

2009.11.2
物性物理学C

拡散方程式とLangevin方程式

拡散方程式

$$\frac{\partial u}{\partial t} = D \nabla^2 u$$

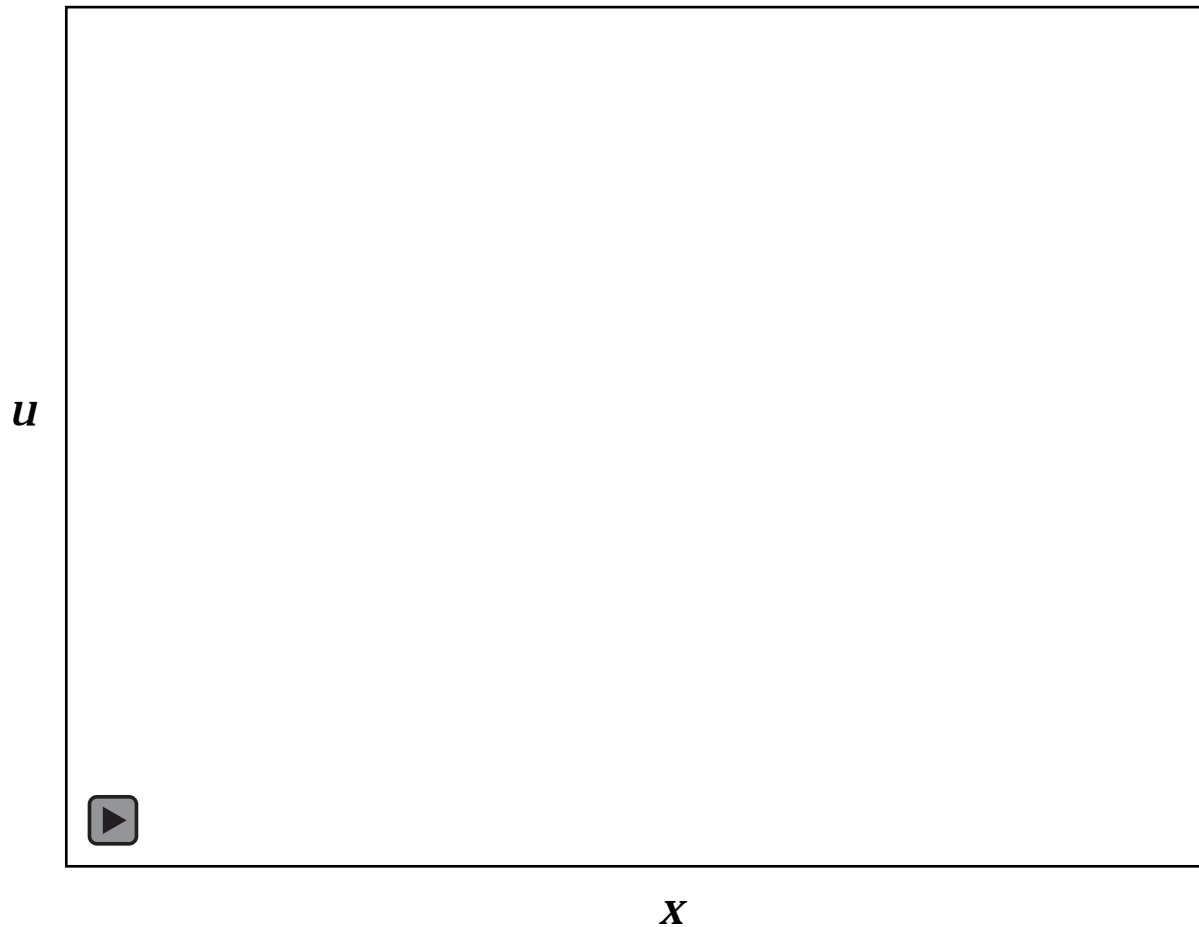
1次元の場合

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

初期値:

