, a])];



        lineIntersectionWithNeighboringSpinesPrev[
           {s0p_, s1p_, s2p_, s3p_, s4p_}, {aP_, a_}, ang_] :=
          lineIntersectionPoint[s1p, s2p, aP, a];
        lineIntersectionWithNeighboringSpinesNext[
           {s0p_, s1p_, s2p_, s3p_, s4p_}, {aP_, a_}, ang_] :=
          lineIntersectionPoint[s2p, s3p, aP, a];

        eucDistVector[v1_, v2_] :=
          Total[(v1 - v2) ^ 2] ^ (1 / 2);
```

```
deltaArea5[{c0x_, c0y_}, {c1x_, c1y_}, {c2x_, c2y_},
  {c3x_, c3y_}, {c4x_, c4y_}, {newc2x_, newc2y_}] :=
 Block[{A1 =
    getPolygonArea[{{c0x, c0y}, {c1x, c1y}, {c2x, c2y}, {c3x, c3y}, {c4x, c4y}}],
   A2 = getPolygonArea[{{c0x, c0y}, {c1x, c1y},
      {newc2x, newc2y}, {c3x, c3y}, {c4x, c4y}}]},
  A2 - A1
 ]

deltaArea4[{c0x_, c0y_}, {c1x_, c1y_}, {c2x_, c2y_},
  {c3x_, c3y_}, {newc1x_, newc1y_}, {newc2x_, newc2y_}] :=
 Block[{A1 = getPolygonArea[{{c0x, c0y}, {c1x, c1y}, {c2x, c2y}, {c3x, c3y}}],
   A2 = getPolygonArea[
     {{c0x, c0y}, {newc1x, newc1y}, {newc2x, newc2y}, {c3x, c3y}}]},
  A2 - A1
 ]
deltaAttArea[{c1x_, c1y_}, {c3x_, c3y_}, {newc2x_, newc2y_}] :=
 getPolygonArea[{{c1x, c1y}, {newc2x, newc2y}, {c3x, c3y}}]

deltaAreaIntMovement[{c0x_, c0y_}, {c1x_, c1y_}, {c2x_, c2y_},
  {c3x_, c3y_}, {newc1x_, newc1y_}, {newc2x_, newc2y_}] :=
 Block[{A1 = getPolygonArea[{{c0x, c0y}, {c1x, c1y}, {c2x, c2y}, {c3x, c3y}}],
   A2 = getPolygonArea[
     {{c0x, c0y}, {newc1x, newc1y}, {newc2x, newc2y}, {c3x, c3y}}]},
  A2 - A1
 ]

pointLineDistance[{Ax_, Ay_}, {Bx_, By_}, {Cx_, Cy_}] :=
 Module[{A, B, C, D, distance},
  (*Define the points*)
  A = {Ax, Ay};
  B = {Bx, By};
  C = {Cx, Cy};

  D = A + (Dot[C - A, B - A] / Dot[B - A, B - A]) (B - A);

  If[Dot[D - A, D - B] ≤ 0,
   distance = Norm[D - C],
   distance = Min[Norm[C - A], Norm[C - B]]
  ];
  distance
 ]
```

