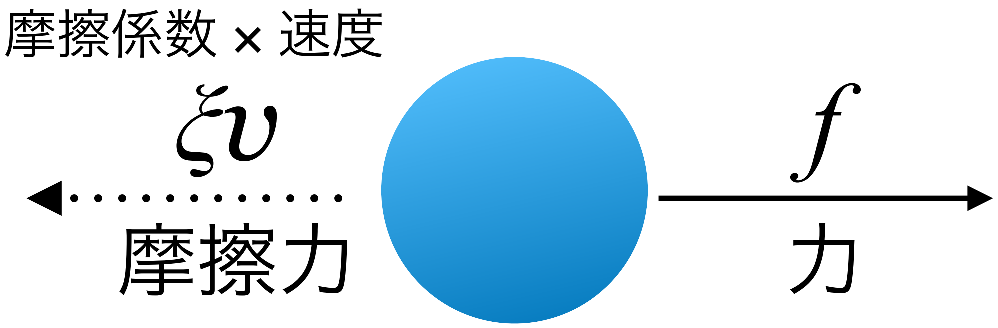



$$f - \xi v = m \frac{\mathrm{d}v}{\mathrm{d}t}$$

$$v = \frac{f}{\xi} \left[ 1 - \exp\left( -\frac{\xi t}{m} \right) \right]$$

$$t = \infty$$

$$f = \xi v_{\infty}$$

流速

$$J \equiv vc, \quad J = \frac{fc}{\xi}$$

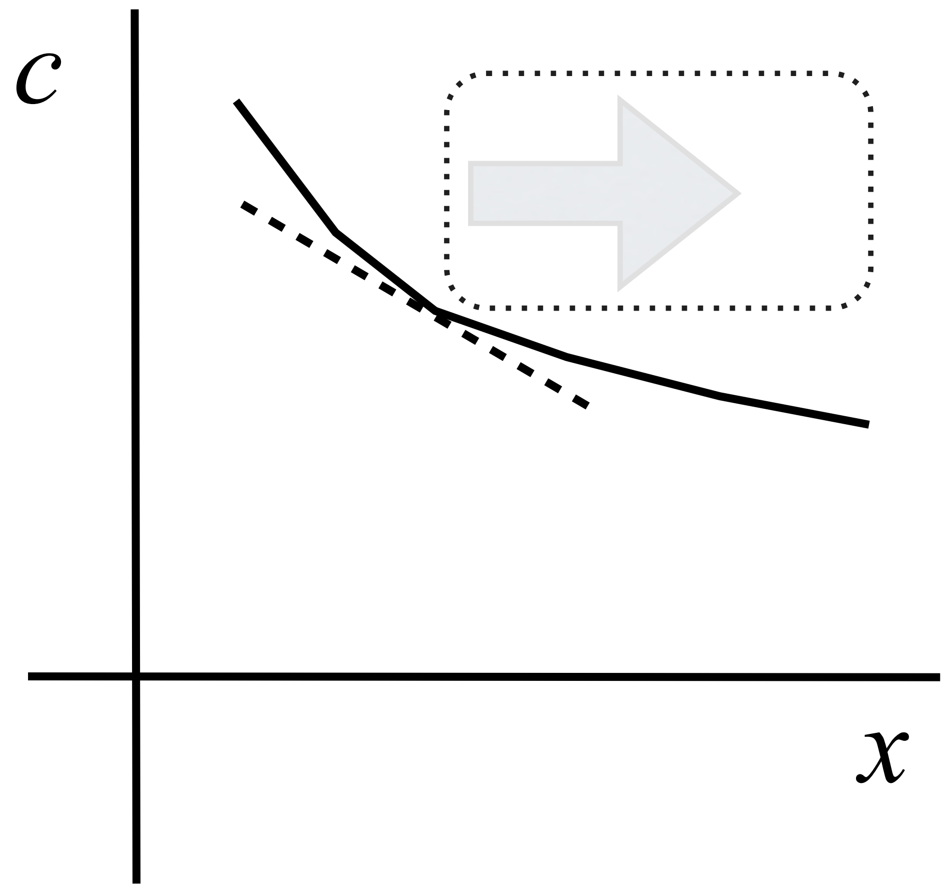
$$F = -\frac{\mathrm{d}\mu}{\mathrm{d}x} = -RT\frac{\mathrm{d}\ln c}{\mathrm{d}x} = -\frac{RT}{c}\frac{\mathrm{d}c}{\mathrm{d}x}$$

$$f \equiv \frac{F}{N_{\mathrm{A}}}$$

$$J = \frac{fc}{\xi} = -\frac{RT}{N_{\mathrm{A}}\xi}\frac{\mathrm{d}c}{\mathrm{d}x} = -D\frac{\mathrm{d}c}{\mathrm{d}x}$$

拡散係数 ($D$)

