2012.10.23
物性物理学C

ランダムウォークと拡散方程式

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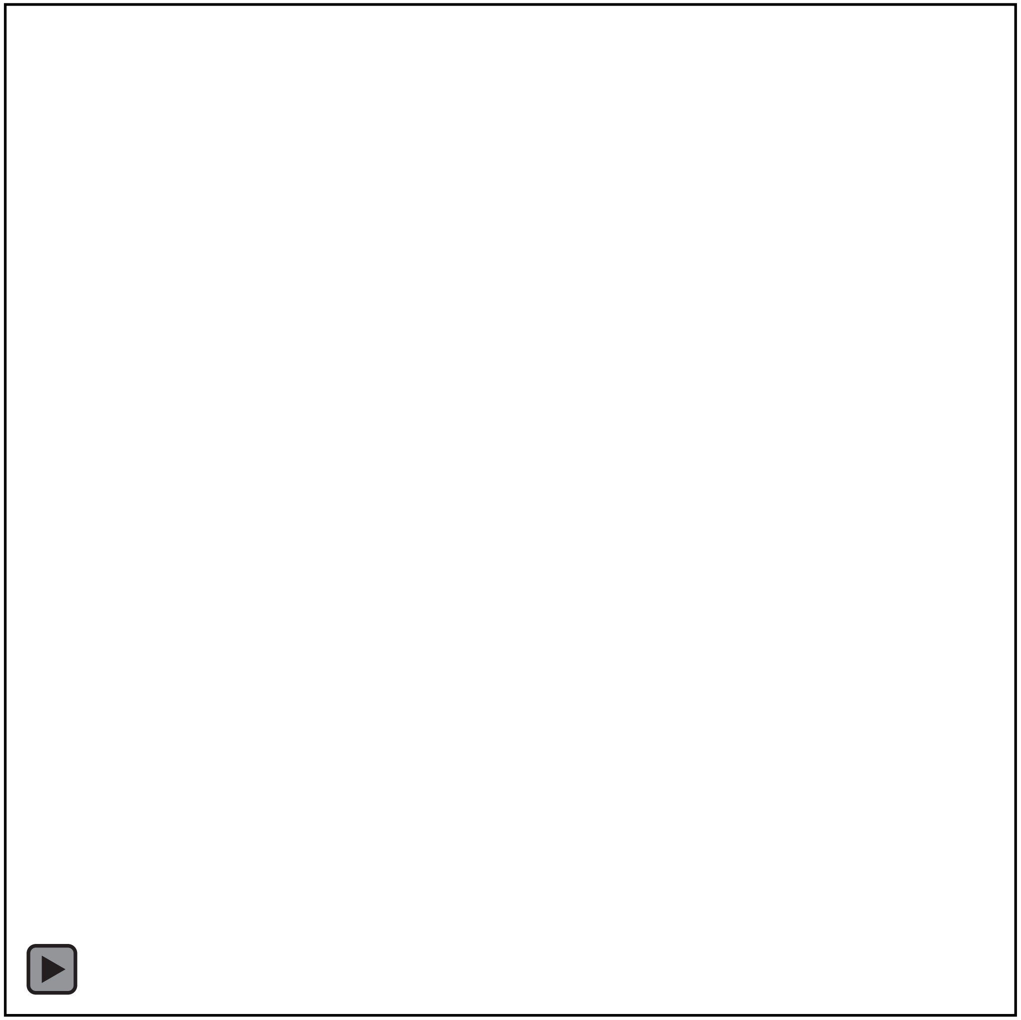
ブラウン運動