```
In[∘]:= rulesSpine := {
```

```
{s0 == spine[centralID0, coords0, adjID0a, centralID1],
  s1 == spine[centralID1, coords1, adjID1a, centralID3],
  s3 == spine[centralID3, coords3, centralID1, adjID3b],
  s4 == spine[centralID4, coords4, centralID3, adjID4b],
  actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP,
   dist, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
  actin[aID, coords, aIDP, aIDN, angle, CL, arpID, end,
   spineID2N, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
  spineHeadArea[area],
  actinATPCount[numActin], spineAtt[aIDP, centralID1, centralID3]
 } → {
  spineAtt[aIDP, centralID1, centralID3],
  actin[aID, coords, aIDP, aIDN, angle, CL, arpID, end, spineID2N,
   ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG], spineHeadArea[area],
  actinATPCount[numActin], actin[aIDP, coordsP, aIDPP, aIDPN, angleP,
   CLP, arpIDP, endP, dist + 1/membraneFactor ((δ (pointGrowthT numActin
          E^(-ωoverf membraneForce[coords0,coords1,coordsP,coords3,coords4,coordsP-coords]) -
         pointRetr))), ATPCountCGP,
   ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP], s0, s1, s3, s4
 },
with[membraneFactor Boole[dist < overgrowthL]],
{
  s0 == spine[centralID0, coords0, adjID0a, centralID1],
  s1 == spine[centralID1, coords1, adjID1a, centralID3],
  s3 == spine[centralID3, coords3, centralID1, adjID3b],
  s4 == spine[centralID4, coords4, centralID3, adjID4b],

  spineAtt[aID, centralID1, centralID3],
  actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, spineID2P,
   ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
  actin[aID, coords, aIDP, aIDN, angle, CL, arpID, BARMEM,
   dist, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
  spineHeadArea[area], actinATPCount[numActin]} →
 {spineAtt[aID, centralID1, centralID3],
  actin[aID, coords, aIDP, aIDN, angle, CL,
   arpID, BARMEM, dist + 1/membraneFactor ((δ (barbGrowthT numActin
          E^(-ωoverf membraneForce[coords0,coords1,coords,coords3,coords4,coords-coordsP]) -
         barbRetr))), ATPCountCG, ADPCountCG, ADPPiCountCG,
   ADPCofCountCG], spineHeadArea[area], actinATPCount[numActin],
   actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP,
    endP, spineID2P, ATPCountCGP, ADPCountCGP,
    ADPPiCountCGP, ADPCofCountCGP], s0, s1, s3, s4
  },
 with[membraneFactor Boole[dist < overgrowthL]],

 {
   s0 ⩵ spine[adjID1a, coords0, adjID0a, adjID0b],
   s1 ⩵ spine[adjID2a, coords1, adjID1a, spineID],
   spine[spineID, coords2, adjID2a, adjID2b],
   s3 ⩵ spine[adjID2b, coords3, spineID, adjID3b],
   s4 ⩵ spine[adjID3b, coords4, adjID4a, adjID4b],
   spineHeadArea[area]
  } →
  {
   s0, s1,
   spine[spineID, membraneDelta[coords0, coords1,
      coords2, coords3, coords4] + coords2, adjID2a, adjID2b]
   , s3, s4,
   spineHeadArea[area + deltaArea5[coords0, coords1, coords2, coords3, coords4,
      membraneDelta[coords0, coords1, coords2, coords3, coords4] + coords2]]
  },
 with[membraneFactor],

 (*Rule for applying working force
  onto a membrane vertex and attached actin object*)
 {
   s0 ⩵ spine[adjID1a, coords0, adjID0a, centralID1],
   spine[centralID1, coords1, adjID1a, centralID3],
   spine[centralID3, coords3, centralID1, adjID3b],
   s4 ⩵ spine[adjID3b, coords4, centralID3, adjID4b],
   actin[aID, coords, attachID2, aIDN, angle, CL, arpID, end,
    membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
   actin[attachID2, coordsP, aIDPP, aID, angleP, CLP, arpIDP, POIMEM,
    dist, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
   spineHeadArea[area], spineAtt[attachID2, centralID1, centralID3]
  } →
  {
   s0, s4,
```

$$\texttt{spine}\left[\texttt{centralID1, coords1} + \left(1 - \frac{\texttt{Norm[coordsP - coords1]}}{\texttt{Norm[coords1 - coords3]}}\right)\right.$$