$$u(x, t = 0) = \delta(x)$$

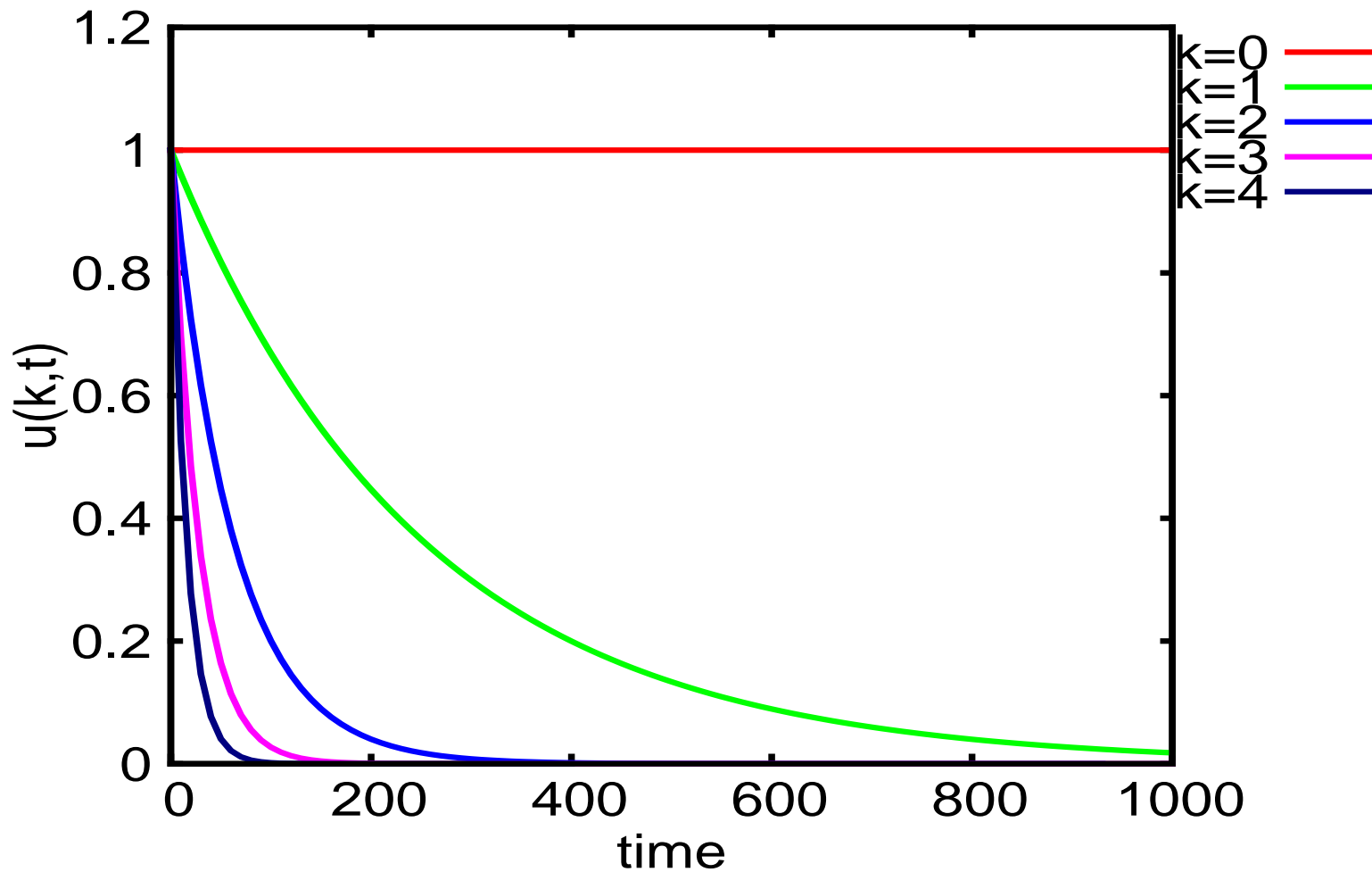
1次元で初期値が δ 関数の解 : Green関数



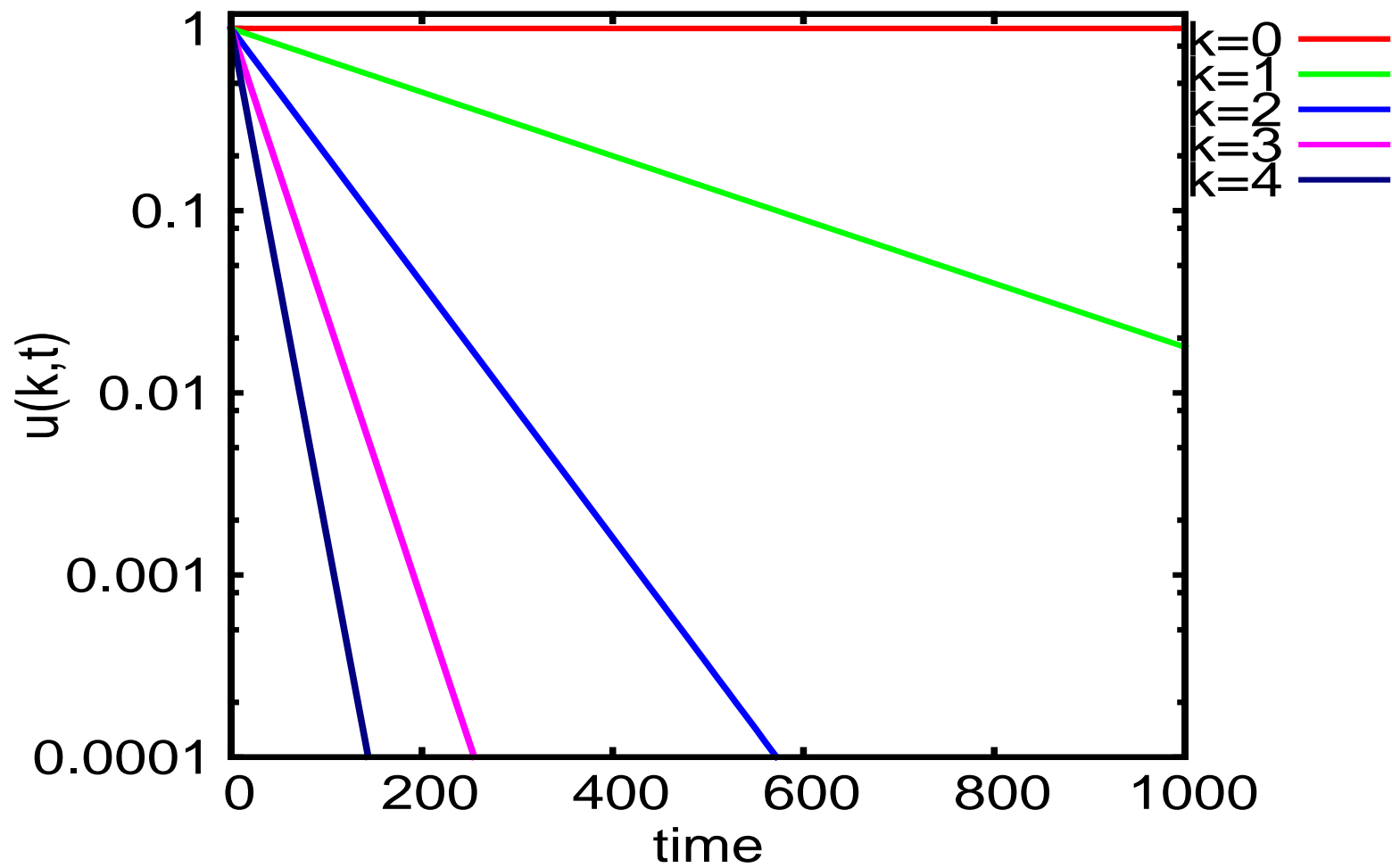
$$u(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

