Supplementary Material

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Cell adhesion and polarization are directly initiated by the molecular dynamics at FA[1], which was theoretically modeled according to the motor-clutch mechanism[2]. Briefly, the motor-clutch model quantifies the stochastic binding dynamics of the ligands anchored at AF and the receptors at interface of cell membrane and ECM surface. The myosin motor pulls the AF back with the force of F_{stall} to move with the retrograde velocity of v^{retro}, whereas the molecular clutches of receptors reversibly engage the ligands at AF to resist the retrograde flow of AF with the binding rate (k_{on}) and the dissociation rate (k_{off}).

The binding rate is changed dynamically with the initial value (k_{on}^0) and a first-order clutch addition rate (k_{add})[3] to capture the FRM at FA[4] as shown in Eq.(1).

$$k_{add} = k_{add}^0 \frac{n_c^{max} - n_c}{n_c^{max}} \bar{n}_c, \tag{1}$$

where k_{add}^0 is the initial clutch addition rate. n_c^{max} is the total number of clutch and clutch candidate in the whole cell. n_c represents current number of clutch at each individual vertex. $\bar{n}_c$ denotes the number of currently bound clutches whose applied force (F_c) exceeds the critical force (F_{cr}) of clutch reinforcement at individual vertex.

Under the pull of myosin motor and the resist of elastic ECM, the clutches are stretched to fail with a force-dependent off rate (k_{off}) as shown in Eq.(2).

$$k_{off} = k_{off}^0 \exp(\frac{F_c}{F_b}), \tag{2}$$

where k_{off}^0 is the clutch unloaded off rate and F_b denotes the clutch bond rupture force.

During myosin loading at AF, the transmitted force induces the simultaneous deformations at clutches (x_c) and ECM (x_{sub}). The force at each clutch is calculated by Eq.(3).

$$F_c = \kappa_c (x_c - x_{sub}), \tag{3}$$

where κ_c is the spring constant of clutch.

After the engagement of clutch is resolved, the ECM displacement is obtained by the force balance between clutches and ECM as shown in Eq.(4).

$$x_{sub} = \frac{\kappa_c \sum_{i=1}^{n_b} x_c(i)}{\kappa_{sub} + n_b \kappa_c}, \tag{4}$$

where n_b is the number of bound clutches and κ_{sub} denotes the spring constant of ECM.

Then, the traction force (F_{trac}) of molecular bond at FA is calculated by Eq.(5).

$$F_{trac} = \kappa_{sub} x_{sub}. \tag{5}$$

The myosin motor loads AF by adjusting the retrograde velocity, and modeled as a linear force-velocity relation against the elastic ECM shown in Eq.(6). Detailed parameter setup of the motor-clutch model is listed in Table 1.

$$v^{retro} = v_u (1 - \frac{F_{trac}}{F_{stall}}), \tag{6}$$

where v_u is the unloaded sliding velocity of myosin motor. F_{stall} is the total stall force of myosin motor, and defined as the product of myosin motor number (n_m) and the stall force of an individual myosin motor (F_m).

Finally, the modeled cells are placed on elastic ECM and the referenced traction forces at the leading vertexes with respect to ECM stiffness are obtained by averaging the traction force (F_{trac}) within 10,000 events based on the above motor-clutch model.

Notes and references

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Table 1 Parameters setup of the motor-clutch model.

Parameter	Value	Reference
the initial number of myosin motor at individual vertex(n_m)	50	[5]
the stall force of a myosin motor (F_m)	2 pN	[5]
the unloaded sliding velocity of myosin motor (v_u)	120 nm/s	[6]
the initial number of clutch at individual vertex (n_c^0)	50	assumed
the maximum number of clutch at individual vertex (n_c^{max})	1,200	assumed
the current number of clutch at individual vertex (n_c)	varied	[3]
the rupture force of clutch (F_b)	2 pN	[5]
the initial binding rate of clutch (k_{on}^0)	0.3 s^{-1}	[5]
the initial addition rate of clutch (k_{add}^0)	1 s^{-1}	[3]
the off rate of unloaded clutch (k_{off}^0)	0.1 s^{-1}	[5]
the spring constant of clutch (κ_c)	0.8 pN/nm	[5]
the critical force of clutch reinforcement (F_{cr})	12 pN	[7]