```
      deltaFuncWF[coords, lineIntersectionPoint[coords1, coords3, coords,
          coordsP], actinRule, dist, ϵ, zeta], adjID1a, centralID3],
    spine[centralID3, coords3 + (1 - Norm[coordsP - coords3]/Norm[coords1 - coords3])
        deltaFuncWF[coords, lineIntersectionPoint[coords1, coords3, coords,
          coordsP], actinRule, dist, ϵ, zeta], centralID1, adjID3b],
    spineHeadArea[area + deltaArea4[coords0, coords1,
        coords3, coords4, coords1 + (1 - Norm[coordsP - coords1]/Norm[coords1 - coords3])
          deltaFuncWF[coords, lineIntersectionPoint[coords1, coords3,
            coords, coordsP], actinRule, dist, ϵ, zeta], coords3 +
          (1 - Norm[coordsP - coords3]/Norm[coords1 - coords3]) deltaFuncWF[coords, lineIntersectionPoint[
            coords1, coords3, coords, coordsP], actinRule, dist, ϵ, zeta]]],
    actin[aID, coords, attachID2, aIDN, angle, CL, arpID, end,
     membraneID, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[attachID2, lineIntersectionPoint[coords1 +
        (1 - Norm[coordsP - coords1]/Norm[coords1 - coords3]) deltaFuncWF[coords, lineIntersectionPoint[
           coords1, coords3, coords, coordsP], actinRule, dist, ϵ, zeta],
       coords3 + (1 - Norm[coordsP - coords3]/Norm[coords1 - coords3]) deltaFuncWF[coords,
          lineIntersectionPoint[coords1, coords3, coords, coordsP],
          actinRule, dist, ϵ, zeta], coords, coordsP],
     aIDPP, aID, angleP, CLP, arpIDP, POIMEM, dist, ATPCountCGP,
     ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    spineAtt[attachID2, centralID1, centralID3]
   },
  with[membraneFactor],

  {
    s0 == spine[adjID1a, coords0, adjID0a, centralID1],
    spine[centralID1, coords1, adjID1a, centralID3],
    spine[centralID3, coords3, centralID1, adjID3b],
    s4 == spine[adjID3b, coords4, centralID3, adjID4b],
    actin[attachID2, coords, aIDP, aIDN, angle, CL, arpID, end,
     dist, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
     ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    spineHeadArea[area], spineAtt[attachID2, centralID1, centralID3]
   } →
```

```
 {
  spine[centralID1, coords1 + (1 - Norm[coords - coords1]/Norm[coords1 - coords3])
     deltaFuncWF[coordsP, lineIntersectionPoint[coords1, coords3, coords,
       coordsP], actinRule, dist, ϵ, zeta], adjID1a, centralID3],
  spine[centralID3, coords3 + (1 - Norm[coords - coords3]/Norm[coords1 - coords3])
     deltaFuncWF[coordsP, lineIntersectionPoint[coords1, coords3, coords,
       coordsP], actinRule, dist, ϵ, zeta], centralID1, adjID3b],
  s0, s4,
  spineHeadArea[area + deltaArea4[coords0, coords1, coords3, coords4,
     coords1 + (1 - Norm[coords - coords1]/Norm[coords1 - coords3]) deltaFuncWF[coordsP,
        lineIntersectionPoint[coords1, coords3, coords, coordsP],
        actinRule, dist, ϵ, zeta], coords3 + (1 - Norm[coords - coords3]/Norm[coords1 - coords3])
       deltaFuncWF[coordsP, lineIntersectionPoint[coords1,
         coords3, coords, coordsP], actinRule, dist, ϵ, zeta]]],
  actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, endP, membraneIDP,
   ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
  actin[attachID2,
   lineIntersectionPoint[coords1 + (1 - Norm[coords - coords1]/Norm[coords1 - coords3])
      deltaFuncWF[coordsP, lineIntersectionPoint[coords1, coords3,
        coords, coordsP], actinRule, dist, ϵ, zeta], coords3 +
     (1 - Norm[coords - coords3]/Norm[coords1 - coords3]) deltaFuncWF[coordsP, lineIntersectionPoint[
        coords1, coords3, coords, coordsP], actinRule, dist, ϵ, zeta],
    coords, coordsP], aIDP, aIDN, angle, CL, arpID, end, dist,
   ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
  spineAtt[attachID2, centralID1, centralID3]
 },
with[membraneFactor],