Fourier modeの時間変化

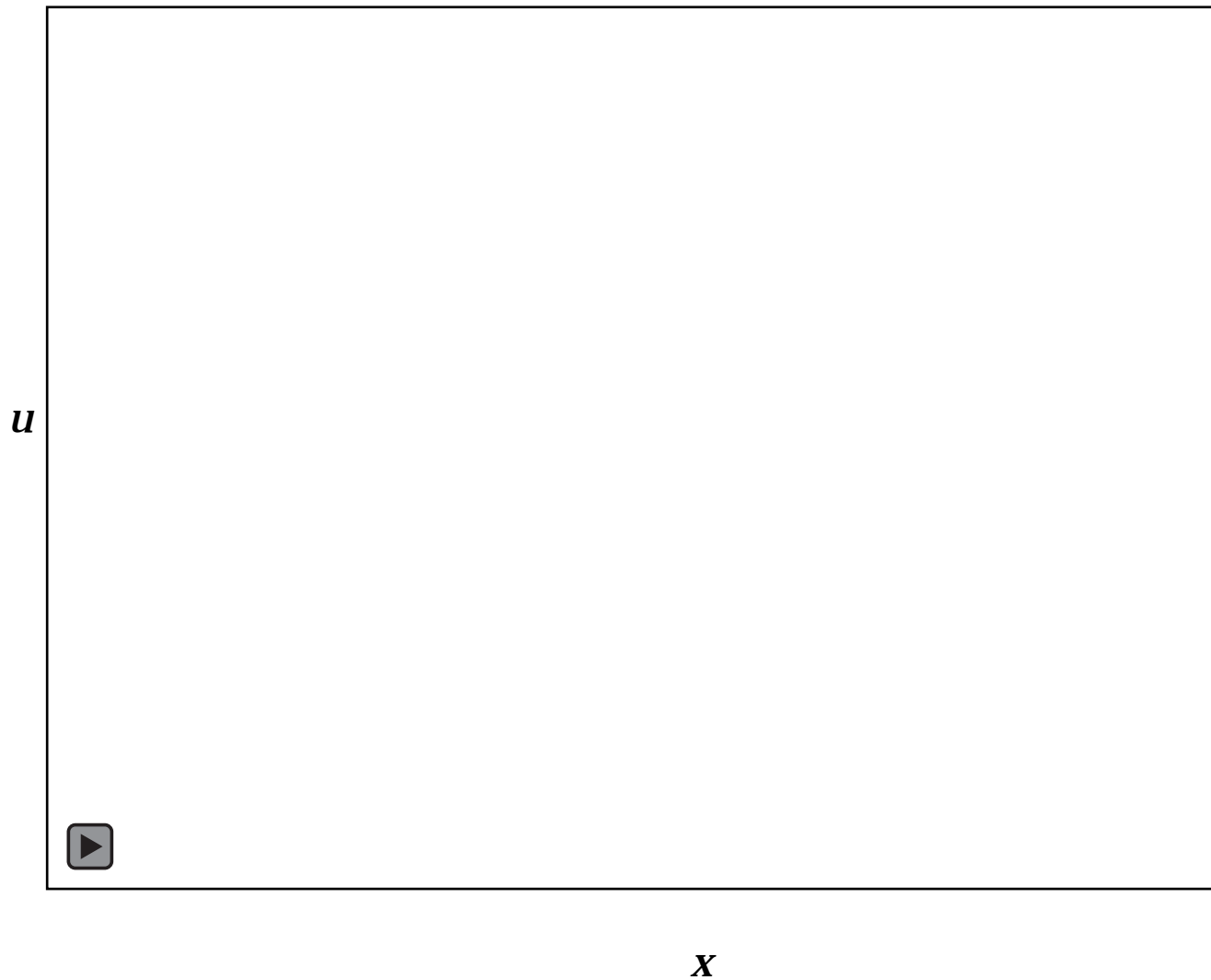
$$u(x,t) = \frac{1}{2\pi} \sum_{k=0}^N \tilde{u}(k,t) \cos\left(\frac{2\pi kx}{NL}\right)$$



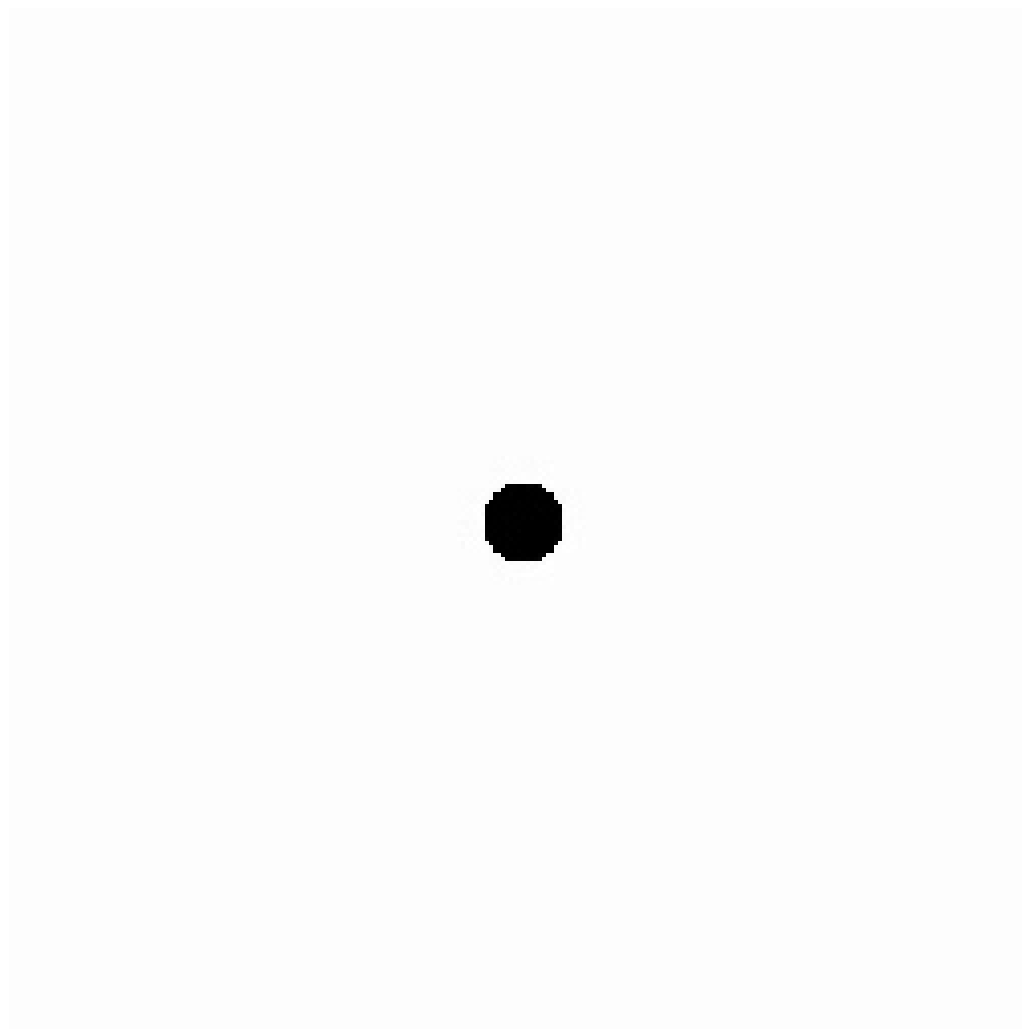
Log scaleでは



初期値が δ 関数ではないとき



2次元で初期値が δ 関数(に近いとき)の解



$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

一般的な溶液、溶質なら

$$D \sim 10^{-9} [\text{m}^2/\text{s}]$$

Green関数のGaussianの特徴的な幅 L は

$$u(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \quad \text{より} \quad L = \sqrt{4Dt}$$

