Recent Advances on Numerical Solution of Fractional PDEs

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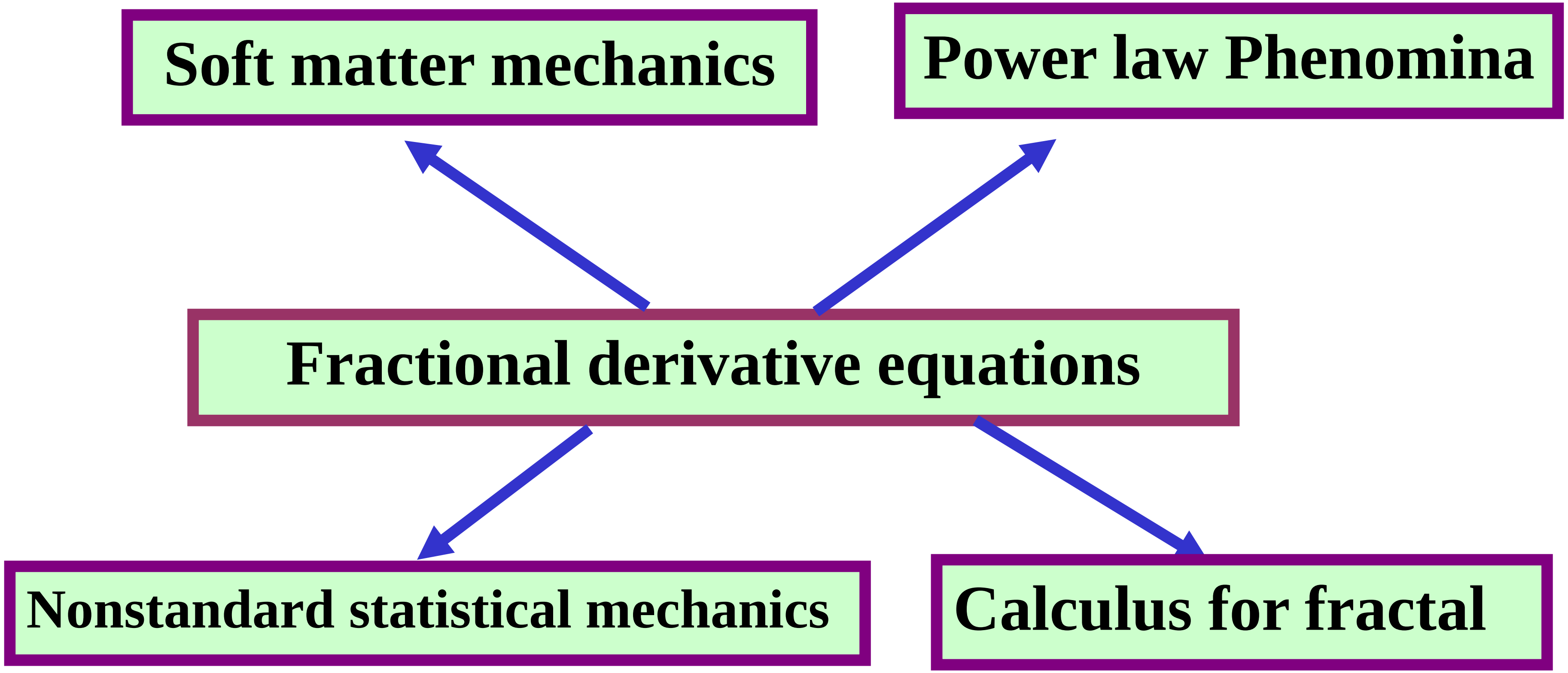
Outline

- **Introduction：underlying physics and mechanics**
- **Advances in numerical simulation**
- **Opening issues**
- **Summary and Outlook**

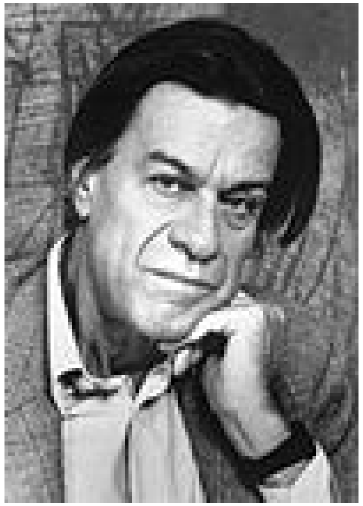
Underlying Physics and Mechanics I



Underlying Physics and Mechanics II

- **Soft matter:** Materials in between ideal solids and Newtonian fluids, such as polymer, emulsions, sediment, biomaterials, oil, et al. Classical models of integer-order derivatives can not properly describe “anomalous” behaviors of soft matter, e.g., **frequency-dependent energy dissipation.**
- **Power law phenomena:** Empirical formula of time- and path-dependent mechanics processes often have a power function expression, whose underlying mechanics constitutive relationship does not obey a variety of standard “gradient” laws, such as granular Darcy law, Fourier heat conduction, Newtonian viscosity, Fickian diffusion, et. al.
- **Calculus description of fractal:** **Differential expression of fractal models.**
- **Calculus description of abnormal statistical mechanics and physics**: Levy stable distribution, fractional Brownian motion.

Soft Matter Physics



Pierre-Gilles de Gennes proposed the term in his Nobel acceptance speech in 1991.