(*Rule for detaching actin from a membrane
 vertex with a barbed actin load due to membrane force*)
{
  spine[spineIDP, coords1, adjID1a, adjID1b],
  spine[spineIDN, coords3, adjID3a, adjID3b],
    actin[aID, coords, aIDP, aIDN, angle, CL, arpID, type,
     dist, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    aP == actin[aIDP, coordsP, aIDPP, aIDPN, angleP, CLP, arpIDP, typeP,
      distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    spineAtt[aID, spineIDP, spineIDN],
    newID[NID]
   } →
   {
    spine[spineIDP, coords1, adjID1a, adjID1b],
    spine[spineIDN, coords3, adjID3a, adjID3b],
    aP, newID[NID + 1],
    actin[aID, (coords - coordsP)/(Norm[coordsP - coords]) + coordsP,
     aIDP, NID, angle, CL, arpID, INT, membraneIDFree,
     ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[NID, coords, aID, aIDFreeB, 0, 0, arpIDFree, type, overgrowthL - 1.,
     ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    spineAtt[NID, spineIDP, spineIDN]
   },
  with[boundarySpineFactor
    Boole[dist ≥ overgrowthL && Norm[coords - coordsP] ≥ overgrowthL]],

  (*Rule for detaching actin from a membrane
   vertex with a pointed actin due to membrane force*)
  {
    spine[spineIDP, coords1, adjID1a, adjID1b],
    spine[spineIDN, coords3, adjID3a, adjID3b],
    a1 == actin[aID, coords, aIDP, aIDN, angle, CL, arpID, end,
      distN, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    actin[aIDP, coordsP, aIDPP, aID, angleP, CLP, arpIDP, POIMEM,
     dist, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    spineAtt[aIDP, spineIDP, spineIDN],
    newID[NID]
   } →
   {
    spine[spineIDP, coords1, adjID1a, adjID1b],
    spine[spineIDN, coords3, adjID3a, adjID3b],
    spineAtt[NID, spineIDP, spineIDN],
    a1, newID[NID + 1],
    actin[aIDP, (coordsP - coords)/(Norm[coordsP - coords]) + coords,
     NID, aID, angleP, CLP, arpIDP, INT, membraneIDFree,
     ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[NID, coordsP, aIDFreeP, aIDP, 0, 0, arpIDFree, POIMEM,
     overgrowthL - 1., ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP]
   },
  with[boundarySpineFactor *
    Boole[dist ≥ overgrowthL && Norm[coords - coordsP] ≥ overgrowthL]],

  (*Fix intersections with spine head membrane*)
  (*Rule for checking if barbed actin rod and membrane rod intersect*)
  {
    s0 == spine[spineID0, coords0, spineIDP, spineID1],
    s1 == spine[spineID1, coords1, spineID0, spineIDN],
    aP == actin[aID, coords, aIDP, aIDN, angle, CL, arpID, INT, distP,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[aIDN, coordsN, aID, aIDNN, angleN, CLN, arpIDN, typeN,
     dist, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG]
   } →
   {
    s0, s1,
    aP, actin[aIDN, lineIntersectionPoint[coords0, coords1,
      overgrowthL (coordsN - coords)/(Norm[coordsN - coords]) + coords, coords], aID, aIDNN, angleN,
     CLN, arpIDN, BARMEM Boole[typeN == BAR] + CAPMEM Boole[typeN == CAP],
     dist Boole[dist ≠ membraneIDFree] +
      pointLineDistance[coords0, coords1, coords] Boole[dist == membraneIDFree],
     ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG],
    spineAtt[aIDN, spineID0, spineID1]
   },
  with[boundarySpineFactor Boole[intersectingLinesQ[coords0,
      coords1, overgrowthL (coordsN - coords)/(Norm[coordsN - coords]) + coords, coords]]
    Boole[typeN == BAR || typeN == CAP]],
  {
    s0 == spine[spineID0, coords0, spineIDP, spineID1],
    s1 == spine[spineID1, coords1, spineID0, spineIDN],
    aP == actin[aID, coords, aIDP, aIDN, angle, CL, NID, end, distP,
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
    actin[NID, coordsN, aID, aIDNN, angleN, CLN, arpIDN,
     BAR, dist, ATPCountCG, ADPCountCG, ADPPiCountCG, ADPCofCountCG]
   } →
```