$$L = \sqrt{4Dt}$$

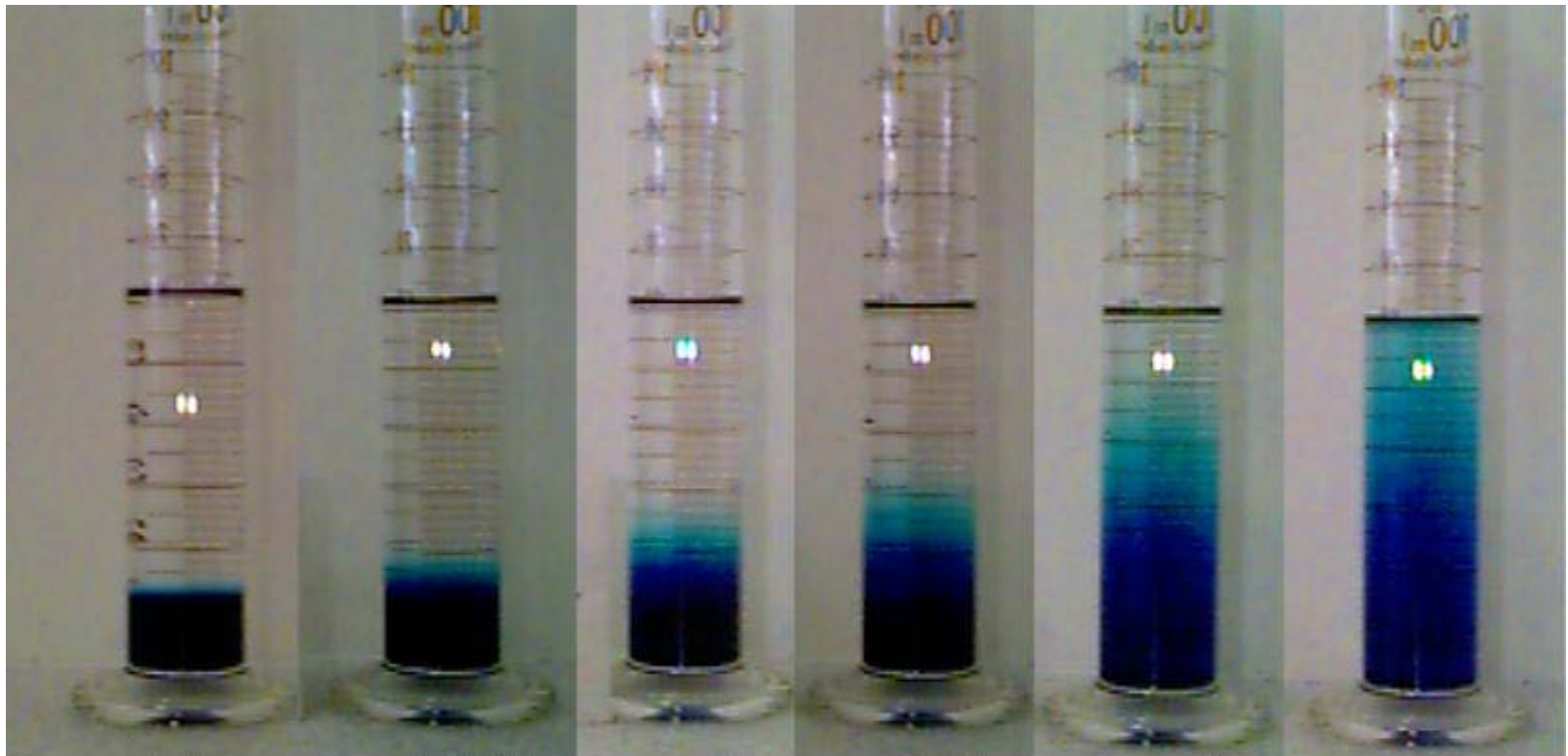
1 mm拡散で広がるには $t \sim 3 \times 10^2 \text{ s} \sim 5 \text{ minutes}$

1 cm拡散で広がるには $t \sim 3 \times 10^4 \text{ s} \sim 8 \text{ hours}$

1 m拡散で広がるには $t \sim 3 \times 10^8 \text{ s} \sim 10 \text{ years!!}$

1 μm 拡散で広がるには $t \sim 3 \times 10^{-4} \text{ s} \sim 0.3 \text{ ms}$

拡散過程



直後

6時間後

1日後

3日後

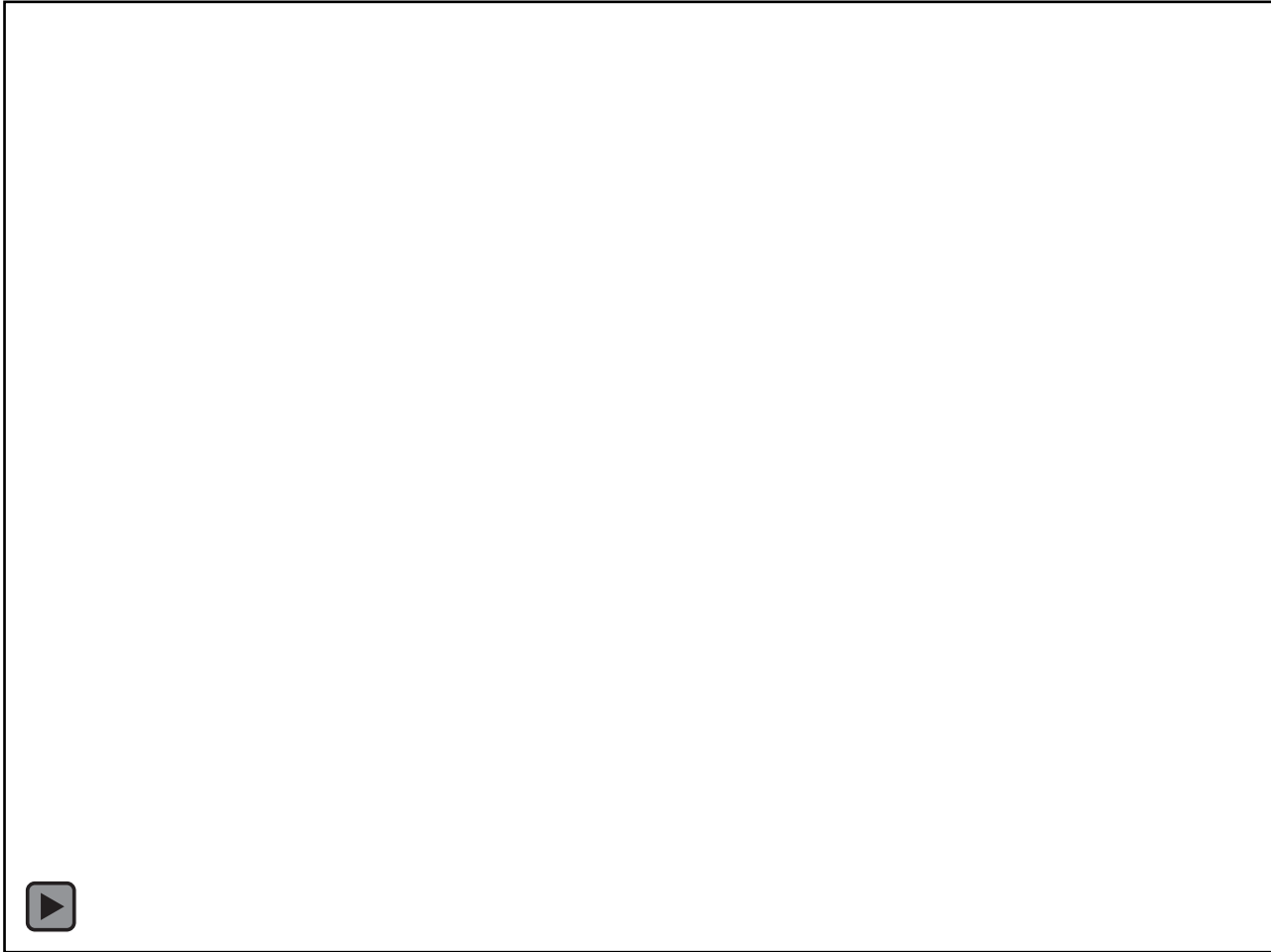
7日後

14日後

水溶液の拡散の様子

ブラウン運動

ナノ粒子



(WEBページより)