ナノ粒子



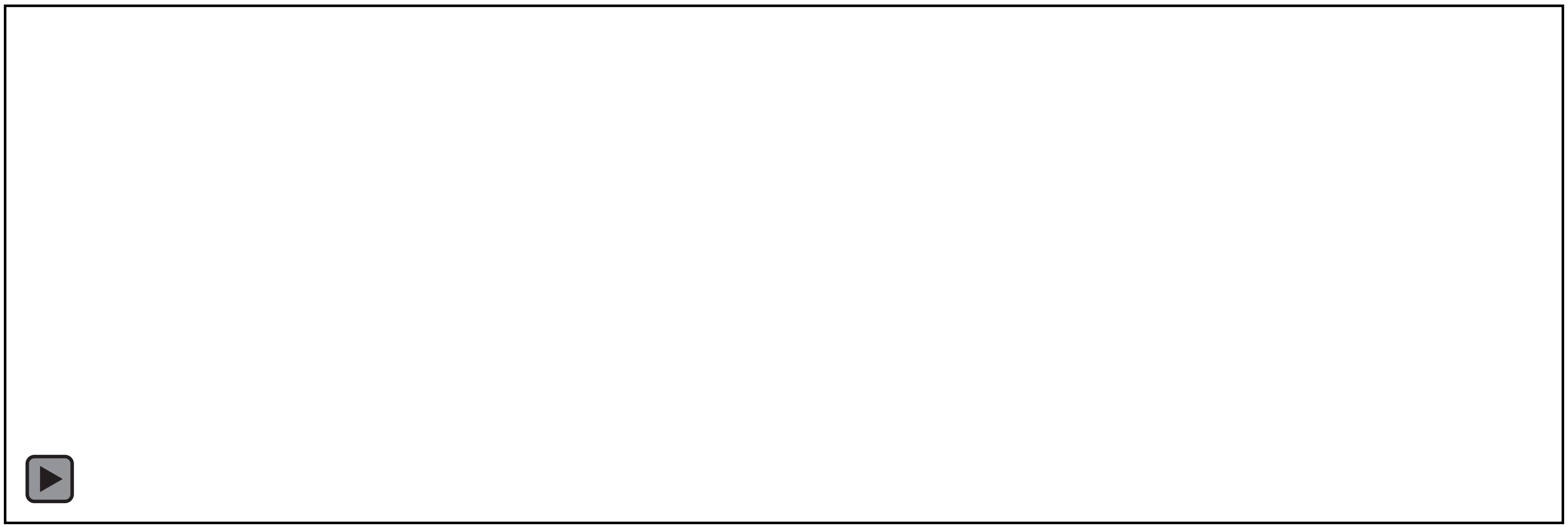
ランダムウォーク

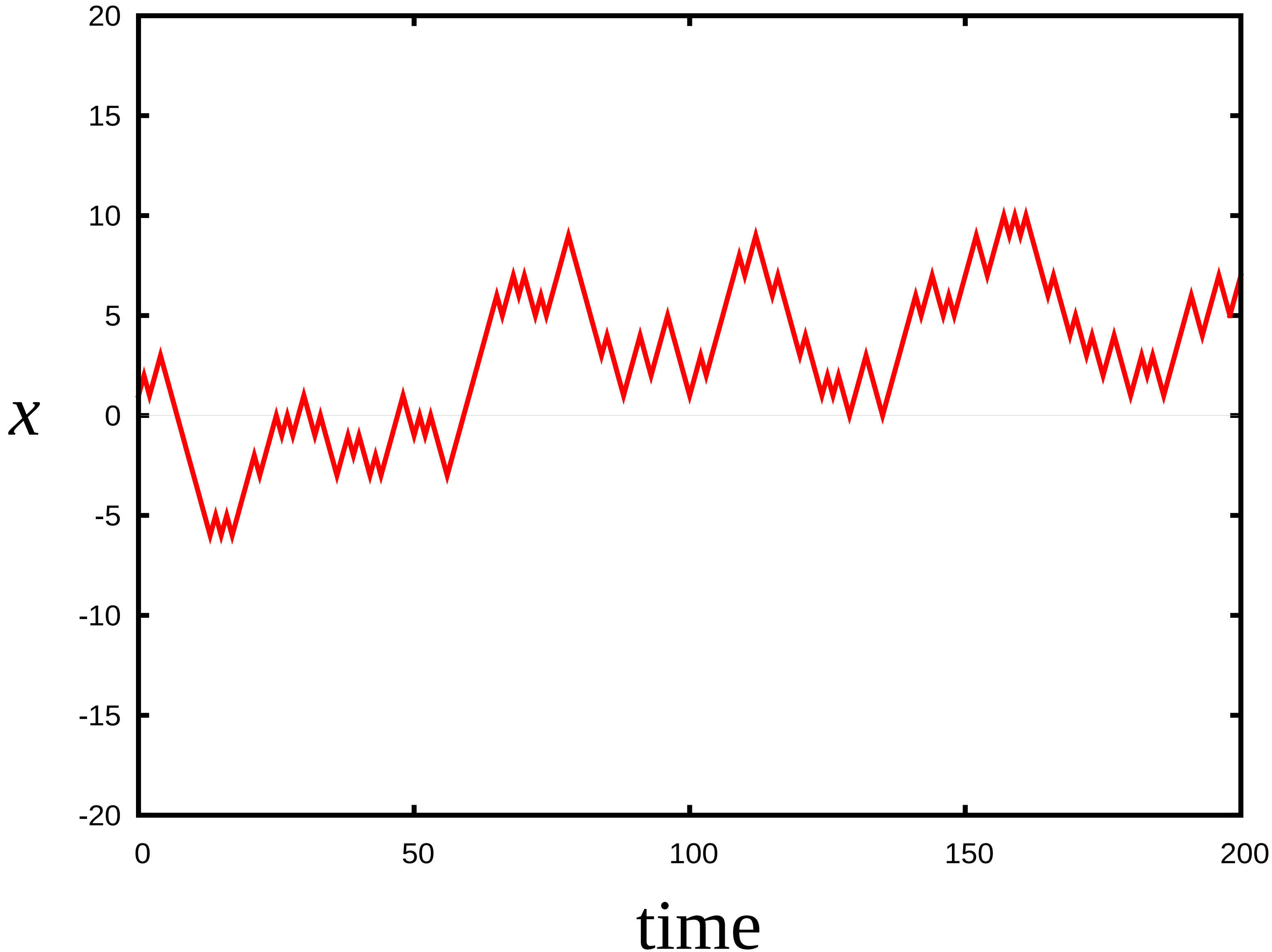
$$x_{i+1} = x_i + \xi_i$$

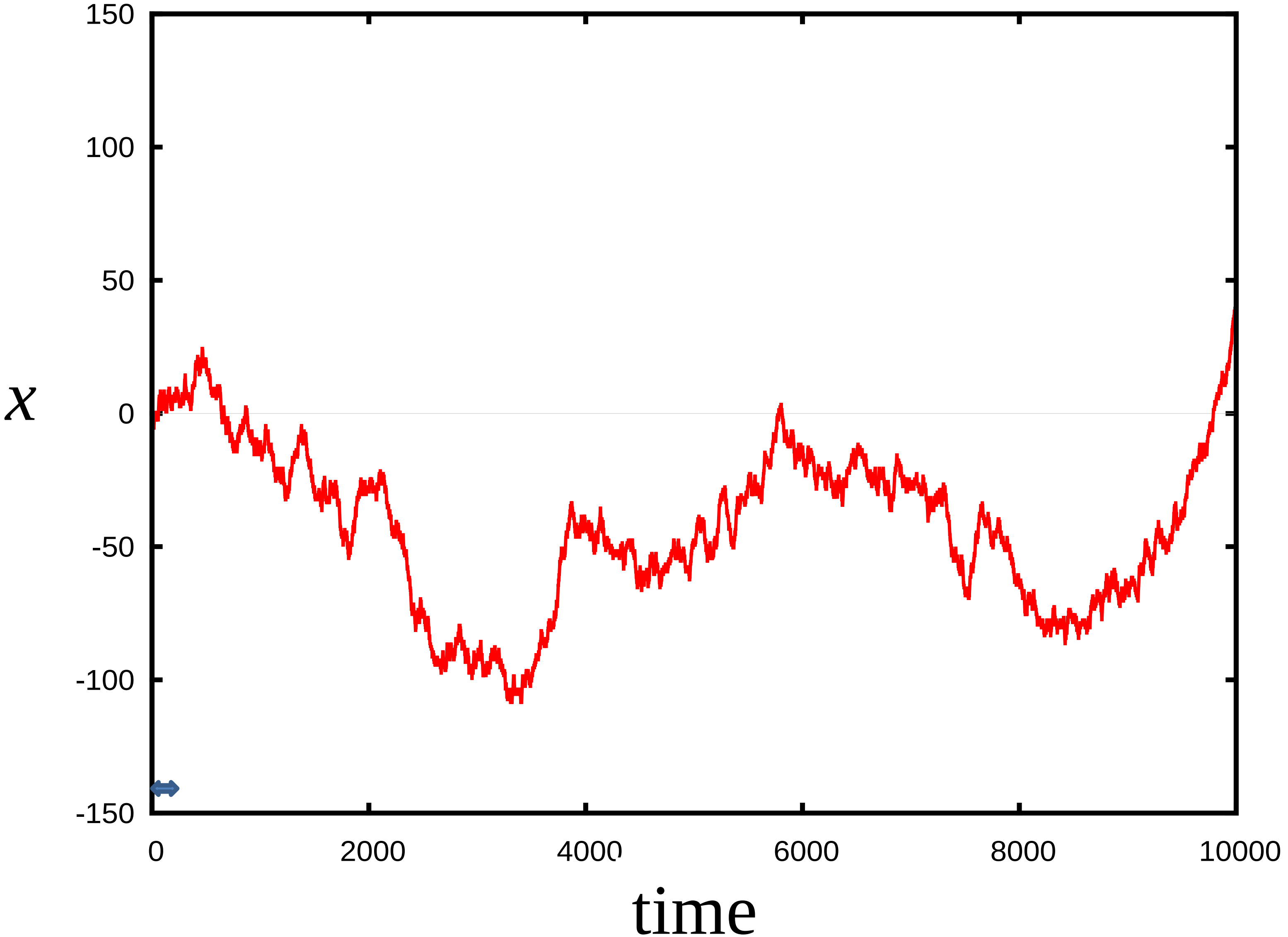
$$\xi_i = \begin{cases} 1 & (\mathrm{Prob.}1/2) \\ -1 & (\mathrm{Prob.}1/2) \end{cases}$$