# 拡散




$$J(x,t) = -D\frac{\partial c(x,t)}{\partial x}$$

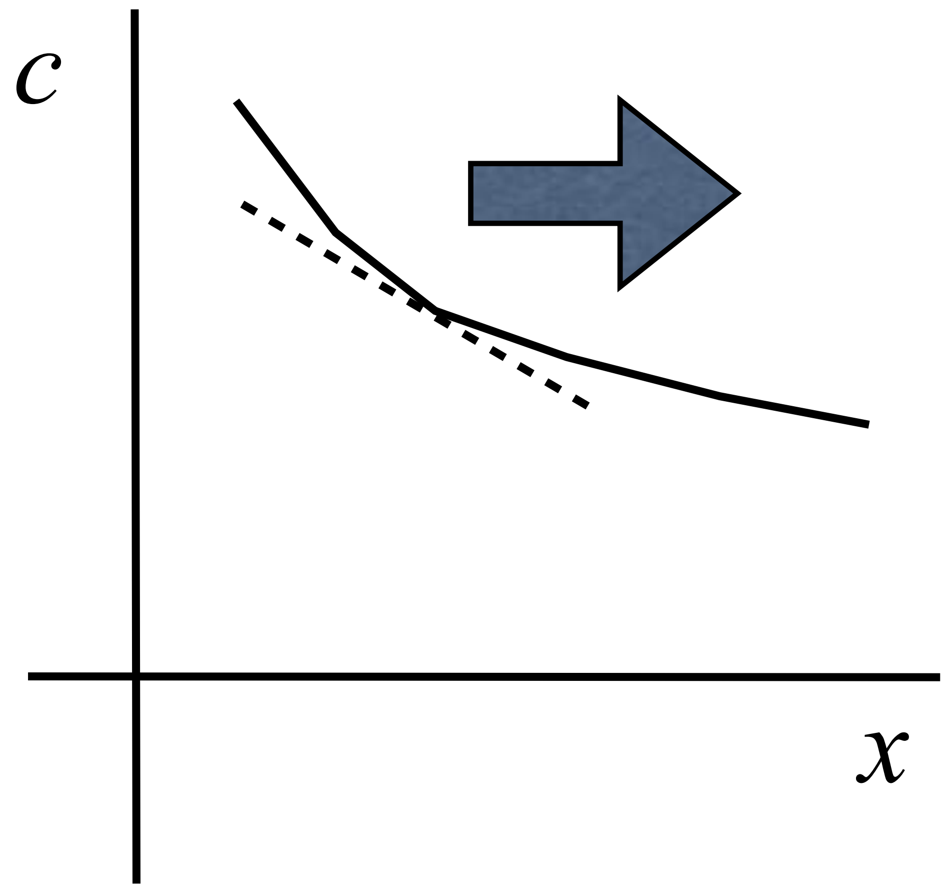
Fickの第一法則

$J$ : 流速(flux) [mol m$^{-2}$ s$^{-1}$]

$D$ : 拡散定数(diffusion constant) [mol m$^{-2}$ s$^{-1}$ mol$^{-1}$ m$^{3}$ m]

= [ m$^{2}$ s$^{-1}$]

# 拡散

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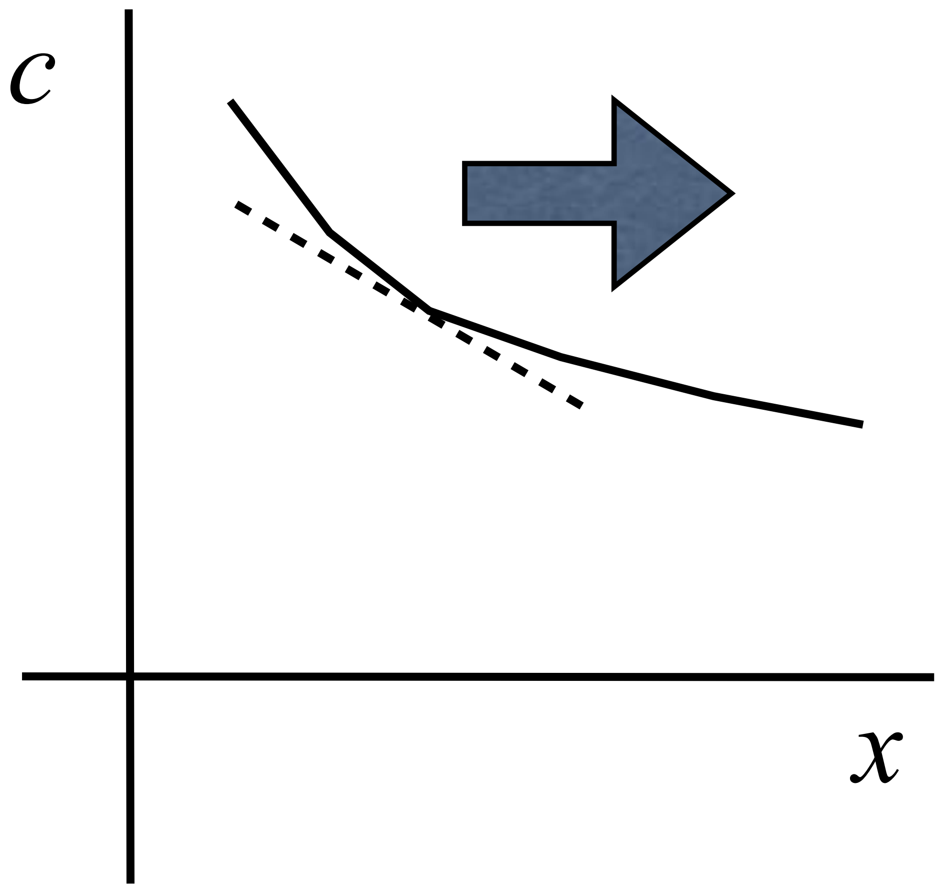


