

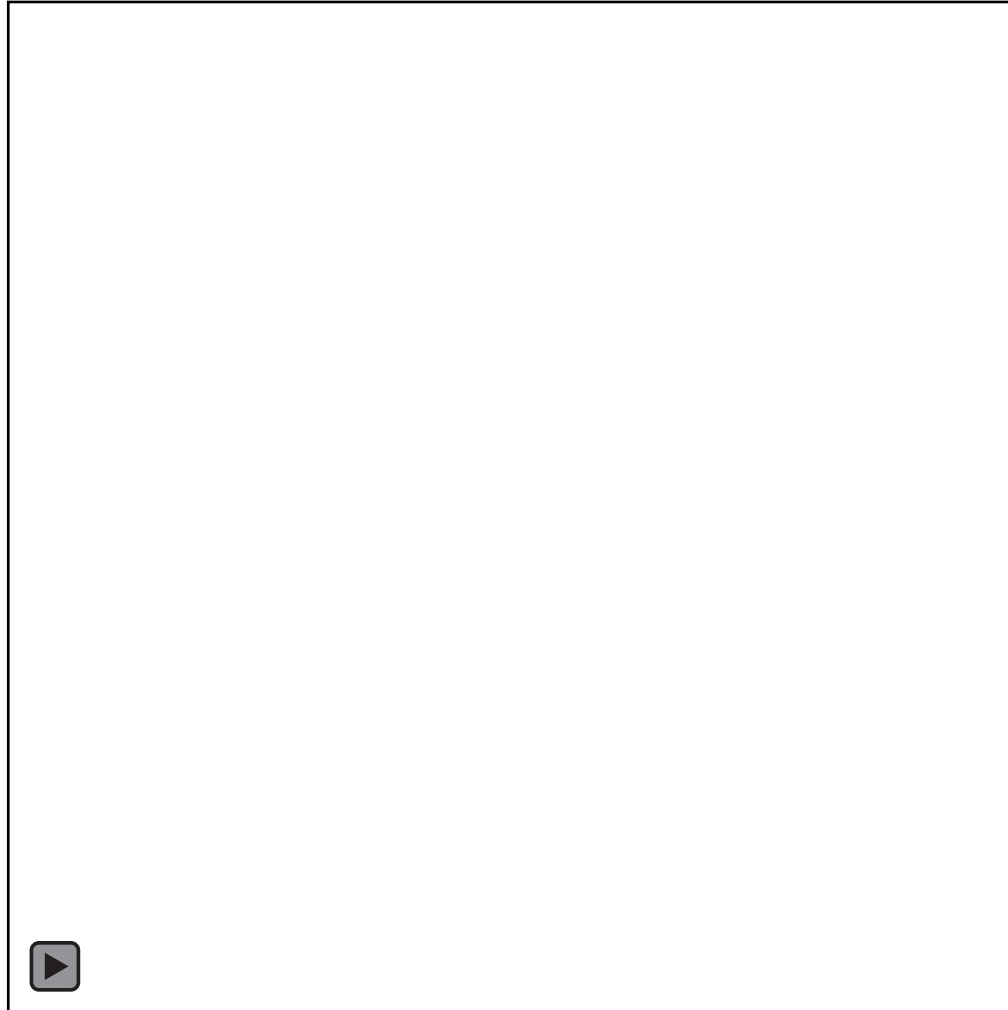
2013.10.22
物性物理学C

ランダムウォークと拡散方程式

北 畑 裕 之

ブラウン運動

ナノ粒子



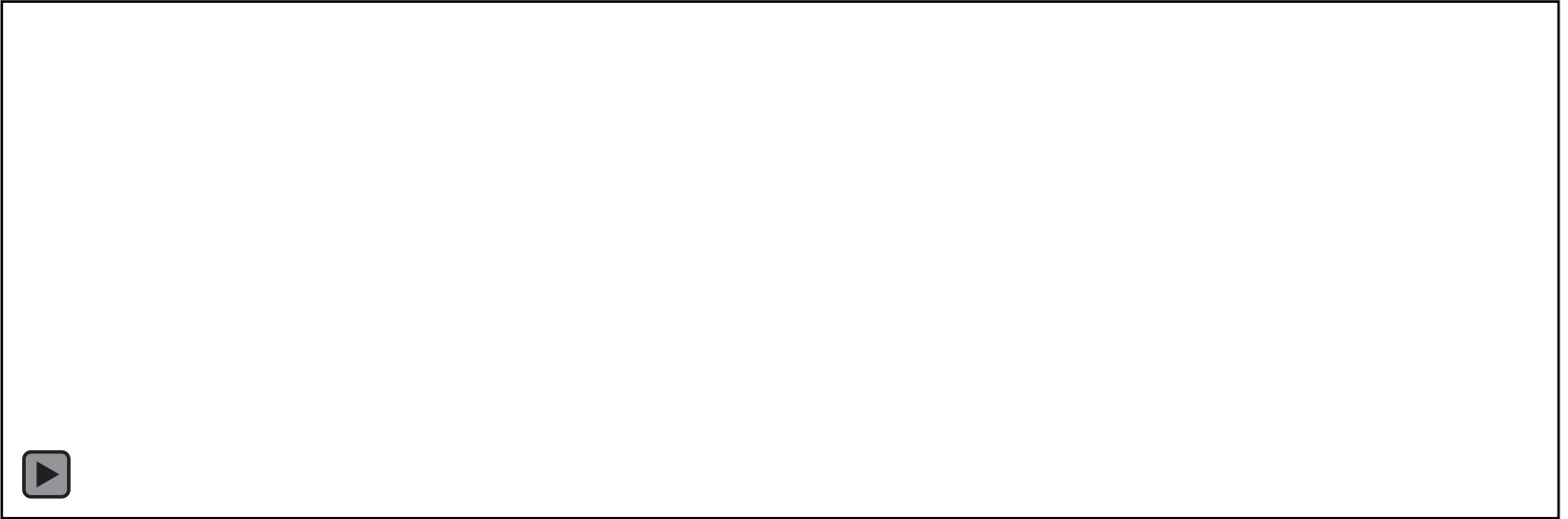
ランダムウォーク

$$x_{i+1} = x_i + \xi_i$$