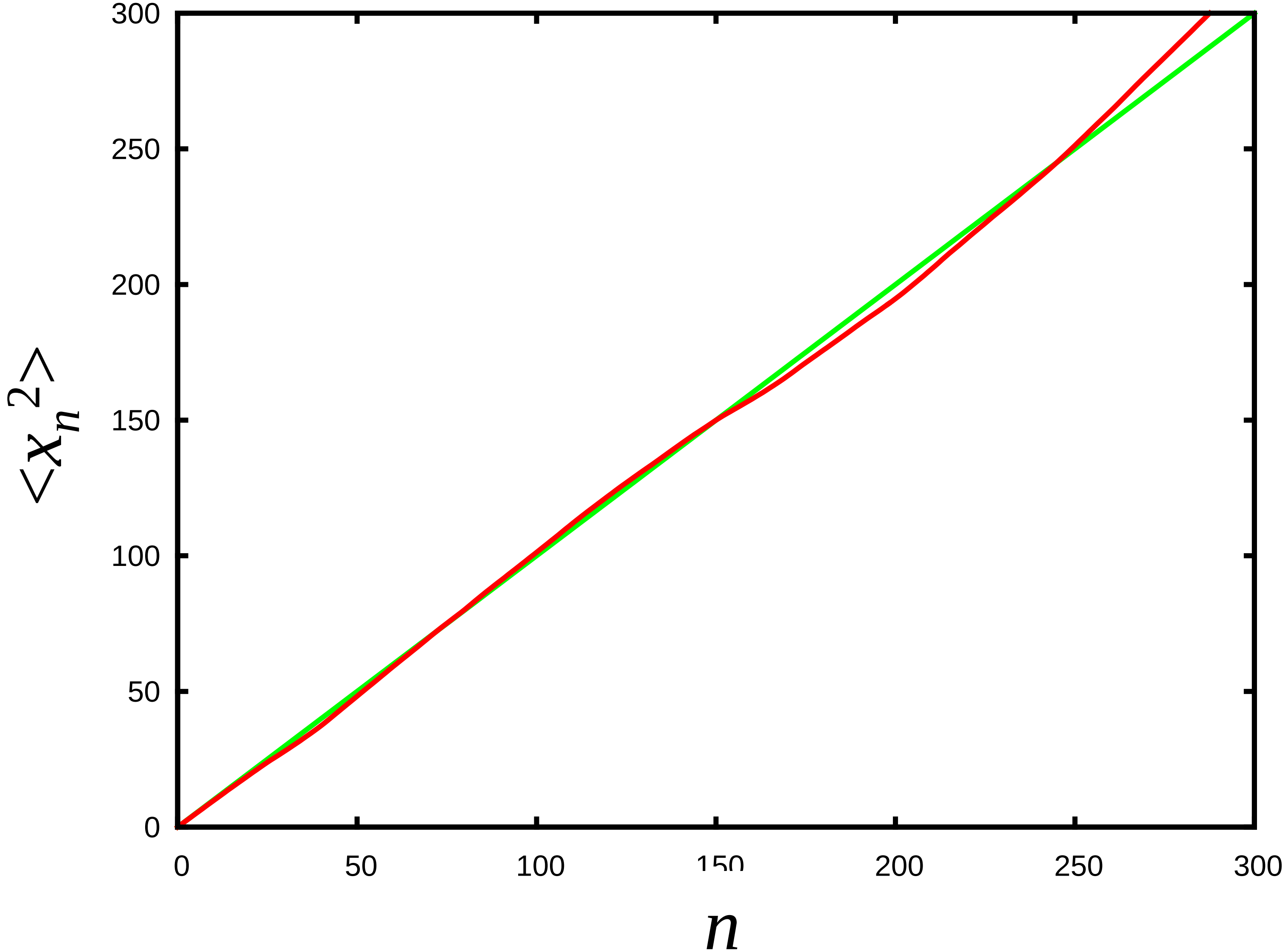
$$\langle \xi_i \xi_j \rangle = \delta_{ij}$$

