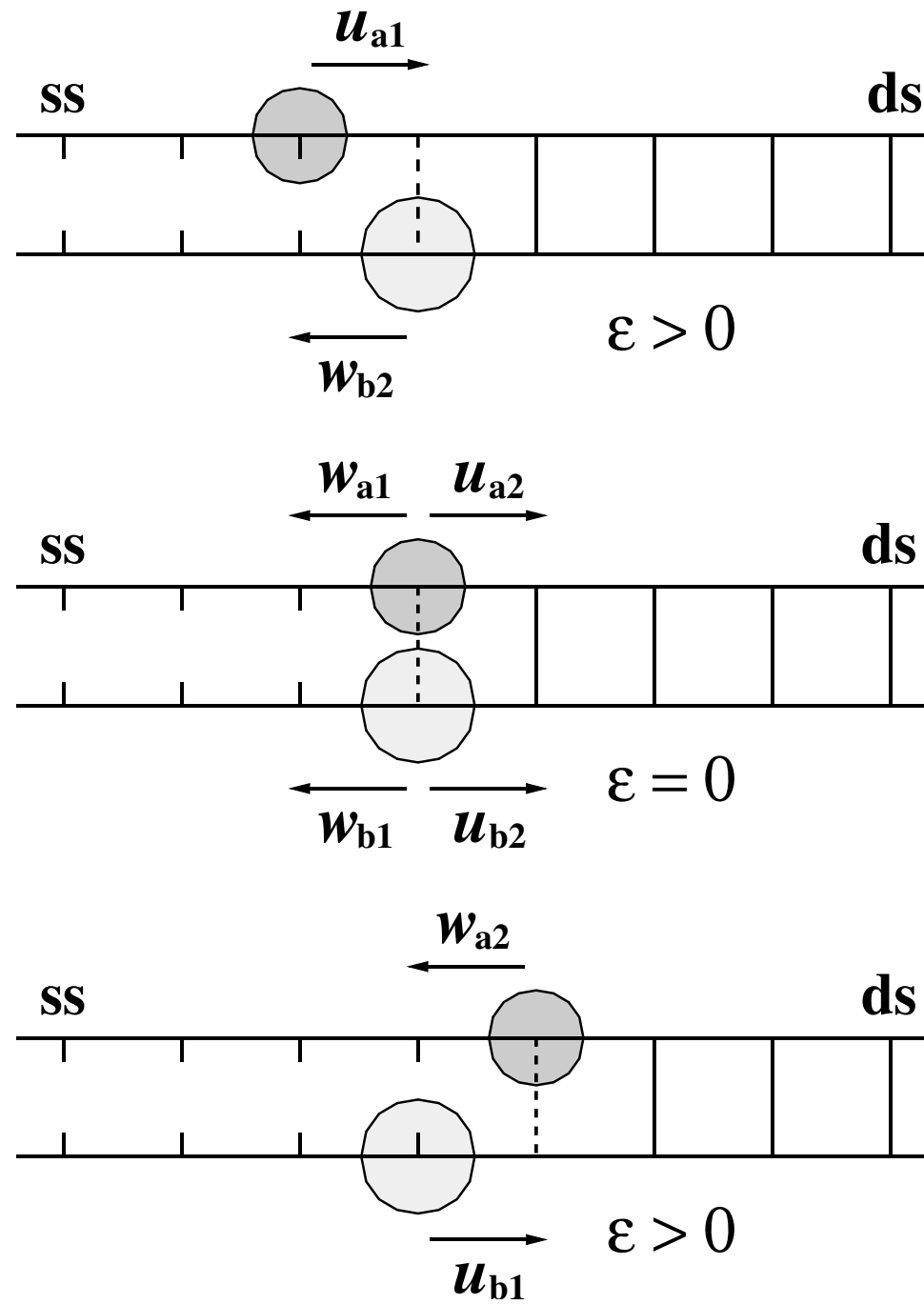