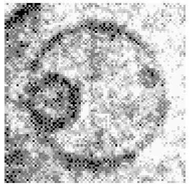
P. G. De Gennes, called Newton of our times

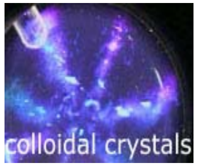
Typical Soft matters Ⅰ

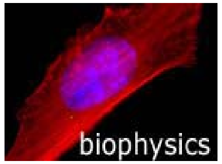
- Granular materials
- Colloids, liquid crystals, emulsions, foams,
- Polymers, textiles, rubber, glass,
- Rock layers, sediments, oil, soil, DNA,
- Multiphase fluids,
- Biopolymers and biological materials

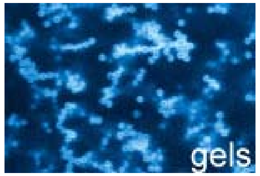
highly deformable, porous, thermal fluctuations play major role, highly unstable

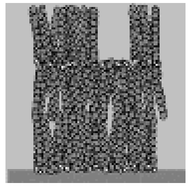
Typical Soft matters II

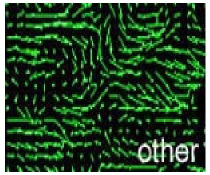


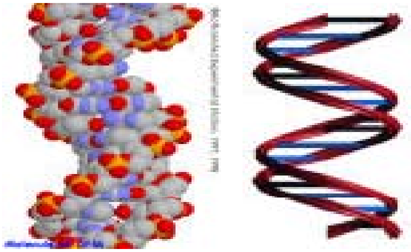


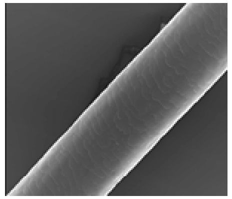


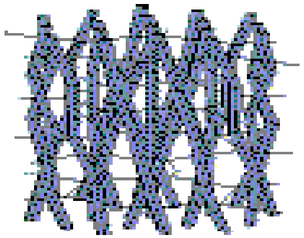


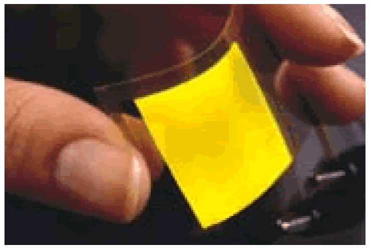


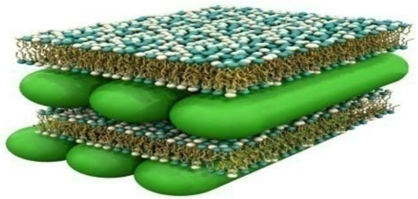












Difficulties with soft matters

- Very slow internal dynamics
- Highly unstable system equilibrium
- Nonlinearity and friction
- Entropy significant

a jammed colloid system, a pile of sand,
a polymer gel, or a folding protein.

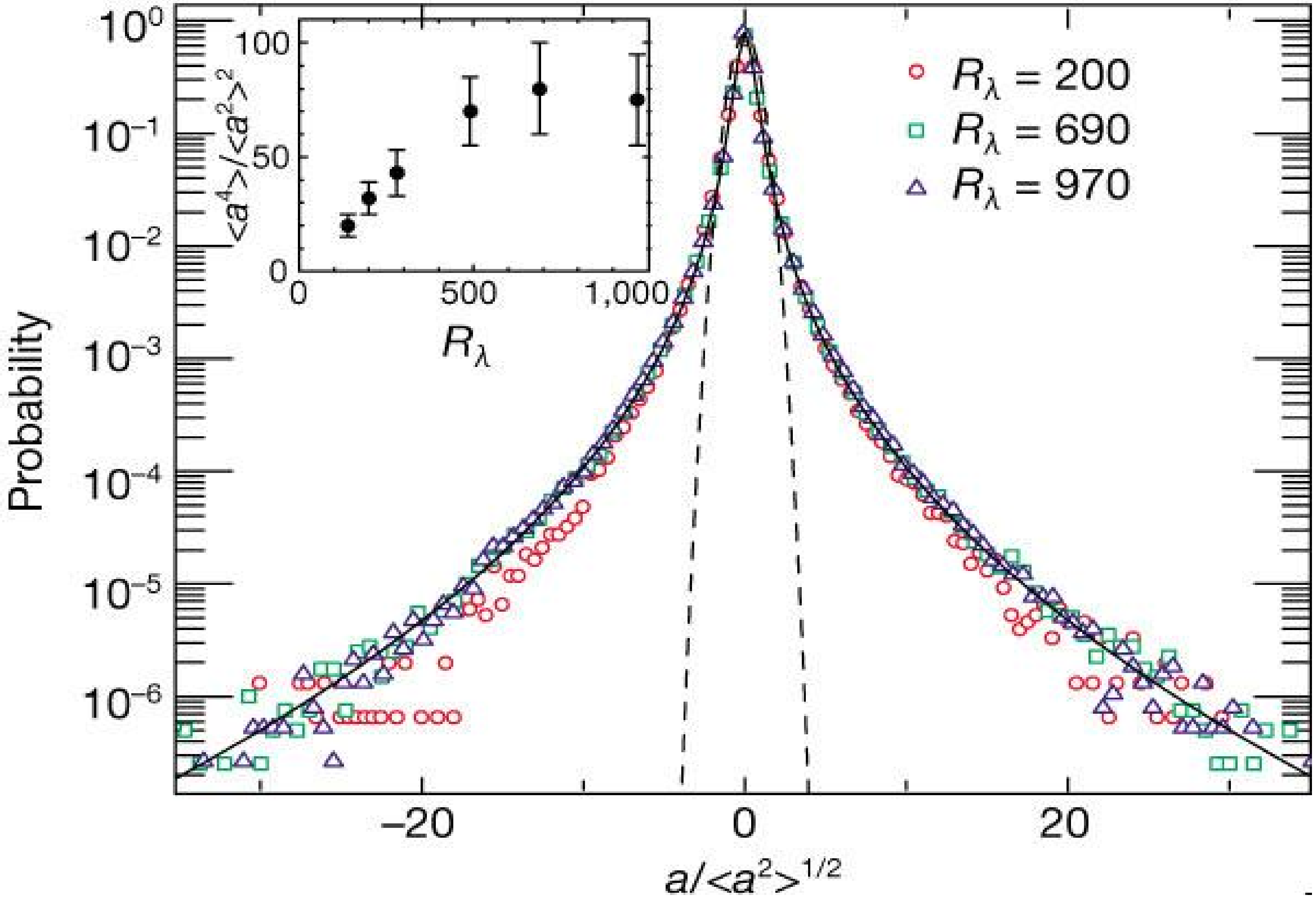
Challenging modeling issues in complex mechanics

