2009.11.10
物性物理学C

# 拡散方程式とLangevin方程式

# 拡散方程式

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

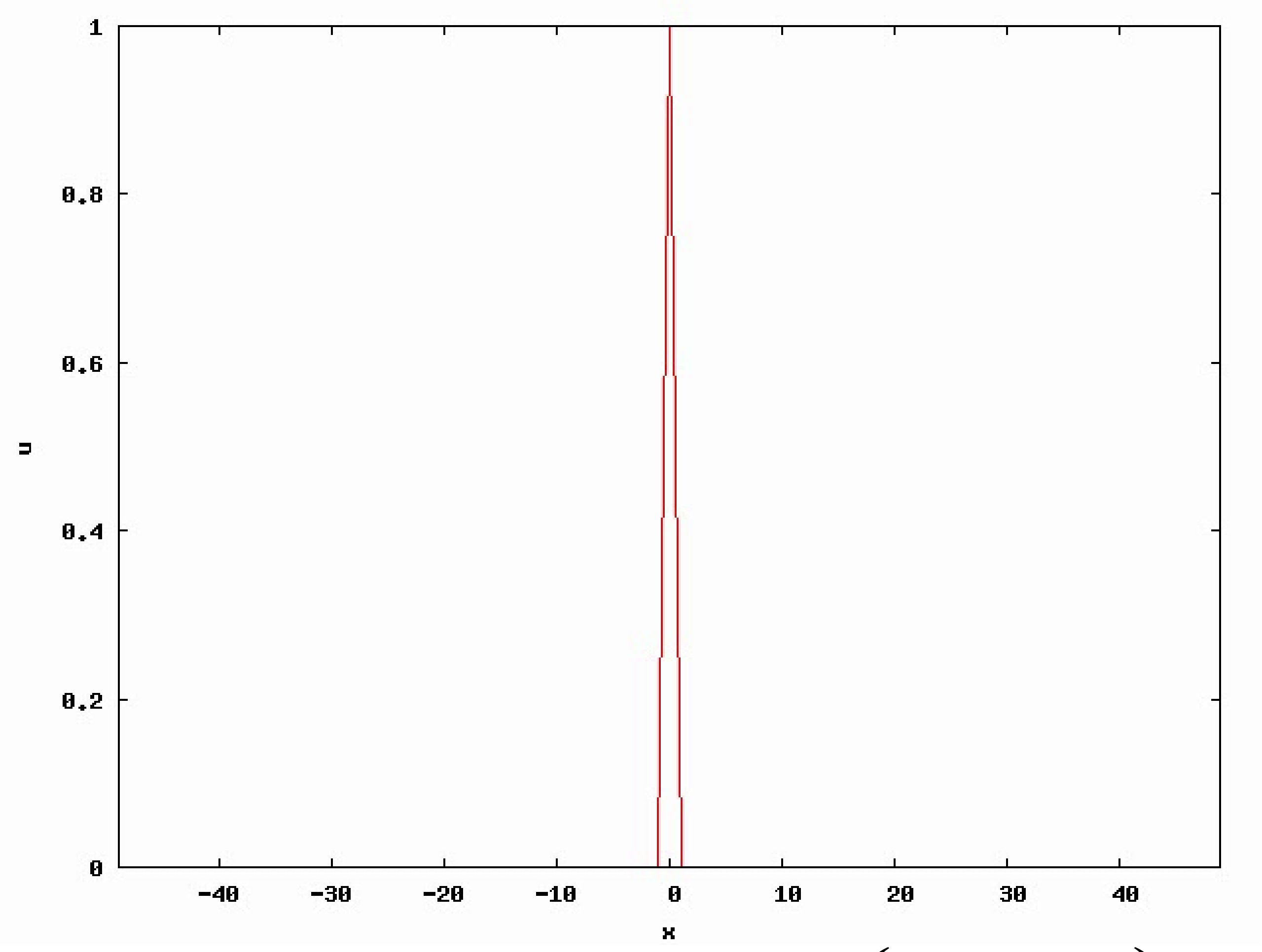
1次元の場合

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

初期値:

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

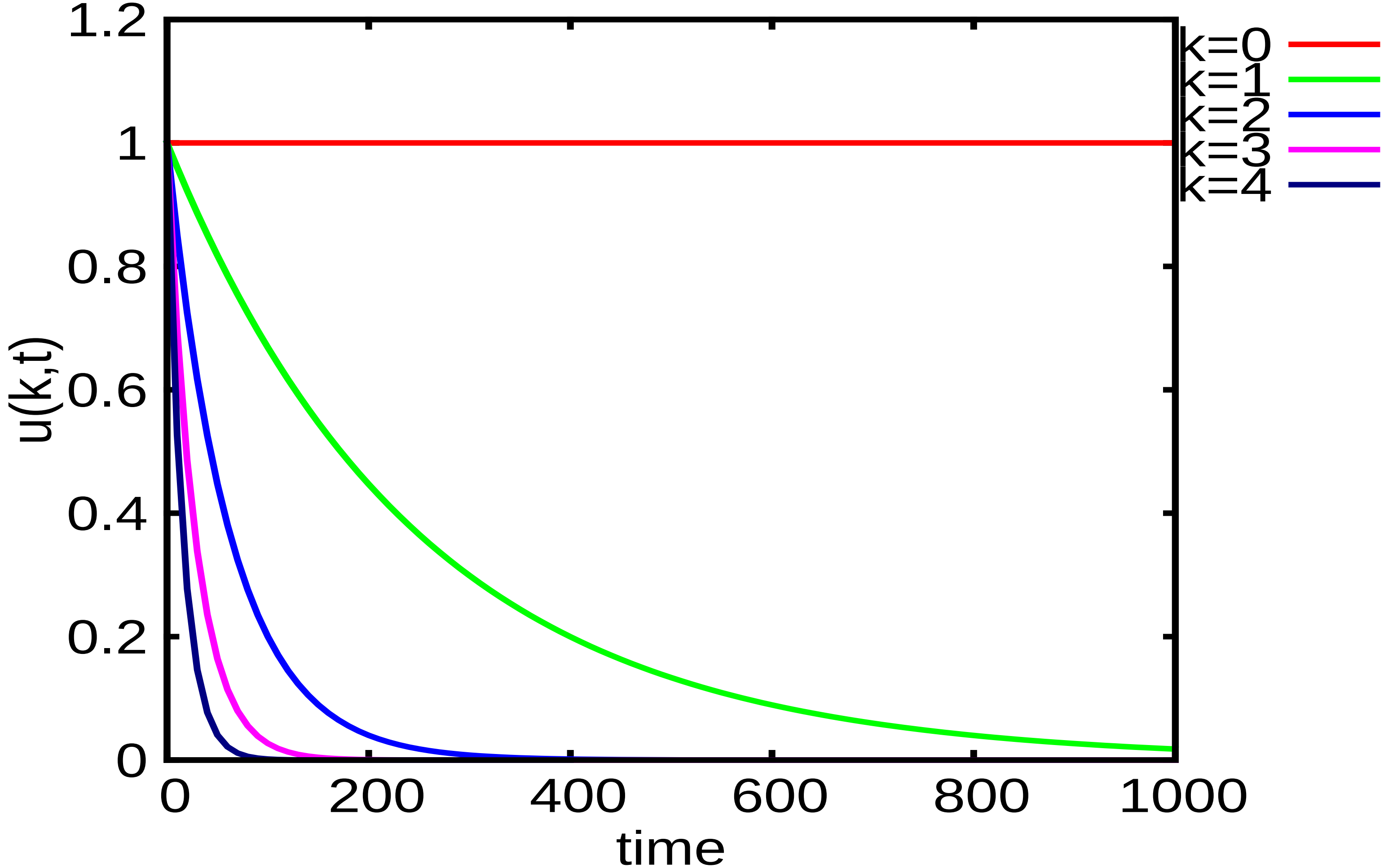
# 1次元で初期値がδ関数の解　：　Green関数



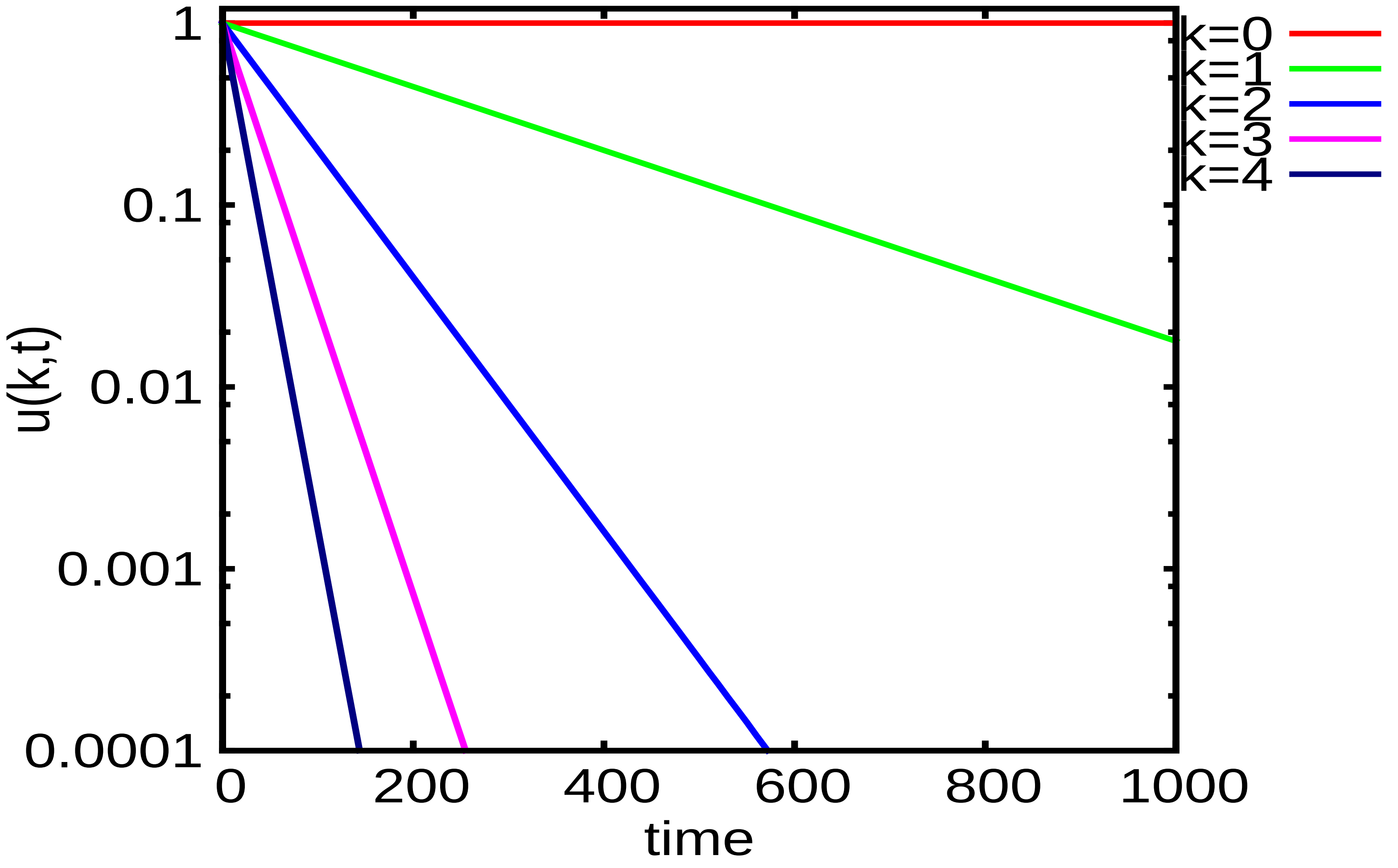

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left( -\frac{x^2}{4Dt} \right)$$