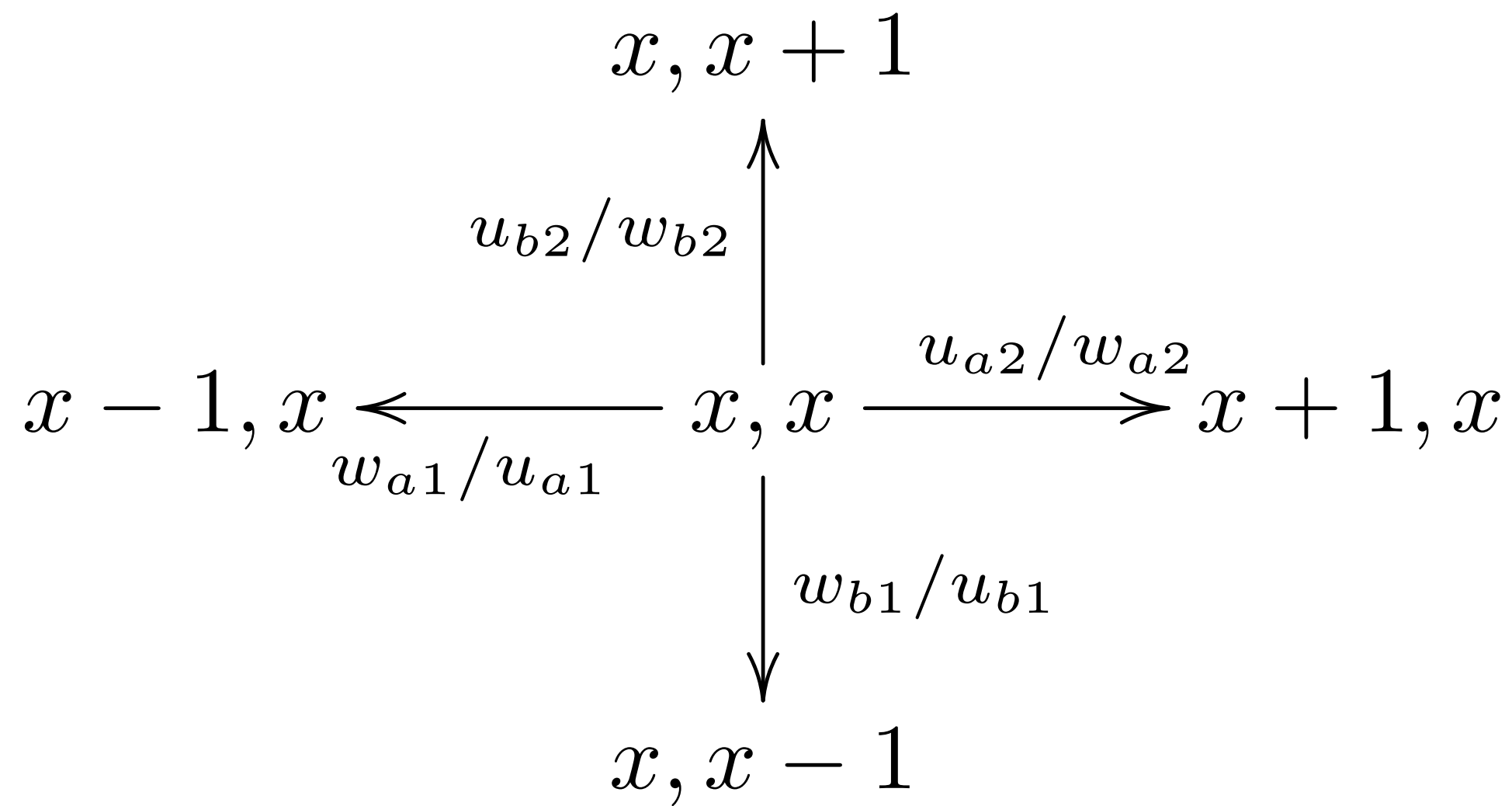


