The 1st Scenario for Getting at Multi-Scale Modeling

Analytical descriptions for explaining mathematically the facts discovered by experiments (a macro-scale viewpoint)

CTRW

Waiting time function

$$w(t) \sim \left(\frac{t}{\tau_0}\right)^{-(\alpha+1)}$$

Discovered by experiments

1. Description of CTRW with PDF

$$P(x,t) = \int_0^t \eta(x,t')\Phi(t-t')dt'$$

PDF for particle existing in time t and space x

1) PDF for particle gathering in time t and space x

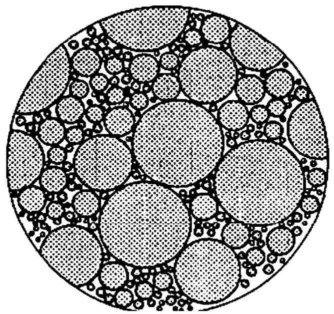
$$\eta(x,t) = \int_{-\infty}^{\infty} dx' \int_0^t dt' \eta(x',t')\varphi(x-x',t-t') + \delta(t)a(x)$$

2) PDF for particle staying by the duration time t

$$\Phi(t) = 1 - \int_0^t w(t')dt' \qquad \varphi(x,t) = \lambda(x)w(t)$$

Microstructure of porous media

Mathematical reasoning behind the observed phenomena in macro-scale

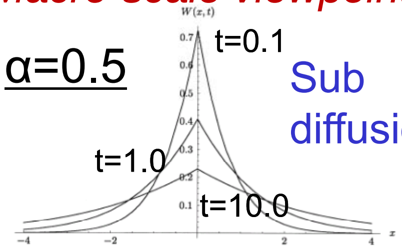


- What are geometric invariants?
- How do we combine the geometric invariants with FDE in a mathematical framework?

Fractional differential equation (FDE)

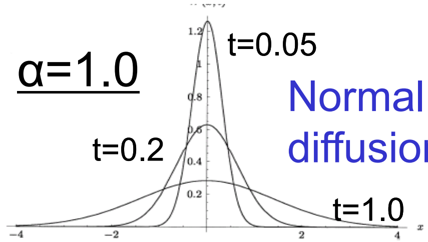
Macro-scale viewpoint

α=0.5



Sub diffusion

α=1.0



Normal diffusion

2. Determination of w(t)

Necessary condition

$$w(t) \sim \left(\frac{t}{\tau_0}\right)^{-(\alpha+1)}, \quad t \to \infty$$

$$w(t) = \frac{1}{\tau_0}\left(\frac{t}{\tau_0}\right)^{\alpha-1} E_{\alpha,\alpha}\left(-\left(\frac{t}{\tau_0}\right)^{\alpha}\right)$$

Mittag-Leffler function

3. Analytic procedures

1) Fourier transformation to x and Laplace transformation to t
2) Approximation taken for only the first term of the infinite series
3) Inverse Fourier transformation to x and Inverse Laplace transformation to t

$$\partial_t^{\alpha} P(x,t) = c\nabla^{\beta}P(x,t) - \gamma_0 \partial_x P(x,t)$$