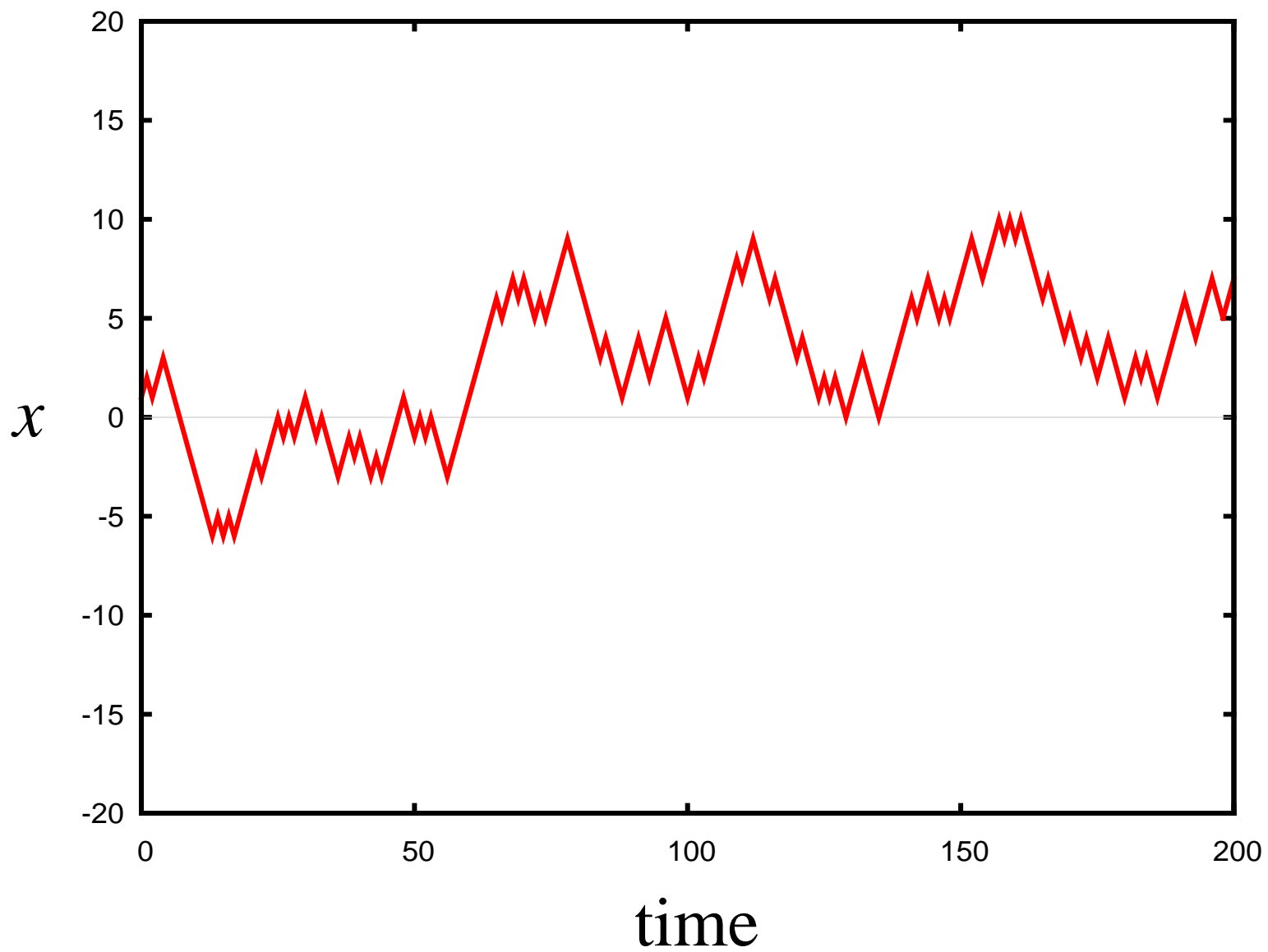
$$\xi_i = \begin{cases} 1 & (\text{Prob. } 1/2) \\ -1 & (\text{Prob. } 1/2) \end{cases}$$

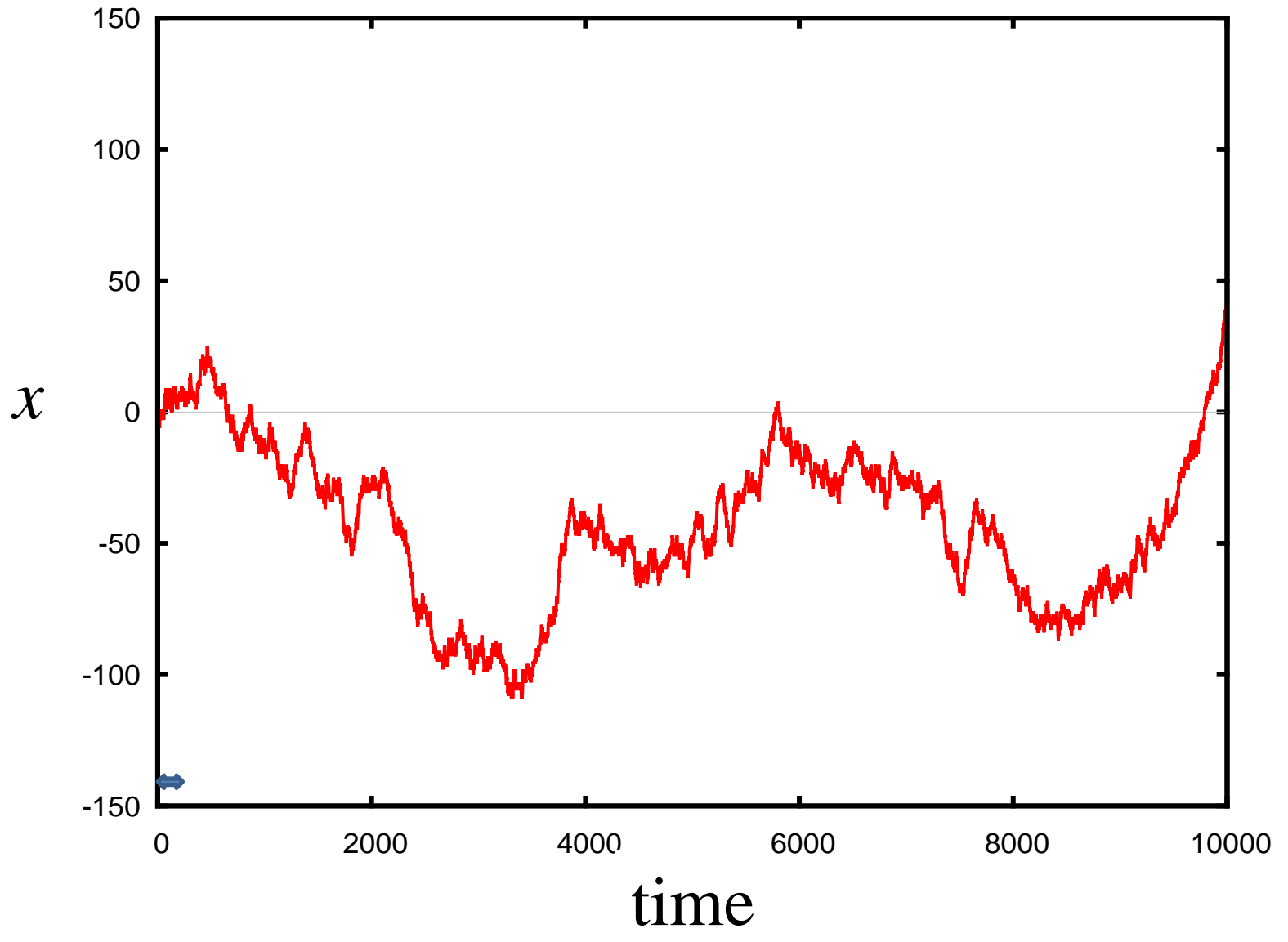
$$\langle \xi_i \xi_j \rangle = \delta_{ij}$$