1次元ランダムウォーク




20
15
10
5
0
-5
-10
-15
-20
x
0
50
100
150
200
time


150
100
50
0
-50
-100
-150
x
0
2000
4000
6000
8000
10000
time



300
250
200
150
100
50
0
0
50
100
150
200
250
300
$<x_n^2>$
n

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

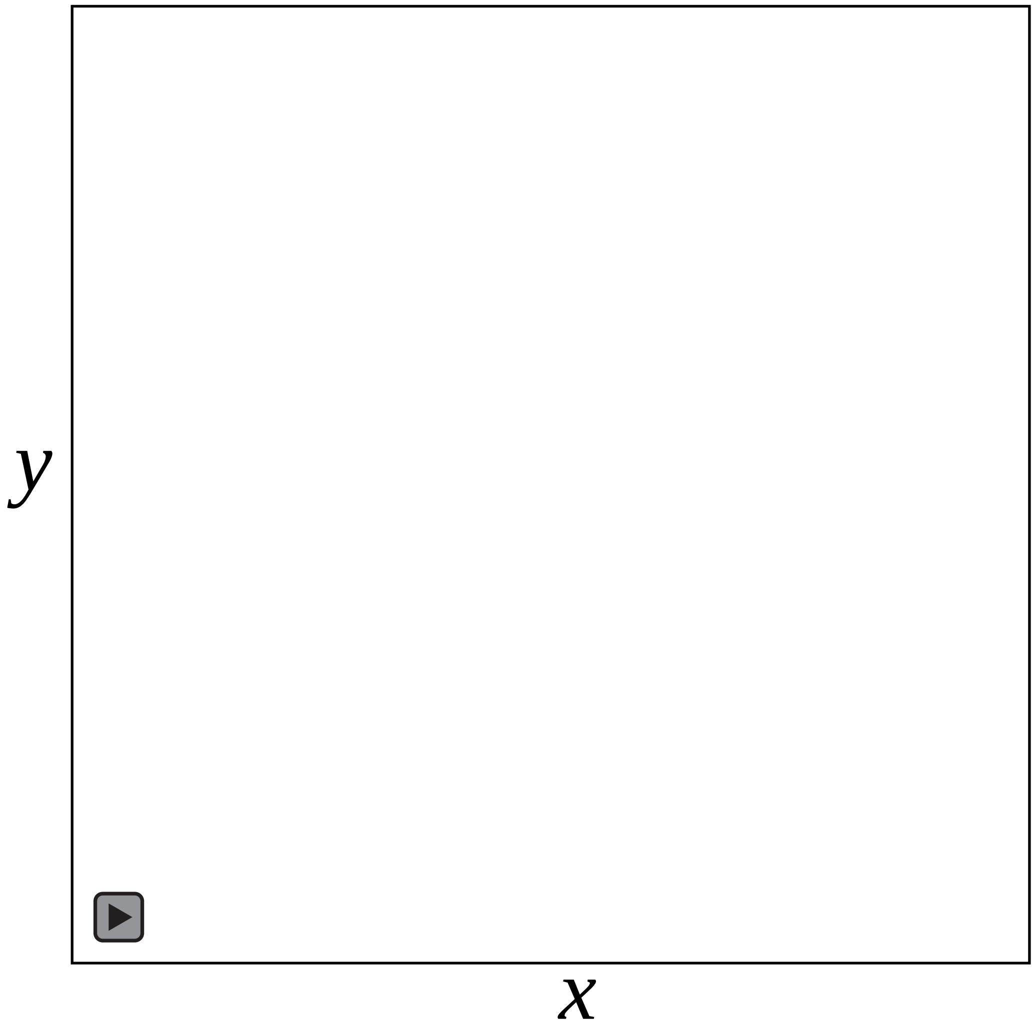
2次元の場合

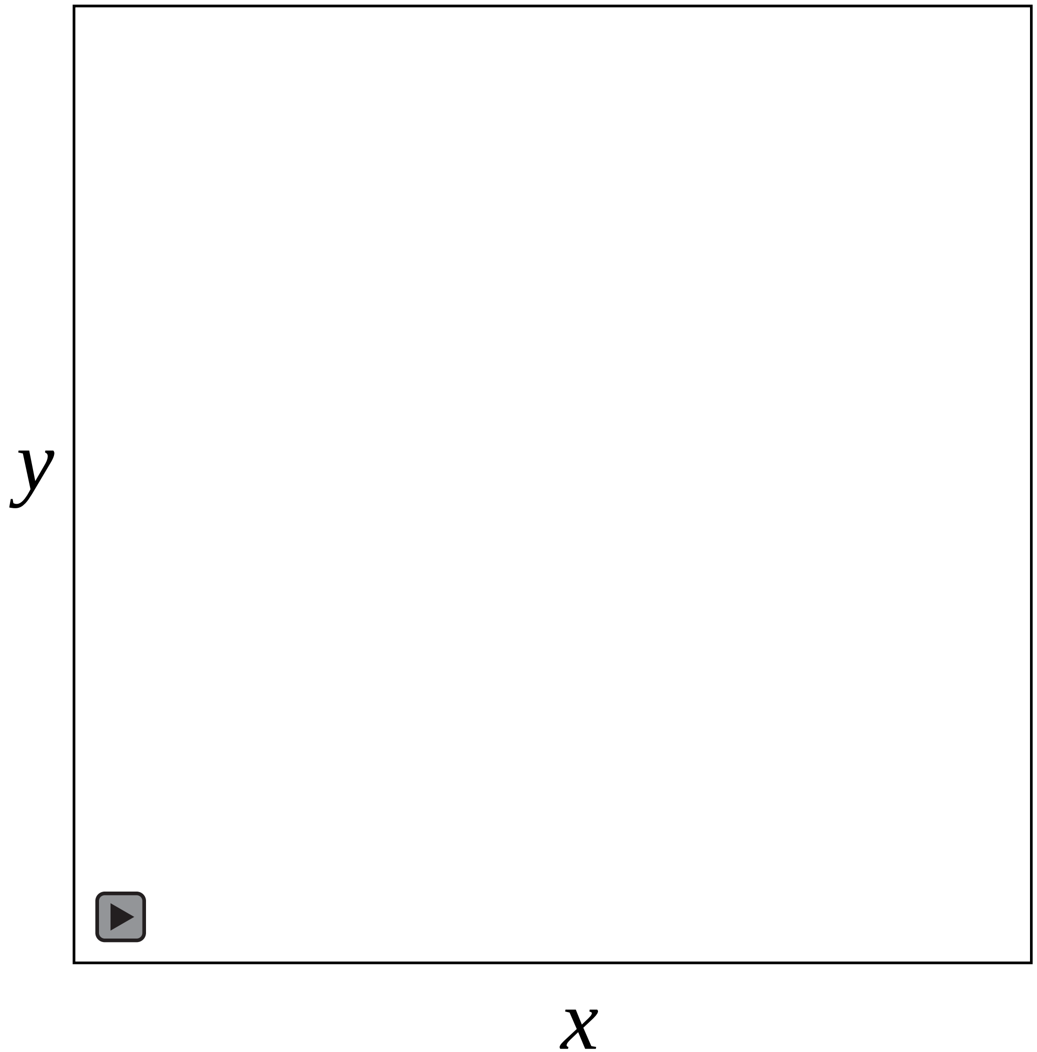
$$\mathbf{r}_{i+1} = \mathbf{r}_i + \boldsymbol{\xi}_i \qquad \mathbf{r}_i = (x_i, y_i)$$