Fourier modeの時間変化

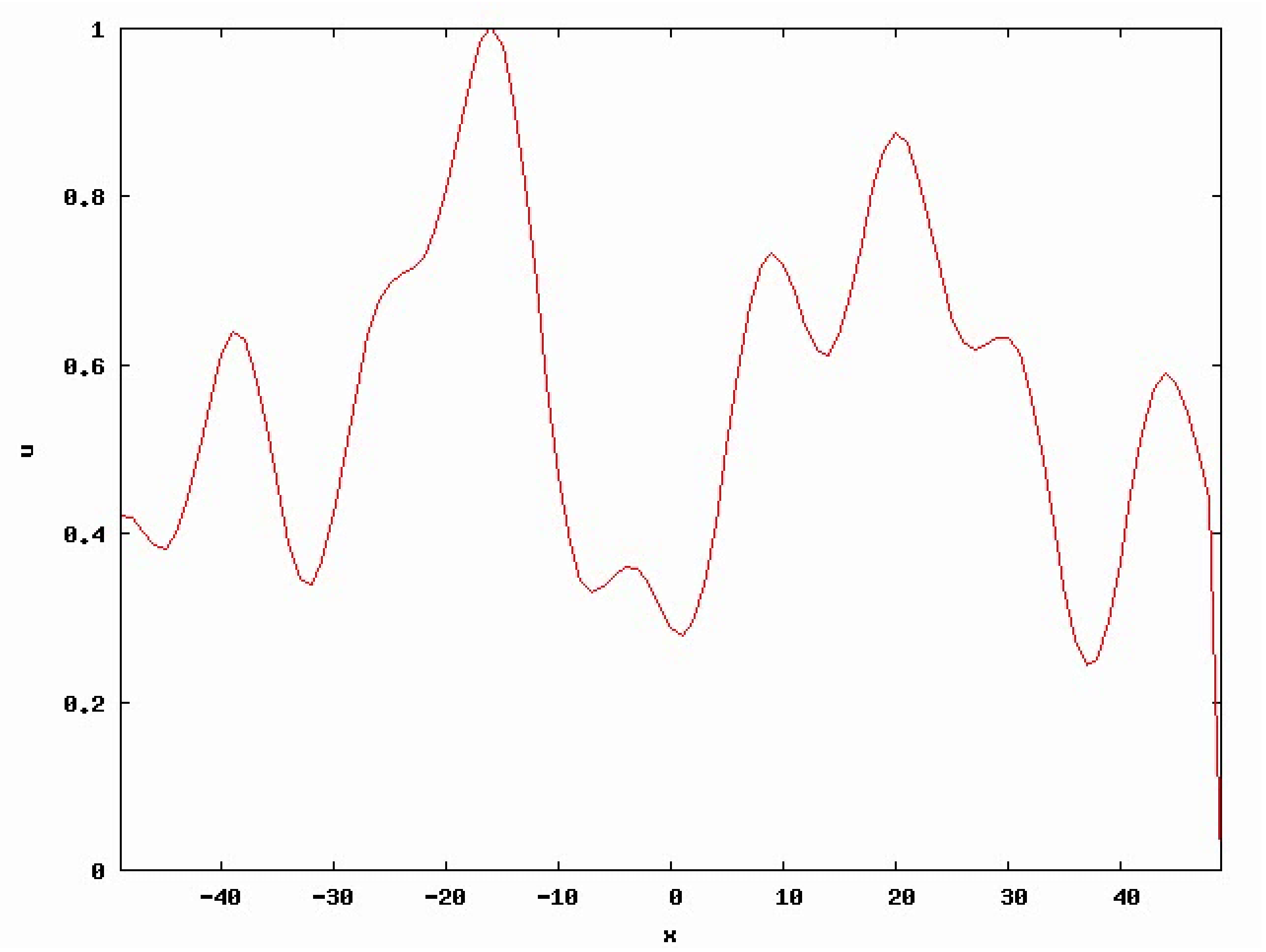
$$u(x,t)=\frac{1}{2\pi}\sum_{k=0}^{N}\tilde{u}(k,t)\cos\left(\frac{2\pi kx}{NL}\right)$$