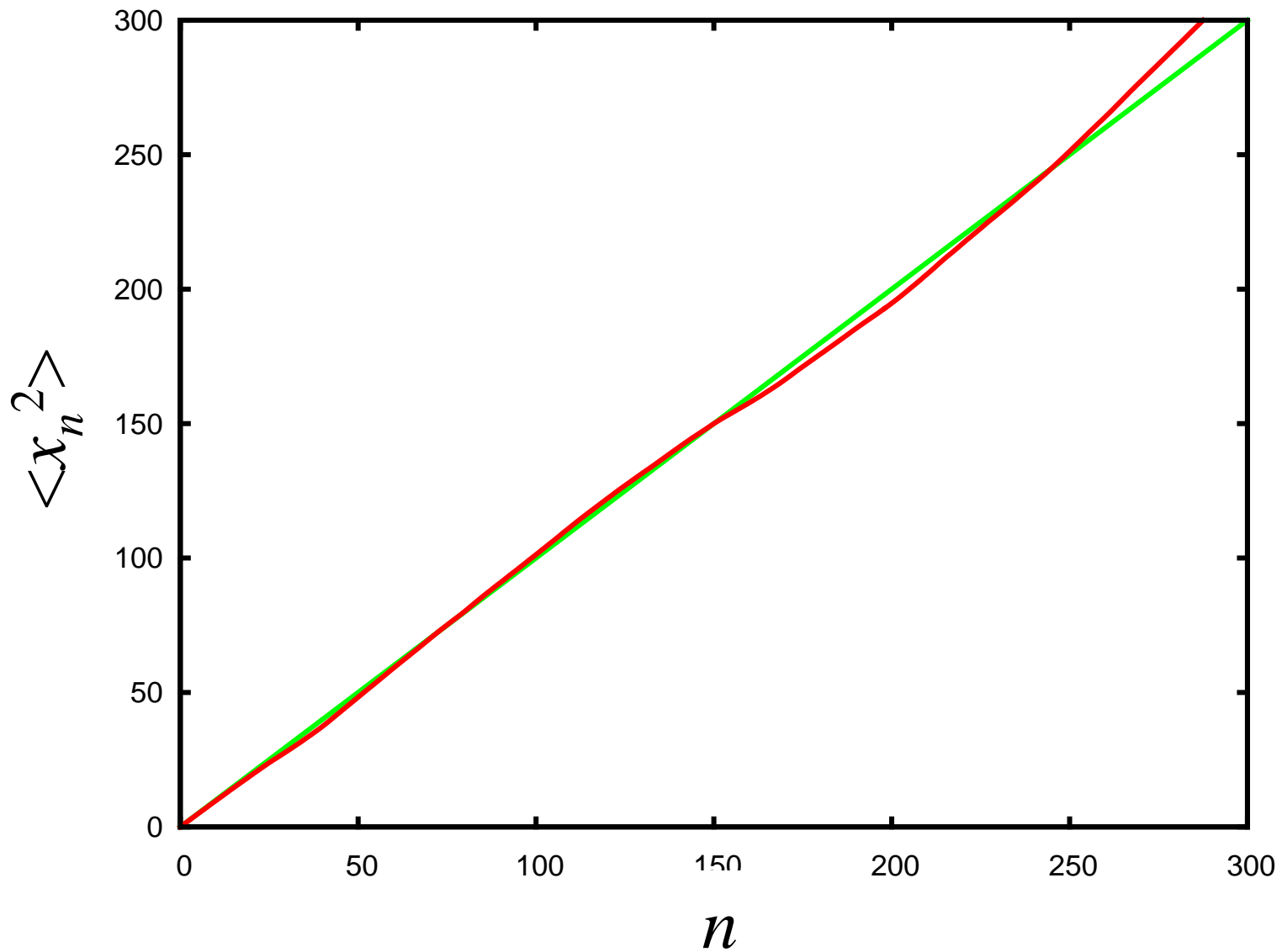
1次元ランダムウォーク



x







$$\begin{aligned}
\langle x_n^2 \rangle &= \left\langle \left[\sum_{k=0}^{n-1} \xi_k \right]^2 \right\rangle \\
&= \left\langle \sum_{k=0}^{n-1} \sum_{k'=0}^{n-1} \xi_k \xi_{k'} \right\rangle \\
&= \sum_{k=0}^{n-1} \sum_{k'=0}^{n-1} \langle \xi_k \xi_{k'} \rangle \\
&= \sum_{k=0}^{n-1} \sum_{k'=0}^{n-1} \delta_{kk'} \\
&= n
\end{aligned}$$