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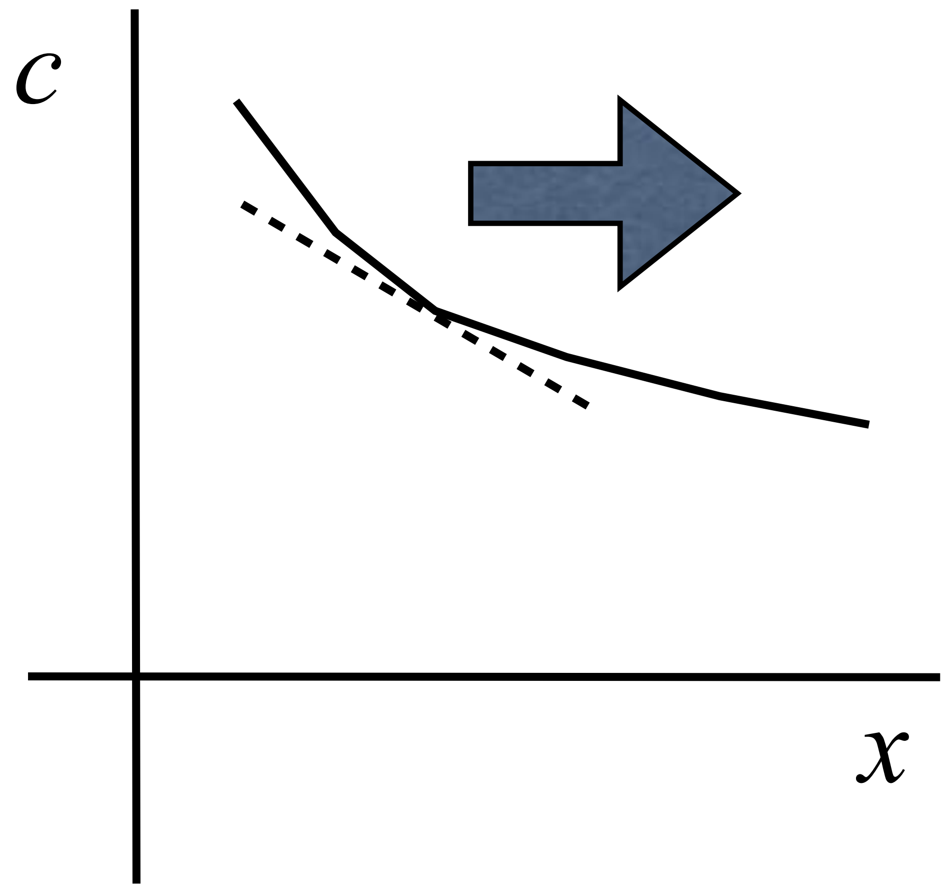
= [ $m^2$ $s^{-1}$]

# 拡散

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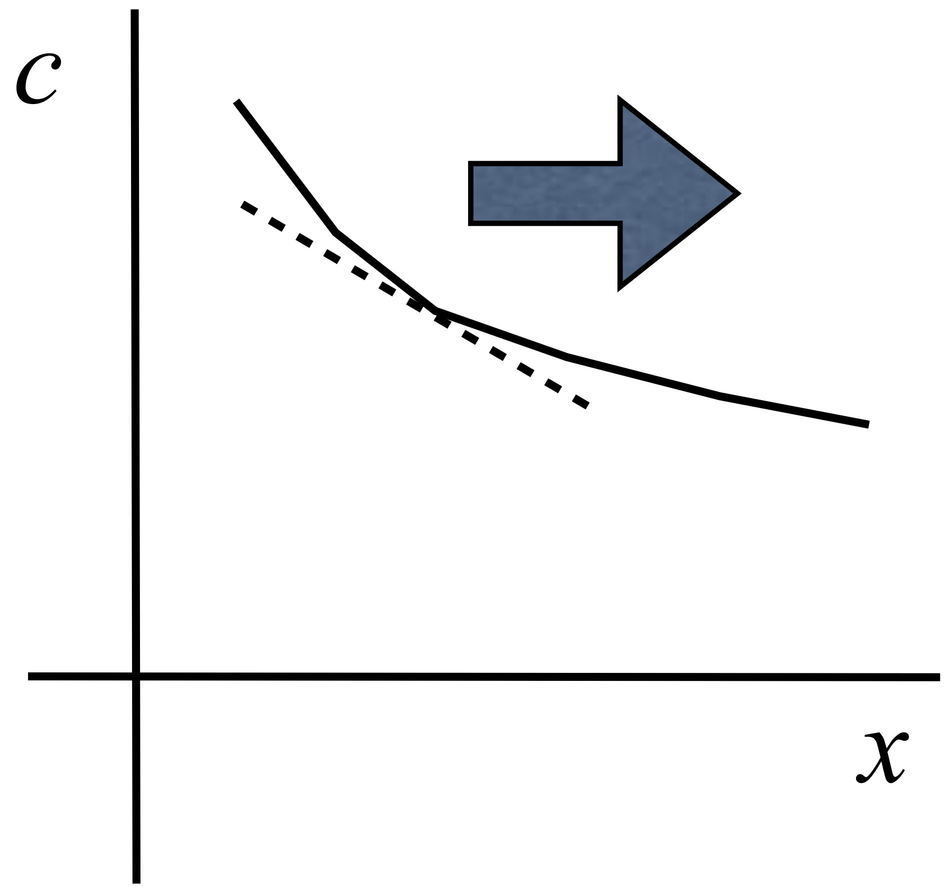
= [ m$^{2}$ s$^{-1}$]