- **Amplitude-dependency**: nonlinear modeling
- **Frequency-dependency**: fractional derivative modeling
- **Hysteresis**: fractional derivative or nonlinear modeling?
- **Stress softening and hardening**?

Mechanics constitutive relationships

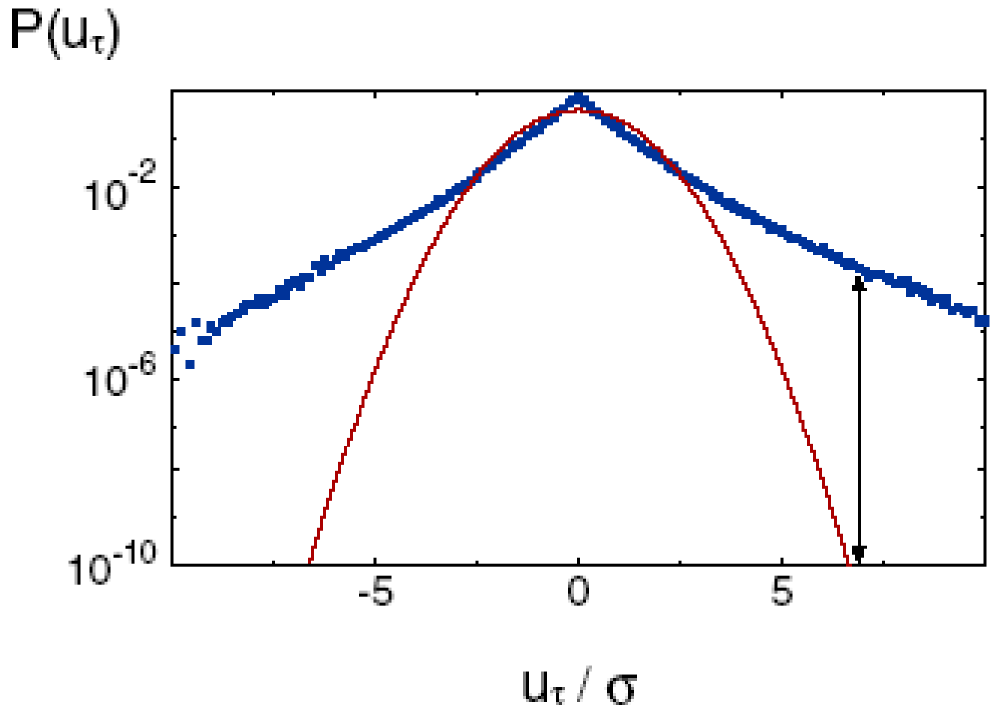
- Hookian law in ideal solids: $F = kx$
- Ideal Newtonian fluids: $F = \upsilon \dfrac{\partial u}{\partial y}$
- Newtonian 2nd law for rigid solids: $F = m\dfrac{d^2 x}{dt^2}$
- Fractional model of soft matter: $F = \rho \dfrac{d^\alpha x}{dt^\alpha} \quad 0 \le \alpha \le 2$