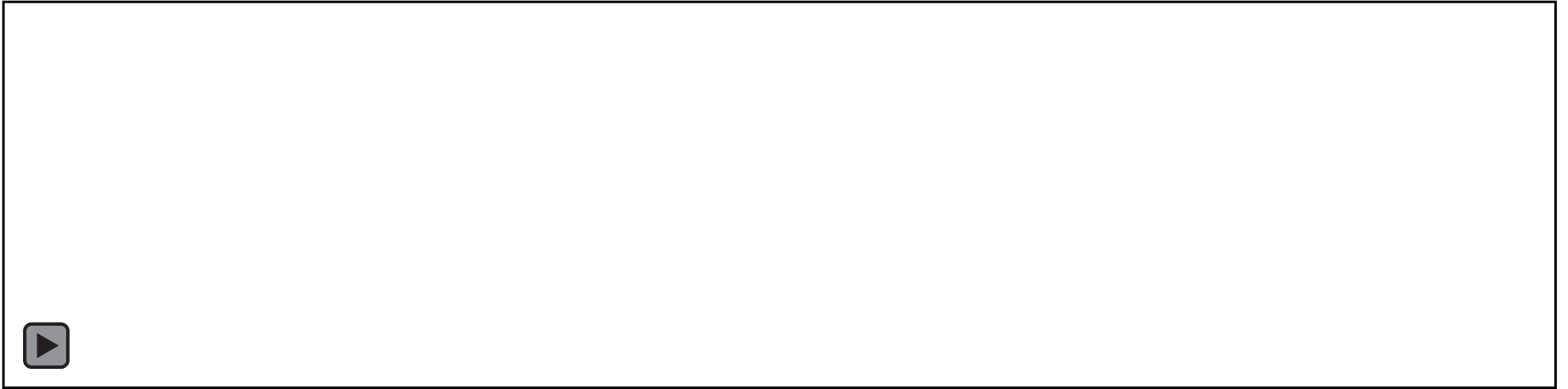
Langevin方程式

$$m \frac{d^2 \mathbf{r}}{dt^2} = -k \frac{d\mathbf{r}}{dt} + \boldsymbol{\xi}(t)$$

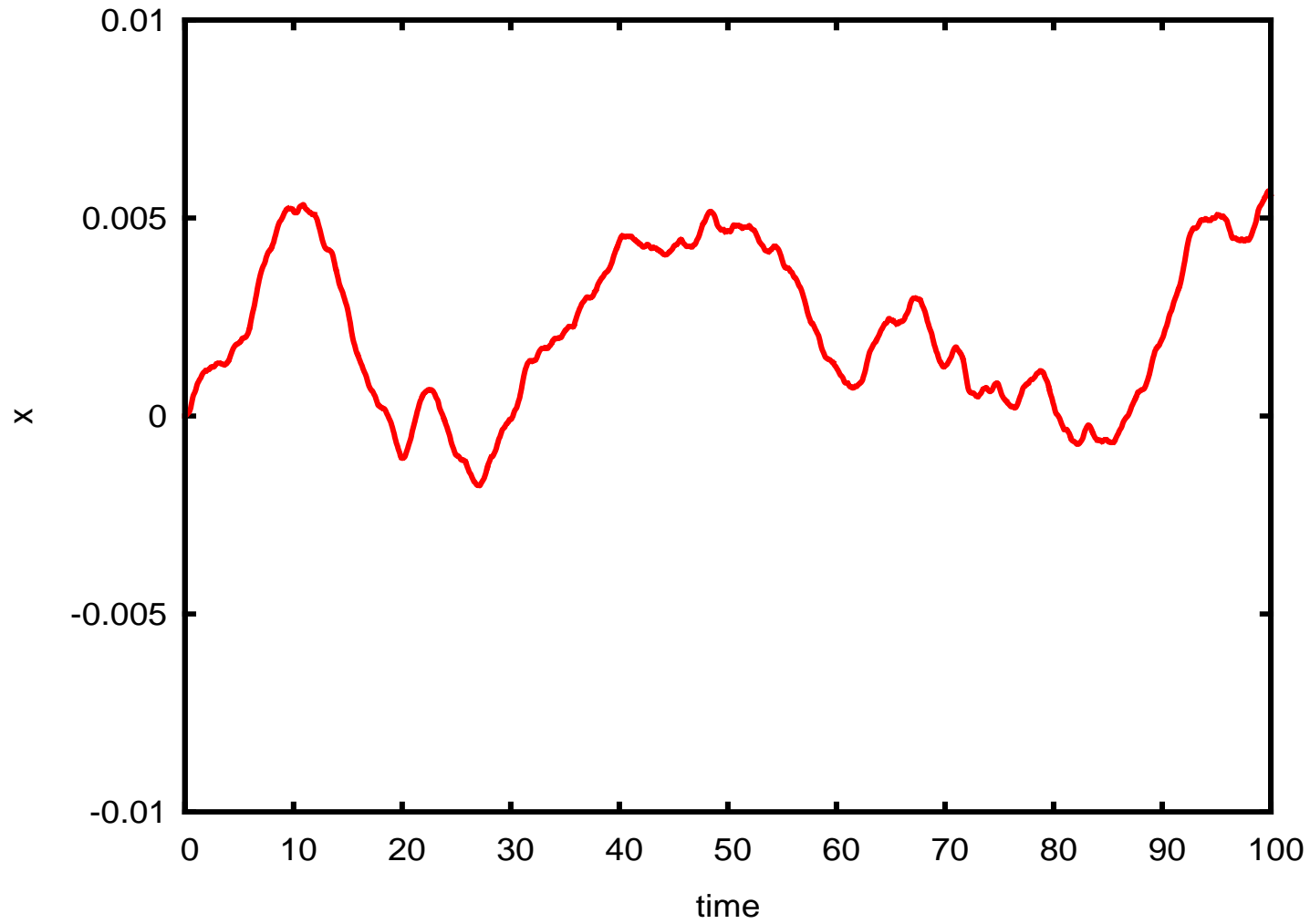
$$\langle \boldsymbol{\xi}(t) \rangle = 0$$