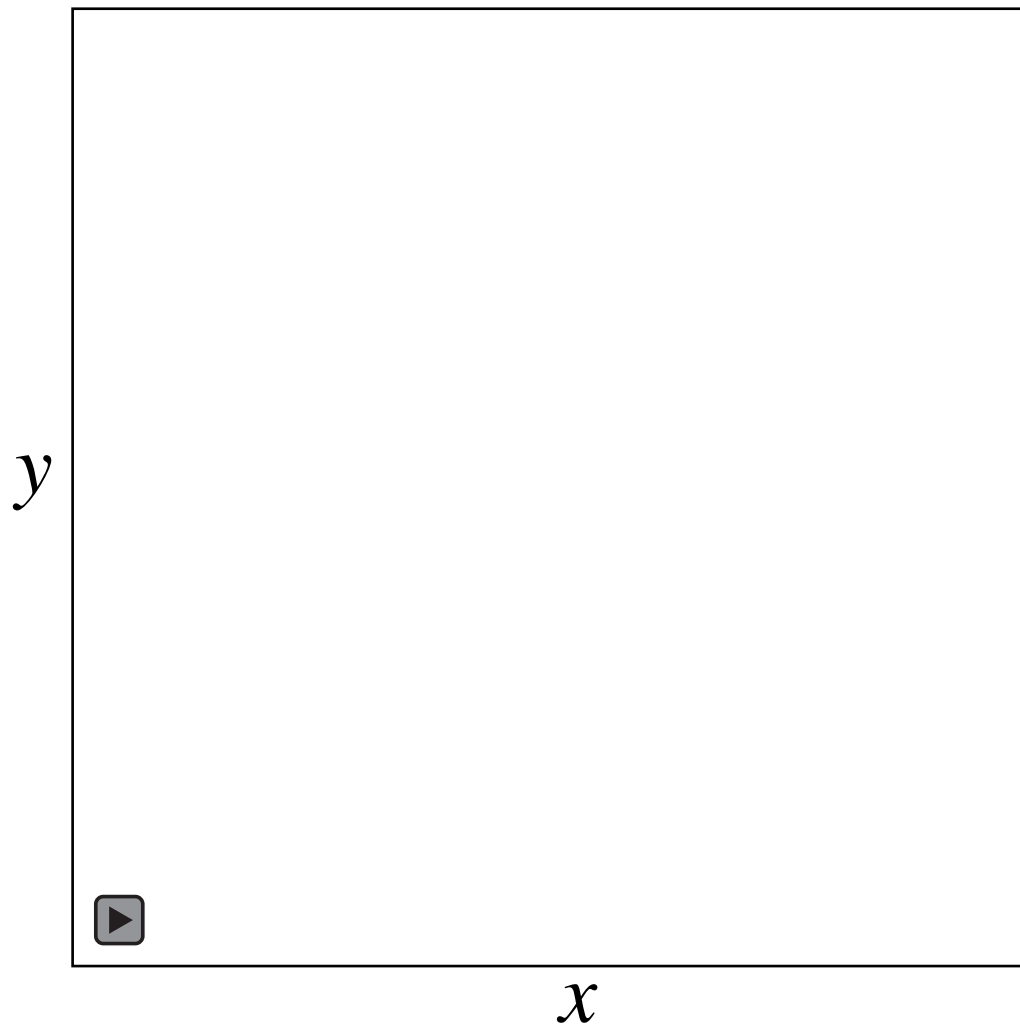
2次元の場合

$$\mathbf{r}_{i+1} = \mathbf{r}_i + \boldsymbol{\xi}_i \quad \mathbf{r}_i = (x_i, y_i)$$

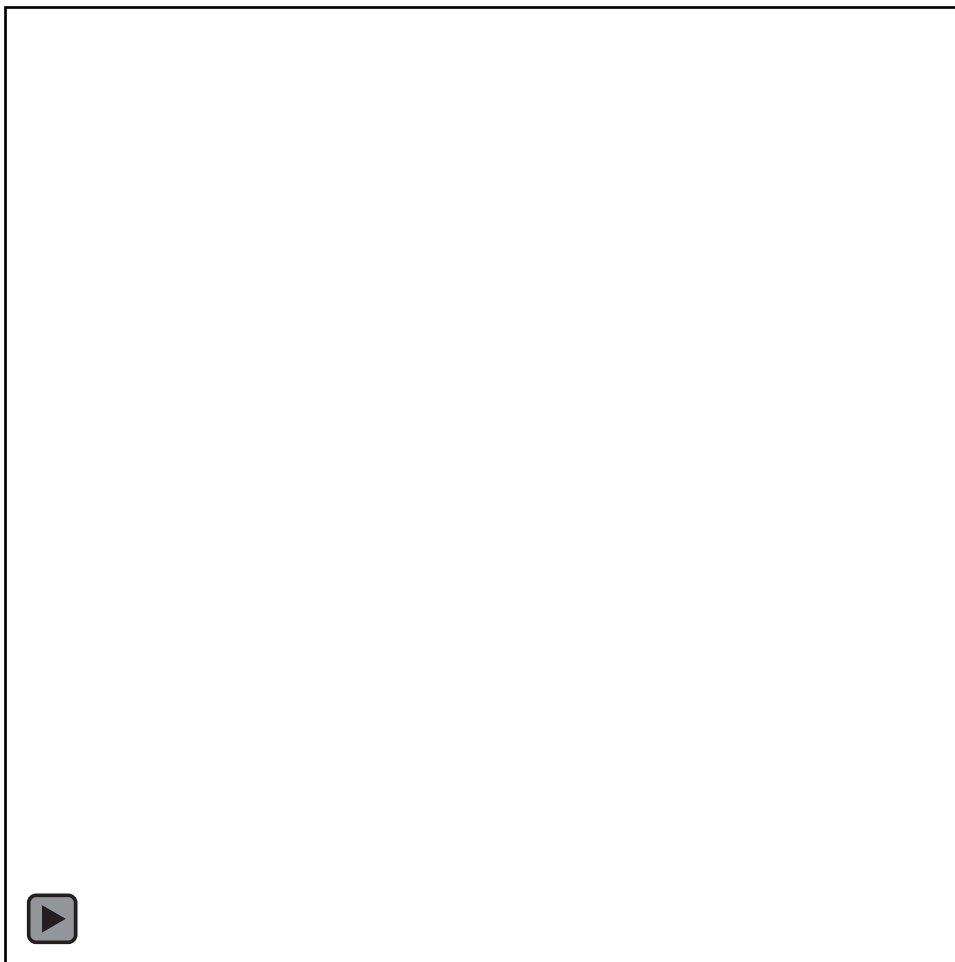
$$\boldsymbol{\xi}_i = \begin{cases} (1, 0) & (\text{Prob. } 1/4) \\ (-1, 0) & (\text{Prob. } 1/4) \\ (0, 1) & (\text{Prob. } 1/4) \\ (0, -1) & (\text{Prob. } 1/4) \end{cases}$$