the Stukalin example (DNA walker)

1. a tale of two engines
 - ring assembly (combat small rings)
 - symmetric motors
 - directional
 - challenge: mean velocity $>$ individual one
2. interested in replacing/scaling micro-CTMC to SDEs ...
3. detailed balance
4. translational invariance

PRL 2005 – Stukalin et al.





$$\begin{array}{ccc}
 x, x+1 & \xrightarrow{u_{a1}} & x+1, x+1 \\
 \uparrow u_{b2} & & \downarrow w_{b1} \\
 x, x & \xleftarrow{w_{a2}} & x+1, x
 \end{array}$$

$$\begin{array}{ccc}
 x, x+1 & \xleftarrow{w_{a1}} & x+1, x+1 \\
 \downarrow w_{b2} & & \uparrow u_{b1} \\
 x, x & \xrightarrow{u_{a2}} & x+1, x
 \end{array}$$

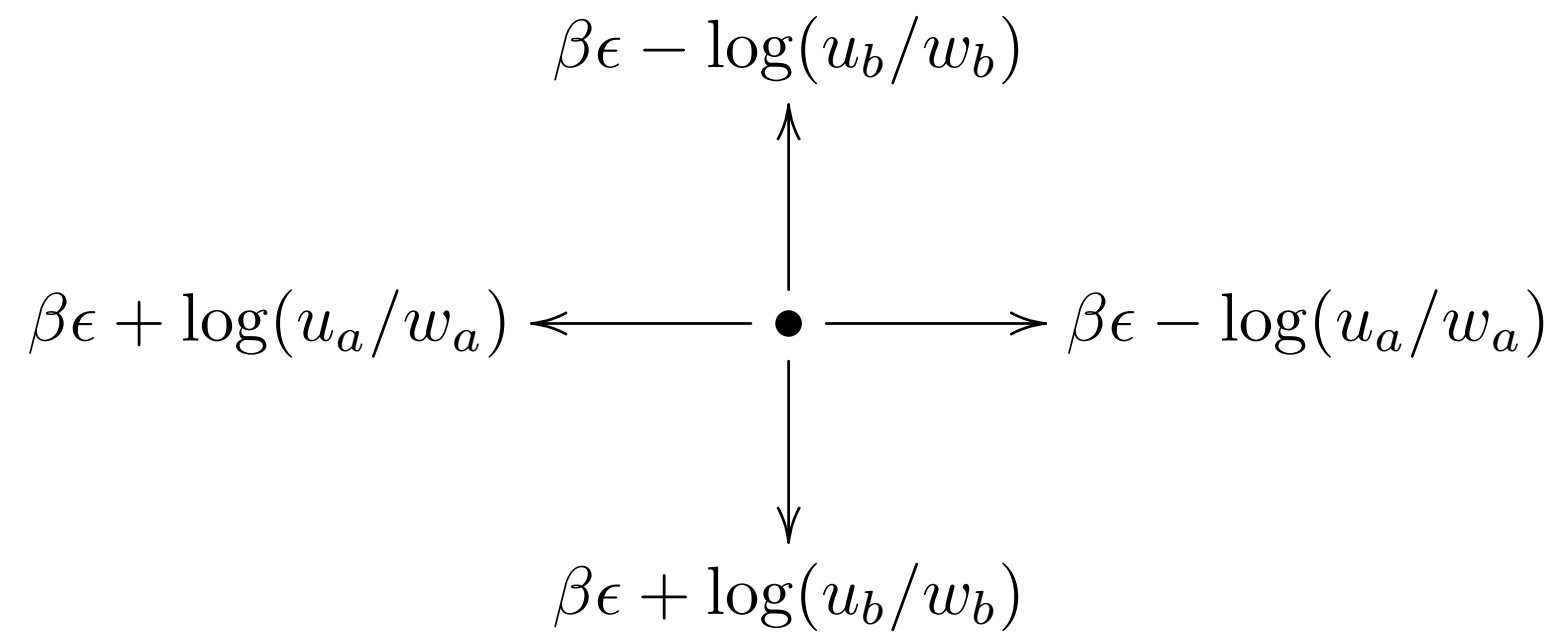
$$\log(w_{b2}/u_{b2}) + \log(w_{a1}/u_{a1}) = \log(w_{a2}/u_{a2}) + \log(w_{b1}/u_{b1})$$

$$\begin{aligned} u_{i1}/w_{i1} &= (u_i/w_i) \gamma \\ u_{i2}/w_{i2} &= (u_i/w_i) \gamma^{-1} \end{aligned}$$

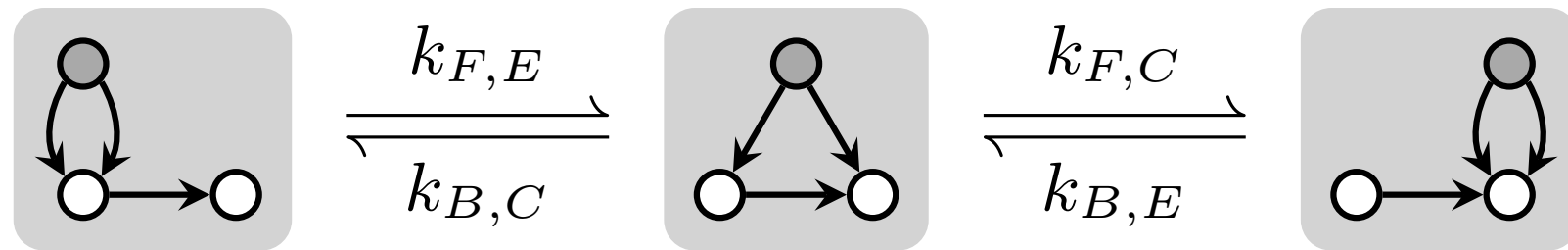
$$\gamma = e^{\beta\epsilon}$$

$$\begin{aligned} \log(u_{a1}/w_{a1}) &= \beta\epsilon + \log(u_a/w_a) \\ \log(w_{a2}/u_{a2}) &= \beta\epsilon - \log(u_a/w_a) \\ \log(u_{b1}/w_{b1}) &= \beta\epsilon + \log(u_b/w_b) \\ \log(w_{b2}/u_{b2}) &= \beta\epsilon - \log(u_b/w_b) \end{aligned}$$