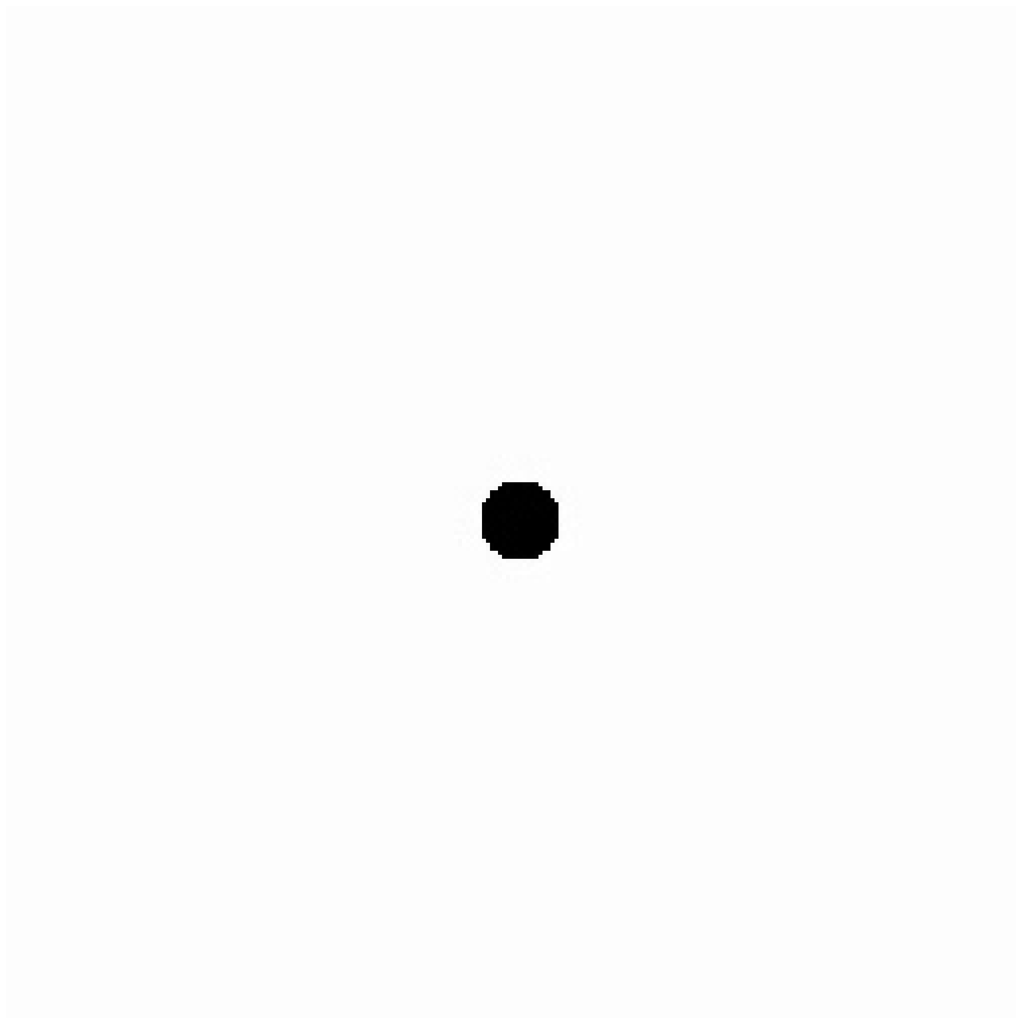
# Log scaleでは



# 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

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

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 $t \sim 3\times10^{2}\,\mathrm{s} \sim 5$ minutes