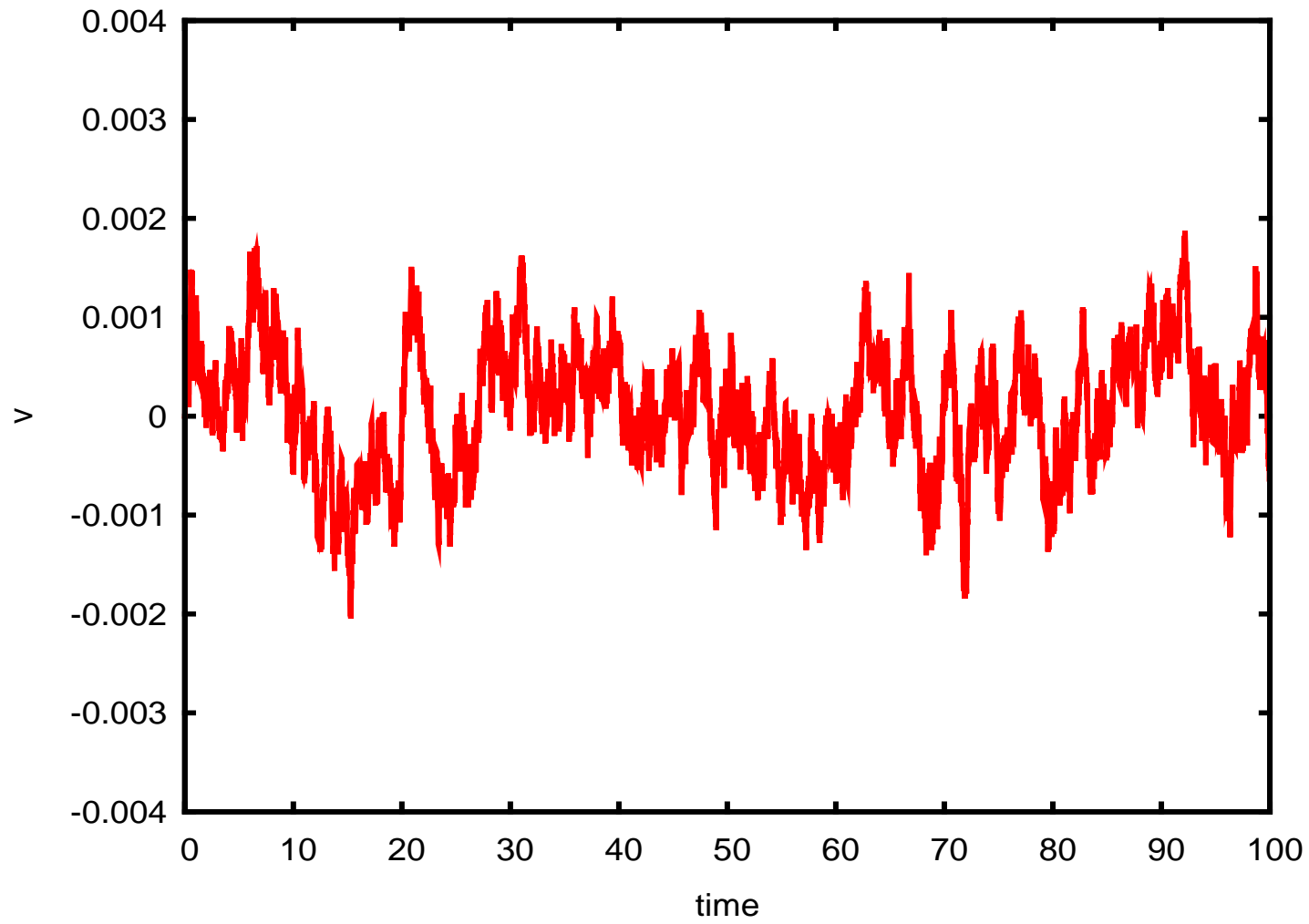
$$\langle \boldsymbol{\xi}(t) \cdot \boldsymbol{\xi}(s) \rangle = 2M\delta(t-s)$$