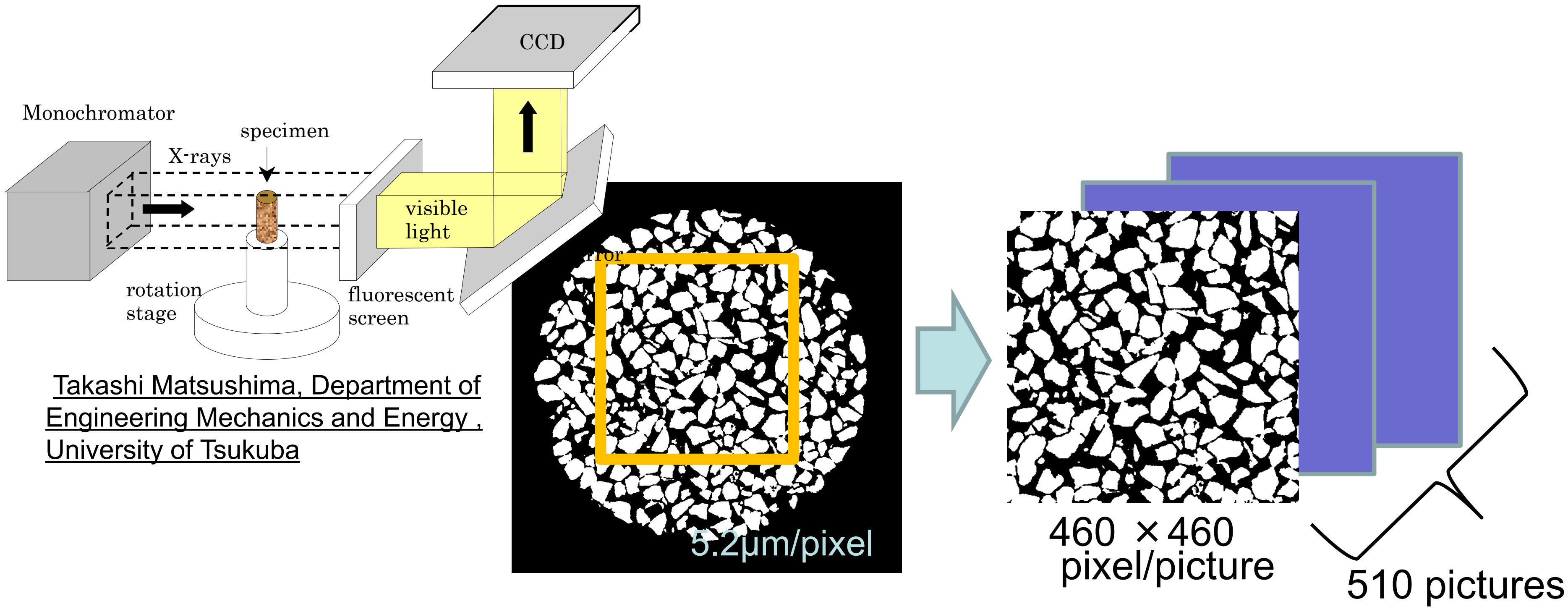
Fractional differential in terms of time

$$\partial_t^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-\tau)^{-\alpha} f'(\tau)d\tau$$

The degree of history to be retained from the initial time (t = 0) to the current time (time t). The smaller α is, the more history will be retained.

The 2nd Scenario for Getting at Multi-Scale Modeling

Characterization of the geometric features of the specimens of 3D CT-image (a micro-scale viewpoint)



Takashi Matsushima, Department of Engineering Mechanics and Energy , University of Tsukuba

1) Geometric dimension ⇒ Fractal dimension d_f

2) Analytic dimension ⇒ Spectral dimension d_s

How do we combine these geometric invariants with FDE(Fractional Differential Equation) in a mathematical framework?

Relationship between d_f, d_s and the Fractional Differential Order α Conjectured by Physicists

Manabu Machida, Department of Mathematics, University of Michigan

Bouchaud, J. P., and A. Georges, 1990, Physics. Reports 195, 127

The behavior of the mean volume V occupies by a diffusion particles initially concentrated on a given site x is given by the mean squared displacement and the fractal dimension.

$$V(x,r) \sim r^{d_f} \sim \left(\sqrt{\langle x(t)^2 \rangle}\right)^{d_f} \qquad (1)$$

$$V(x,r) := \mu(B(x,r))$$
$$B(x,r) := \{y \in V \mid d(x,y) < r\}$$

V(x, r) is the Riemannian volume of a geodesic ball B(x,r).