# 拡散

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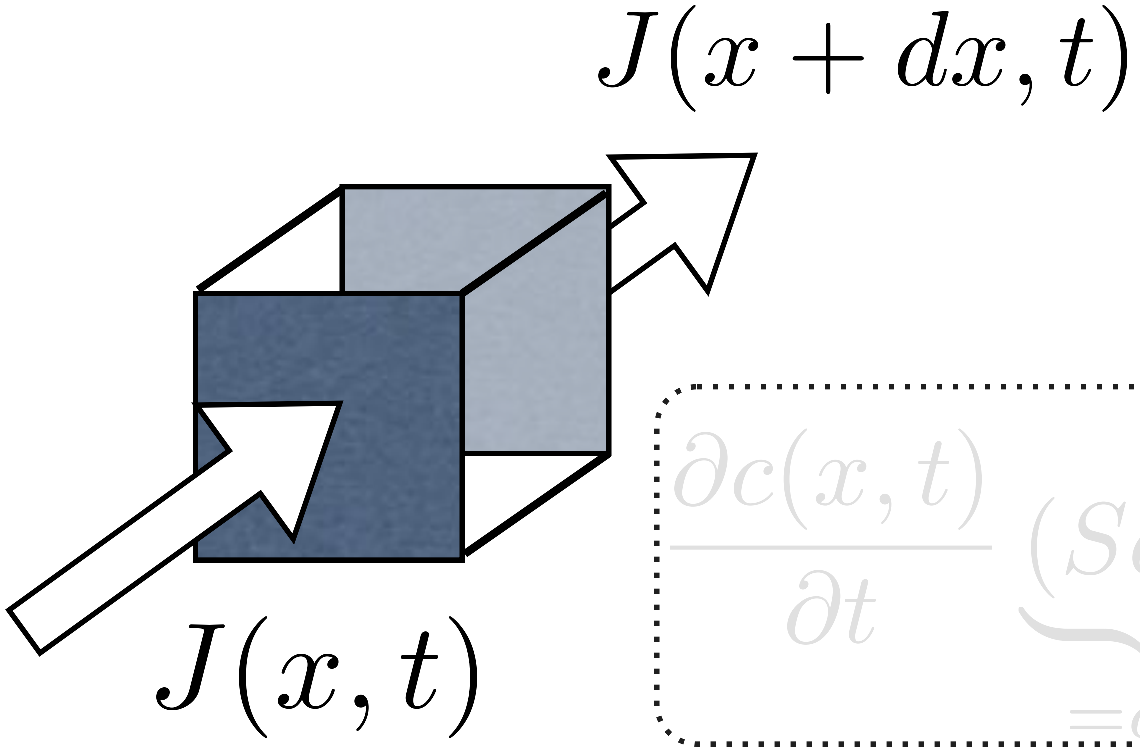


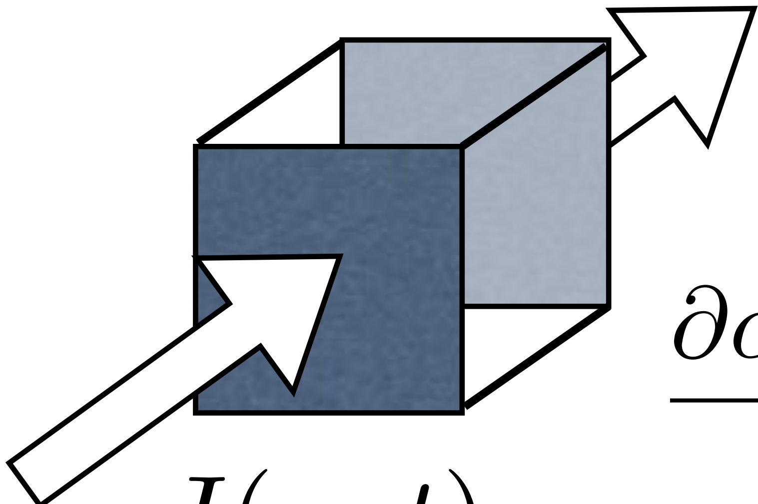

$$\frac{\partial c(x,t)}{\partial t}\underbrace{(S dx)}_{=dV} = [\underbrace{J(x,t)}_{\text{flux in}} - \underbrace{J(x+dx,t)}_{\text{flux out}}]S$$

$$J(x+dx,t) = J(x,t) + \frac{\partial J}{\partial x}dx$$

$$J(x,t) = -D\frac{\partial c(x,t)}{\partial x}$$

$$\frac{\partial c(x,t)}{\partial t} = \frac{1}{dx}\left(-\frac{\partial J}{\partial x}\right)dx = D\frac{\partial^2 c}{\partial x^2}$$

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2}$$

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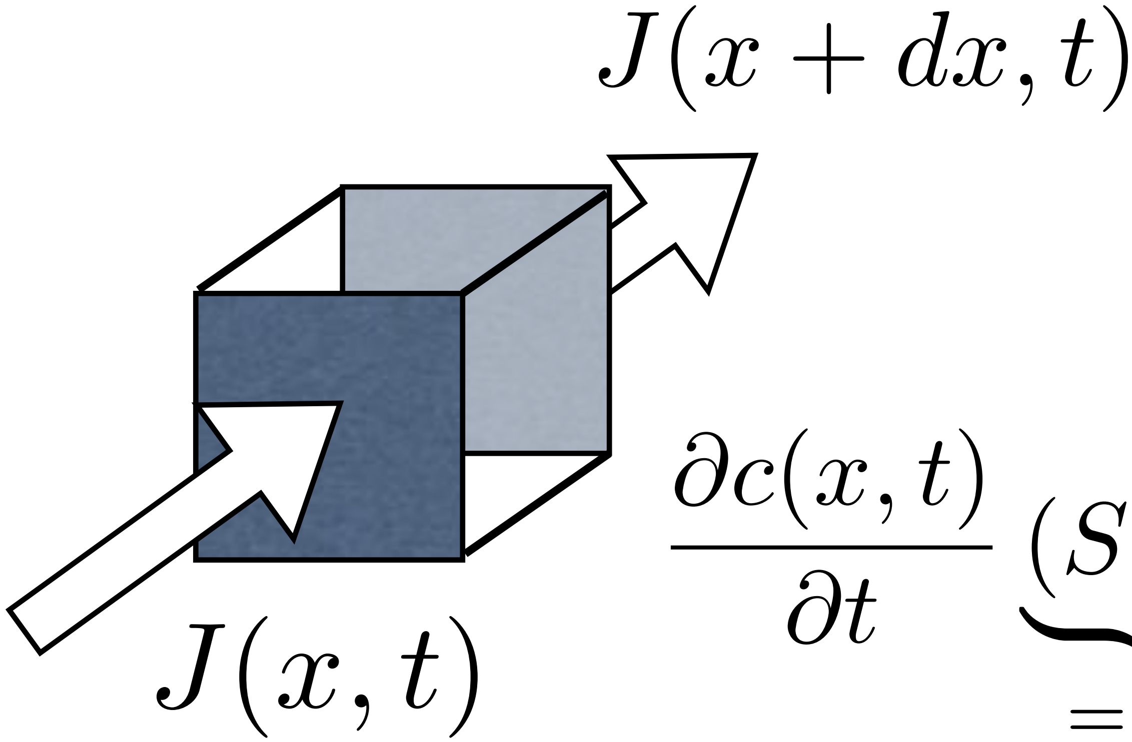