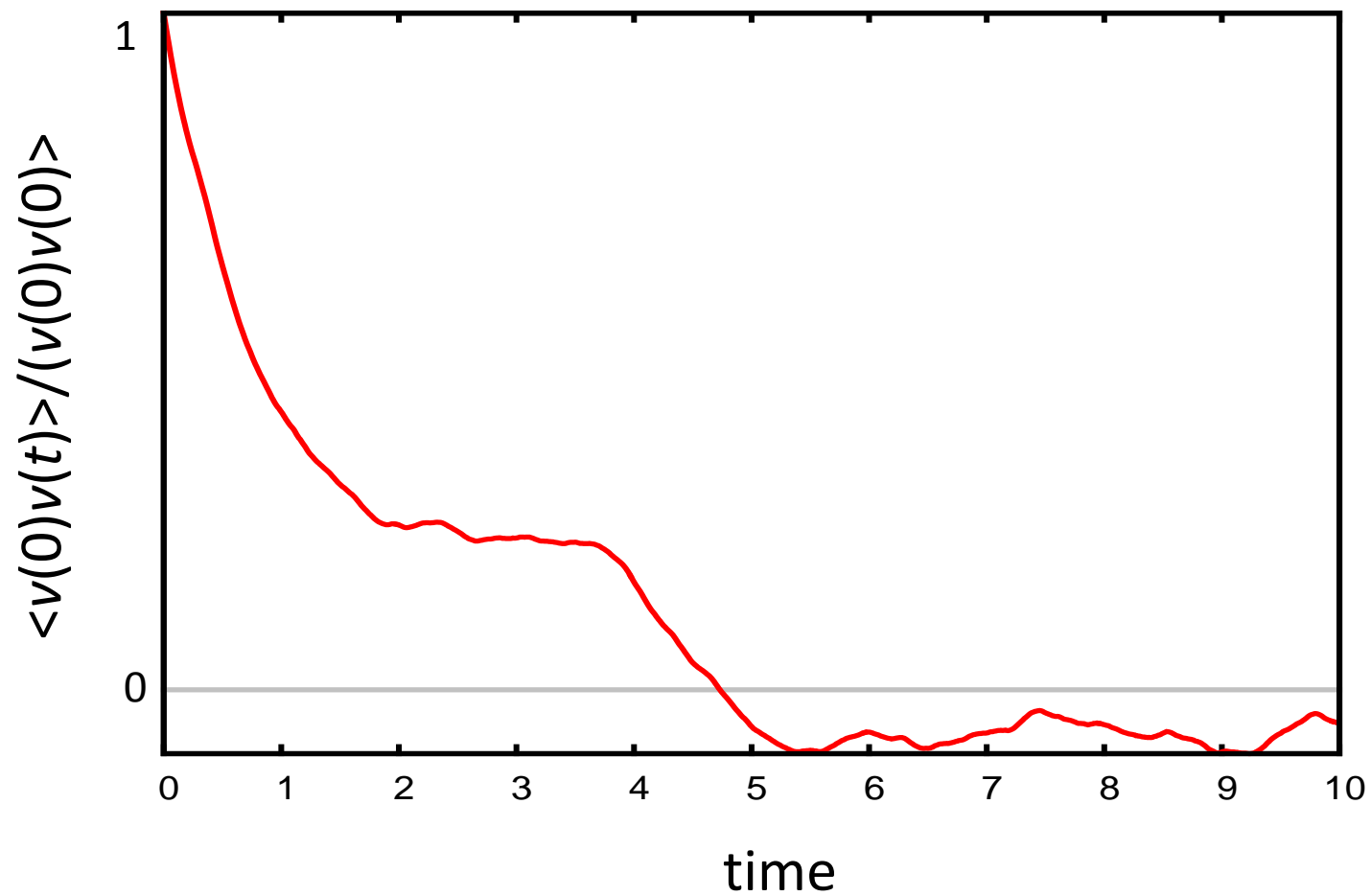
1次元系でのLangevin方程式による挙動



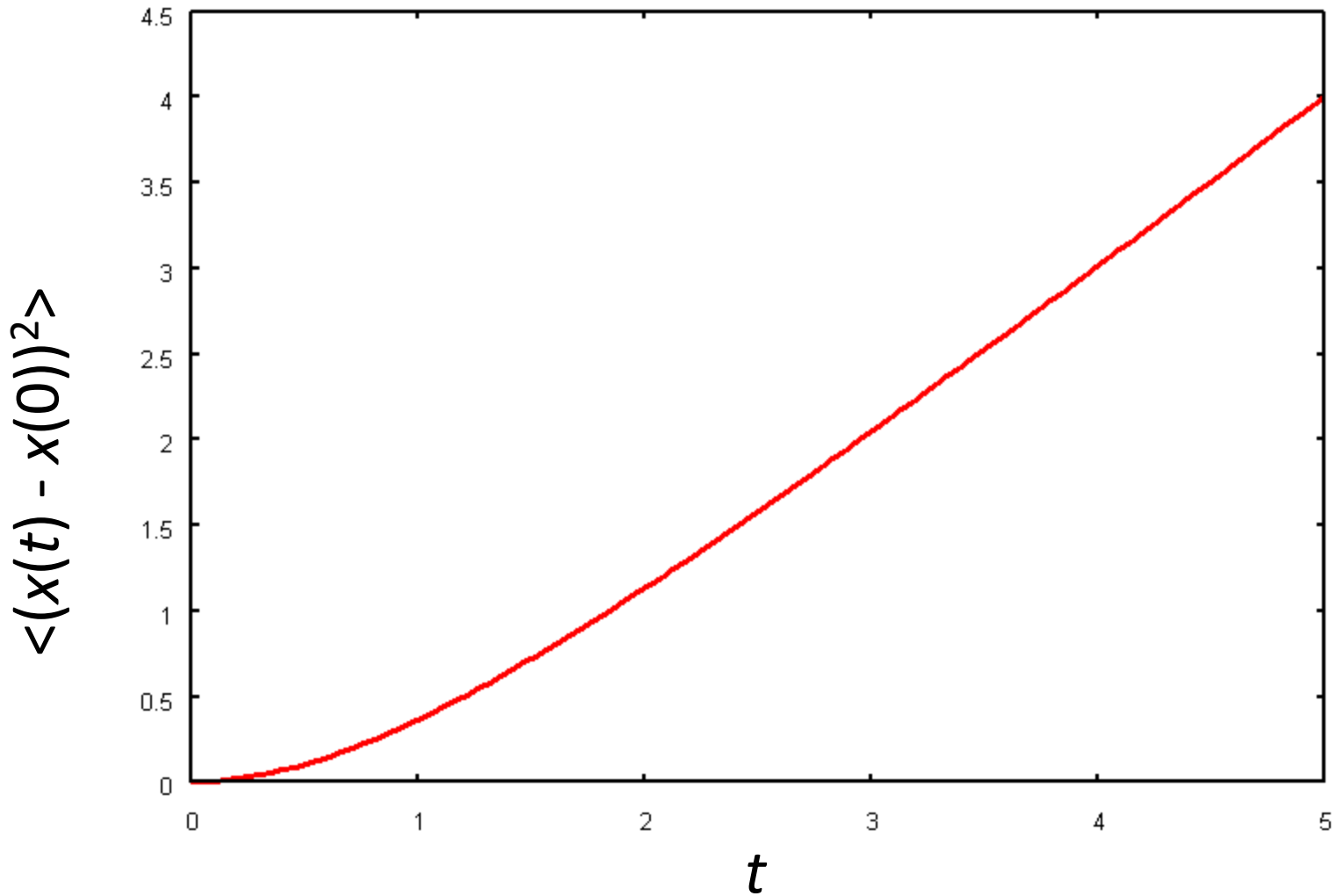
x





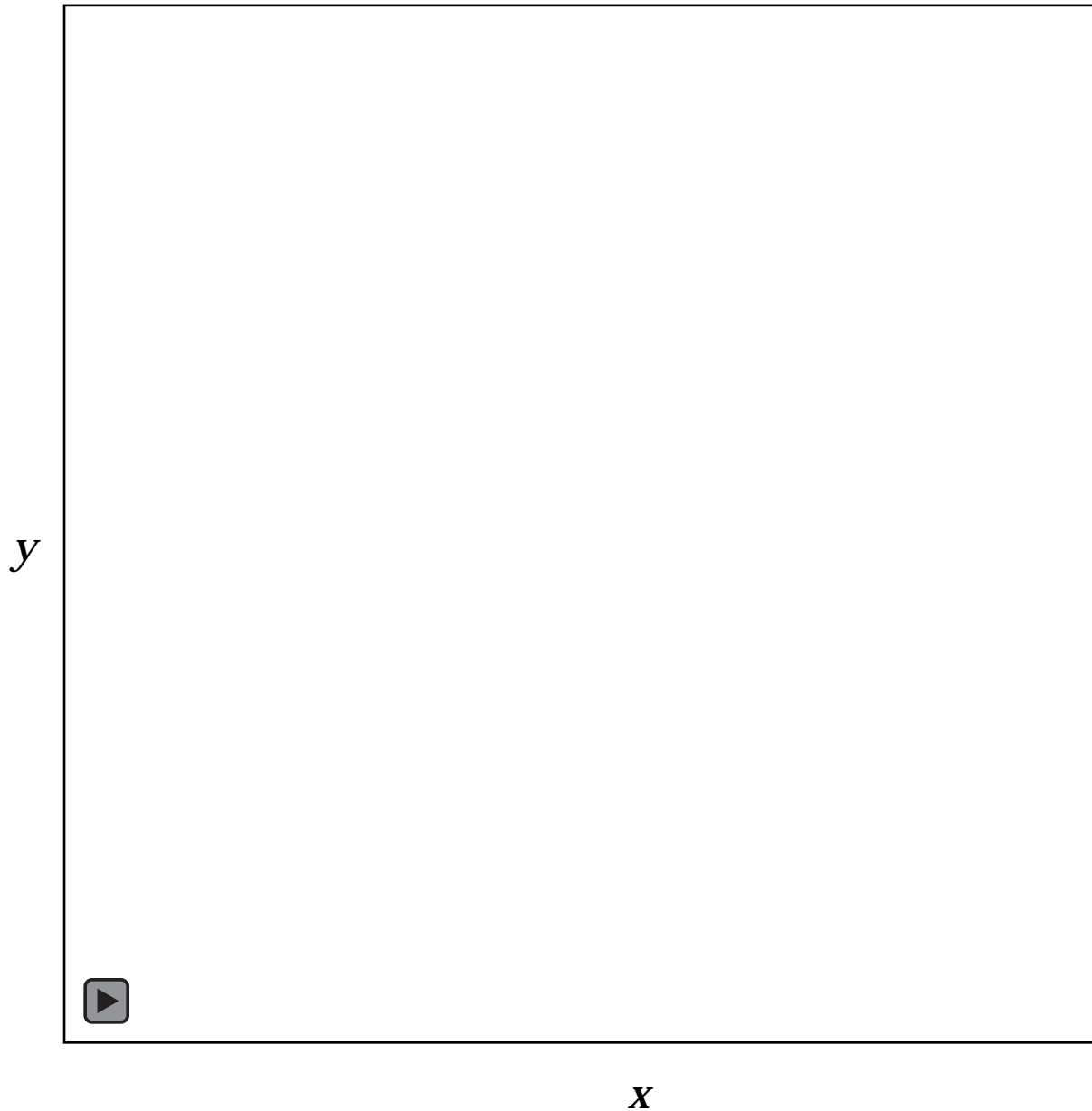


$$\langle v(0)v(t) \rangle / \langle