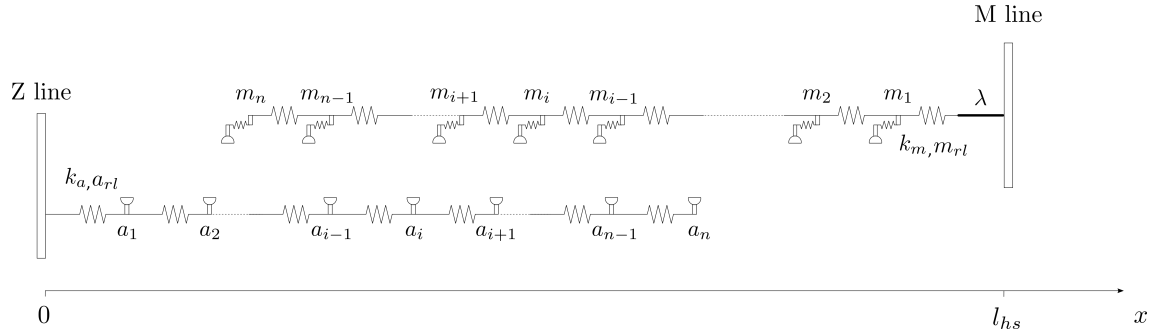


# Force-balance in FiberSim

## 1 Compliant myofilaments

FiberSim is a spatially-explicit model of a half-sarcomere. It describes a compliant network of protein filaments, which is detailed below.



Geometry and mechanical arrangement of the thick and thin filament in FiberSim.

### 1.1 Actin filaments

Thin filaments are composed of nodes joined by linear springs of stiffness  $k_a$  with a resting length  $a_{rl}$ . If the position of the  $i^{th}$  node along an x-axis is noted  $a_i$ , then the force-balance equations for the thin filament can be written as:

$$\begin{aligned} 2 k_a a_1 - k_a a_2 &= 0 \\ -k_a a_{i-1} + 2 k_a a_i - k_a a_{i+1} &= 0 \quad (\text{for } 1 < i < n) \\ -k_a a_{n-1} + k_a a_n &= k_a a_{rl} \end{aligned} \tag{1}$$

### 1.2 Myosin filaments

Thick filaments are composed of nodes joined by linear springs of stiffness  $k_m$  with a resting length  $m_{rl}$ . A rigid link of length  $\lambda$  connects the thick

filament to the M-line. If the position of the  $i^{th}$  node along an x-axis is noted  $m_i$ , and the half-sarcomere length is noted  $l_{hs}$ , then the force-balance equations for the thick filament can be written as:

$$\begin{aligned} 2k_m m_1 - k_m m_2 &= k_m (l_{hs} - \lambda) \\ -k_m m_{i-1} + 2k_m m_i - k_m m_{i+1} &= 0 \quad (\text{for } 1 < i < n) \\ k_m m_{n-1} - k_m m_n &= k_m m_{rl} \end{aligned} \quad (2)$$

The system of equations (1)-(2) can be written in matrix form:

$$Kx = F \quad (3)$$

where  $K$  is a matrix containing the springs stiffness,  $x$  is a vector containing the positions of the actin and myosin nodes ( $a_i$  and  $m_i$ , respectively) and  $F$  is a vector containing the constant terms (independent of nodes positions).  $K$  is a tridiagonal matrix:

$$K = \begin{bmatrix} \# & \# & & 0 \\ \# & \ddots & \ddots & \\ & \ddots & \ddots & \# \\ 0 & & \# & \# \end{bmatrix}$$

and numerical methods exist to solve Eq.(3) for  $x$ .

Crossbridges can bind during contraction, and thus induce crossbridge links between actin and myosin filaments. This will bring new force contributions to Eqs.(1)-(2), and "non-tridiagonal" elements inside  $K$ . This is described in the next section.

## 2 Crossbridge links

Myosin heads located at the thick filament nodes can attach to neighboring binding sites at the thin filament nodes, thus affecting the filament lattice framework.

A crossbridge located at the  $j^{th}$  thick filament node which attaches to the  $i^{th}$  node of the thin filament generates a force  $f_{cb}$  given by:

$$f_{cb} = k_{cb} (m_j - a_i + x_{ps}) \quad (4)$$

where  $k_{cb}$  is the crossbridge spring stiffness and  $x_{ps}$  is the crossbridge extension when deploying the power stroke.

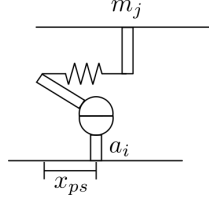


Figure 2: Schematic representation of a crossbridge link.

This additional force on the filaments should be added to the force-balance equations (1)-(2):

$$-k_a a_{i-1} + 2k_a a_i - k_a a_{i+1} - k_{cb} a_i + k_{cb} m_j = f_{cb} x_{ps} \quad (5)$$

$$-k_m m_{j-1} + 2k_m m_j - k_m m_{j+1} + k_{cb} a_i - k_{cb} m_j = -f_{cb} x_{ps} \quad (6)$$

The terms in red will add non-tridiagonal, opposite elements to the  $K$  matrix:

$$K = \begin{bmatrix} \# & \# & \# & 0 \\ \# & \ddots & \ddots & \\ -\# & \ddots & \ddots & \# \\ 0 & & \# & \# \end{bmatrix}$$

while the blue terms will contribute to the  $F$  vector.

Crossbridge linking toughen the numerical solving of Eq.(3), which notably requires an iterative procedure to find a solution  $x$  that satisfies a certain precision.

### 3 Titin

Titin is responsible for the passive force developing within the half-sarcomere when it is stretched, and for the recoil force when it is shortened. In the model, it is assumed that titin is a linear spring of stiffness  $k_t$  and rest length  $t_{rl}$ . This spring is attached at both ends, on a particular thick and thin filament node respectively. Similar to crossbridge links, titin adds some force contribution  $f_t$  to Eqs.(1)-(2):

$$f_t = k_t (m_l - a_k + t_{rl}) \quad (7)$$

## 4 Myosin-binding Protein C