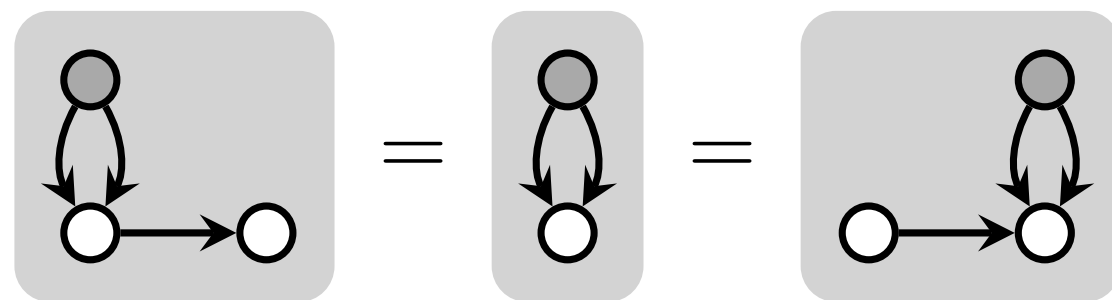
$$\beta\epsilon - \log(u_b/w_b) - \beta\epsilon - \log(u_a/w_a) = \beta\epsilon - \log(u_a/w_a) - \beta\epsilon - \log(u_b/w_b)$$



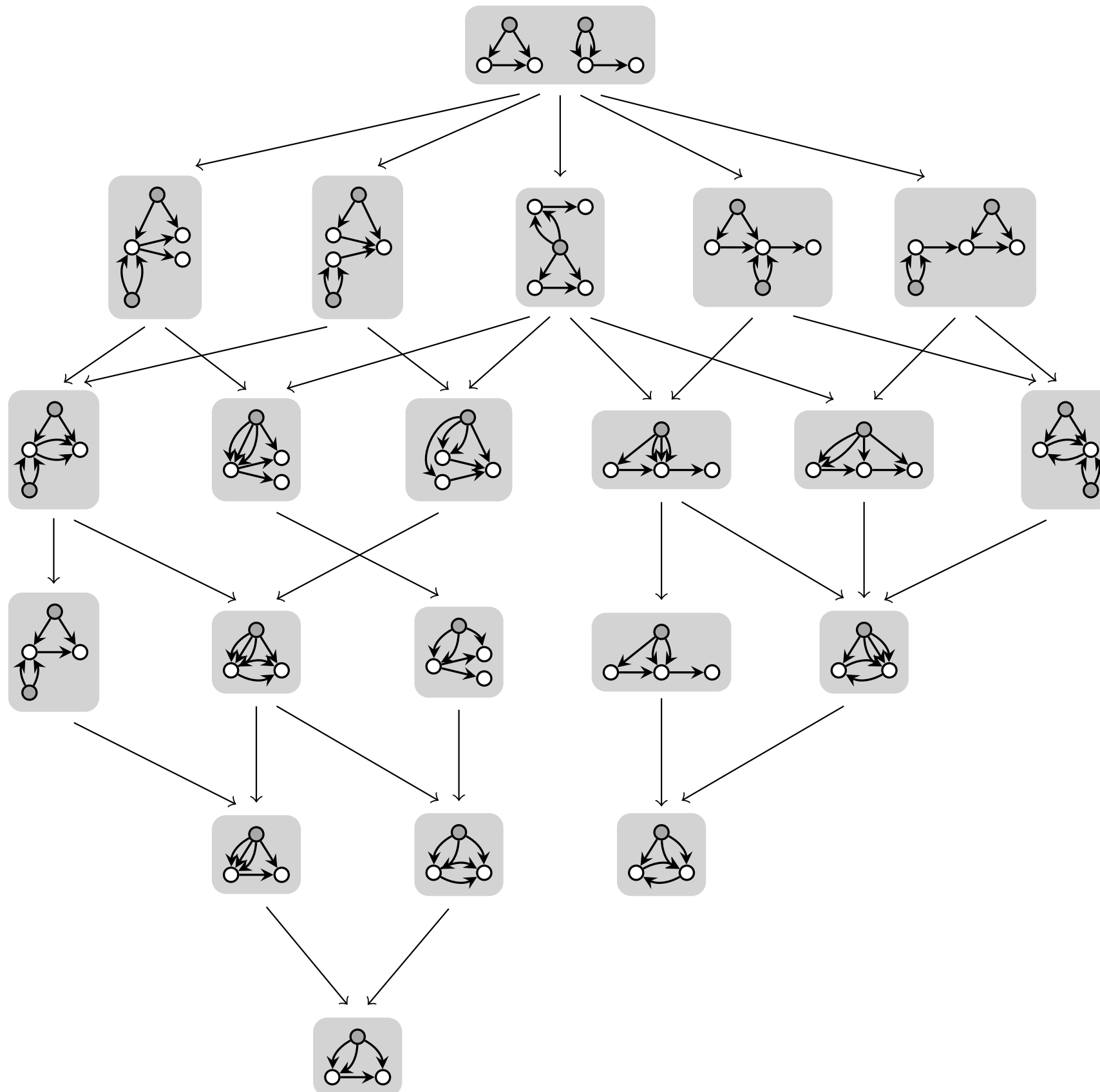
$$\tau := \log(u_b/w_b) + \log(u_a/w_a) = 0$$