$$\langle \boldsymbol{\xi}_i \cdot \boldsymbol{\xi}_j \rangle = \delta_{ij}$$

2次元ランダムウォーク

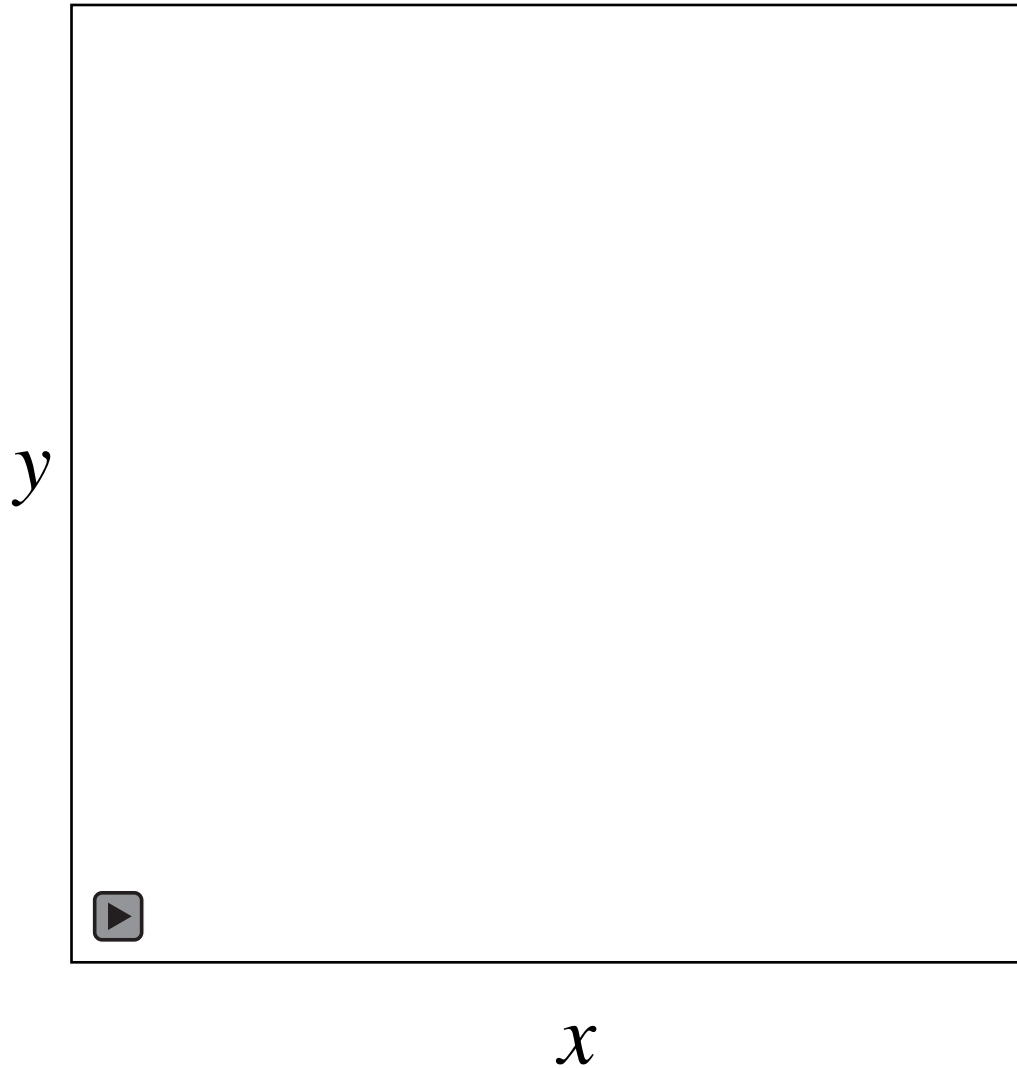


y

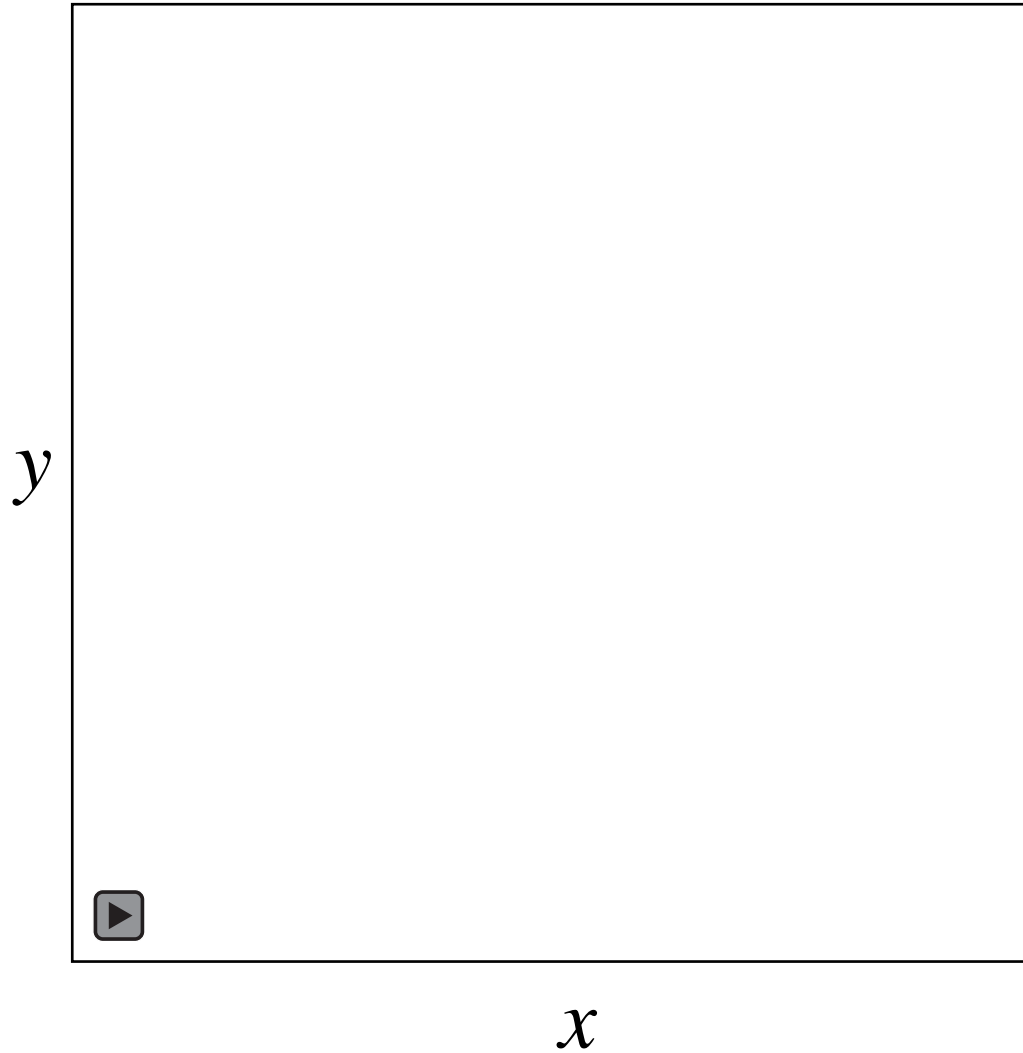


x

100個の粒子



1000個の粒子



拡散方程式

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

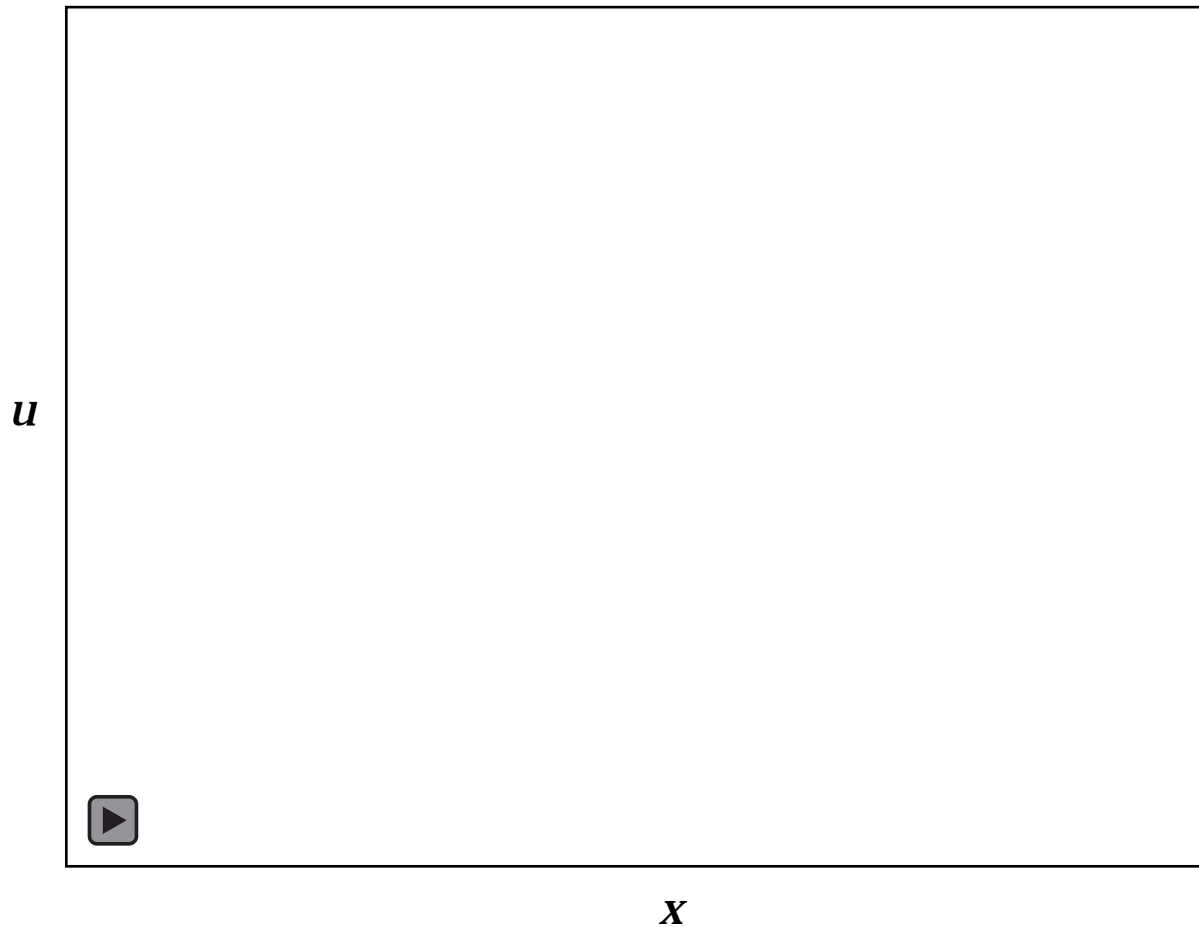
1次元の場合

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

初期値:

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

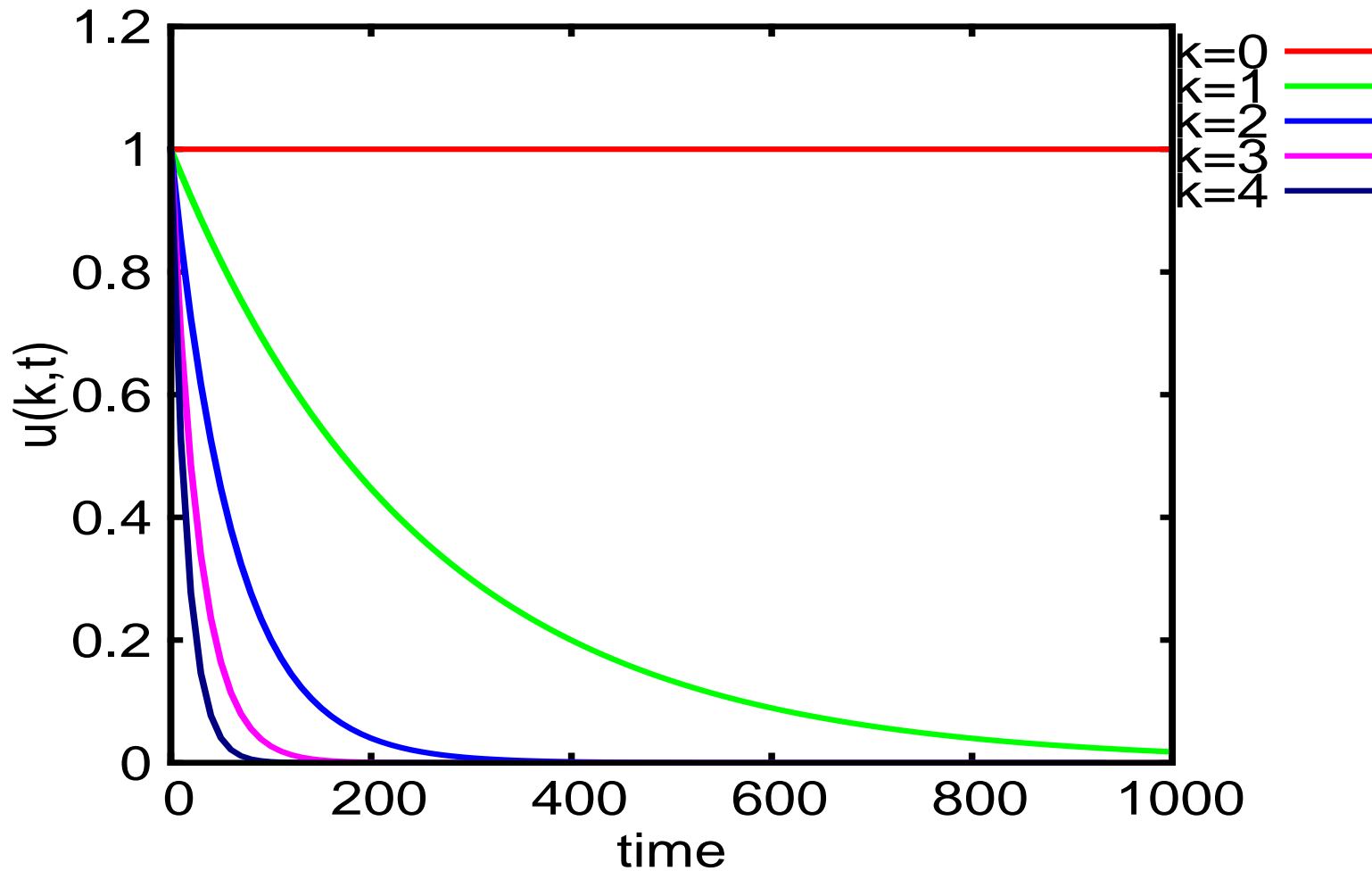
1次元で初期値が δ 関数の解 : Green関数



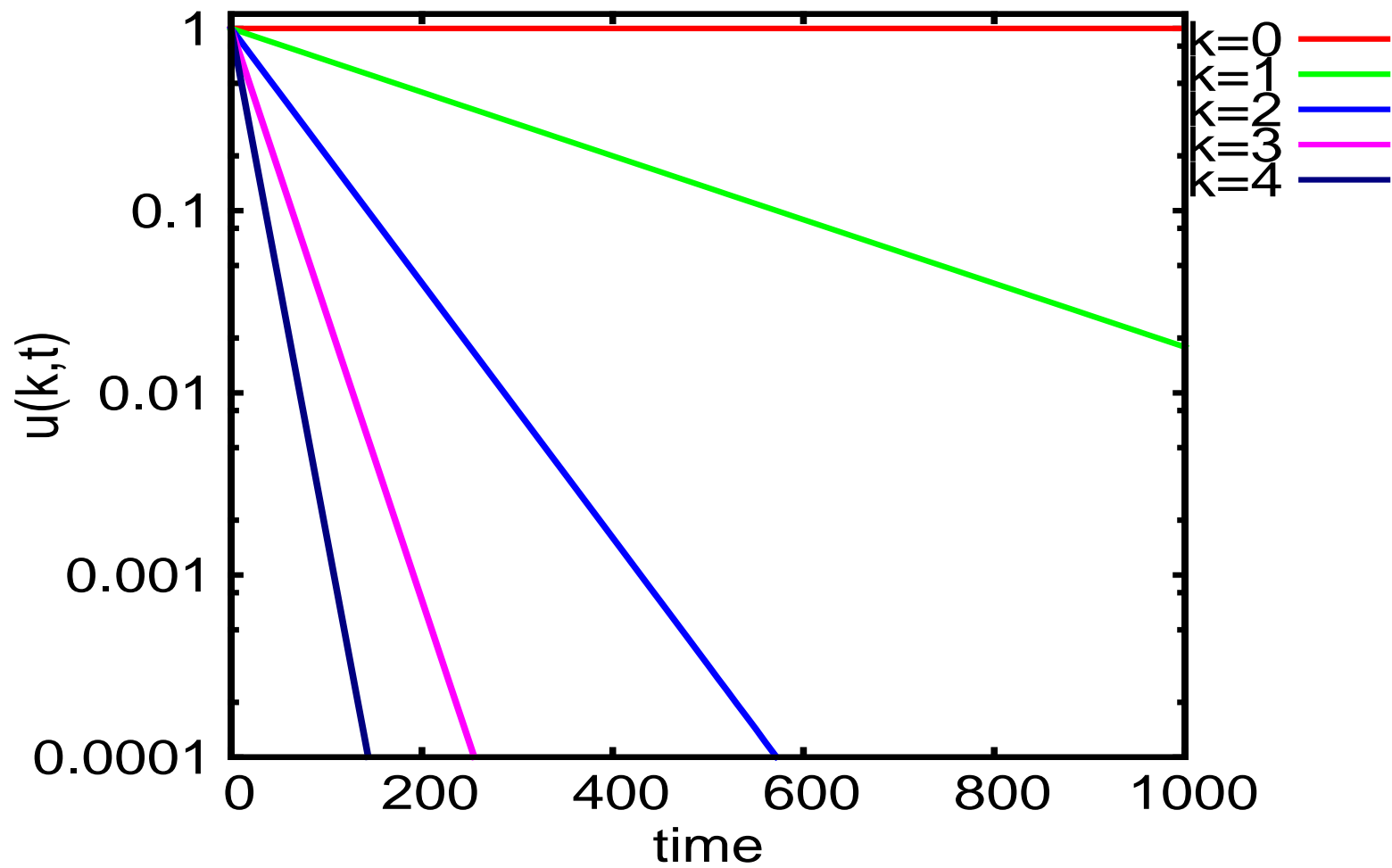