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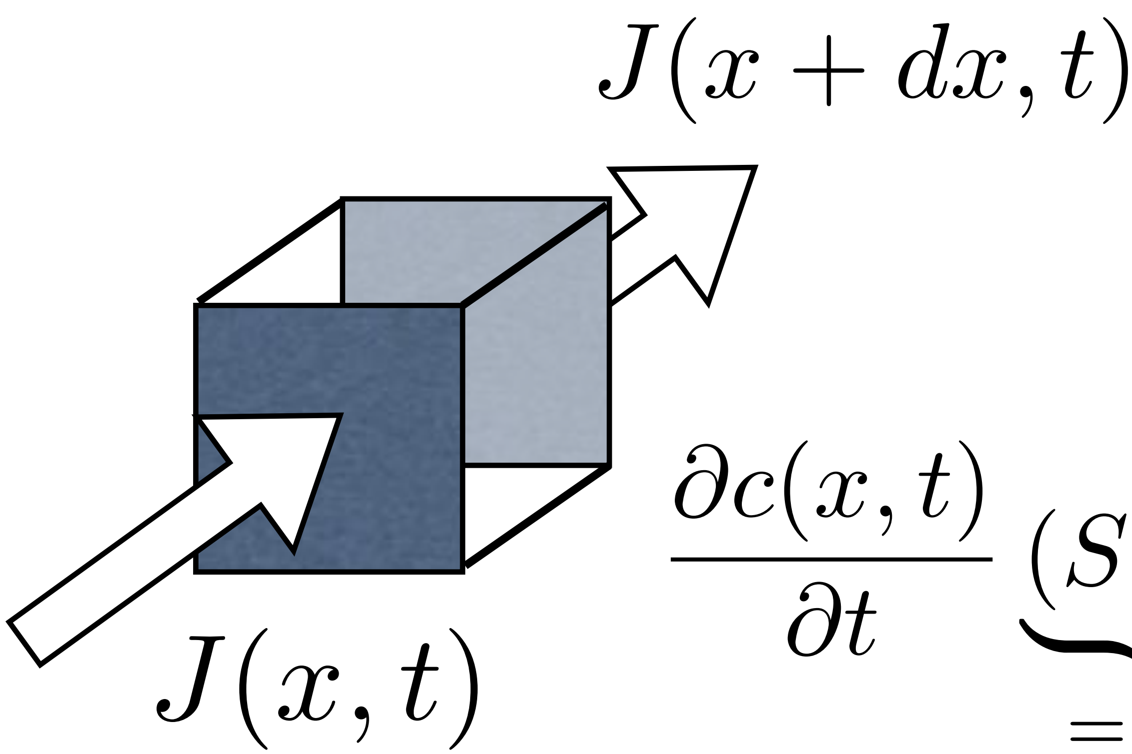


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$$\boxed{\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2}}$$

# 拡散方程式のFTによる解法

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2}$$

$$\mathcal{F}[c(x,t)] \equiv c(k,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} c(x,t)e^{-ikx}dx$$

$$\mathcal{F}[\frac{\partial c(x,t)}{\partial t}] = D\mathcal{F}[\frac{\partial^2 c(x,t)}{\partial x^2}]$$