no- or cyclic-boundary invariants



minimal gluings/minimal unions



infinite ODE

$$\frac{d}{dt} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \end{array} = k_{F,E} \begin{array}{c} \circ \\ \downarrow \\ \circ \rightarrow \circ \end{array} - k_{B,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \end{array} - k_{F,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \end{array} + k_{B,E} \begin{array}{c} \circ \rightarrow \circ \\ \uparrow \\ \circ \end{array}$$

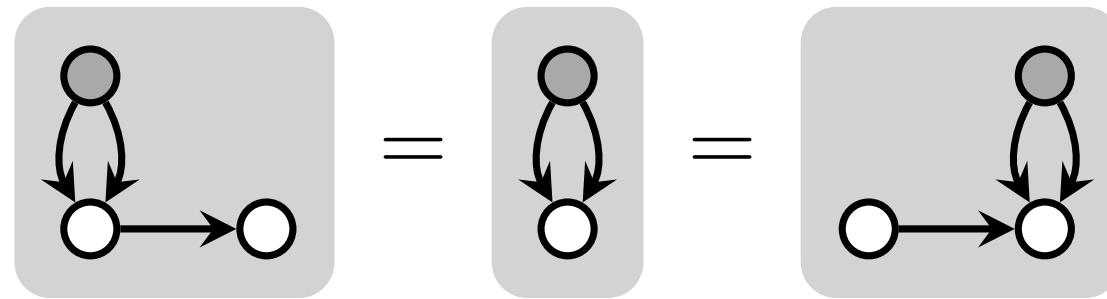
$$\frac{d}{dt} \begin{array}{c} \circ \\ \downarrow \\ \circ \rightarrow \circ \end{array} = -k_{F,E} \begin{array}{c} \circ \\ \downarrow \\ \circ \rightarrow \circ \end{array} + k_{B,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \end{array} + k_{F,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} - k_{B,E} \begin{array}{c} \circ \rightarrow \circ \\ \uparrow \\ \circ \rightarrow \circ \end{array}$$

$$\frac{d}{dt} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} = k_{F,E} \begin{array}{c} \circ \\ \downarrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} - k_{B,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} - k_{F,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} + \dots$$

$$\frac{d}{dt} \begin{array}{c} \circ \\ \downarrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} = -k_{F,E} \begin{array}{c} \circ \\ \downarrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} + k_{B,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \rightarrow \circ \end{array} + k_{F,C} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \rightarrow \circ \rightarrow \circ \end{array} - \dots$$

$$\frac{d}{dt} \begin{array}{c} \circ \\ \swarrow \searrow \\ \circ \rightarrow \circ \rightarrow \circ \rightarrow \circ \end{array} = \dots$$

