

# 1 SUPPLEMENTARY TEXT

A Monte-Carlo approach is used in both models, where the state and position of each myosin is followed at each time step  $\Delta t = 10^{-6}s$ . At each time step, the algorithm updates the position  $x_i$  of the  $i$ -th myosin with respect to its anchor on the thick filament, considering the current position of the actin filament, the coupling factor for the myosin motors. In this way, the total force generated is given by:

$$F_{Tot} = \sum_{j=1}^{N_{fil}} \sum_{i=1}^{N_{XB}} kx_{ij} \quad (S1)$$

where  $x_{ij}$  refers to the  $i$ -th myosin motor in the  $j$ -th filament,  $N_{XB}$  is the total number of myosin heads, and  $N_{fil}$  is the number of filaments in the sarcomere, while  $k$  is the stiffness of the myosin motor. The position of the myosin head is first updated based on the position of the actin filament,  $z$ , in the previous time step:

$$x_i(t) = z(t) - z_i^a + x_i^a + n_{ps}d \quad (S2)$$

Here  $z_i^a$  and  $x_i^a$  are the positions of the actin filament and the myosin pre-stretch, respectively, at the time of attachment of the  $i$ -th myosin head.  $n_{ps}$  equals 0, 1 and 2 when the myosin head resides in the S0, S1 and S2 minimum, respectively. Having updated the position of each myosin head, the algorithm updates the position of the actin filament by the NewtonRaphson method. In each iteration, the total force is computed by Equation S1.

In both models, rate constants in the attached state are computed through a Kramers-Smoluchovsky approximation of the corresponding Langevin equation of a diffusing, over-damped particle with drag coefficient  $\eta$  in the sinusoidal energy landscape  $E_c(x) + 1/2k(x - x_0)^2$  (see Matherials and Methods):

$$\eta\dot{x}_i = -\omega_i(t)E'(x_i) - k(x_i - x_0^i) + \sqrt{\eta\kappa_b T}\Gamma(t). \quad (S3)$$

$\omega$  is zero when the myosin head is detached and one when it is attached.  $\Gamma(t)$  is a random term satisfying  $\langle \Gamma(t) \rangle = 0$  and  $\langle \Gamma(t_1), \Gamma(t_2) \rangle = 2\delta(t_1 - t_2)$  (white noise).

The algorithm for the model requires a pre-step outside the time loop::

0. Generate a matrix of rate constants for each stretching level between -80 nm and 20 nm through a numerical integration of the Kramers-Smoluchivsky approximation of the Langevin equation describing the motion of a particle in the defined potential energy.

Then:

1. Compute the tension acting on each thin filament and computing the new value of  $k_{01}$
2. Define the new stable state of each myosin (OFF, ON, Pre or post power stroke) using the rate constants for the transitions  $k_{01}$ ,  $k_{10}$ ,  $k_{12}$ ,  $k_{21}$ ,  $k_f$  and  $k_b$ .
3. Update the positions of each myosin head and the actin filament, depending on the setup and external conditions, and calculate the total force.
4. Update the position of the actin filament through an implicit method
5. Increment the time by one time step and return to Step 1 until total time is less than the prescribed

**Table S1. Parameter values and their descriptions**

Parameter	Value	Description
$k$	$2 \text{ pN/nm}$	myosin stiffness
$\eta$	$70 \text{ pNns/nm}$	myosin drag coefficient
LB	$50 \text{ nm}$	half-bare zone
LM	$825 \text{ nm}$	half-myosin filament length
LA	$1224 \text{ nm}$	actin filament length
$\Delta t$	$1 \mu\text{s}$	time step
$\bar{T}$	$277.15\text{K}$	Temperature
$K$	$0.0138 \text{ pNnm/K}$	Boltzmann constant
$k_{01} \text{ MS}$	$596.8 * ON_f s^{-1}$	OFF-ON rate
$k_{10} \text{ MS}$	$206.5 \text{ s}^{-1}$	ON-OFF rate
$k_{12} \text{ MS}$	$92.1 \text{ s}^{-1}\text{nm}^{-1}$	ON to attached rate
$k_{21}^+ \text{ MS}$	$19.1 \text{ s}^{-1}\text{nm}^{-1}$	attached to ON rate when $x > 0$
$k_{21}^- \text{ MS}$	$490 \text{ s}^{-1}$	attached to ON rate when $x < 0$
$k_{01}^0 \text{ conv}$	$17.0\text{s}^{-1}$	OFF-ON rate
$k_{10}^0 \text{ conv}$	$7500 \text{ s}^{-1}$	ON-OFF rate
$\gamma \text{ conv}$	40	cooperativity factor
$k_{12} \text{ conv}$	$30.0 \text{ s}^{-1}\text{nm}^{-1}$	ON to attached rate
$k_{20}^+ \text{ conv}$	$6.2 \text{ s}^{-1}\text{nm}^{-1}$	attached to ON rate when $x > 0$
$k_{20}^- \text{ conv}$	$500 \text{ s}^{-1}$	attached to ON rate when $x < 0$
$m$	0.01	minimum $ON_f$
$t_f$	$200 \text{ pN}^2$	inflection factor for $ON_f$
$d$	$4.6 \text{ nm}$	first and second power stroke step
$F_{atp}$	$8 K\bar{T}/d \text{ pN}$	ATP bias of the energy
$H$	$5.7 K\bar{T} \text{ pNnm}$	Barrier between minima