v(0)v(0) \rangle \propto \exp(-t/\tau)$$



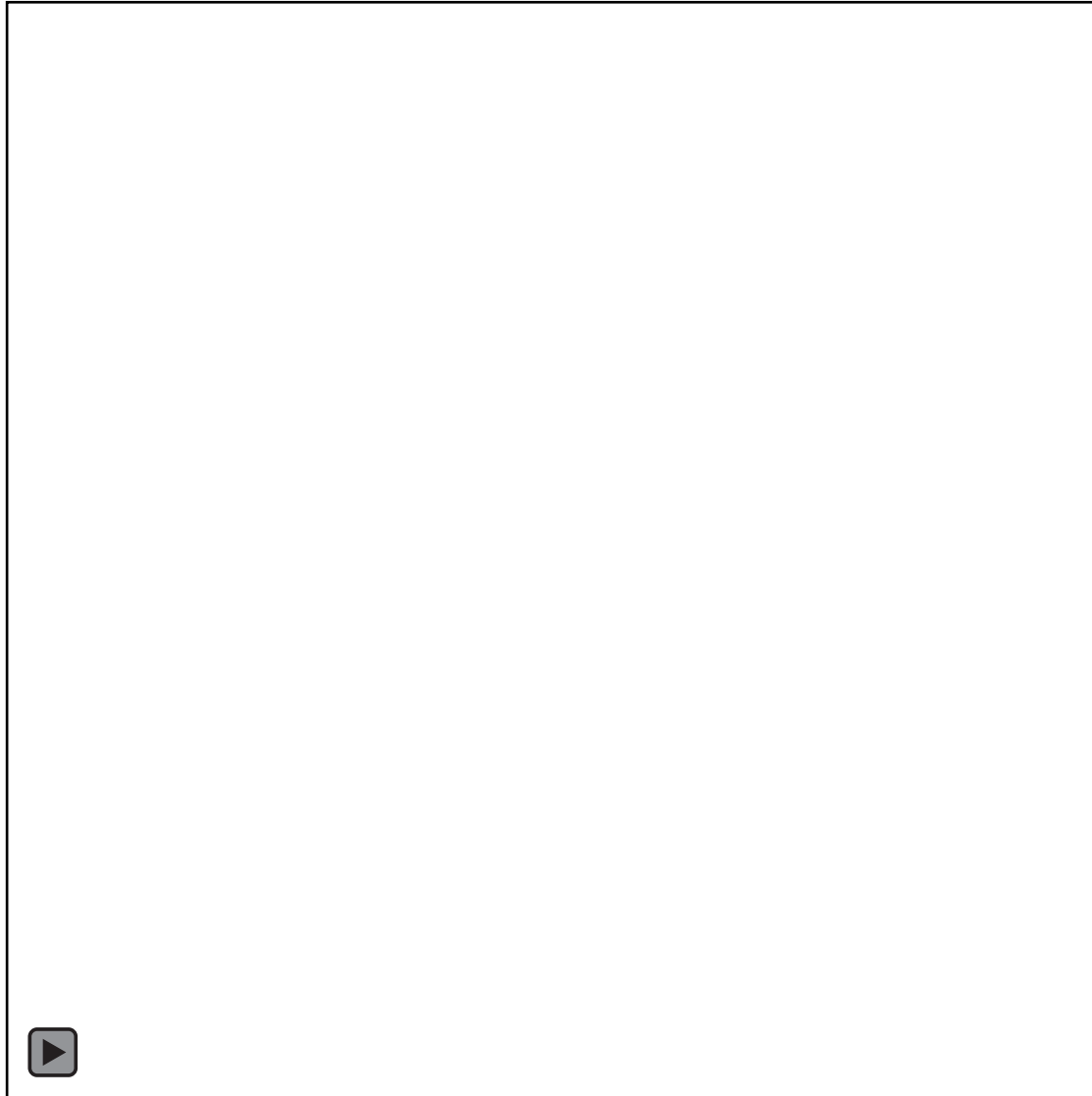
$$\langle (x(t) - x(0))^2 \rangle = (2Mt/\gamma) [t - (m/\gamma) \exp(-\gamma t/m)]$$

2次元での数値計算



軌跡を残すと

y



x