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

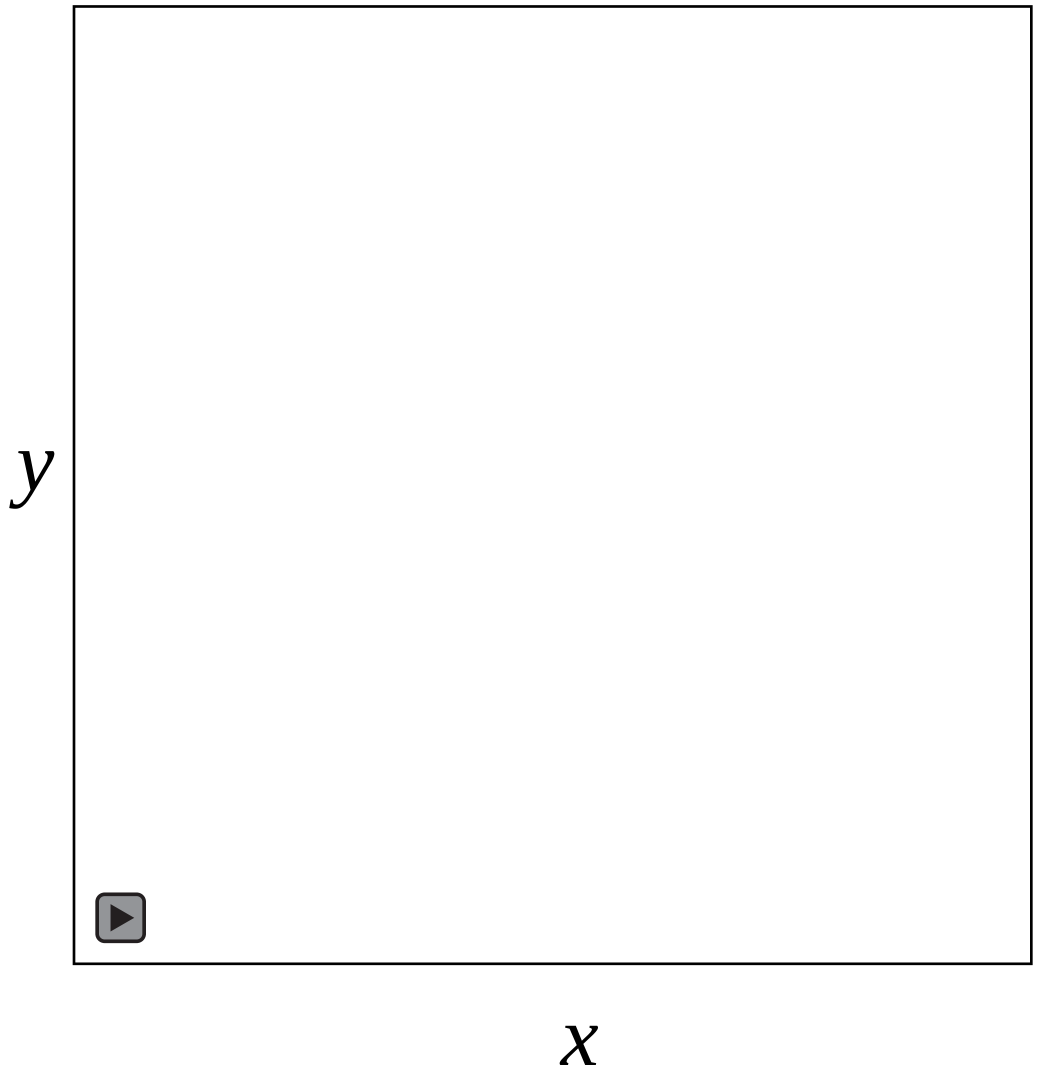
$$\langle \boldsymbol{\xi}_i \cdot \boldsymbol{\xi}_j \rangle = \delta_{ij}$$