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

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

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

# 拡散過程

拡散の写真は

http://www.geocities.jp/kagakulabo/4.html

より

# ブラウン運動

ナノ粒子

ブラウン運動の動画は

http://spie.org/documents/newsroom/videos/1429/100+200c.wmv

より

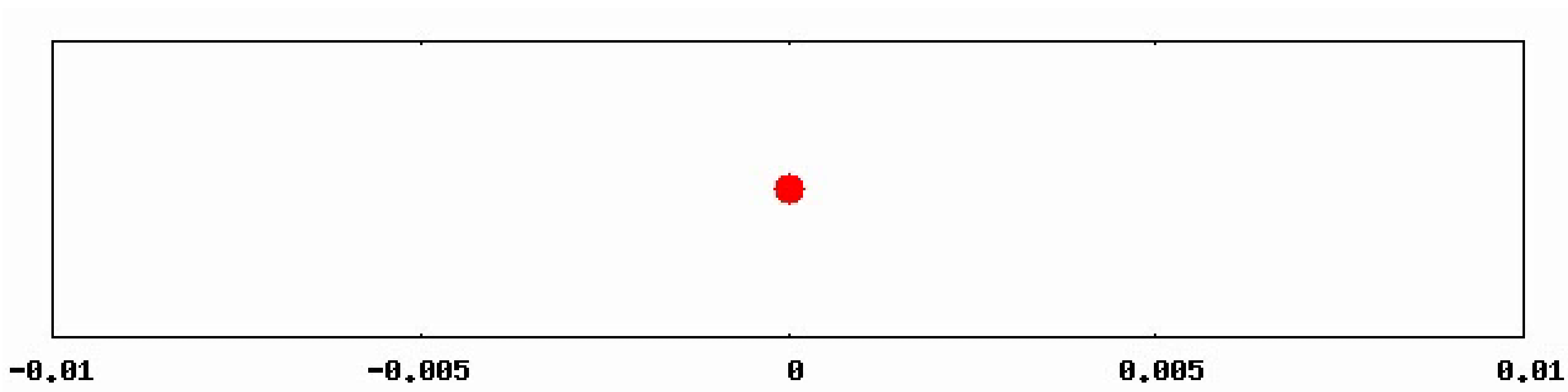
