METHODS S2: Detailed description of the computational model of actomyosin mechanics, related to Figure 6.

Brownian dynamics via the Langevin equation

In our agent-based model, F-actin is simplified into serially connected cylindrical segments with barbed and pointed ends. Motors have a backbone structure with eight arms ($N_a = 8$) attached, and each of the motor arm represents four myosin heads. Therefore, the total number of myosin heads represented by one motor is 32, which is not quite different from 56 myosin heads in one non-muscle myosin thick filament (Tyska et al, 1999). The backbone and arms of the motors are also described by cylindrical segments. ACPs are comprised of two cylindrical arm segments.

The displacements of all the cylindrical segments are determined by the Langevin equation with the negligence of inertia:

$$\dot{\mathbf{r}}_i - \zeta_i \frac{d\mathbf{r}}{dt} + F_i^T = 0 \quad (S1)$$

where $\mathbf{r}_i$ is a position vector of the $i$th element, $\zeta_i$ is a drag coefficient, $t$ is time, $F_i$ is a deterministic force, and $F_i^T$ is a stochastic force satisfying the fluctuation-dissipation theorem (Underhill and Doyle, 2004):

$$\langle F_i^T(t) F_j^T(t) \rangle = \frac{2k_B T \zeta_i \delta_{ij}}{\Delta t} \delta \quad (S2)$$

where $\delta$ is a second-order tensor, $\delta_{ij}$ is the Kronecker delta, and $\Delta t = 1.15 \times 10^{-5}$ s is a time step.

The drag coefficients are calculated via an approximated form for cylindrical objects (Clift, Grace and Weber, 2005):
\[ \zeta_i = 3\pi \mu r_{c,i} \frac{3+2r_{0,i}/r_{c,i}}{5} \quad (S3) \]

where \( \mu \) is the viscosity of surrounding medium, and \( r_{0,i} \) and \( r_{c,i} \) are the length and diameter of segments, respectively. The positions of all the cylindrical segments are updated at each time step via the Euler integration scheme:

\[
\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \frac{d\mathbf{r}_i}{dt} \Delta t = \mathbf{r}_i(t) + \frac{1}{\zeta_i} \left( \mathbf{F}_i + \mathbf{F}_i^T \right) \Delta t \quad (S4)
\]

**Deterministic forces**

Deterministic forces include extensional forces maintaining equilibrium lengths, bending forces maintaining equilibrium angles, and repulsive forces accounting for volume-exclusion effects between actin segments. The extensional and bending forces originate from the following potentials:

\[
U_s = \frac{1}{2} \kappa_s (r - r_0)^2 \quad (S5)
\]

\[
U_b = \frac{1}{2} \kappa_b (\theta - \theta_0)^2 \quad (S6)
\]

where \( \kappa_s \) and \( \kappa_b \) are extensional and bending stiffnesses, \( r \) and \( r_0 \) are the instantaneous and equilibrium lengths of cylindrical segments, and \( \theta \) and \( \theta_0 \) are instantaneous and equilibrium angles formed by segments. The equilibrium length of actin segments (\( r_{0,A} = 140 \text{ nm} \)) and an equilibrium angle formed by two adjacent actin segments (\( \theta_{0,A} = 0 \text{ rad} \)) are maintained by extensional (\( \kappa_{s,A} \)) and bending (\( \kappa_{b,A} \)) stiffnesses of actins, respectively. The reference value of \( \kappa_{b,A} \) corresponds to the persistence length of \( \sim 9 \mu \text{m} \) (Isambert et al, 1995). The equilibrium length of ACP arms (\( r_{0,ACP} \)}
= 23.5 nm) and an equilibrium angle formed by the two arm segments of each ACP ($\theta_{0,\text{ACP}} = 0$ rad) are regulated by extensional ($\kappa_{s,\text{ACP}}$) and bending ($\kappa_{b,\text{ACP}}$) stiffnesses of ACPs, respectively. The equilibrium length of motor backbone segments ($r_{s,M1} = 42$ nm) and an equilibrium angle formed by adjacent backbone segments ($\theta_{0,M} = 0$ rad) are maintained by extensional ($\kappa_{s,M1}$) and bending ($\kappa_{b,M}$) stiffnesses, respectively. The value of $\kappa_{s,M1}$ is equal to that of $\kappa_{s,A}$, whereas the value of $\kappa_{b,M}$ is larger than that of $\kappa_{b,A}$. The extension of each motor arm is regulated by the two-spring model with stiffnesses of transverse ($\kappa_{s,M2}$) and longitudinal ($\kappa_{s,M3}$) springs. The transverse spring maintains an equilibrium distance ($r_{0,M2} = 13.5$ nm) between the endpoint of a motor backbone and an actin segment where the arm of the motor binds, whereas the longitudinal spring maintains a right angle between the motor arm and the actin segment ($r_{0,M3} = 0$ nm).