M. Barlow and E. Perkins, Brownian motion on the Sierpinski gasket, Probab. Th. Rel. Fields, 79 (1988), showed that the following heat kernel takes place for a large variety of fractal sets;

$$p(x,y,t) \sim t^{-\frac{d_s}{2}} \exp\left(-\left(\frac{d(x,y)^{d_w}}{ct}\right)^{\frac{1}{d_w-1}}\right) \qquad (2)$$

In the case of y=x,

$$\Rightarrow \quad p(x,x,t) \sim t^{-\frac{d_s}{2}} \qquad (3)$$

We assume that

$$p(x,x,t) \sim V(x,r)^{-1} \qquad (4)$$

With Eq. (1), Eq. (4) and Eq. (3), we obtain that

$$\langle x(t)^2 \rangle \sim V(x,r)^{\frac{2}{d_f}} \sim p(x,x,t)^{-\frac{2}{d_f}} \sim \left(t^{-\frac{d_s}{2}}\right)^{-\frac{2}{d_f}} \sim t^{\frac{d_s}{d_f}} \qquad (5)$$

Numerical experiments using CTRW say that

$$\langle x(t)^2 \rangle \sim t^{\alpha} \qquad (6)$$

By comparing Eq. (5) and Eq. (6), we have

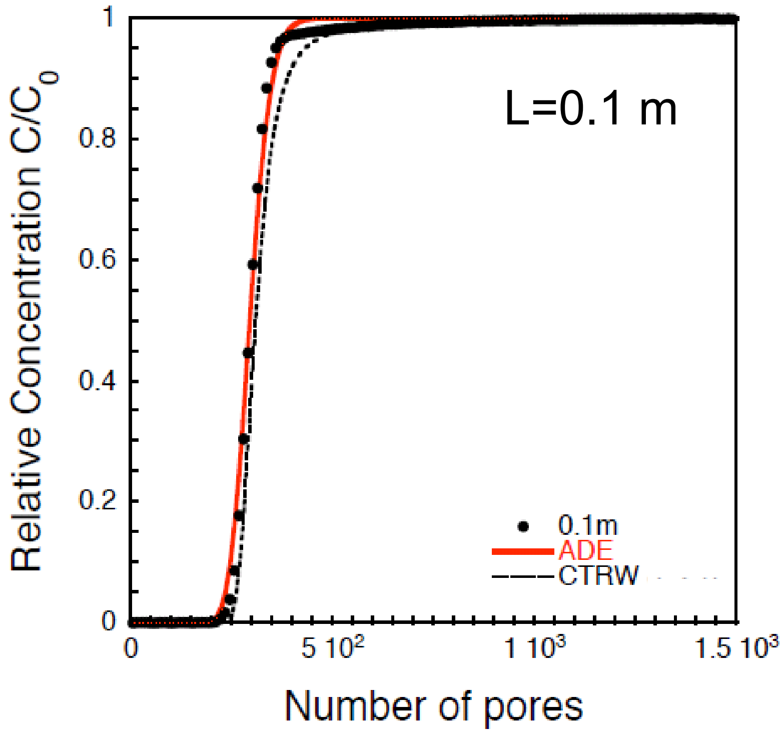
$$\alpha = \frac{d_s}{d_f} \qquad (7)$$

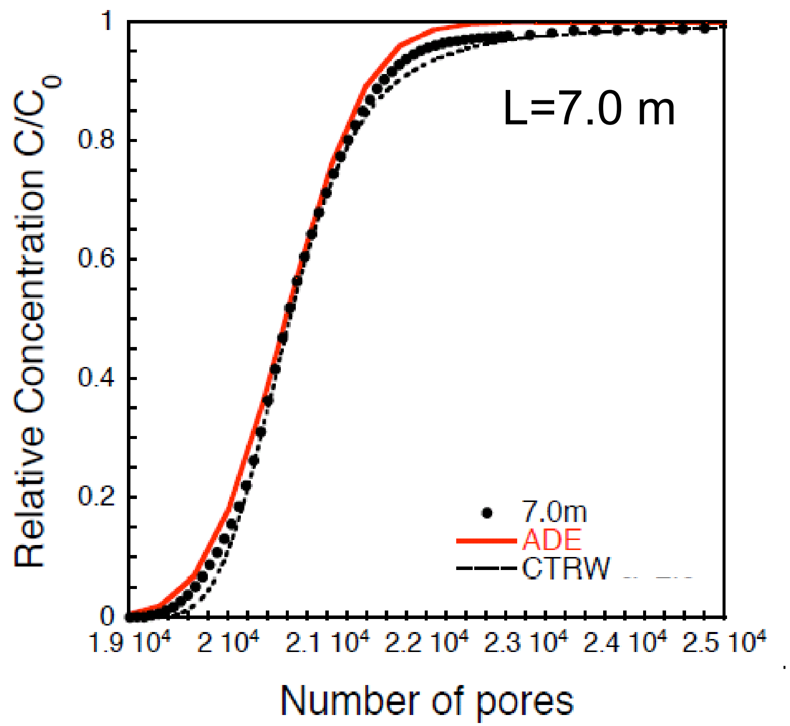
Comparison of Diffusion Behavior between Small Scale Experiment and Large Scale One