# Langevin方程式

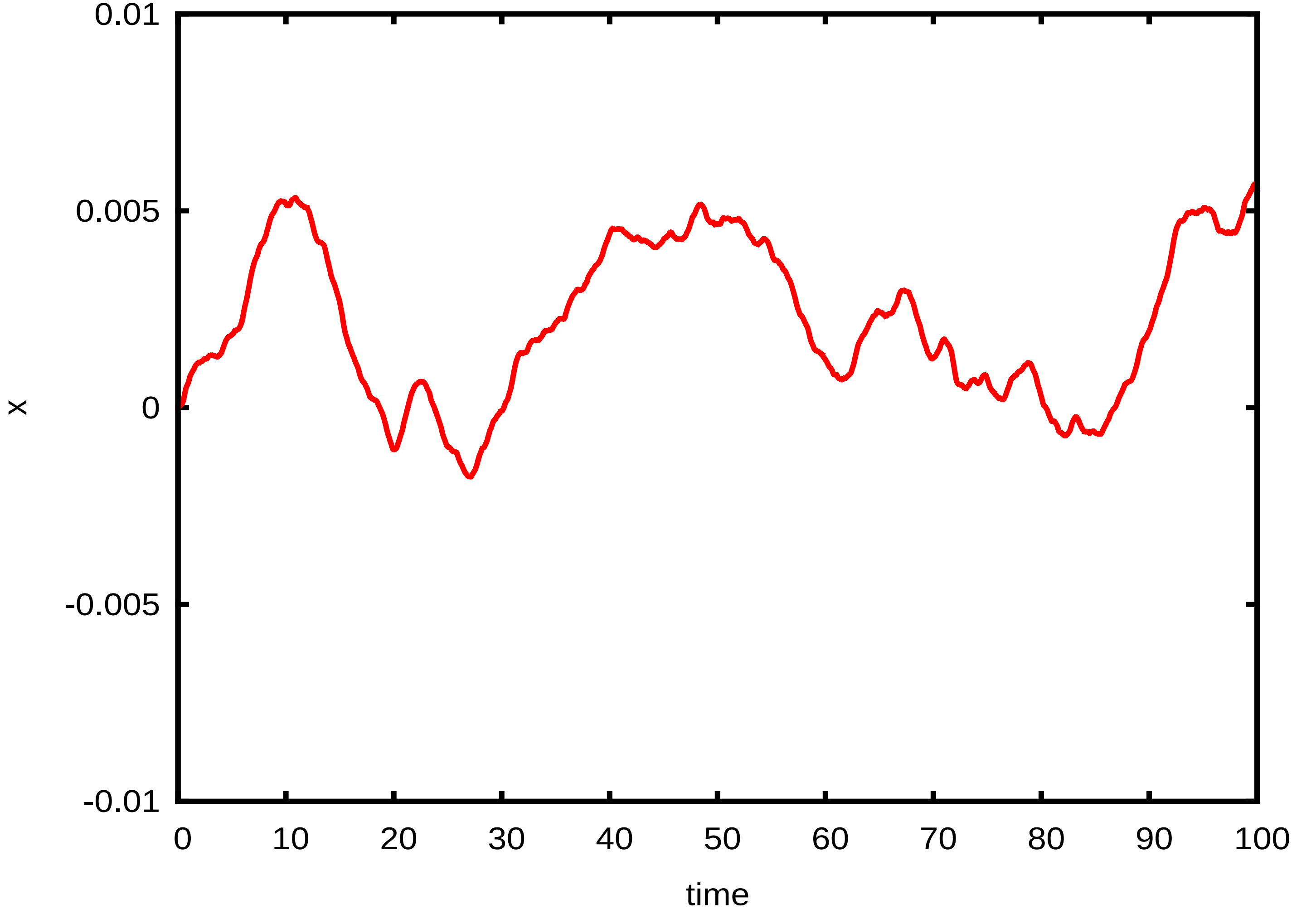
$$m\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = -k\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} + \boldsymbol{\xi}(t)$$

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

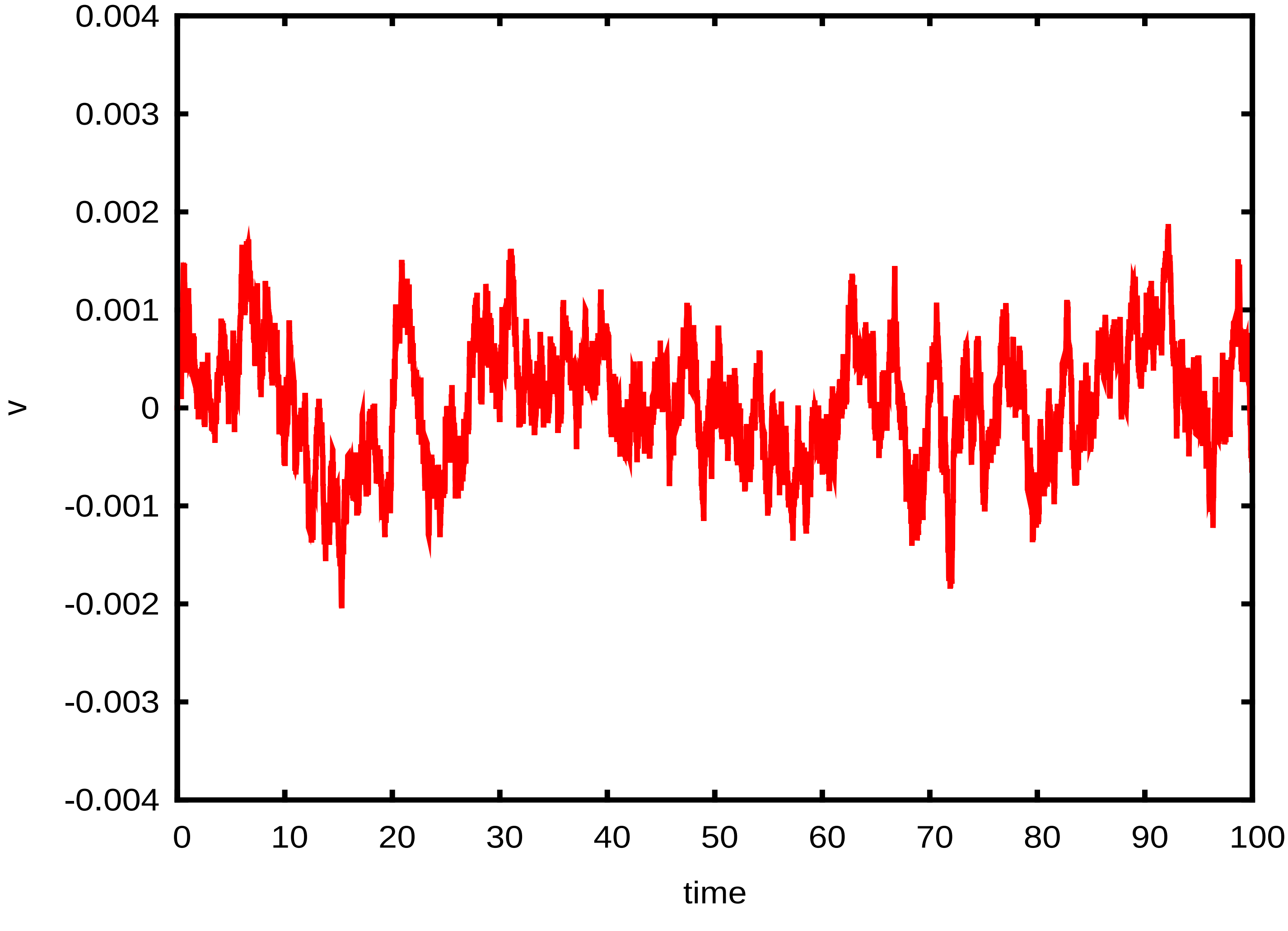
$$\langle \boldsymbol{\xi}(t)\cdot\boldsymbol{\xi}(s) \rangle = 2M\delta(t-s)$$