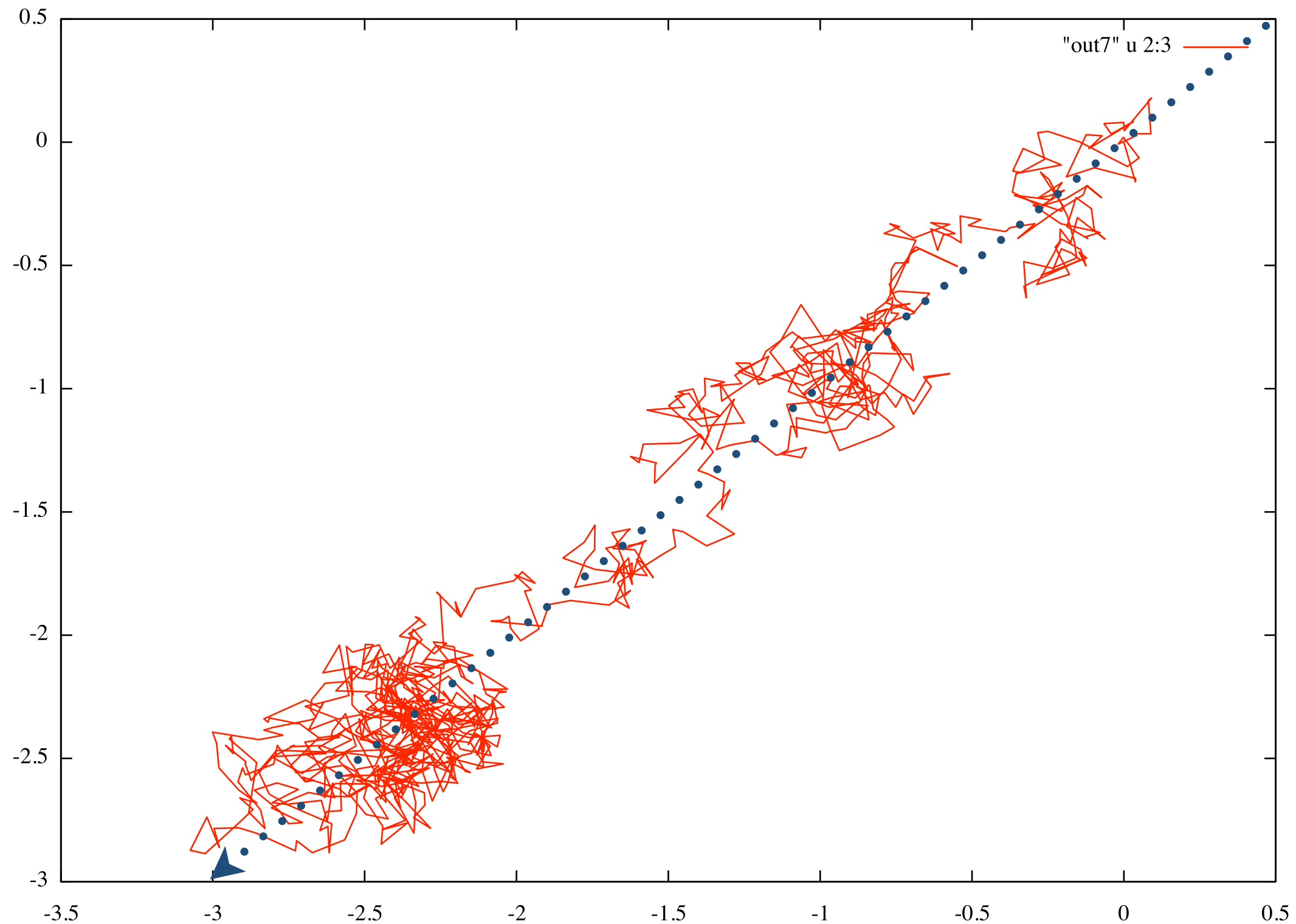
no- or cyclic-boundary invariants



The Stukalin MFA equations

$$\begin{aligned}
 \frac{d}{dt} \begin{array}{|c|} \hline \text{triangle} \\ \hline \end{array} &= k_{F,E} \begin{array}{|c|} \hline \text{cycle}_{BL} \\ \hline \end{array} - k_{B,C} \begin{array}{|c|} \hline \text{triangle} \\ \hline \end{array} - k_{F,C} \begin{array}{|c|} \hline \text{triangle} \\ \hline \end{array} + k_{B,E} \begin{array}{|c|} \hline \text{cycle}_{BL} \\ \hline \end{array} \\
 \frac{d}{dt} \begin{array}{|c|} \hline \text{cycle}_{BL} \\ \hline \end{array} &= -k_{F,E} \begin{array}{|c|} \hline \text{cycle}_{BL} \\ \hline \end{array} + k_{B,C} \begin{array}{|c|} \hline \text{triangle} \\ \hline \end{array} + k_{F,C} \begin{array}{|c|} \hline \text{triangle} \\ \hline \end{array} - k_{B,E} \begin{array}{|c|} \hline \text{cycle}_{BL} \\ \hline \end{array}
 \end{aligned}$$

same thing with SDEs?