Yuko Hatano, Department of Risk Engineering, University of Tsukuba

✓The result of the small scale experiment shows that the diffusion follows ADE (normal diffusion).

✓The result of the large scale one not only differs from ADE, but CTRW also can't explain the behavior completely. We need a scaling law to combine laboratory experiments with field scale.





The 3rd Scenario for Getting at Multi-Scale Modeling

Deductive reasoning to derive the fractional differential equation using the homogenization method (a multi-scale viewpoint)

Masaaki Uesaka, Graduate School of Mathematical Science, The University of Tokyo

J.L. Auriault and J. Lewandowska, Non-Gaussian Diffusion Modeling in Composite Porus Media by Homogenization: Tail Effect, Transport in Porous Media, 21:47-70,1995

$$\begin{cases} \partial_t c^\varepsilon - \nabla \cdot \left(D(x/\varepsilon) \nabla c^\varepsilon \right) = 0 & in\ \Omega \times (0,T) & (1) \\ c^\varepsilon(x,0) = c_0(x) & in\ \Omega & (2) \\ \partial_\nu c^\varepsilon = 0 & on\ \partial\Omega \times (0,T) & (3) \end{cases}$$

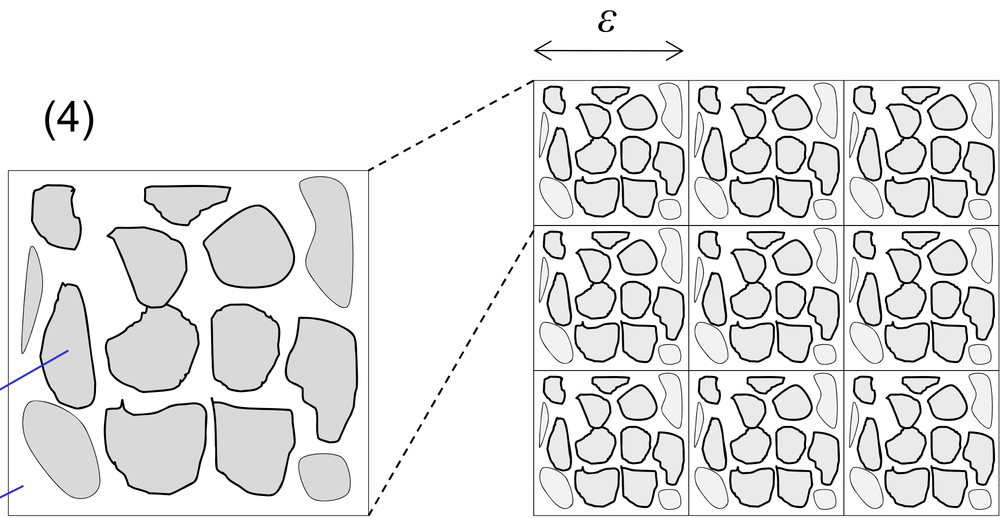
Ω is composed of periodic components of a microcell.

where

$$D(y) = D_f(y) 1_F(y) + D_m(y) 1_M(y) \qquad (4)$$

$$D_m / D_f \cong \varepsilon^2 \qquad (5)$$

The ratio of the two effective diffusion coefficients is defined in terms of the power of the homogenization parameter.