$$\frac{\partial c(k,t)}{\partial t} = -Dk^2 c(k,t)$$

$$c(k,t) = c(k,0)\exp(-Dk^2 t)$$

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2}$$

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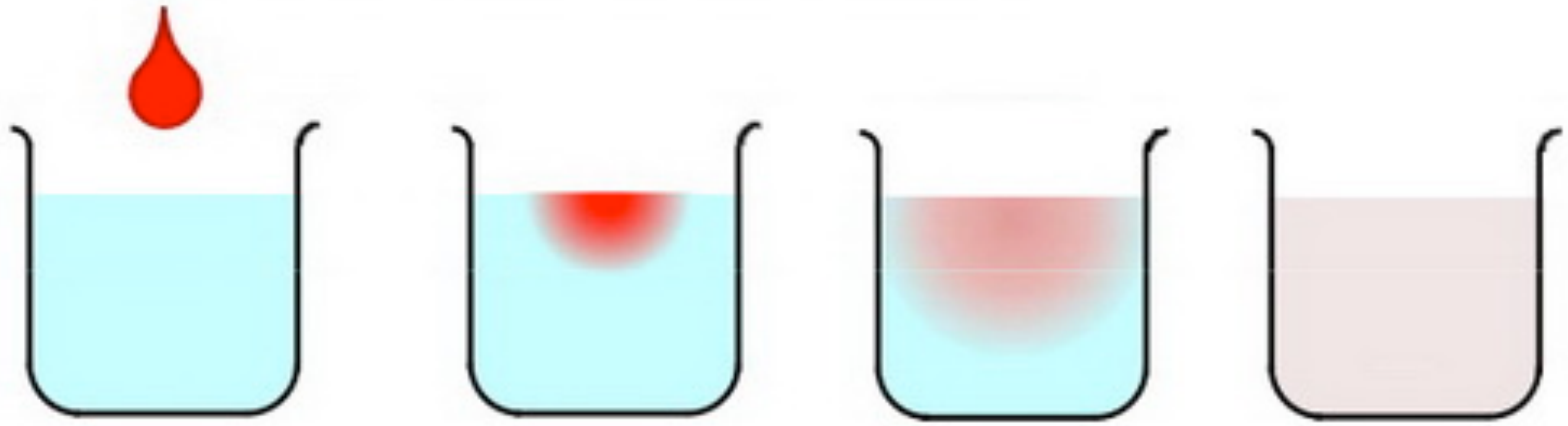
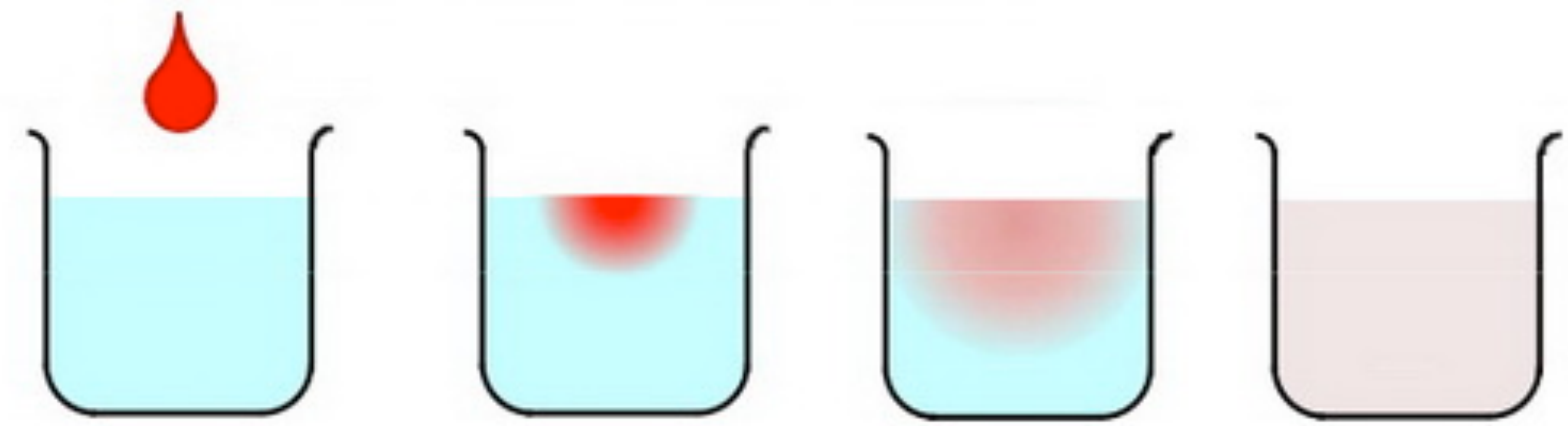


$$c(k,0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} c(x,0)e^{-ikx}dx$$

$$c(x,0) = c_0\delta(x)$$

$$c(k,0) = \frac{c_0}{2\pi}\int_{-\infty}^{\infty} \delta(x)e^{-ikx}dx = \frac{c_0}{2\pi}e^{-ik0} = \frac{c_0}{2\pi}$$

$$c(k,t) = \frac{c_0}{2\pi}\exp(-Dk^2t)$$



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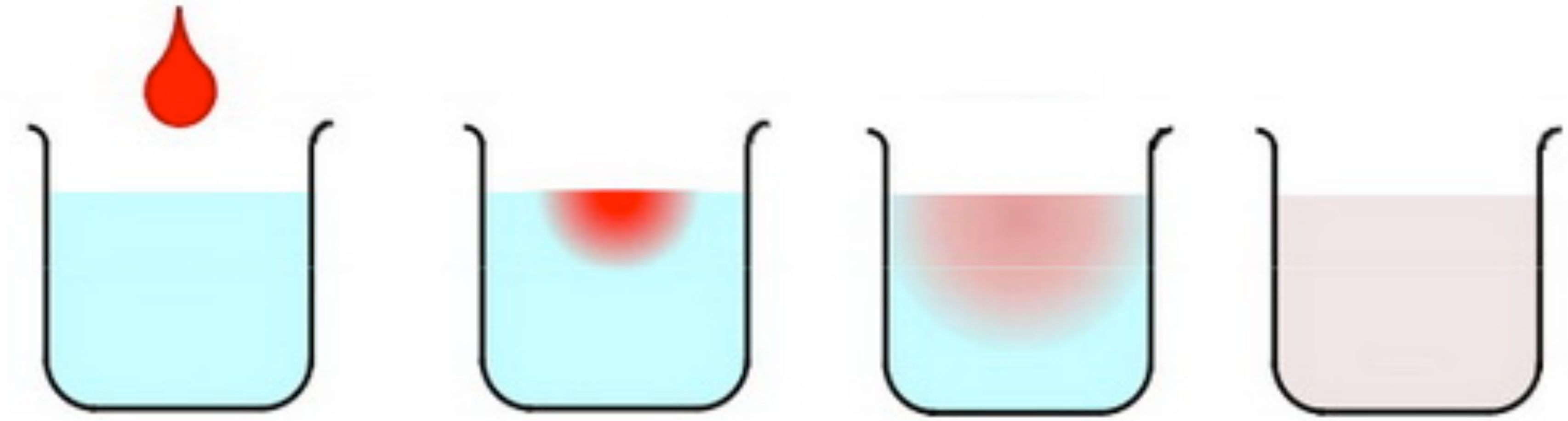