Non-Gaussian distribution of Turbulence



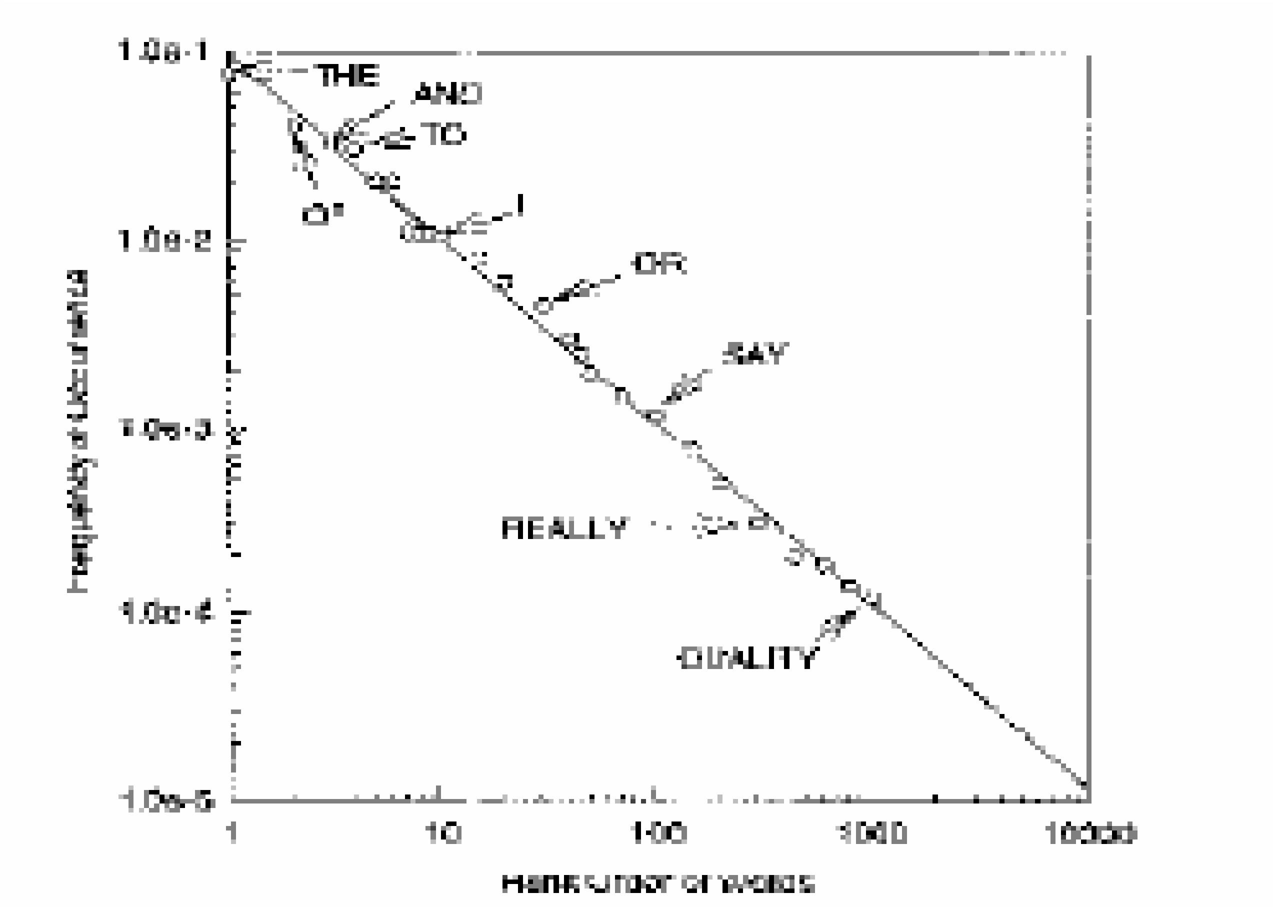
A. La Porta, et al.. *Nature* 409(2001), 1017–1019

Measured probability density of changes of the wind speed over 4 sec



J. Peinke, et al, Ann. Phys. (Leipzig) **13**, No. 7–8, 450 – 460 (2004)

Power law of English vocabulary



Bruce J. West, University of Illinois at Urbana-Champaign, May 15, 2006.

Fractional derivative modeling vs. Nonlinear modeling

- History- and path-dependency (**non-Markovian**)
- Global interaction
- Fewer physical parameters (**simple= beautiful**)
- **Competition or complementary**？

Definitions of fractional time derivative

（1）Gruwald-Letnikov fractional derivative:

$$\frac{d^p f(t)}{dt^p} = \lim_{\substack{h\to 0\\ nh=t-a}} h^{-p} \sum_{r=0}^{n} (-1)^r \binom{p}{r} f(t-rh)$$

（2）Riemann-Liouville fractional derivative:

$$\frac{d^p f(t)}{dt^p} = \frac{1}{\Gamma(1-p)} \frac{d}{dt} \int_a^t (t-\tau)^{-p} f(\tau) d\tau \quad (0 < p < 1)$$

（3）Caputo fractional derivative:

$$\frac{d^p f(t)}{dt^p} = \frac{1}{\Gamma(n-p)} \int_a^t \frac{f^{(n)}(\tau)}{(t-\tau)^{p+1-n}} d\tau \quad (n-1 < p < n)$$

Fourier transform of fractional time derivative

$$FT^{+}\left(\frac{d^{\eta}p}{dt^{\eta}}\right)=\left(-i\omega\right)^{\eta}P$$

Examples: fractional derivative operation and equation

Operation:

$$\frac{d^{1/2}t}{dt^{1/2}} = \frac{2}{\sqrt{\pi}} t^{1/2}$$

Initial value problems:

$$\begin{cases} \frac{d^{1/2}p(t)}{dt^{1/2}} + p = 0 \\ p(0) = A \end{cases}$$

Fractional Hamiltonian:

$$\dot{x}^{\alpha} = \frac{\partial H}{\partial p} \qquad \dot{p}^{\alpha} = \frac{\partial H}{\partial x}$$

$$\dot{x}^{\alpha} = \frac{dx^{\alpha}}{dt^{\alpha}} = p \qquad \dot{p}^{\alpha} = \frac{d^{\alpha}p}{dt^{\alpha}}$$