# 1次元系でのLangevin方程式による挙動

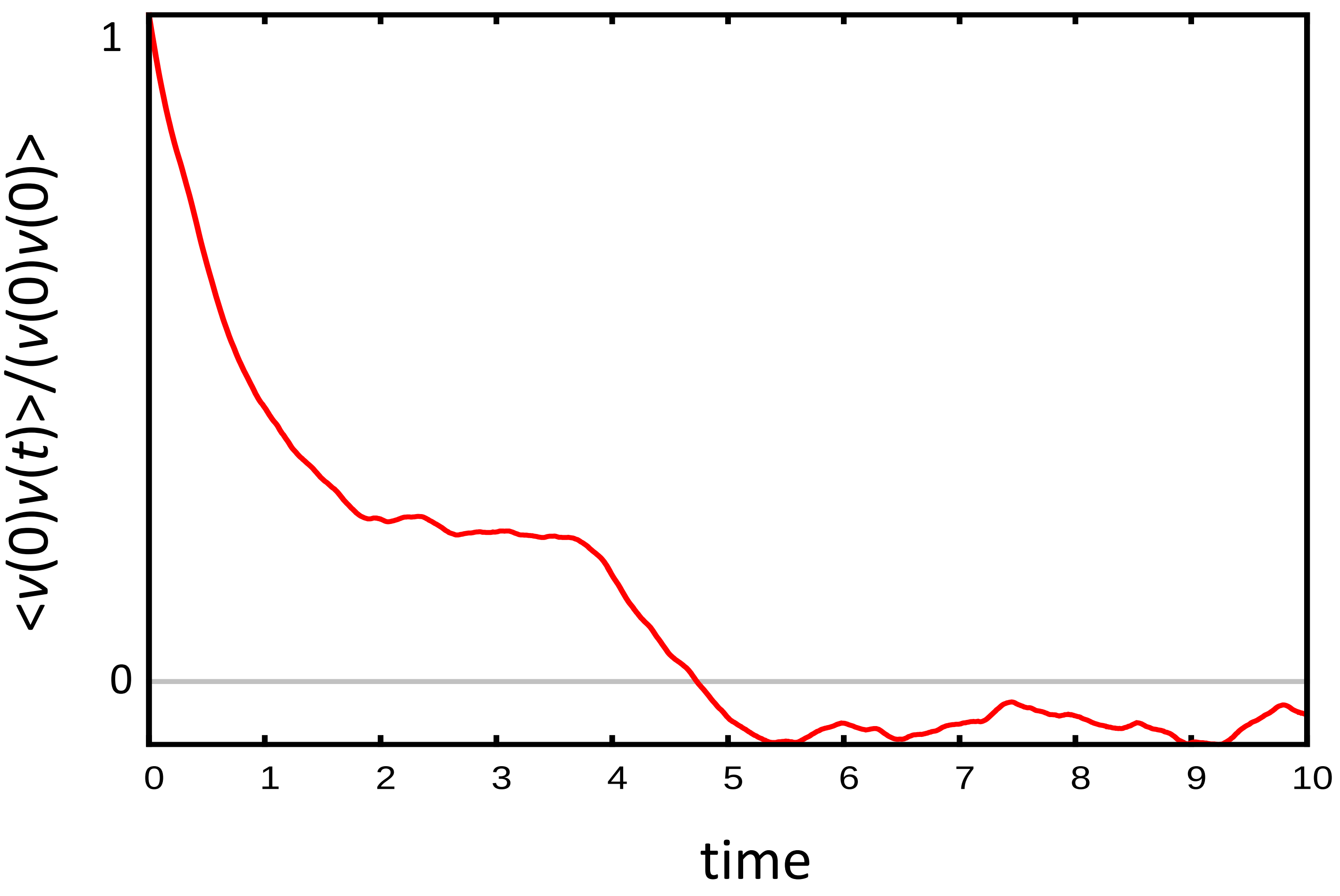




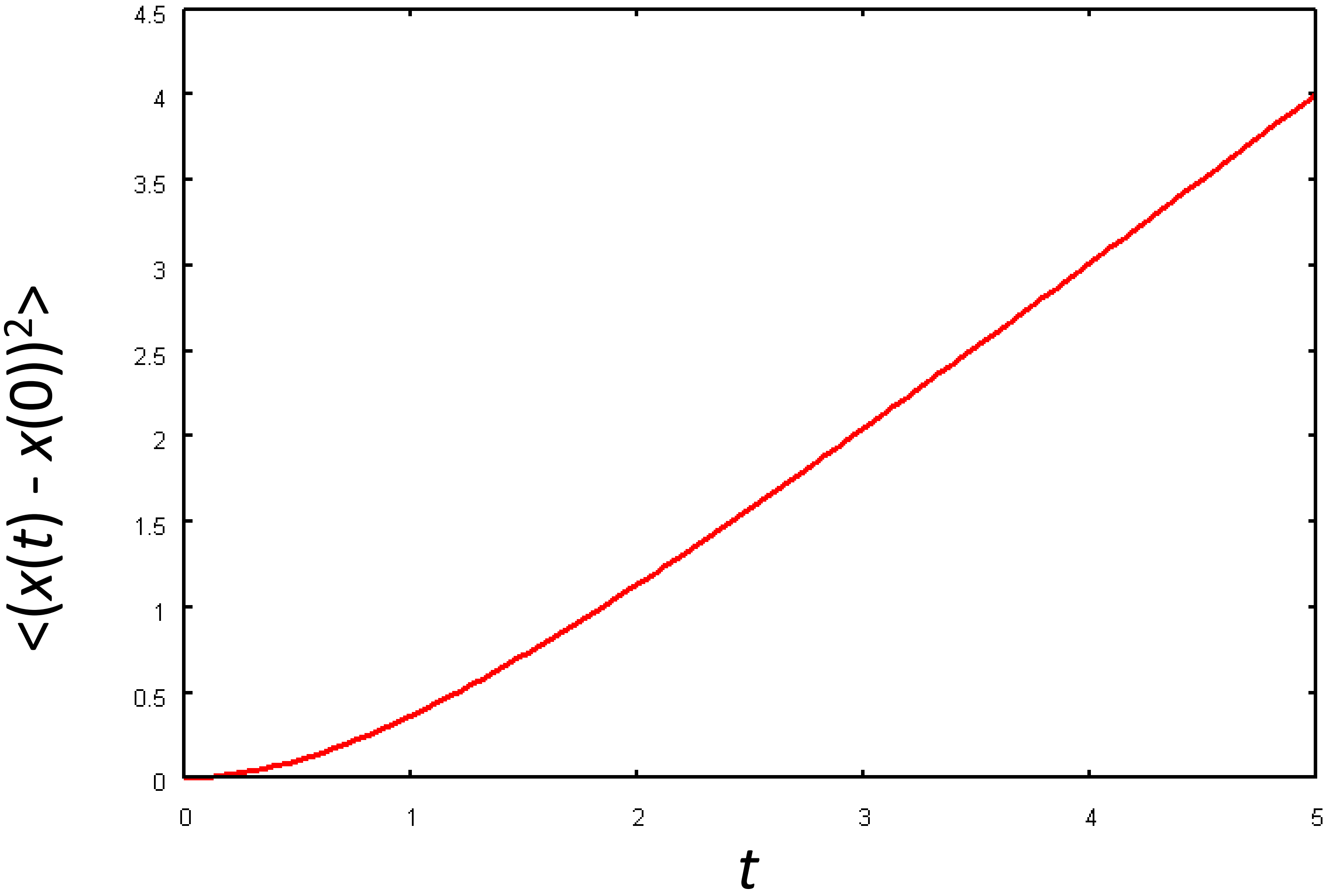
0.01
0.005
0
-0.005
-0.01
x
0
10
20
30
40
50
60
70
80
90
100
time



0.004
0.003
0.002
0.001
0
-0.001
-0.002
-0.003
-0.004
v
0
10
20
30
40
50
60
70
80
90
100
time

