Mathematical Modeling Lecture 5

Crossbridge populations: transition kinetics and mechanical force

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Attached and detached populations

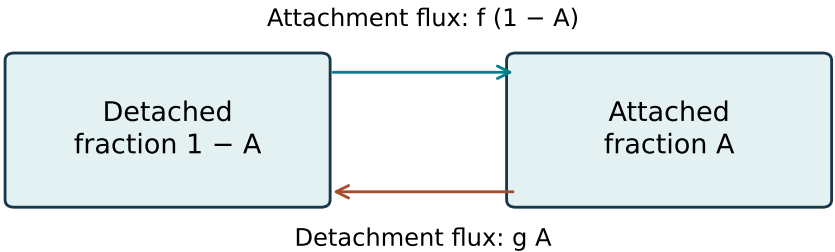
$A + D = 1$, with $A, D \in [0, 1]$.

A fixed population of heads changes category; filaments slide relative to one another.

Occupancy retains chemical state but discards displacement.

Transition fluxes

Two categories; one conserved population



Transition fluxes

$$J_{D\to A} = fD, \qquad J_{A\to D} = gA.$$

$[f] = [g] = \mathrm{s}^{-1}$; both fluxes are population fraction per second.

A transition requires a head in its source category.

The conserved two-state system

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} D \\ A \end{pmatrix} = \begin{pmatrix} -f & g \\ f & -g \end{pmatrix}\begin{pmatrix} D \\ A \end{pmatrix}.$$

$$\dot{D} + \dot{A} = 0, \qquad \dot{A} = f - (f+g)A.$$

Invariant fraction interval

$$\dot{A}\big|_{A=0} = f \geq 0, \qquad \dot{A}\big|_{A=1} = -g \leq 0.$$

The vector field points into the admissible interval at both endpoints.

A negative computed fraction is not an alternative biological state.

Equilibrium with continuing turnover

$$f(1 - A_\infty) = gA_\infty \quad \Longrightarrow \quad A_\infty = \frac{f}{f+g}.$$

For $f = 3$, $g = 1\,\mathrm{s}^{-1}$:

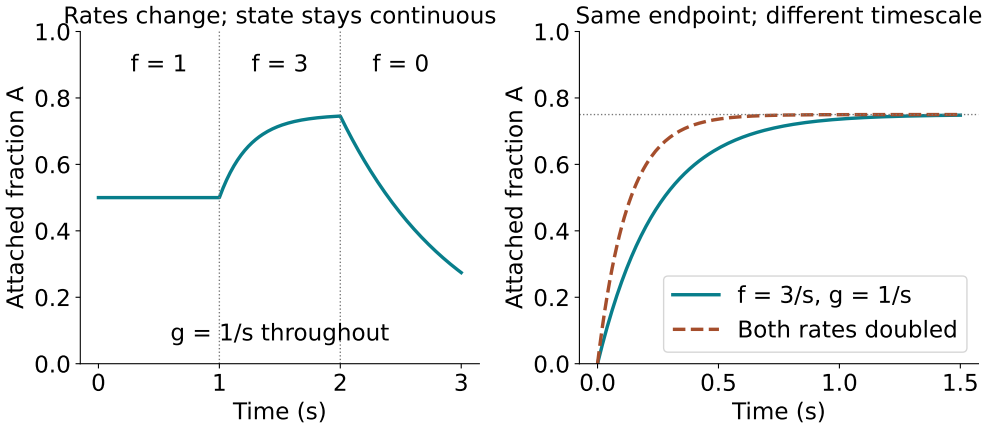
$$A_\infty = 0.75, \qquad J_{D\to A} = J_{A\to D} = 0.75\,\mathrm{s}^{-1}.$$

Derivation of the relaxation law

$$\frac{\mathrm{d}}{\mathrm{d}t}(A - A_\infty) = -(f + g)(A - A_\infty).$$

$$A(t) = A_\infty + (A_0 - A_\infty)e^{-t/\tau}, \qquad \tau = (f + g)^{-1}.$$

Endpoint and timescale identify different parameters



Endpoint and timescale identify different parameters

$$(f, g) \mapsto (cf, cg): \qquad A_\infty \mapsto A_\infty, \quad \tau \mapsto \tau/c.$$

$$f = A_\infty/\tau, \qquad g = (1 - A_\infty)/\tau.$$

An endpoint alone cannot identify both rates.

Exact updates across rate switches

$$A_{n+1} = A_\infty + (A_n - A_\infty)e^{-(f+g)h}.$$

Carry A_{n+1} into the next interval.

A rate switch changes the slope, not the current attached fraction.

A three-stage calculation

$$
\begin{aligned}
A(1) &= 0.5, \\
A(2) &= 0.75 - 0.25e^{-4} \simeq 0.74542, \\
A(3) &= A(2)e^{-1} \simeq 0.27422.
\end{aligned}
$$

Attachment is first balanced, then increased, then switched off.

Euler accuracy and admissibility

$$A_{n+1} = A_n + h\{f(1 - A_n) - gA_n\}.$$

$A_n = 0.5$, $f = 3$, $g = 1$, $h = 0.05$ gives 0.55; exact: 0.54532.

$hf \leq 1$ and $hg \leq 1$ preserve $[0, 1]$; smaller steps may still be needed for accuracy.

The zero-rate and one-way limits

$$\begin{array}{c|c} f = g = 0 & A(t) = A_0 \\ f = 0,\ g > 0 & A(t) = A_0 e^{-gt} \\ g = 0,\ f > 0 & A(t) = 1 - (1 - A_0)e^{-ft} \end{array}$$

A fixed-force closure

$$F = NAF_{\text{head}}.$$

$$1000 \times 0.75 \times 2\,\text{pN} = 1.5\,\text{nN}.$$

All attached heads are assumed to exert the same aligned force.

Occupancy and force are different moments

$$A = \int u(x,t)\ \mathrm{d}x, \qquad F = N \int p(x)u(x,t)\ \mathrm{d}x.$$

If $p(x) = \kappa x$, equal attached fractions may have different mean strains and different forces.

Reduction of a displacement model

$$\partial_t u - v\partial_x u = f(1-A)\delta(x-x_a) - gu.$$

Integrate over displacement, with vanishing endpoint flux:

$$\dot{A} = f(1-A) - gA.$$

Rate experiments in the companion

Compare $(f, g) = (3, 1)$ and $(6, 2)$.

Check exact interval composition, fraction bounds, and pure detachment.

Report endpoint, relaxation time, and the assumed force per head separately.

Mechanical and chemical power

$$P_{\text{mechanical}} = Fv.$$

At $v = 0$, force and transition fluxes may remain nonzero.

ATP consumption requires chemical stoichiometry and free energy per cycle.