$$u(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

Fourier modeの時間変化

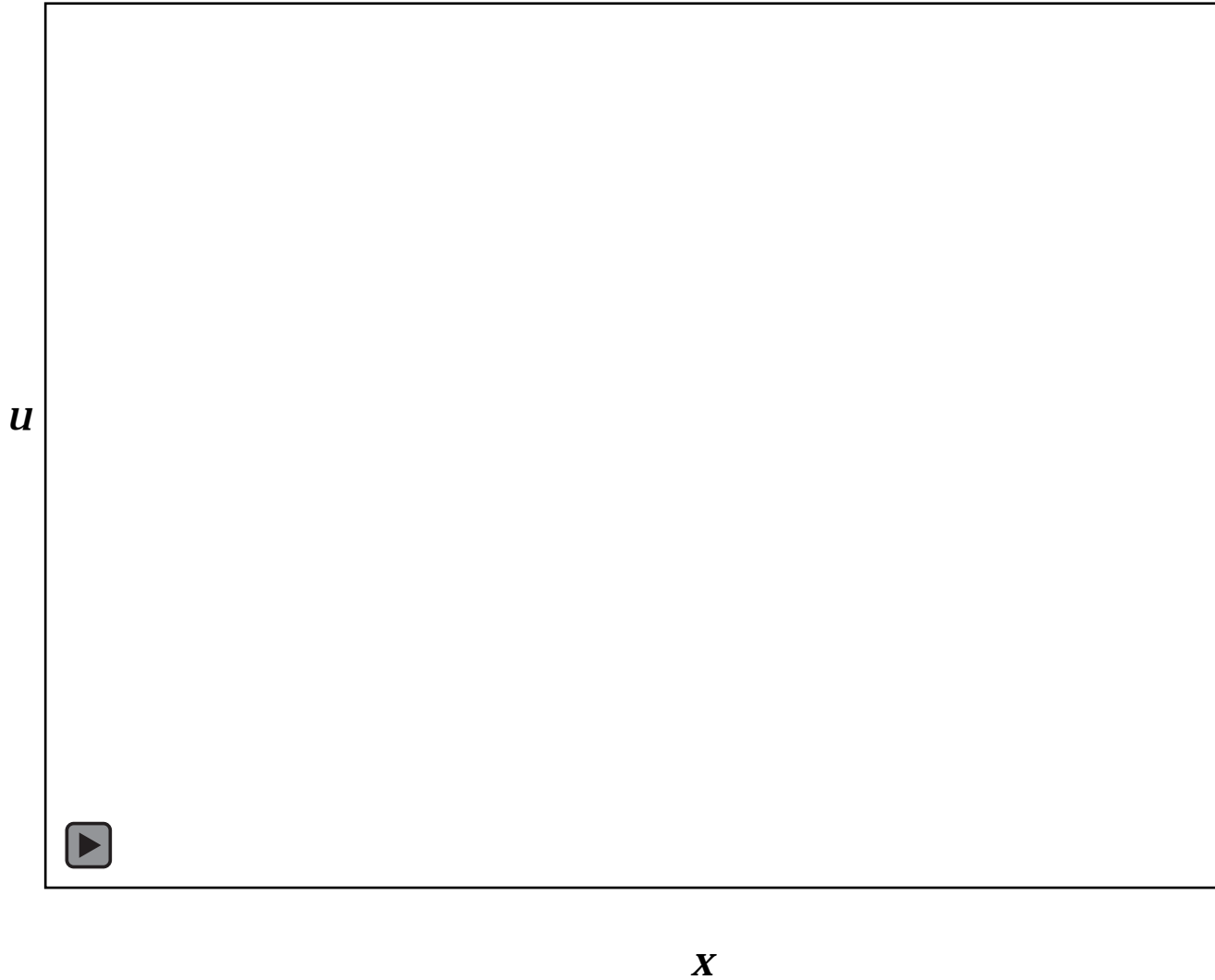
$$u(x,t) = \frac{1}{2\pi} \sum_{k=0}^N \tilde{u}(k,t) \cos\left(\frac{2\pi kx}{NL}\right)$$



