# Stochastic Simulations for DREAM4

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## 1 ODE model (DREAM3)

$$\frac{dx_i}{dt} = F_i^{RNA}(\boldsymbol{x}, \boldsymbol{y}) = m_i \cdot f_i(\mathbf{y}) - \lambda_i^{RNA} \cdot x_i \quad (1)$$

$$\frac{dy_i}{dt} = F_i^{Prot}(\boldsymbol{x}, \boldsymbol{y}) = r_i \cdot x_i - \lambda_i^{Prot} \cdot y_i \quad (2)$$

where $m_i$ is the maximum transcription rate, $r_i$ the translation rate, $\lambda_i^{\mathrm{RNA}}$ and $\lambda_i^{\mathrm{Prot}}$ are the mRNA and protein degradation rates, and $f_i(\cdot)$ is the so-called input function of gene $i$. The input function computes the *relative activation* of the gene, which is between 0 (the gene is shut off) and 1 (the gene is maximally activated), given the transcription-factor (TF) concentrations $\mathbf{y}$.

## 2 SDE model (DREAM4)

$$\frac{dx_i}{dt} = F_i^{RNA}(\boldsymbol{x}, \boldsymbol{y}) + \sigma_i^{RNA} \cdot \eta_i \quad (3)$$

$$\frac{dy_i}{dt} = F_i^{Prot}(\boldsymbol{x}, \boldsymbol{y}) + \sigma_i^{Prot} \cdot \zeta_i \quad (4)$$

where each $\eta_i$ and $\zeta_i$ is an independent Gaussian white noise with zero mean and unit variance. $\sigma_i^{RNA}$ and $\sigma_i^{Prot}$ represent the amplitude (standard deviation) of the noise.

## 3 Numerical simulation of SDEs

For notational simplicity, we consider here only a single equation and not a system of equations. Equations (3) and (4) are of the following, general form (note that we use the Stratonovich scheme)

$$dX_t = F(X_t)dt + G(X_t)dW_t \quad (5)$$

$$dX_t = \underline{F}(X_t)dt + G(X_t) \circ dW_t \quad (6)$$

$$\underline{F} = F - \frac{1}{2}G'G \quad (7)$$

where $dW_t$ is a Wiener process. The Itô scheme is defined by (5) and the equivalent Stratonovich scheme is given by (6) and (7).[1,5] In (3) and (4) the amplitude of the noise $G(X_t)$ is a constant $\sigma_i$.

We propose to use the Milstein scheme for the numerical integration, which is better than the basic Euler-Marumaya method, but still easy to implement.[1,3,5,6] Given $X(n) = X_n$, the value at the next discrete time point $X_{n+h}$ is approximated by

$$X_{n+h} = X_n + \underline{F}(X_n)h + G(X_n)\Delta W_n + \frac{1}{2}G'(X_n)G(X_n)[\Delta W_n]^2 \quad (8)$$

$$\Delta W_n = [W_{t+h} - W_t] \sim \sqrt{h}\mathcal{N}(0,1) \quad (9)$$

where $h$ is the step size.

# References


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[5] H. Lamba, *Stepsize control for the Milstein scheme using first-exit-times.*

[6] Umberto Picchini, *Sde toolbox: Simulation and estimation of stochastic differential equations with matlab.*