G. Turchetti, Hamiltonian systems with fractional time derivative, 2000.

Definitions of fractional Laplacian

Fourier transform: $F^{+}\left\{(-\Delta)^{\beta} p\right\} = k^{2\beta} P \qquad 0<\beta<1$

Difference definition: $(-\Delta p)^{\beta} = \dfrac{1}{d(\beta)} \int_{\Omega} \dfrac{p(x) - p(\xi)}{\|x-\xi\|^{d+2\beta}} d\Omega(\xi)$

Integral definition:

$$(-\Delta)^{\beta} p(x) = (-\Delta)_{*}^{\beta} p(x) + h\int_{S} \left[D(\xi) \frac{\partial}{\partial n}\left(\frac{1}{\|x-\xi\|^{d+2\beta-2}} \right) - \frac{N(\xi)}{\|x-\xi\|^{d+2\beta-2}} \right] dS(\xi)$$

W.Chen and S. Holm, Journal of Acoustic Society of America, 115(4), 1424-1430, 2004

Fractional Laplacian model of dissipative acoustic wave

Damped wave equation(β=0): $$\Delta p = \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + \frac{2\alpha_0}{c_0}\frac{\partial p}{\partial t}$$

Thermoviscous equation(β=1): $$\Delta p = \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + 2\alpha_0 c_0 \frac{\partial}{\partial t}\left(-\Delta p\right)$$

Modified Szabo's wave equation: $$\Delta p = \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + \frac{2\alpha_0}{c_0 \cos\frac{\eta\pi}{2}}\frac{\partial^{\eta+1} p}{\partial t^{\eta+1}}$$

$$\beta = \frac{\omega}{c_0} + \alpha_0 \omega^{\eta} \tan\frac{\eta\pi}{2}$$

$$(0 < \eta < 2,\ \ \eta \neq 1)$$

Fractional Laplacian wave equation: $$\Delta p = \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + \frac{2\alpha_0}{c_0^{1-y}}\frac{\partial}{\partial t}\left(-\Delta\right)^{\beta} p$$

($0<\beta<1$)

Anomalous diffusion equation of fractional time-space derivatives

$$\partial^{\alpha} p / \partial t^{\alpha} + \gamma(-\Delta)^{\beta} p = 0$$

$0 \prec \alpha \leq 1$ $\qquad$ $0 \prec \beta \leq 1$

Advances of numerical simulations

- **Numerical methods for fractional time derivative equations**
- **Numerical methods for fractional space derivative equations**

Numerical methods for fractional time derivative equations I

➢ Finite difference methods

- Explicit methods
- Implicit methods
- Crank-Nicholson method

➢ Volterra integral equation method

- Prediction-correction method
- Block by block method

…….

Numerical methods for fractional time derivative equations II

- Homotopy perturbation method
- Laplace transform method
- Variational iteration method
- Differential transformation method
- Adomian decomposition method
- Random walker methods
- Finite element method
- Discontinuous Galerkin method
- Meshless methods
  - Kansa’s method
  - Laplace transformed boundary particle method