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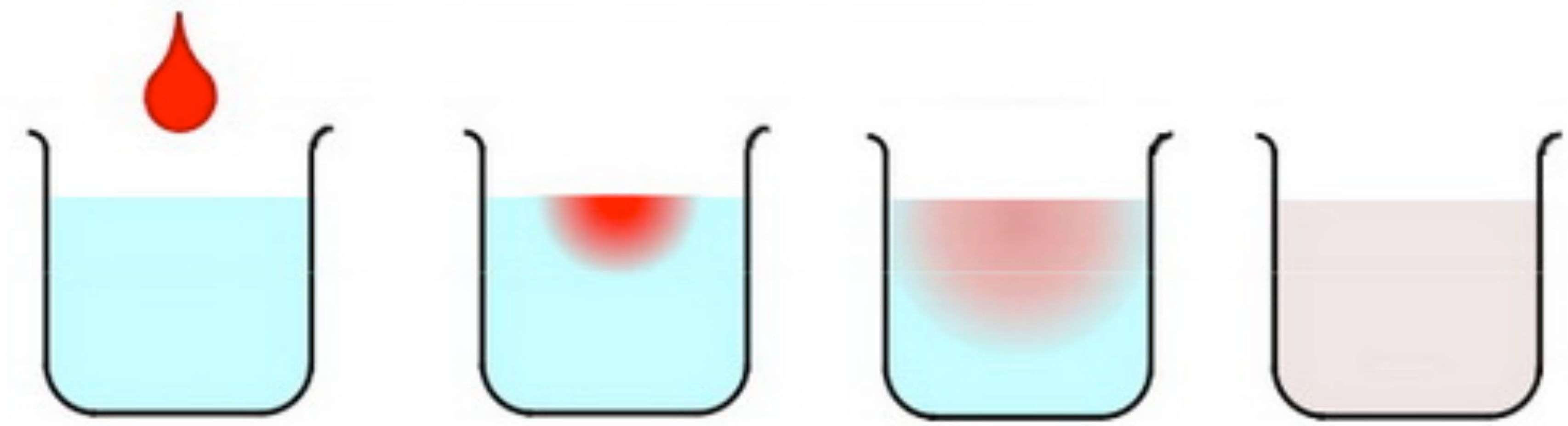

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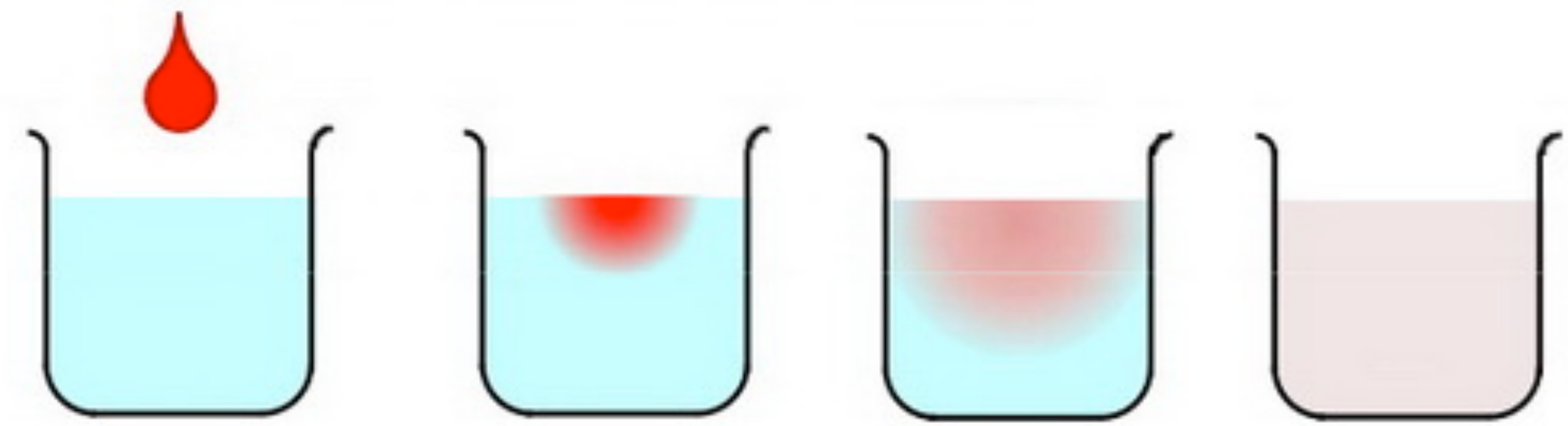