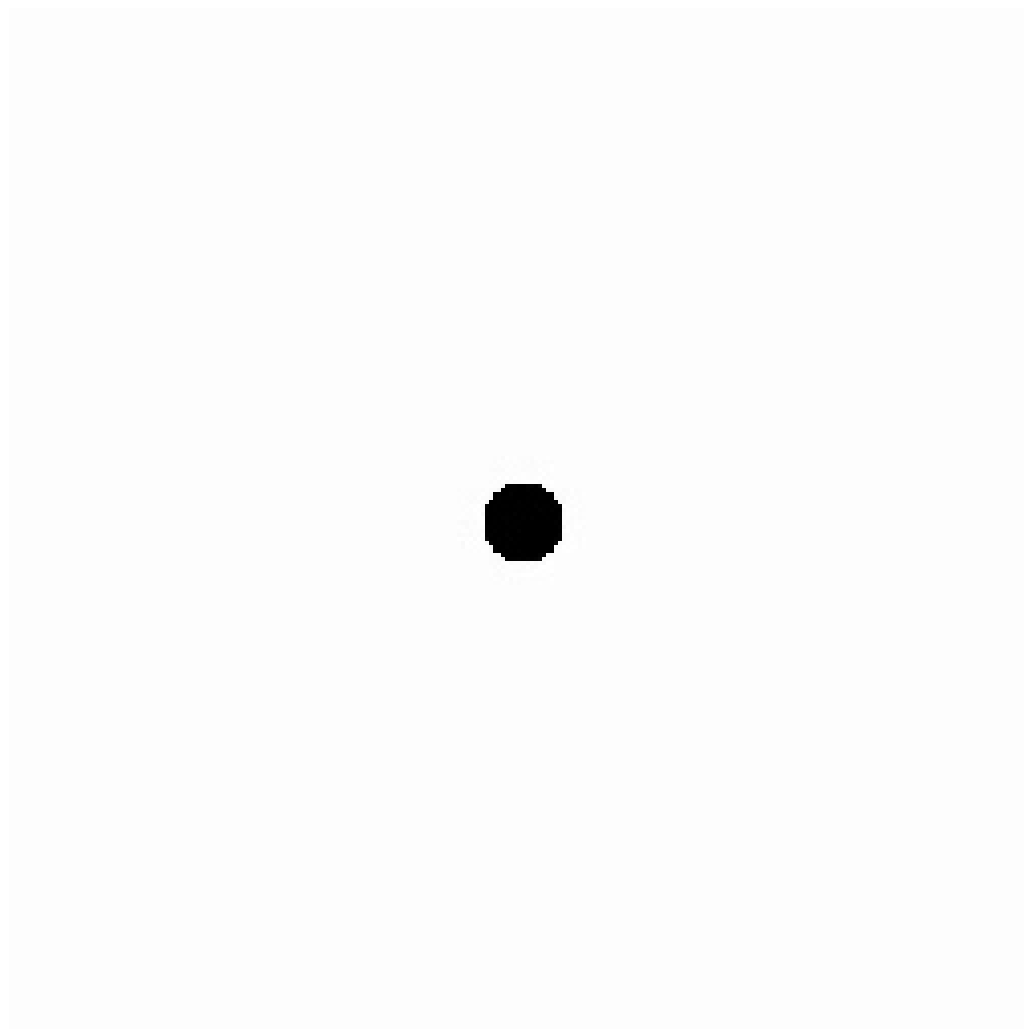
Log scaleでは



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

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

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

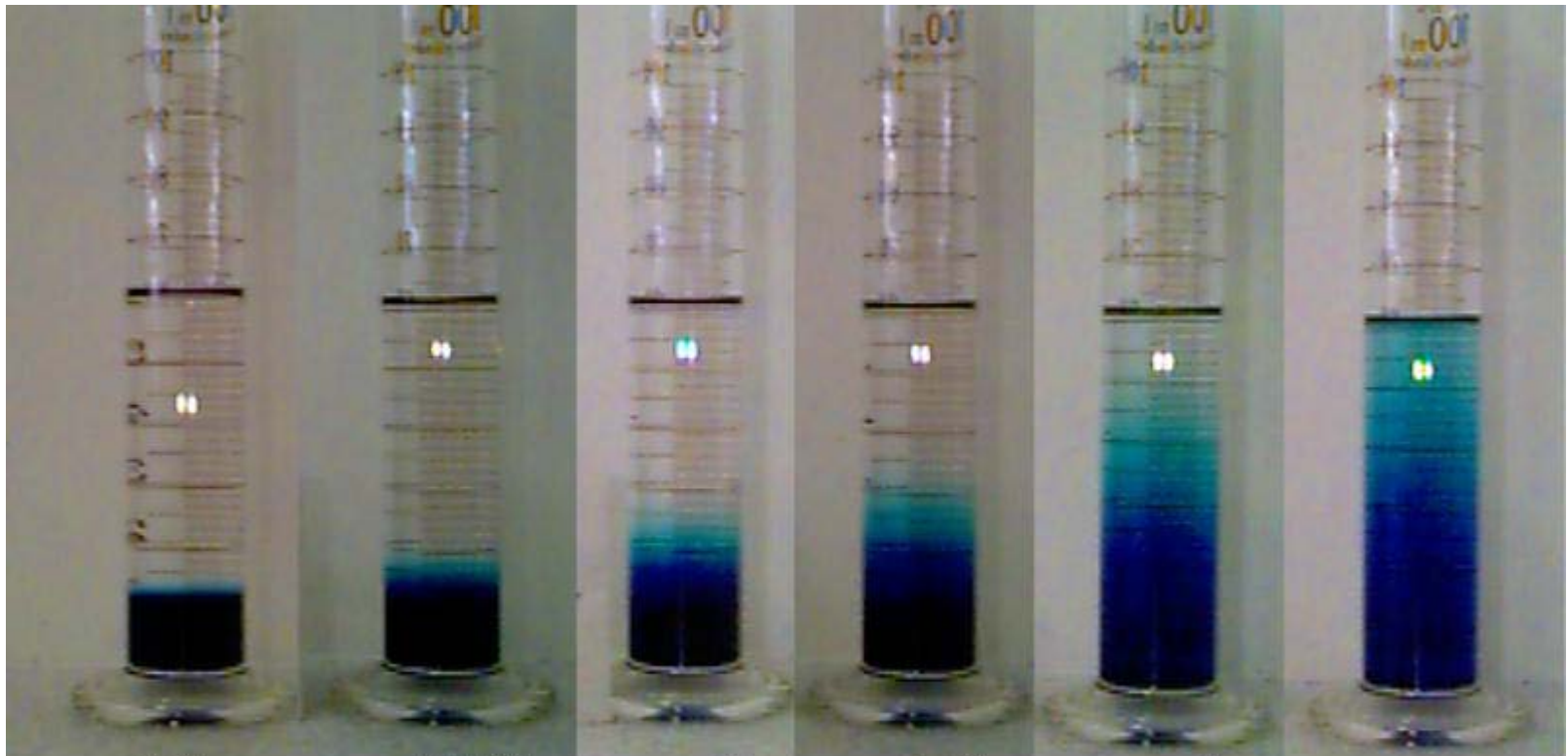
1 mm拡散で広がるには $t \sim 3 \times 10^2 \text{ s} \sim 5 \text{ minutes}$

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