The repulsive force is represented by a harmonic potential (Kim et al, 2009):

$$U_r = \begin{cases} \frac{1}{2} \kappa_r \left( r_{12} - r_{c,A} \right)^2 & \text{if } r_{12} < r_{c,A} \\ 0 & \text{if } r_{12} \geq r_{c,A} \end{cases}$$

(S7)

where $\kappa_r$ is the strength of repulsive force, and $r_{12}$ is a minimum distance between two actin segments. Forces exerted on actin segments by bound motors and ACPs or by the repulsive force are distributed onto the barbed and pointed ends of the actin segments as described in our previous work (Young, Murrell, Kim, 2015).

**Dynamics of ACPs**

ACP bind to binding sites located on actin segments every 7 nm without preference for cross-linking angles at a constant rate and also unbind from F-actin at a force-dependent rate determined by Bell’s law (Bell, 1978):
\[
 k_{u,ACP} = \begin{cases} 
 k_{u,ACP}^0 \exp \left( \frac{x_{u,ACP} |\bar{F}_{u,ACP}|}{k_BT} \right) & \text{if } r \geq \eta_{0,ACP} \\
 k_{u,ACP}^0 & \text{if } r < \eta_{0,ACP} 
\end{cases}
\]  

where $|\bar{F}_{u,ACP}|$ is a spring force acting on an ACP arm, $k_{u,ACP}^0$ is the zero-force unbinding rate constant, $x_{u,ACP}$ is sensitivity to an applied force, and $k_BT$ is thermal energy. The values of $k_{u,ACP}^0 (= 0.115 \text{ s}^{-1})$ and $x_{u,ACP} (= 1.04\times10^{-10} \text{ m})$ are determined based on filamin A (Ferrer et al, 2008).

**Dynamics of motors**

Motor arms bind to binding sites on actin segments at the rate of $40N_h \text{ s}^{-1}$, where $N_h = 8$ is the number of myosin heads represented by each motor arm. The walking ($k_w,M$) and unbinding ($k_u,M$) rates of the motor arms are determined by the parallel cluster model to mimic the mechanochemical cycle of non-muscle myosin II (Erdmann, Albert, Schwartz, 2013, Erdmann, Schwartz, 2012). The details of implementation and benchmarking of the parallel cluster model in our models are described in detail in our previous study (Kim, 2015). Note that $k_w,M$ and $k_u,M$ are smaller with larger applied loads because motors exhibit a catch-bond behavior. The unloaded walking velocity and stall force of motors are $\sim$$140 \text{ nm/s}$ and $\sim$$5.7 \text{ pN}$, respectively.

**Actin dynamics**

The formation of F-actin is initiated from a nucleation event with the appearance of one cylindrical segment with polarity (i.e., with barbed and pointed ends) in a random orientation.
perpendicular to the z direction. The polymerization and depolymerization of actins are simulated by the addition and removal of cylindrical segments, respectively, as in our previous studies (Mak et al, 2016). The average length of F-actin ($<L_f>$) used in simulations is ~1 μm. This value is comparable to that estimated in our in vivo experiments. In addition, with the reference values of the rate constants for actin dynamics, each F-actin turns over every ~10 s.

**Contraction of actin**

In order to quantitatively analyze the network morphology, we evaluate the contraction of F-actin, using the spatial distribution of F-actins in activated regions whose dimension is 5×5 μm in x and y directions. First, the activated region is divided into $N_G \times N_G$ grids. We found that the optimal level of $N_G$ is 15. All grids are indicated by their own coordinate, $(i, j)$. In each grid, we measure the intensity of actin segments at time $t$, $\rho_{\lambda,j}^{i,j}$. Then, the standard deviation of $\rho_{\lambda,j}^{i,j}$ in all $N_G^2$ grids is calculated and normalized by the initial mean value of actin density, $\rho_{\lambda,0}$. The normalized value represents the extent of actin contraction at each time point, $t$:

$$\text{Actin contraction at } t = \frac{1}{\rho_{\lambda,0}} \sqrt{\sum_{i,j=1}^{N_G} (\rho_{\lambda,j}^{i,j} - \rho_{\lambda,j})^2 \over N_G}$$  \hspace{1cm} (Eq. S9)

We calculate the time evolution of actin contraction by subtracting the initial value of actin contraction from the instantaneous value at each time step. As F-actins aggregate more within the activated region (i.e., more contraction), the spatial distribution of F-actins will become more heterogeneous, increasing the standard deviation of $\rho_{\lambda,j}^{i,j}$ and thus enhancing the extent of actin
contraction. From the time evolution curve (Fig. 6b, inset), we obtain the maximal extent of actin contraction and contraction level at a plateau phase.