Media M: D_m

Media F: D_f

$Y = (0,1)^n$

$\Omega = \Omega_f^\varepsilon \cup \Omega_m^\varepsilon$

Masaaki Uesaka, Graduate School of Mathematical Science, The University of Tokyo

J.L. Auriault and J. Lewandowska, Non-Gaussian Diffusion Modeling in Composite Porus Media by Homogenization: Tail Effect, Transport in Porous Media, 21:47-70,1995

When ε goes to zero, c^ε converges to the solution of the following homogenized equations.

$$\begin{cases} \partial_t c - \boxed{\int_0^t K(t-\tau)\partial_\tau^2 c\, d\tau} = \nabla\cdot\left(D^{eff}\nabla c\right) & in\ \Omega\times(0,T) \quad (6) \\ c(x,0)=c_0(x) & in\ \Omega \quad (7) \\ \partial_\nu c = 0 & on\ \partial\Omega\times(0,T) \quad (8) \end{cases}$$

Where D^{eff} and K are determined by D_m, D_f, and the shape of M;

The memory function $K(t)$ is an inverse Laplace transform of the function (9), where $k(y,p)$ is a solution of Eq. (10) and (11)

$$(\mathcal{L}\,K)(p) = \frac{1}{p}\int_M k(y,p)dy \quad (9)$$

$$\begin{cases} \nabla_y\cdot\left(D_m\nabla_y k(\cdot,p)\right) = p\left(k(\cdot,p)-1\right) & in\ M \quad (10) \\ k(\cdot,p)=0 & in\ \partial M. \quad (11) \end{cases}$$

What shape of M leads to a similar effect like the fractional differential?

Summary and Discussion

- *<u>The 1st scenario</u>*: Analytical descriptions for explaining mathematically the facts discovered by experiments (a macro-scale viewpoint)
  - CTRW → The α fractional differential in terms of time
  - Levy flights → The β fractional differential in terms of space

- *<u>The 2nd scenario</u>*: Characterization of the geometric features of the specimens of 3D-CT image (a micro-scale viewpoint)
  - The equality $\alpha = d_s/d_f$ based on the hypothesis: $p(x,x,t) \sim V(x,r)^{-1}$ exists.
  - If d_s *and* d_f can be determined by the geometric features, we will be able to combine the fractional differential equation with the geometric features in the observed region.
  - Experimental results say that we need a scaling law to connect laboratory experiments with field scale's observations.

- *<u>The 3rd scenario</u>*: Deductive reasoning to derive the fractional differential equation using the homogenization method (a multi-scale viewpoint)
  - Geometric conditions M in a microcell
    - → The memory function generates the long-tail effect
    - → Our concern is 'what shape of M leads to a similar effect like the fractional differential'?

Relationship among CTRW, FDE and d_s/d_f in terms of α, between Levy flight, FDE in terms of β

CTRW

$$\langle x(t)^2 \rangle \sim t^{\alpha}$$

Geometric index

$$\alpha = \frac{d_s}{d_f}$$

Levy symmetric alpha stable distribution

$$(\mathcal{F}\lambda)(k) = \exp(-c|k|^{\beta} + i\gamma_0)$$

FDE (Fractional Differential Equation)

The α fractional differential in terms of time

The β fractional differential in terms of space

$$\partial_t^{\alpha} P(x,t) = c\nabla^{\beta} P(x,t) - \gamma_0 \partial_x P(x,t)$$

The sub-Gaussian heat kernel on graphs

$$p(x,y,t) \sim \boxed{t^{-\frac{d_s}{2}}} \exp\left(-\left(\frac{d(x,y)^{d_w}}{ct}\right)^{\frac{1}{d_w-1}}\right) \; ?$$

Let E(x, R) be the mean exit time from the ball B(x,R).
Consider the hypothesis

$$E(x,R) \sim R^{d_w}$$

walk dimension $d_w \geq 2$

$d_w = 2$ → normal

$d_w > 2$ → sub-diffusion

Thank you for your attention!

異分野連携の場「数学イノベーションプラットフォーム（仮称）」へ、ようこそ！

数学・数理科学により、諸科学・工学・産業界で得られている一連の実験的事実または経験的事実を<u>一貫性のある論理で統合できる理論を構築</u>し、同理論に基づく数理モデルを介し、<u>諸科学・工学・産業における未解決問題のブレークスルー</u>と<u>当該分野の研究・開発工期の驚異的短縮</u>ができたという実績を示してゆくことを目指します。

数学イノベーションを目指す有志の皆様の参加を歓迎します。

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