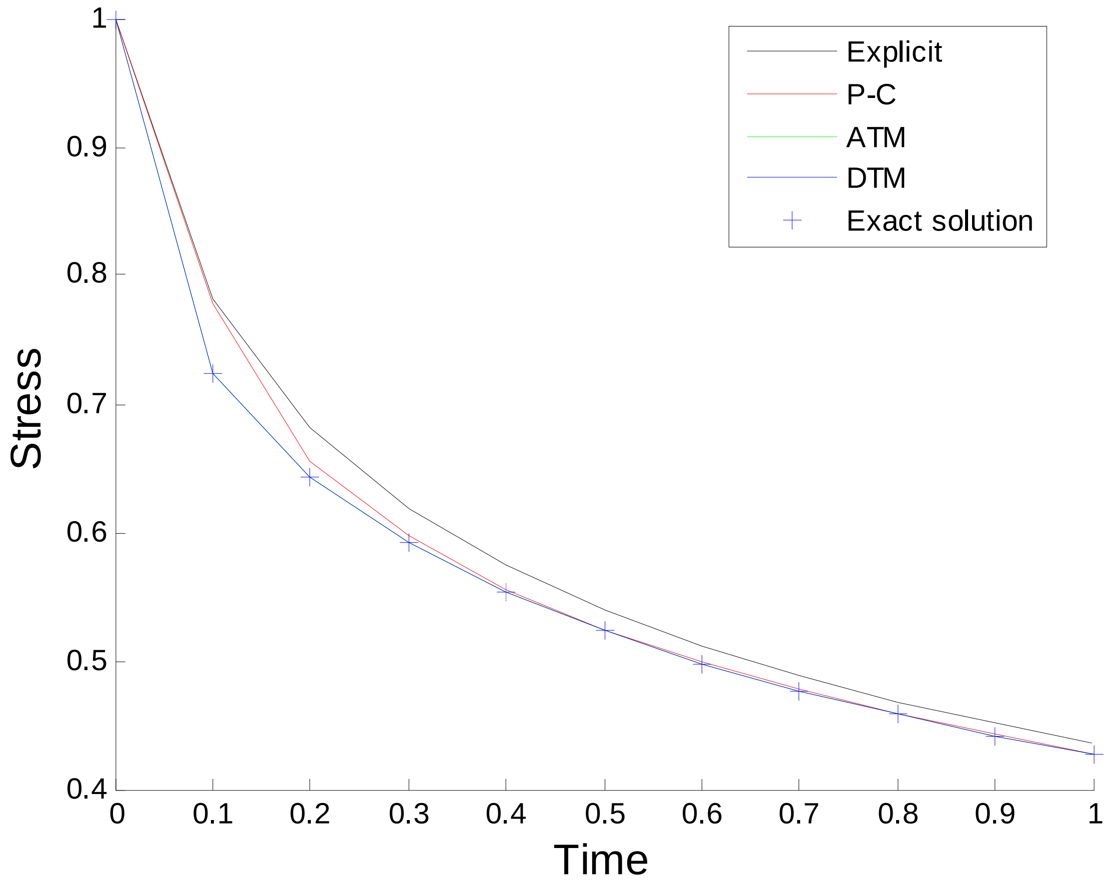
……

Numerical examples

$$\frac{d^p u(t)}{dt^p} + Bu(t) = f(t) \ (0 < p \le 2)$$
$$u(0) = C$$

- **0<p<1**: fractional relaxation equation for concrete, colloid, soil, et. al; creep under known stress. $u(t)$ stress, $f(t)$ strain function, C initial condition.
- **1<p<2**： fractional damped vibration equation for complex viscous. $u(t)$ displacement, $f(t)$ external force, C initial displacement.

A comparison of four different kinds of numerical method



p=0.5; time step 0.1; initial stress (B=1， $u(0)$=1)

Meshless method-Kansa's method

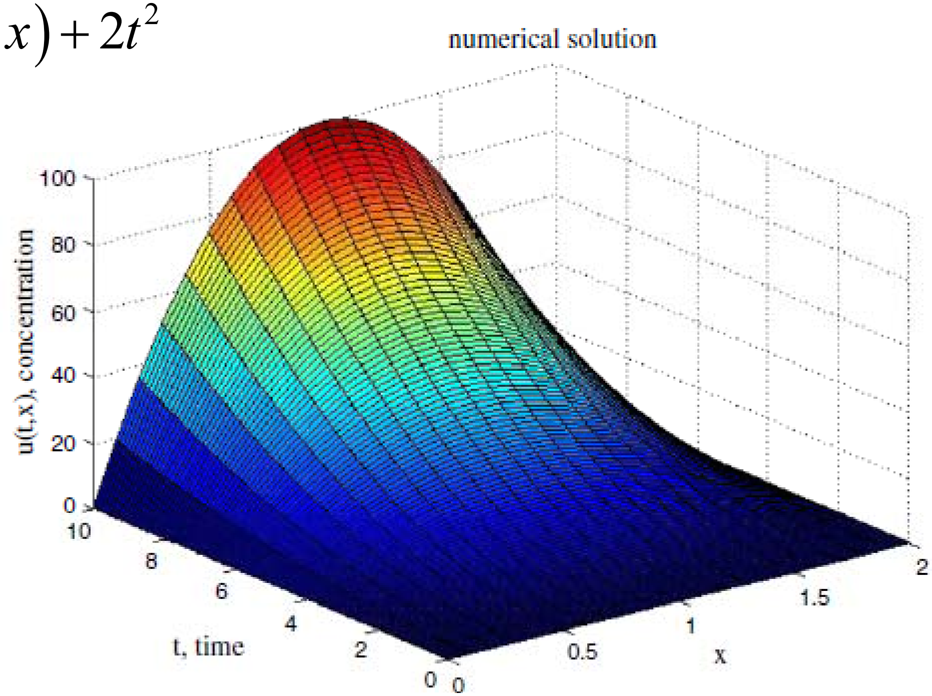
1D time fractional diffusion problem

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}+u(x,t)=\frac{\partial^2 u(x,t)}{\partial x^2}+Q(x,t),\quad 0<\alpha<1, 0\le x\le 2, t\ge 0$$

$$Q(x,t)=\frac{2}{\Gamma(3-\alpha)}t^{2-\alpha}x(2-x)+t^2x(2-x)+2t^2$$

$$u(0,t)=u(2,t)=0,\quad t\ge 0$$

$$u(x,0)=0,\quad 0\le x\le 2$$



Interpolation basis (MQ function)

$$\phi(x_i,x_j)=\sqrt{(x_i-x_j)^2+c^2}$$

Convergence order $\mathrm{O}(\Delta t^{2-\alpha})$

Chen W et al. Computer and Mathematics with Applications, 2010, 59 (5):1614-1620.