**Contraction of myosin motors**

We calculate the extent of motor contraction using the center position of motor thick filaments, \((x_{M_i}, y_{M_i})\), where \(i\) is the index of motors, and \(t\) is time. At each time step, we calculate a distance between the center position of each thick filament and the center position of a currently activated region, \((x_{reg,t}, y_{reg,t})\). We assume that the average of all the distances represents the approximate size of motor clusters. The average is further divided by an initial value:

\[
\text{Motor contraction} = \frac{\sum_{i=1}^{N_M} \sqrt{(x_{M_i,t} - x_{reg,t})^2 + (y_{M_i,t} - y_{reg,t})^2} / N_M}{\sum_{i=1}^{N_M} \sqrt{(x_{M_i,0} - x_{reg,0})^2 + (y_{M_i,0} - y_{reg,0})^2} / N_M}
\]  
(Eq. S10)

In the time evolution of motor contraction, we average the maximum values of the motor contraction in all pulse periods to use it as an indicator for the extent of motor contraction.
Table S4. List of parameters employed in the model. For some of the parameters, references are provided if the parameters were determined based on specific previous studies.

| Symbol | Definition | Value |
|--------|------------|-------|
| $r_{0,A}$ | Length of an actin segment | $1.4 \times 10^{-7} [m]$ |
| $r_{c,A}$ | Diameter of an actin segment | $7.0 \times 10^{-9} [m]$ (Kishino and Yanagida, 1988) |
| $\theta_{0,A}$ | Bending angle formed by adjacent actin segments | 0 [rad] |
| $\kappa_{s,A}$ | Extensional stiffness of F-actin | $1.69 \times 10^{-2} [N/m]$ |
| $\kappa_{b,A}$ | Bending stiffness of F-actin | $2.64 \times 10^{-19} [N \cdot m]$ (Isambert et al, 1995) |
| $r_{0,ACP}$ | Length of an ACP arm | $2.35 \times 10^{-8} [m]$ (Meyer and Aebi, 1990) |
| $r_{c,ACP}$ | Diameter of an ACP arm | $1.0 \times 10^{-8} [m]$ |
| $\theta_{0,ACP}$ | Bending angle formed by two ACP arms | 0 [rad] |
| $\kappa_{s,ACP}$ | Extensional stiffness of ACP | $2.0 \times 10^{-3} [N/m]$ |
| $\kappa_{b,ACP}$ | Bending stiffness of ACP | $1.04 \times 10^{-19} [N \cdot m]$ |
| $r_{0,M1}$ | Length of a motor backbone segment | $4.2 \times 10^{-8} [m]$ |
| $r_{0,M2}$ | Length of a motor arm | $1.35 \times 10^{-8} [m]$ |
| $r_{c,M}$ | Diameter of a motor arm | $1.0 \times 10^{-8} [m]$ |
| $\theta_{0,M}$ | Bending angle formed by motor backbone segments | 0 [rad] |
| $\kappa_{s,M1}$ | Extensional stiffness of a motor backbone | $1.69 \times 10^{-2} [N/m]$ |
| $\kappa_{s,M2}$ | Extensional stiffness 1 of a motor arm | $1.0 \times 10^{-3} [N/m]$ |
| $\kappa_{s,M3}$ | Extensional stiffness 2 of a motor arm | $1.0 \times 10^{-3} [N/m]$ |
| $\kappa_{b,M}$ | Bending stiffness of a motor backbone | $5.07 \times 10^{-18} [N \cdot m]$ |
| $N_h$ | Number of heads represented by a motor arm | 4 |
| $N_a$ | Number of arms per motor | 8 |
| $k_{n,A}$ | Nucleation rate of actin | $0.001 [\mu M^{-1} s^{-1}]$ |
| $k_{p,A}$ | Polymerization rate of actin at the barbed end | $5 [\mu M^{-1} s^{-1}]$ |
| $k_{d,A}$ | Depolymerization rate of actin at the pointed end | $50 [s^{-1}]$ |
| $k_0^{ACP}$ | Zero-force unbinding rate constant of ACP | $0.115 [s^{-1}]$ (Ferrer et al, 2008) |
| $x_u^{ACP}$ | Sensitivity of ACP unbinding to applied force | $1.04 \times 10^{-10} [m]$ (Ferrer et al, 2008) |
| $\kappa_r$ | Strength of repulsive force | $1.69 \times 10^{-3} [N/m]$ |
| $\Delta t$ | Time step | $1.15 \times 10^{-5} [s]$ |
| $\mu$ | Viscosity of surrounding medium | $8.6 \times 10^{-3} [kg/m \cdot s]$ |
| $k_B T$ | Thermal energy | $4.142 \times 10^{-21} [J]$ |
| $C_A$ | Actin concentration | $200 [\mu M]$ |
| $R_M$ | Ratio of myosin concentration to $C_A$ | 0.08 |
| $R_{ACP}$ | Ratio of ACP concentration to $C_A$ | 0.01 |
| $\langle L_f \rangle$ | Average length of F-actins | $\sim 1 [\mu m]$ |
| $\rho_f$ | Enhancement factor for faster actin polymerization | 10 |
| $\tau_f$ | Duration of faster actin polymerization | 10 s |
| $d_M$ | Time delay of myosin activation | 5 s |
| $\tau_M$ | Duration of myosin activation | 15 s |