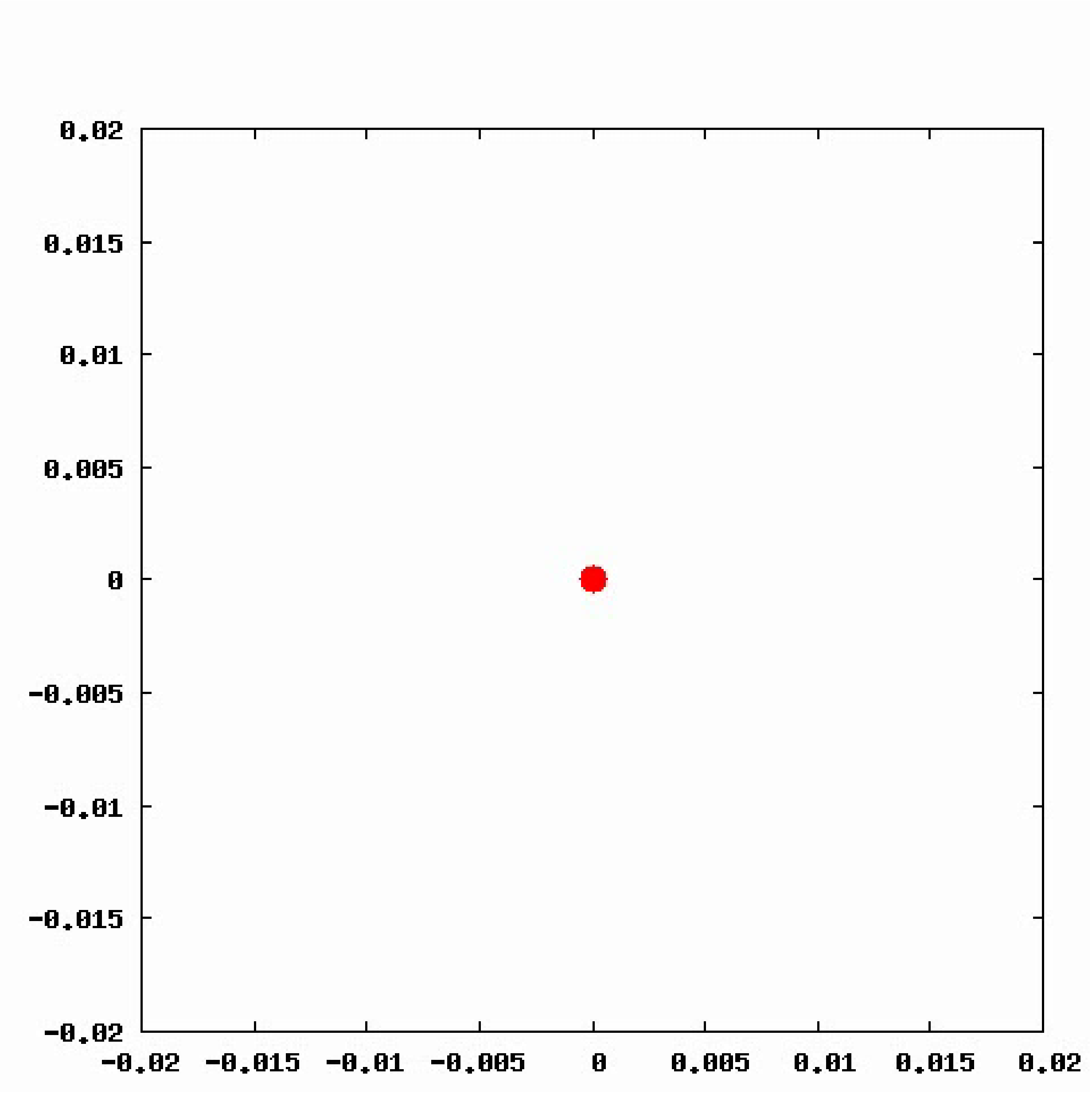



$\langle v(0)v(t)\rangle / (v(0)v(0)\rangle \propto \exp(-t/\tau)$

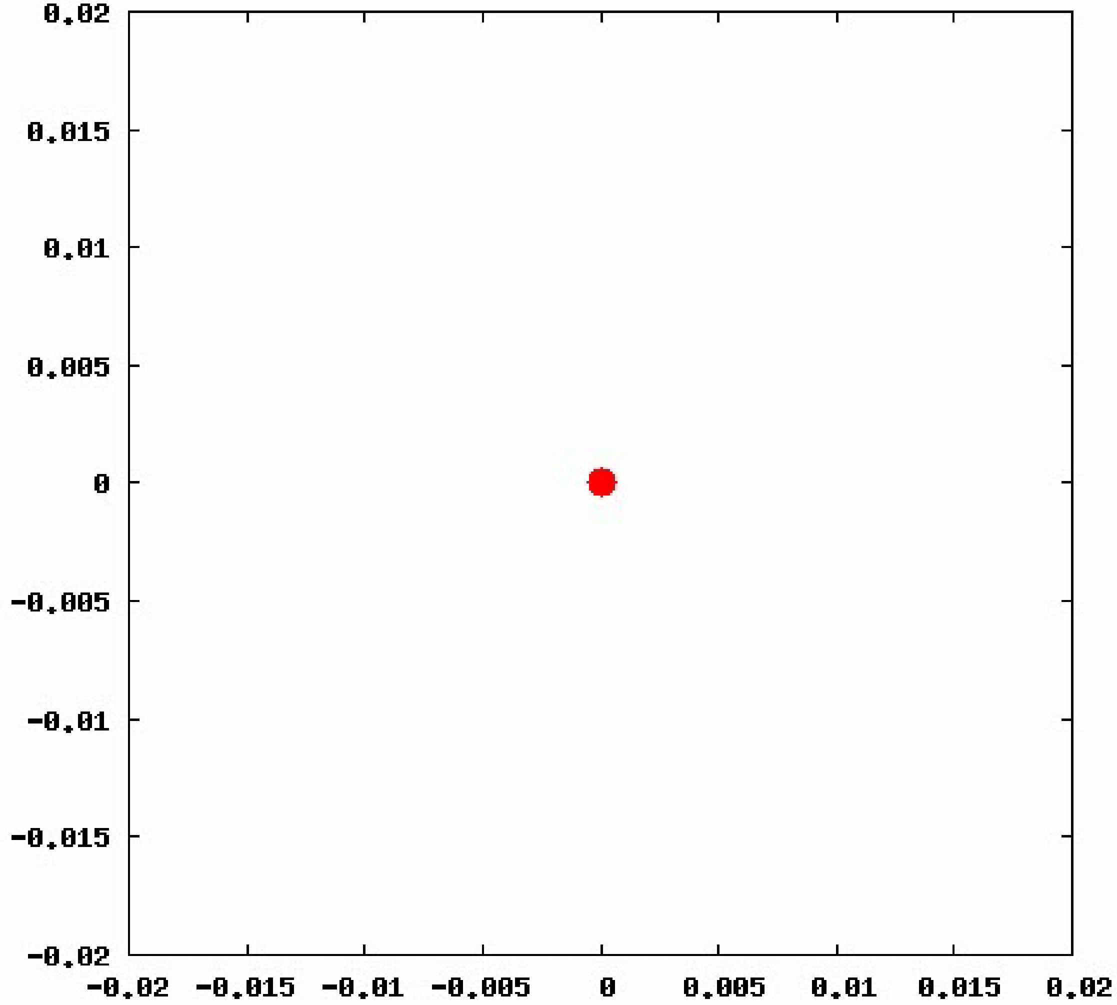



$$<(x(t) - x(0))^2> = (2Mt/\gamma)\ [t - (m/\gamma)\exp(-\gamma t/m)]$$

# 2次元での数値計算


0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.02
-0.015
-0.01
-0.005
0
0.005
0.01
0.015
0.02

# 軌跡を残すと


0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.02
-0.015
-0.01
-0.005
0
0.005
0.01
0.015
0.02