2次元ランダムウォーク

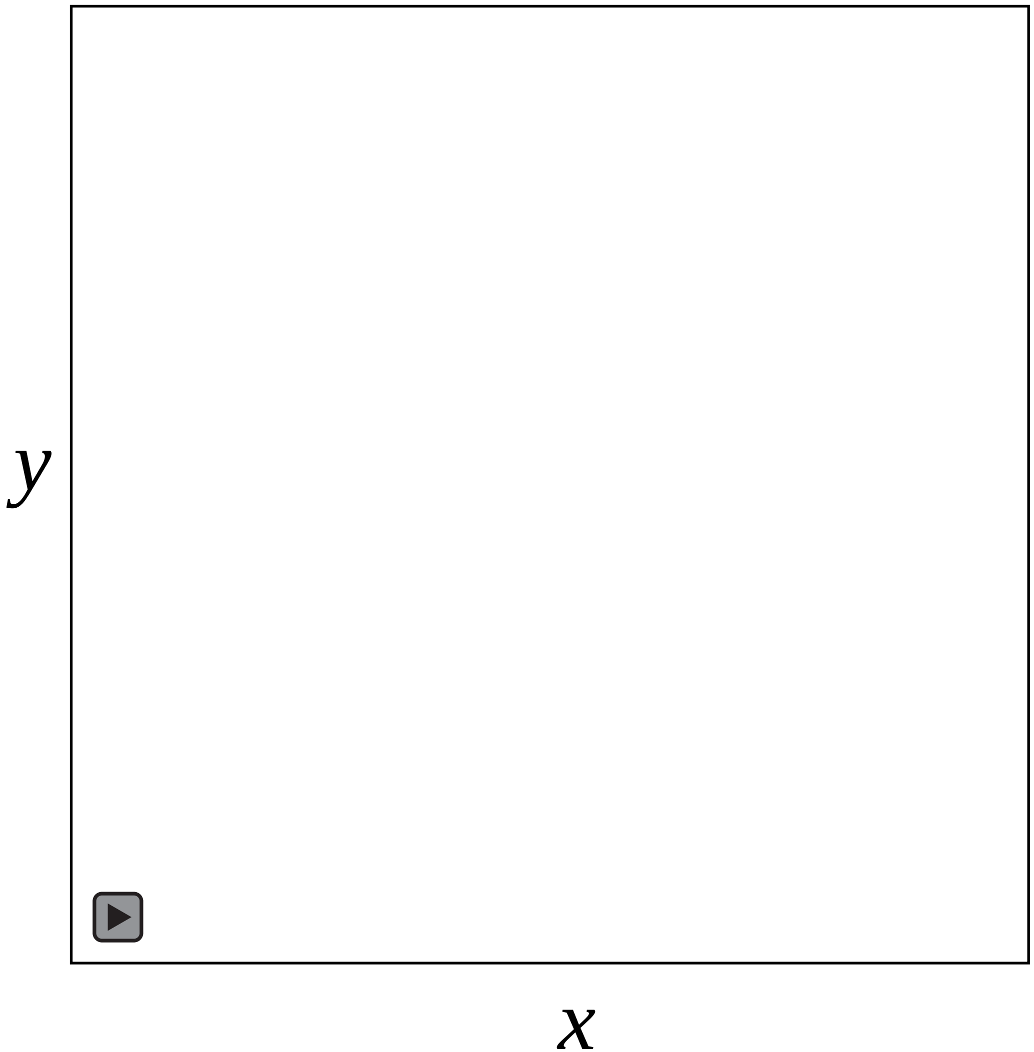



y
x

100個の粒子



1000個の粒子



拡散方程式

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

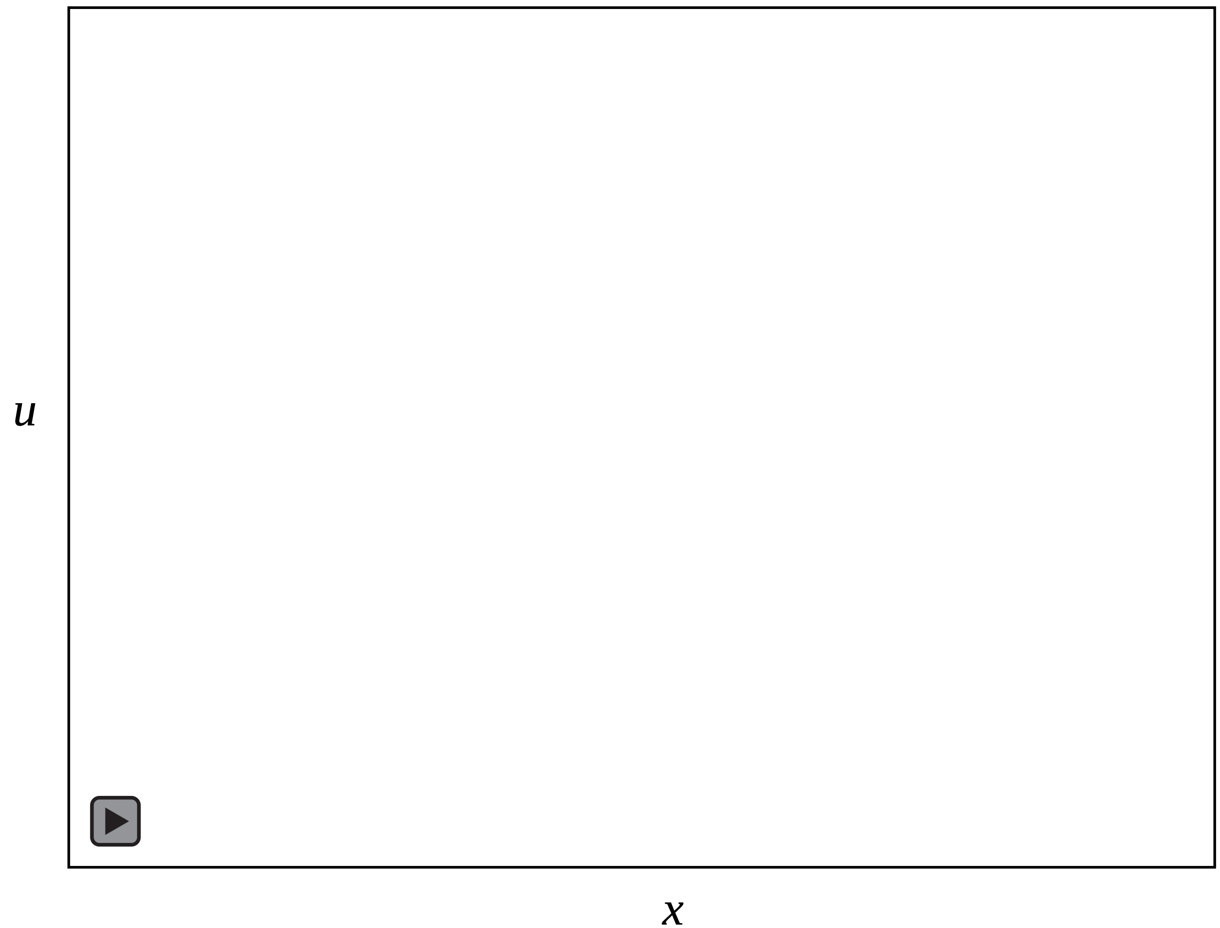
1次元の場合

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

初期値:

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

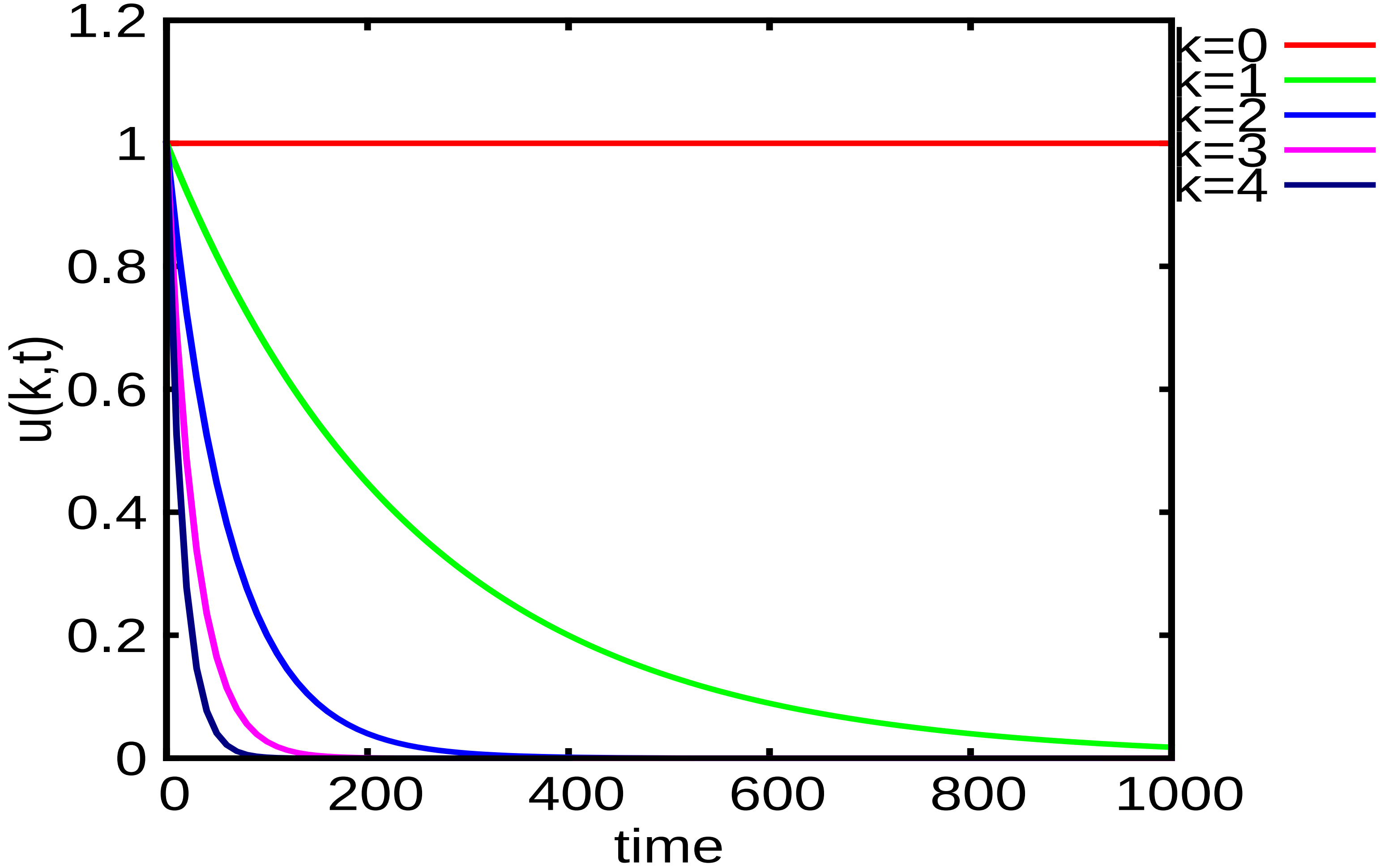
1次元で初期値がδ関数の解　：　Green関数



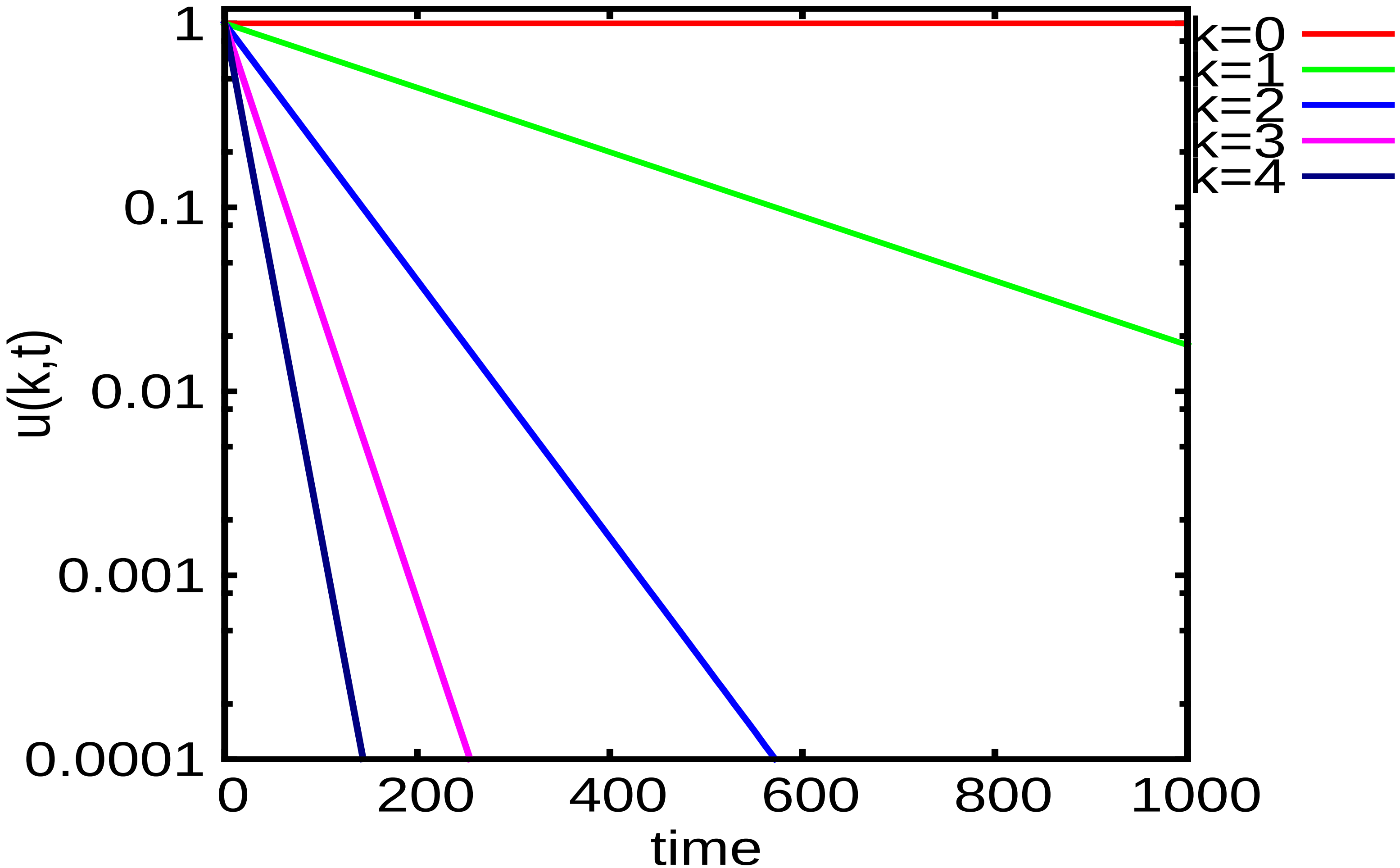
$$u(x,t)=\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