```
    {
     s0, s1,
     actin[aID, coords, aIDP, aIDN, angle, CL, arpIDFree, end,
      distP, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP]
    },
   with[boundarySpineFactor Boole[intersectingLinesQ[coords0,
       coords1, overgrowthL (coordsN - coords)/Norm[coordsN - coords] + coords, coords]]],
   (*Rule for checking if pointed actin rod and membrane rod intersect*)
   {
     s0 == spine[spineID0, coords0, spineIDP, spineID1],
     s1 == spine[spineID1, coords1, spineID0, spineIDN3],
     actin[aIDP, coordsP, aIDPP, aIDN, angleP, CLP, arpIDP, POI,
      dist, ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP],
     aN == actin[aIDN, coordsN, aIDP, aIDNN, angleN, CLN, arpIDN, INT,
       distN, ATPCountCGN, ADPCountCGN, ADPPiCountCGN, ADPCofCountCGN]
    } →
    {
     spineAtt[aIDP, spineID0, spineID1], s0, s1,
     aN, actin[aIDP, lineIntersectionPoint[coords0, coords1,
       overgrowthL (coordsP - coordsN)/Norm[coordsP - coordsN] + coordsN, coordsN],
      aIDPP, aIDN, angleP, CLP, arpIDP, POIMEM,
      dist Boole[dist ≠ membraneIDFree] + pointLineDistance[
         coords0, coords1, coordsN] Boole[dist == membraneIDFree],
      ATPCountCGP, ADPCountCGP, ADPPiCountCGP, ADPCofCountCGP]
    },
   with[boundarySpineFactor Boole[intersectingLinesQ[coords0,
       coords1, overgrowthL (coordsP - coordsN)/Norm[coordsP - coordsN] + coordsN, coordsN]]]
  };
```

Reduced Test

```
parameter = NOR;
currSynthRate = Log10[
   Boole[parameter === Arp] arpSynthRate + Boole[parameter === Cam] camSynthRate +
    Boole[parameter === Cof] cofilinSynthRate + Boole[parameter === NOR]];
synthRates = Table[x, {x, currSynthRate - 1.5, currSynthRate + 1.5, 3. / 9}];
```

```
modelSpine =
  Grammar[rules → Join[rulesBarb, rulesPoint, rulesMolVanilla, rulesNuc, rulesCof,
        rulesCap, rulesBranch, rulesAnisotropic, rulesEndPairwiseAnisotropic,
        rulesBending, rulesEndPairwiseBending, rulesHessian, rulesHessianEnds,
        rulesBundling, rulesBundlingMovement, rulesBundlingMovementHessian,
        rulesSpine] /. potentialVars /. rateVars /. membraneRules];
```

$$\text{Norm}'[\text{d\_}] := \frac{\text{d}}{\text{Norm}[\text{d}]};$$

