Thin filament regulation – Run example

The code calculates (1) the dynamics of myosin binding to actin filaments in a solution, and (2) the "titration". Equilibrium is reached by stochastic transitions of tropomyosin between the states blocked, closed and open, and myosin transition between unbind, bind, and rigid states.

(1) Select an output file;
(2) Setup the parameters on the text-boxes. The first box indicate the number of block of 7 monomers per actin fiber and the second box indicate the number of fibers. Thus the total number of possible binding sites are 7 x BOX1 x BOX2. Next choose the time step and the total time of the simulation. Note that a too small time step increase the CPU time, and a too large add errors, thus at the bottom of the page there is a button which suggest a time step. We strong recommend do not select a time step greater than the suggest time. Smaller time steps are always welcome. In the next 8 boxes is possible to select all rates constants. The molar concentration of actin can be selected at box 13;
(3) Select the type of simulation between (a) time course and (b) titration. For time course you have to add the myosin concentration while for titration you have to add the initial and the final concentration of myosin and the number of steps between them. The number of steps will determine the accuracy of the titration curve;
(4) The last text box is the random seed. The random seed can be changed to have different stochastic process. The same random seed with the same parameters will reproduce exactly the same result. However, the overall result should be very similar, almost identical, for different random seeds in a large system;
(5) Then press run to run;
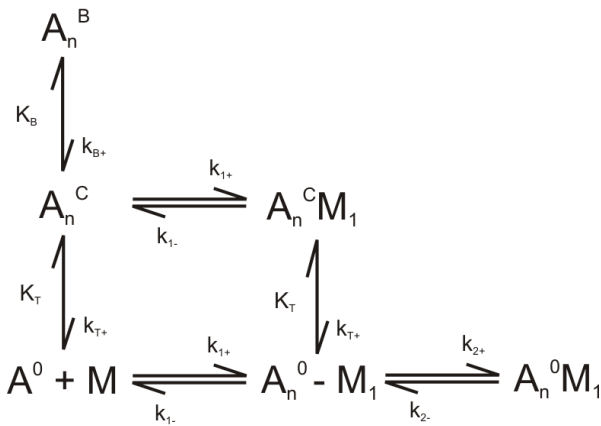(6) Press graphs to see results (several data files, with header, are also stored in the same directory);

Time course frame:

Titration frame:

Used constant rates scheme:

Typical titration graphical result:

A_n^B

K_B , k_{B+}

$A_n^C \rightleftharpoons[k_{1-}]{k_{1+}} A_n^C M_1$

K_T , k_{T+} K_T , k_{T+}

$A^0 + M \rightleftharpoons[k_{1-}]{k_{1+}} A_n^0 - M_1 \rightleftharpoons[k_{2-}]{k_{2+}} A_n^0 M_1$
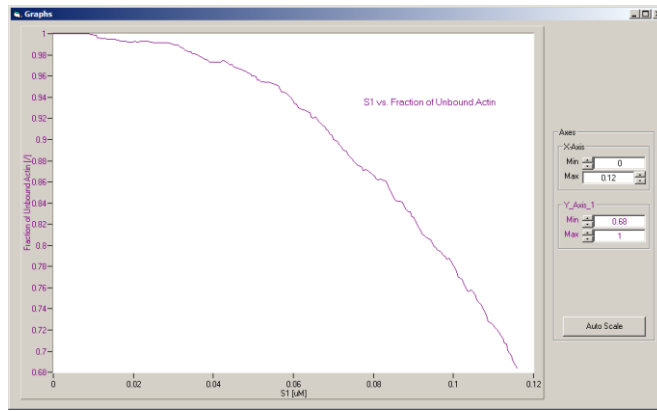
Typical histogram of the occupancy of myosin in the actin filament. The y-axes of each column indicate the fraction of tropomyosin is occupied with 1, 2, … or 7 myosins. Typical time course graphical output is on the right side (picture below)