A comparison of FDM and LTBPM

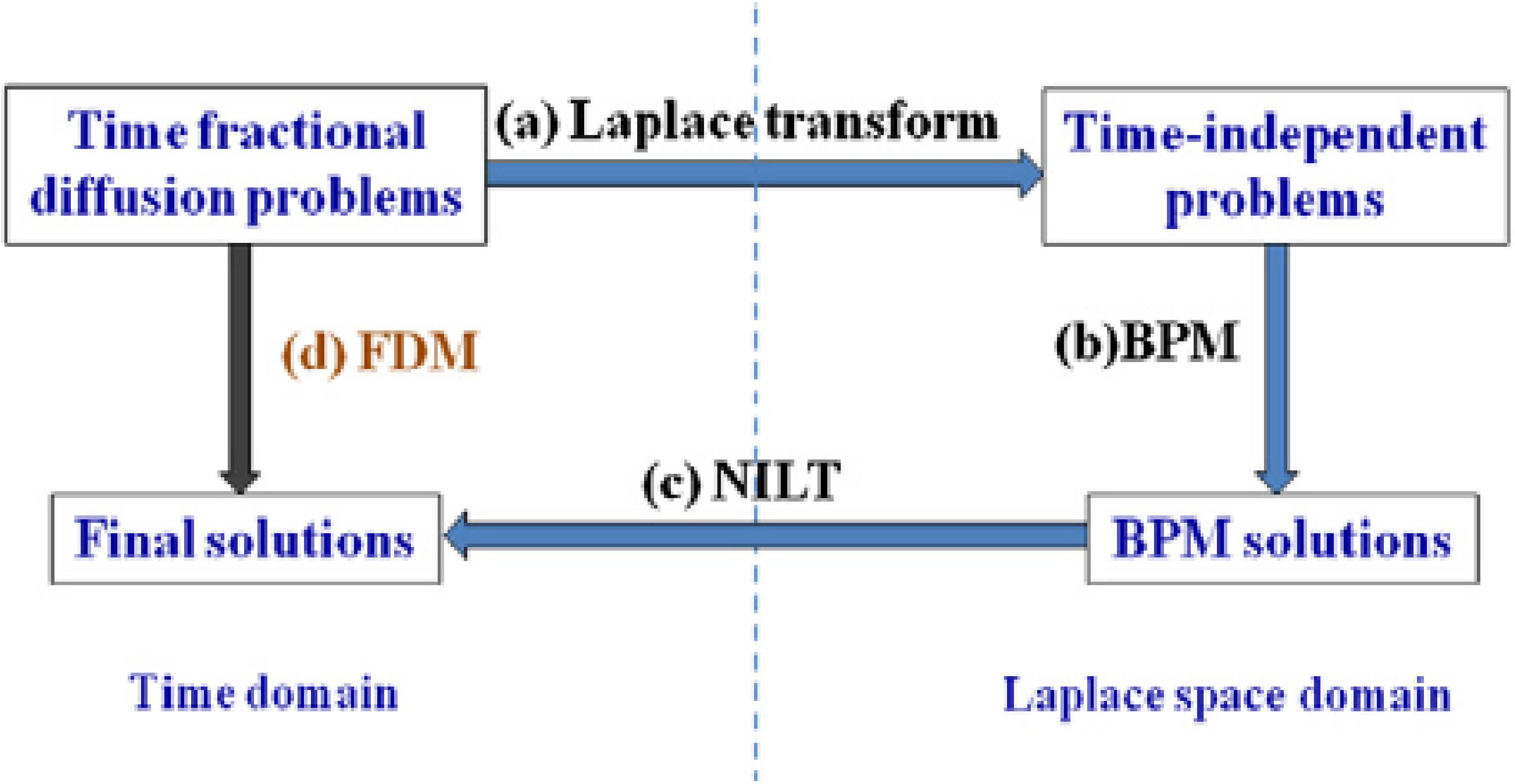


Fig. 1. The roadmaps of the LTBPM and the FDM for time fractional diffusion problems.

Fu ZJ et al. Journal of Computational Physics, 2013, 235: 52-66.

2D time fractional diffusion problem

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \Delta u(x,t) + Q(x,t), \quad x \in [0,1]^2, t \in (0,T)$$

$$u(x,t) = t^2 e^{x+y}, \quad x \in \partial\Omega, t \in (0,T)$$

$$u_0(x) = 0, \quad x \in \Omega, t=0$$

$$Q(x,t) = \left[\frac{2t^{2-\alpha}}{\Gamma(3-\alpha)} - 2t^2\right] e^{x+y}$$

$$\alpha = 0.85$$

$$\text{Merr}(u) = \max_{1\le i\le NT} \left|u(i) - \bar{u}(i)\right|,$$

$$\text{Rerr}(u) = \sqrt{\frac{\sum_{i=1}^{NT}\left(u(i) - \bar{u}(i)\right)^2}{\sum_{i=1}^{NT}\left(u(i)\right)^2}},$$

Table 1 Errors at T=1: LTBPM($\Delta h = 0.2$) vs domain-type RBF method($\Delta h = 0.1$)

	Merr(u)	Rerr(u)	Rerr($u_{,x}$)	Rerr($u_{,y}$)
LTBPM(M=10)	4.135e-4	5.596e-5	5.596e-5	5.596e-5
DRBF($\Delta t = 0.1$)	1.234e-2	2.073e-3	6.864e-3	6.864e-3
DRBF($\Delta t = 0.004$)*	3.046e-4	5.116e-5	1.694e-4	1.694e-4

* Calculated from the formula $O\left(\Delta t^{2-\alpha}\right)$ in reference（*Computational Mechanics*, 48,1-12,2011)