diffusion limits – here a 2d OU

$$dX_t = -\theta(X_t - \mu)dt + \sigma dB_t$$

$$dX_1 = -\theta_1(X_1 - \mu_1)dt + dB_t^1$$

$$dX_2 = -\theta_2(X_2 - \mu_2)dt + dB_t^2$$

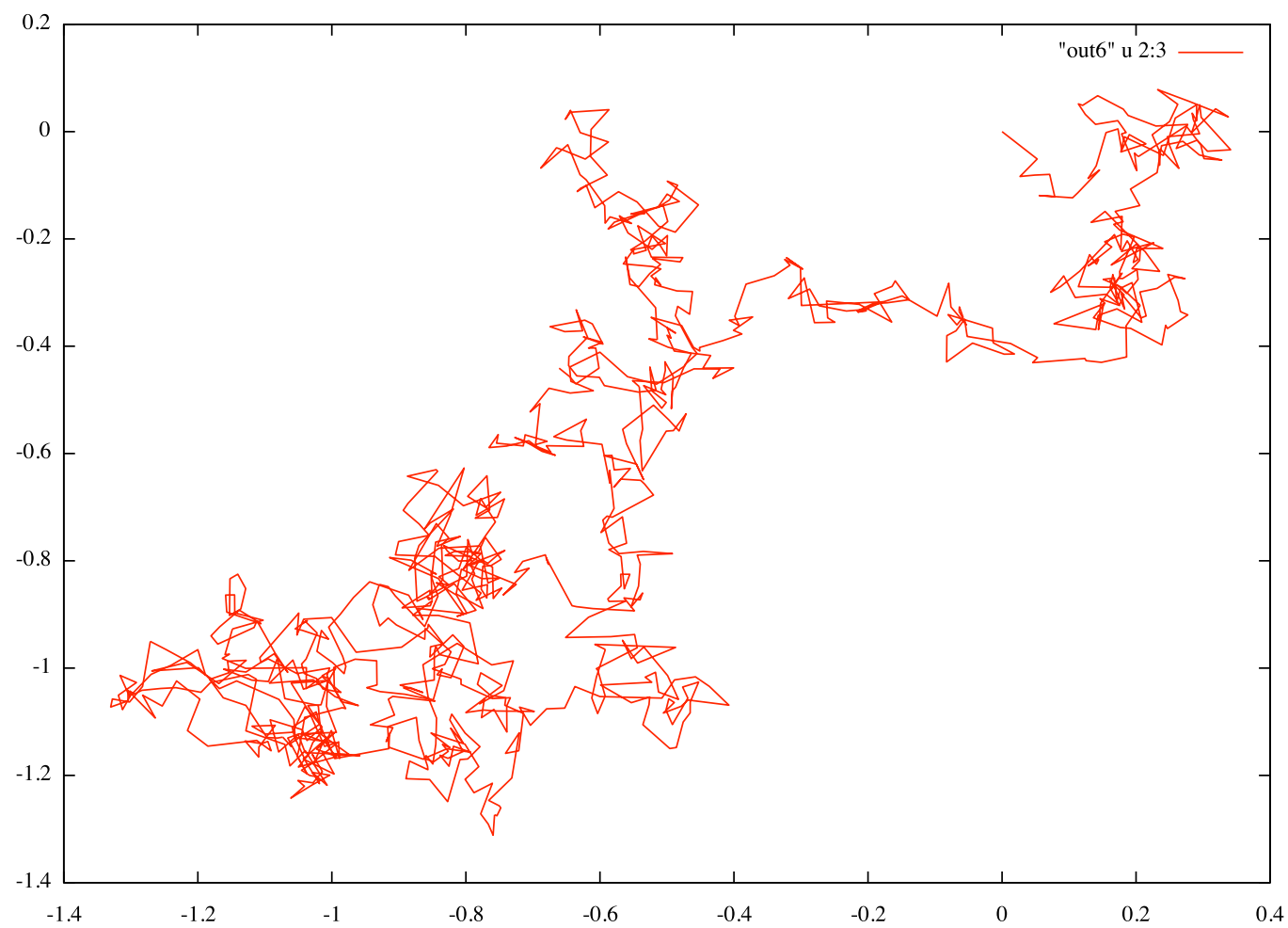


Figure 2: The OU SDE above, starting at 0, 0 and run with $\mu_1 = \mu_2 = 0$, $\theta_1 = \theta_2 = 1.0$, $\Sigma = I$, $e = 1000$, $dt = 0.01$

$$dX_t = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} dt + \begin{pmatrix} -\theta_1 & \theta_1 \\ \theta_2 & -\theta_2 \end{pmatrix} X_t dt + \Sigma dB_t$$