```
Re'[d_] := Re[d];
<< Plenum.m;
meshSize = 20;
spineCoords = generateSpinePoints[meshSize, 3.];
reducedSpineic = {};
spineic = myic;
For[i = 2, i ≤ Length[spineCoords] + 1, i++,
  AppendTo[reducedSpineic,
   spine[i, newPos[spineCoords⟦i - 1⟧, 360 Degree / meshSize],
    Mod[i - 3, Length[spineCoords]] + 2, If[i == Length@spineCoords + 1, 2, i + 1]]]
 ];
AppendTo[reducedSpineic, spineIDMax[Length@spineCoords + 3]];

rate = 10 ^ (synthRates⟦Mod[it, 10] + 1⟧);
myRates = {arpRate → rate Boole[parameter === Arp] +
     arpSynthRate Boole[! (parameter === Arp)], cofilinRate →
    rate Boole[parameter === Cof] + cofilinSynthRate Boole[! (parameter === Cof)],
   cofilinDeg → cofilinDegRate, barbGrowthT → kPlusBarbedT / nCG,
   barbGrowthD → kPlusBarbedD / nCG,
```

$$\text{barbRetr} \to \frac{1}{\frac{1}{\frac{\text{kMinusBarbedT}}{\text{ATPCountCG+10}^{-8}}} + \frac{1}{\frac{\text{kMinusBarbedD}}{\text{ADPCountCG+ADPPiCountCG+10}^{-8}}} + \frac{1}{\frac{\text{kMinusBarbedCof}}{\text{ADPCofCountCG+10}^{-8}}}},$$

```
   pointGrowthT → kPlusPointedT / nCG, pointGrowthD → kPlusBarbedD / nCG,
```

$$\text{pointRetr} \to \frac{1}{\frac{1}{\frac{\text{kMinusPointedT}}{\text{ATPCountCG+10}^{-8}}} + \frac{1}{\frac{\text{kMinusPointedD}}{\text{ADPCountCG+ADPPiCountCG+10}^{-8}}} + \frac{1}{\frac{\text{kMinusPointedCof}}{\text{ADPCofCountCG+10}^{-8}}}}, \text{cap} \to \text{kcapon},$$

```
   capoff → kcapoff, sever → ksev, branchAng → θArp, sdGrowth → θp,
   arpDeg → arpDegRate , actinRate → actinSynthRate , actinDeg → actinDegRate ,
   bundle → koncamKIIβ / nCG, unbundle → koffcamKIIβ / nCG,
   actinPhos → actinNucPhos, actinATPDc → actinATPDissociation,
   cofBindEdge → kOnCofEdge, cofUnbind → kOffCof, cofBindSingle → kOnSingleCof,
   branchGrowthAct → keqk2 * nCG, branchRetrAct → kminus2,
   branchGrowthDeact → k1 / nCG, branchRetrDeact → kminus1 / nCG,
   capRate → cappingSynthRate, capDeg → cappingDegRate, camRate →
    rate Boole[parameter === Cam] + camSynthRate Boole[! (parameter === Cam)],
    camDeg → camDegRate, capoffcof → kcofcapoff, caponcof → kcofcapon,
    cofBindPiEdge → kOnCofEdgeADPPi};

reducedSpineic = Join[reducedSpineic , ( {
        actin[1, { -1., 0}, aIDFreeP, 2, 0.0, 0., arpIDFree, POI,
         membraneIDFree, nCG, 0, 0, 0], (* new node at the pointed end *)
        actin[2, {0., 0.}, 1, 3, 0., 0., 4, INT,
         membraneIDFree, nCG - 1., 0, 0, 1], (* new internal node *)
        actin[3, {1., 0.}, 2, aIDFreeB, 0.0, 0., arpIDFree, BAR,
         membraneIDFree, nCG, 0, 0, 0], (* new node at the pointed end *)