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$$c(k,0) = \frac{c_0}{2\pi}\int_{-\infty}^{\infty} \delta(x)e^{-ikx}dx = \frac{c_0}{2\pi}e^{-ik0} = \frac{c_0}{2\pi}$$

$$c(k,t) = \frac{c_0}{2\pi}\exp(-Dk^2t)$$

$$c(x,t) = \mathcal{F}^{-1}[c(k,t)]$$

$$= \frac{c_0}{2\pi}\mathcal{F}^{-1}[\exp(-Dtk^2)]$$

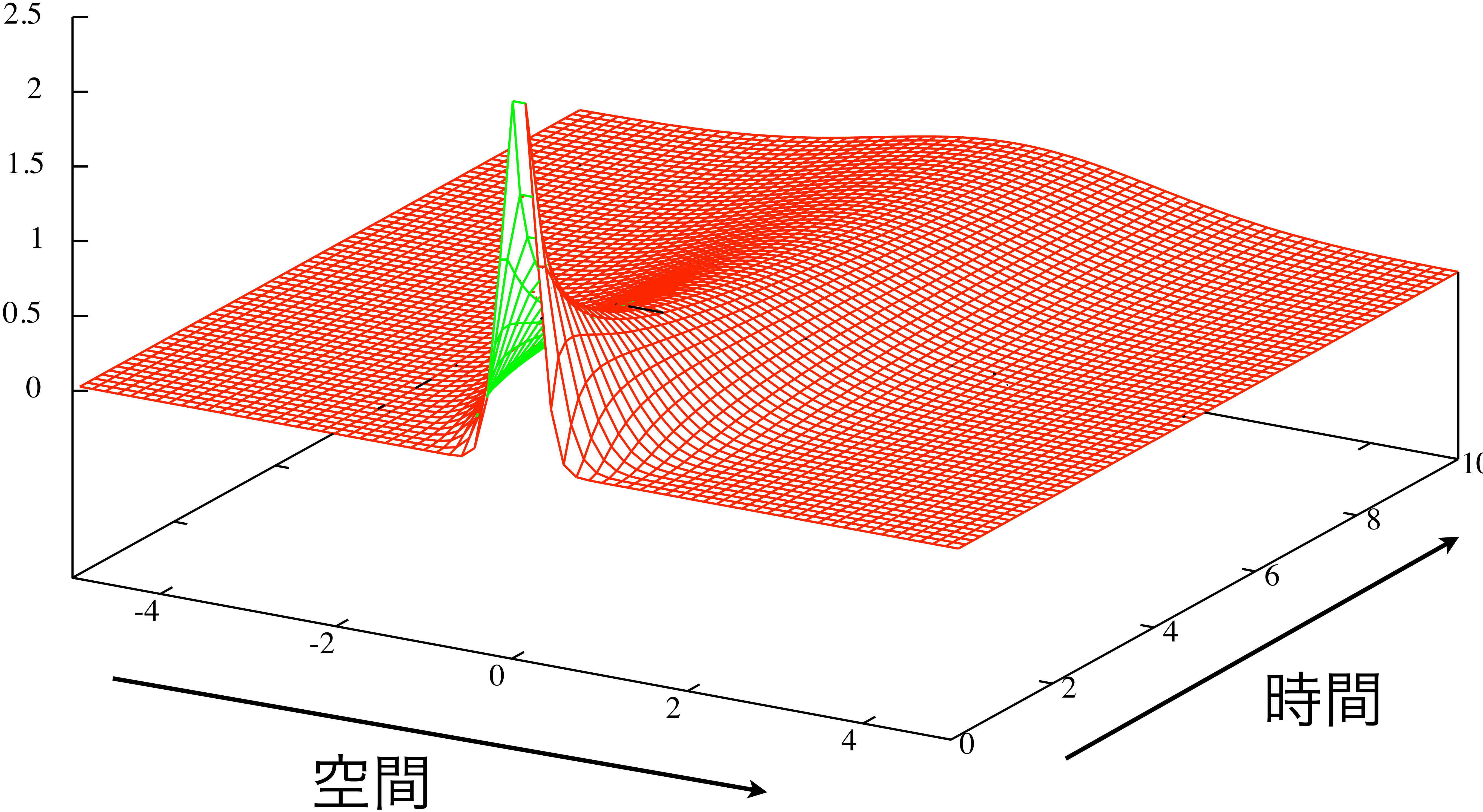
$$= \frac{c_0}{2\pi}\int_{-\infty}^{\infty} \exp(-Dtk^2)e^{ikx}dk$$

$$= \frac{c_0}{2\pi}\exp(-\frac{x^2}{4Dt})\int_{-\infty}^{\infty} \exp\{-Dt[k+ix/(2Dt)]^2\}dk$$

$$= \frac{c_0}{2\pi}\exp(-\frac{x^2}{4Dt})\sqrt{\frac{\pi}{Dt}}$$

$$= \frac{c_0}{\sqrt{4\pi Dt}}\exp(-\frac{x^2}{4Dt})$$

$$
\begin{aligned}
c(x,t) &= \mathcal{F}^{-1}[c(k,t)] \\
&= \frac{c_0}{2\pi}\mathcal{F}^{-1}[\exp(-Dtk^2)] \\
&= \frac{c_0}{2\pi}\int_{-\infty}^{\infty}\exp(-Dtk^2)e^{ikx}dk \\
&= \frac{c_0}{2\pi}\exp(-\frac{x^2}{4Dt})\int_{-\infty}^{\infty}\exp\{-Dt[k+ix/(2Dt)]^2\}dk \\
&= \frac{c_0}{2\pi}\exp(-\frac{x^2}{4Dt})\sqrt{\frac{\pi}{Dt}} \\
&= \frac{c_0}{\sqrt{4\pi Dt}}\exp(-\frac{x^2}{4Dt})
\end{aligned}
$$



2.5
2
1.5
1
0.5
0
-4
-2
0
2
4
0
2
4
6
8
10
空間
時間