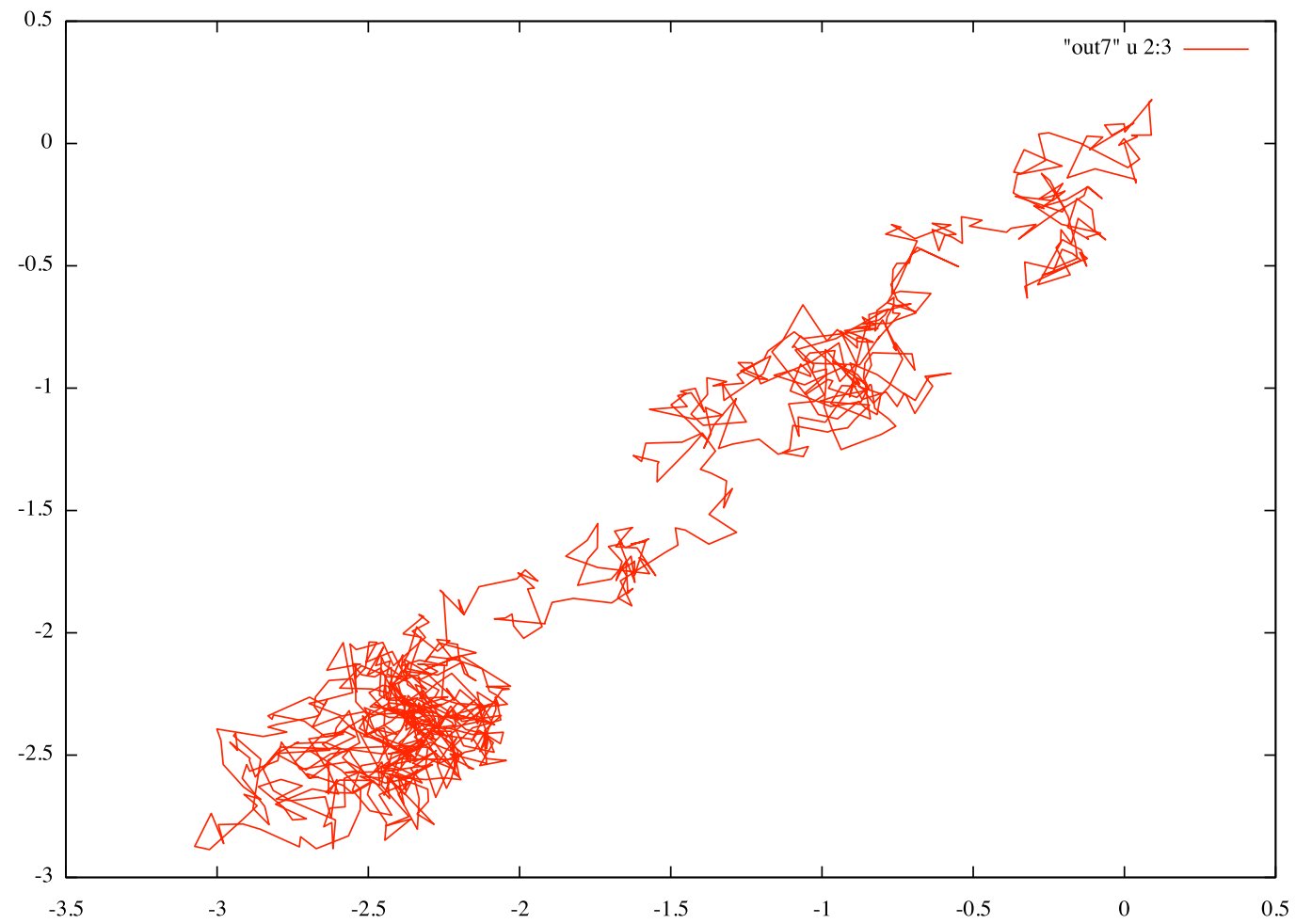


Figure 3: The OU SDE above, starting at 0, 0 and run with $\mu_1 = \mu_2 = 0$, $\theta_1 = \theta_2 = 1.0$, $\Sigma = I$, $e = 1000$, $dt = 0.05$; the concentration on $y = x$ is noticeable on this longer time.