Fourier modeの時間変化

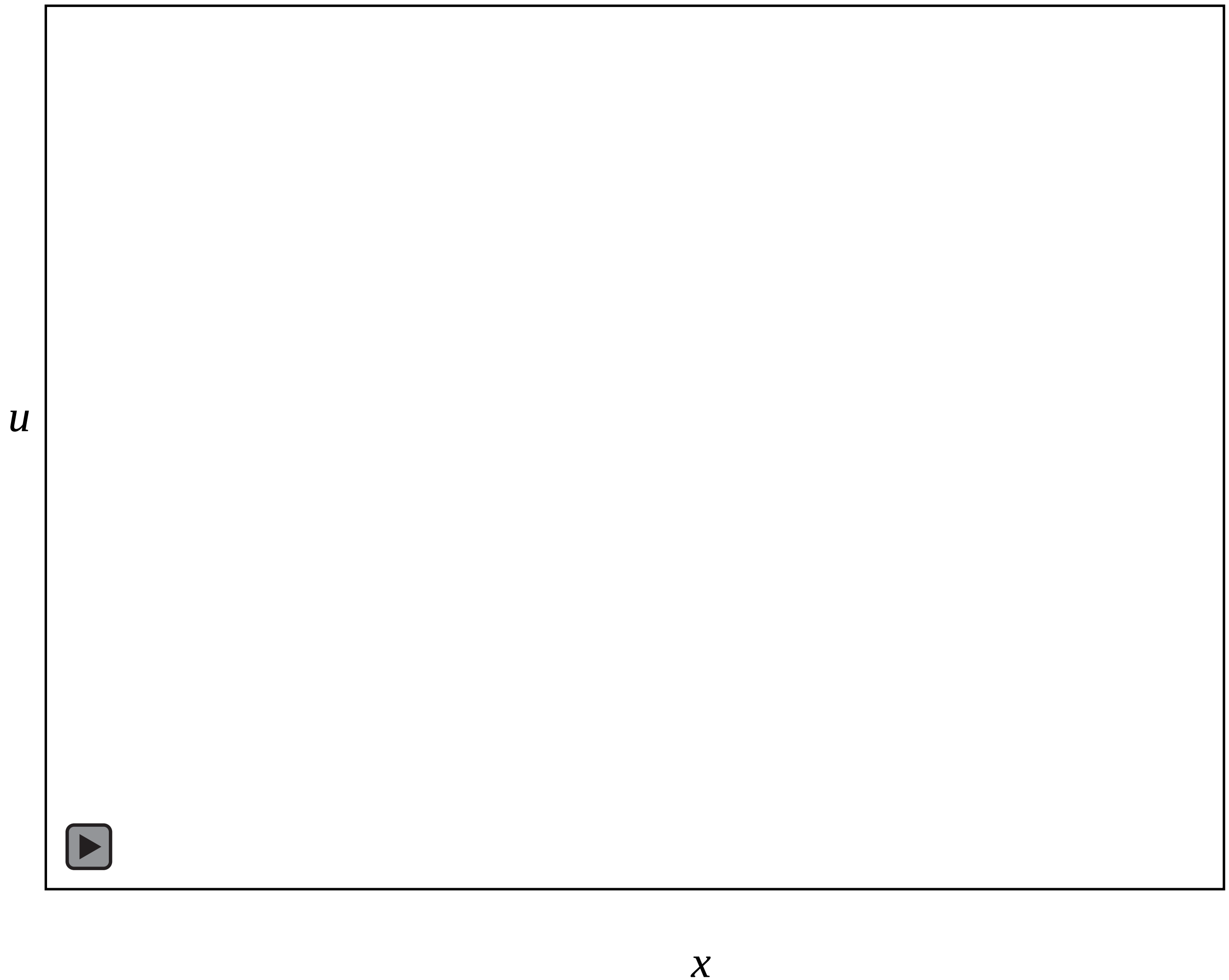
$$u(x,t)=\frac{1}{2\pi}\sum_{k=0}^{N}\tilde{u}(k,t)\cos\left(\frac{2\pi kx}{NL}\right)$$



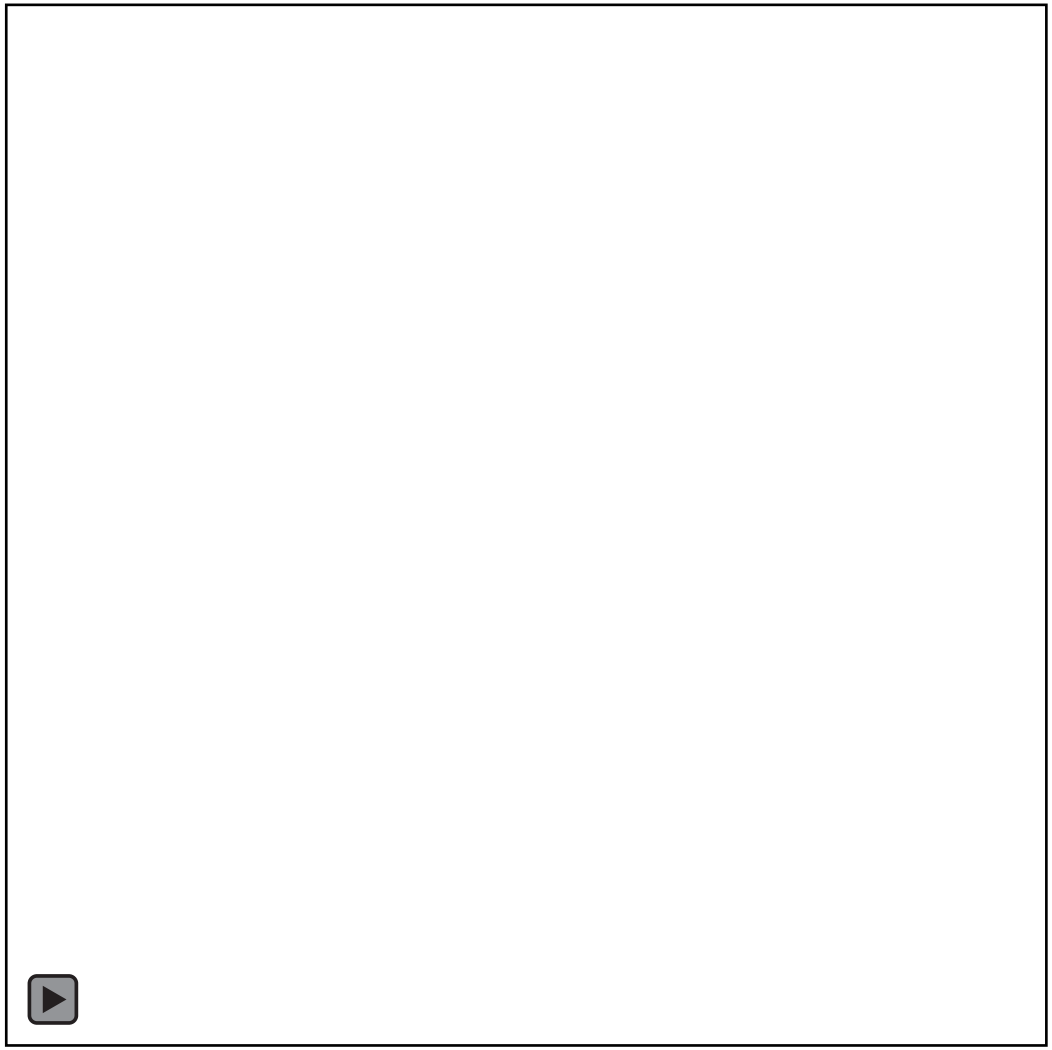
Log scaleでは



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

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

Green関数のGaussianの特徴的な幅Lは

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

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1 mm拡散で広がるには $t \sim 3\times10^{2}\,\mathrm{s} \sim 5\,\mathrm{minutes}$

1 cm拡散で広がるには $t \sim 3\times10^{4}\,\mathrm{s} \sim 8\,\mathrm{hours}$

1 m拡散で広がるには $t \sim 3\times10^{8}\,\mathrm{s} \sim 10\,\mathrm{years!!}$

1 μm拡散で広がるには $t \sim 3\times10^{-4}\,\mathrm{s} \sim 0.3\,\mathrm{ms}$