        (* place a branch to begin with and see how it works *)
        actin[4, { Cos[70 Degree], Sin[70 Degree]}, 2,
         5, 0., 0.0, arpIDFree, INT, membraneIDFree, nCG, 0, 0, 0],
        actin[5, {2 Cos[70 Degree], 2 Sin[70 Degree]}, 4, aIDFreeB,
         0.0, 0.0, arpIDFree, BAR, membraneIDFree, nCG, 0, 0, 0],

        newID[11], (* counter for new ids to be generated *)
        arpCount[
         (rate Boole[parameter === Arp] + arpSynthRate Boole[! (parameter === Arp)]) /
          arpDegRate], (* counter for the amount of ARP
         floating in the system at any given point in the sim *)
        actinATPCount[initActinATPNum],
        actinADPCount[initActinADPNum],
        cofilinCount[(rate Boole[parameter === Cof] +
            cofilinSynthRate Boole[! (parameter === Cof)]) / cofilinDegRate],
        spineHeadArea[area],
        cappingCount[initCappingNum],
        camCount[(rate Boole[parameter === Cam] +
            camSynthRate Boole[! (parameter === Cam)]) / camDegRate]
      }) // N] /. {area → getPolygonArea[spineCoords] // N};

modelSpine = modelSpine /. myRates;

simdir = "~/simNew" <> ToString[parameter] <> "_3-13-25/" <> ToString[it] <> "/";
CreateDirectory[simdir];
SetDirectory[simdir];
simSpine = {{0, reducedSpineic}};
Export[simdir <> "simSpine0.wls", {0., simSpine}];
transformedRate = N@(rate * speciesToMol // FullSimplify);
Export[simdir <> "param.wls", transformedRate];
SeedRandom[it^2];
Clear[sims];
```

```
Clear[frames];
files =
  SortBy[FileBaseName[#] & /@ FileNames[simdir <> "/simSpine*"], processFileNames];
files = simdir <> # <> ".wls" & /@ files;
simSpine = Import[files⟦-1⟧]⟦2⟧;
lastSavedIt = (processFileNames[FileBaseName[files⟦-1⟧]] // ToExpression);
For[j = 1, j ≤ 100 000 000., j++,
  lastTime = simSpine⟦-1, 1⟧;
  ic = simSpine⟦-1, 2⟧;
  Clear[simSpine];
  {t1, b1} = AbsoluteTiming[
    executeGrammar[modelSpine, ic, 20, False, saveAllSimulation → True]];
  simSpine = getSimulationStruct[] /. {} → Nothing;
  simSpine⟦ ;; , 1⟧ += lastTime;
  Export[
   simdir <> "/simSpine" <> ToString[lastSavedIt + j] <> ".wls", {t1, simSpine}];
 ];
```

Utilities

In[ ]:=
```
checkAngles[snapshot_] :=
 Block[{trueAngle, simAngle, a, prevActin, nextActin, nextAng, prevAng, i,
   actins = Join[Cases[snapshot⟦2⟧, actin[__], Cases[snapshot⟦2⟧, arp[__]]]]},
  For[i = 1, i ≤ Length@actins, i++,
   a = actins⟦i⟧;
   prevActin = Select[actins, #⟦1⟧ == a⟦PREV⟧ &];
   nextActin = Select[actins, #⟦1⟧ == a⟦NEXT⟧ &];
   If[Length@prevActin ≠ 0 && Length@nextActin ≠ 0,
    prevActin = prevActin⟦1⟧;
    nextActin = nextActin⟦1⟧;
    nextAng = ArcTan @@ (nextActin⟦POS⟧ - a⟦POS⟧);
    prevAng = ArcTan @@ (a⟦POS⟧ - prevActin⟦POS⟧);
    If[Abs[nextAng] > Pi / 2 && Sign[nextAng] ≠ Sign[prevAng],
     trueAngle = Mod[nextAng, 2 Pi] - Mod[prevAng, 2 Pi],
     trueAngle = nextAng - prevAng
    ];
    simAngle = a⟦ANGLE⟧;
    If[Abs[trueAngle - simAngle] > 10 ^ (-5),
     Print["Anomaly"];
     Print[prevActin];
     Print[a];
     Print[nextActin];
     Print[Abs[trueAngle - simAngle]];
     Print[trueAngle];
    ]
   ]
  ]
 ]
```