Save the computing cost for long-range time simulation

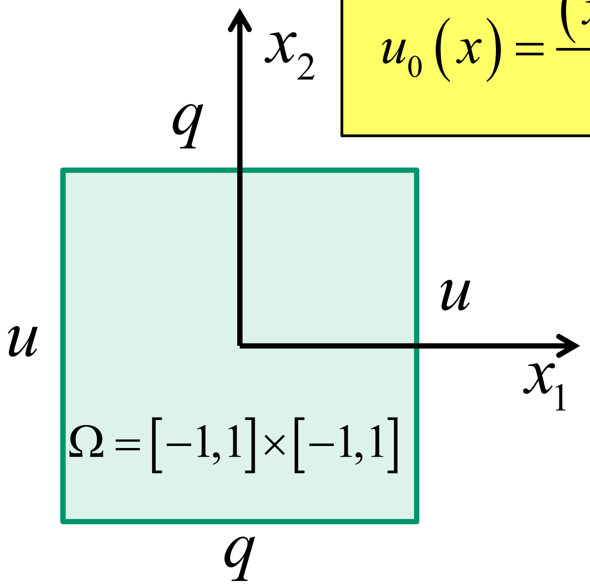
2D subdiffusion convection problem

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \Delta u(x,t) + 0.005\frac{\partial u(x,t)}{\partial x_1}, \quad x\in[-1,1]^2, t\in(0,T)$$

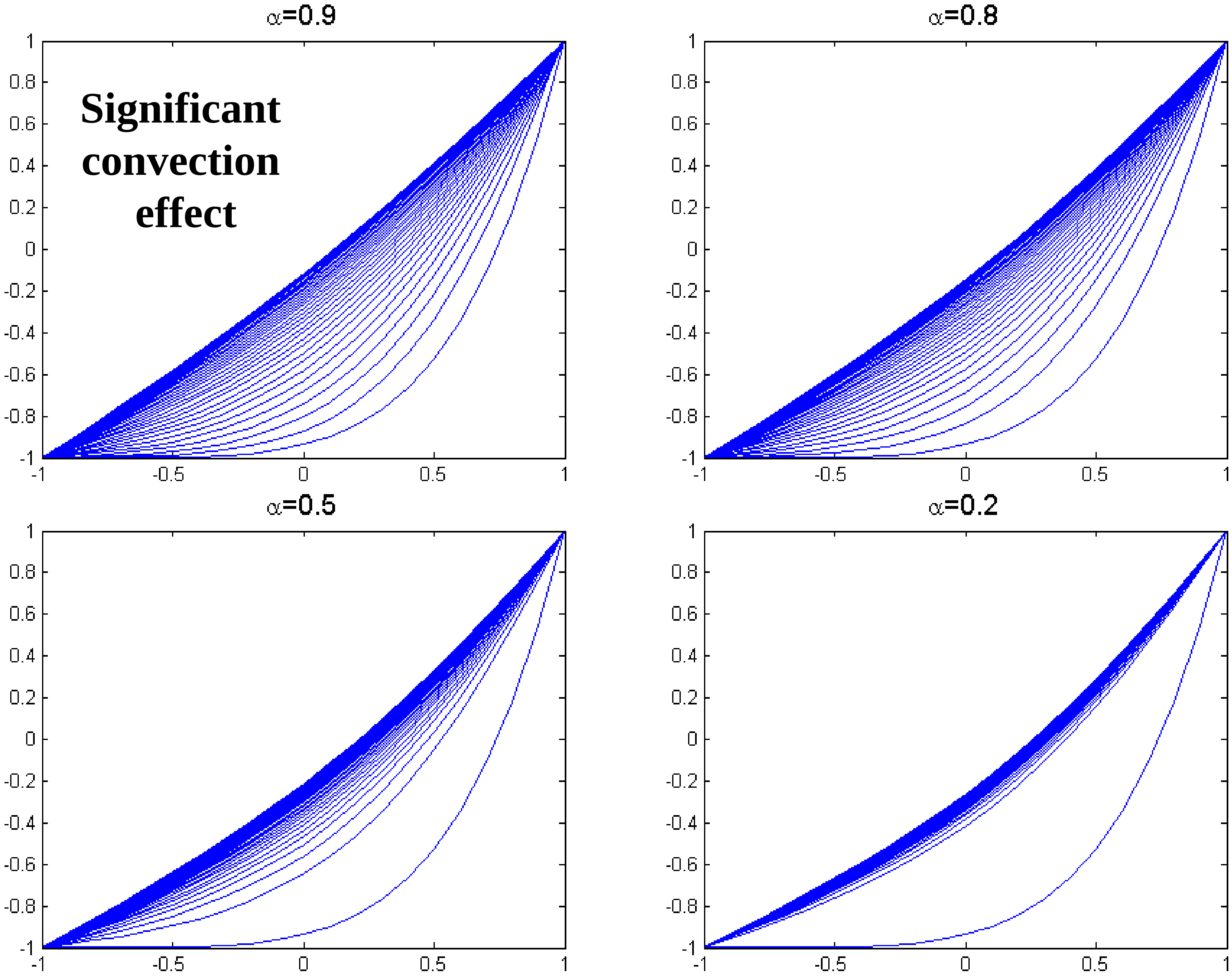
$$u(x,t) = x_1 + 1, x\in\{(x_1,x_2)\,|\,x_1=-1,1; -1\le x_2\le 1\}, t\in(0,T)$$

$$q(x,t) = \frac{\partial u(x,t)}{\partial n} = 0, x\in\{(x_1,x_2)\,|\,x_2=-1,1; -1\le x_1\le 1\}, t\in(0,T)$$

$$u_0(x) = \frac{(x+1)^5 - 16}{16}, \quad x\in\Omega, t=0$$



Numerical solution

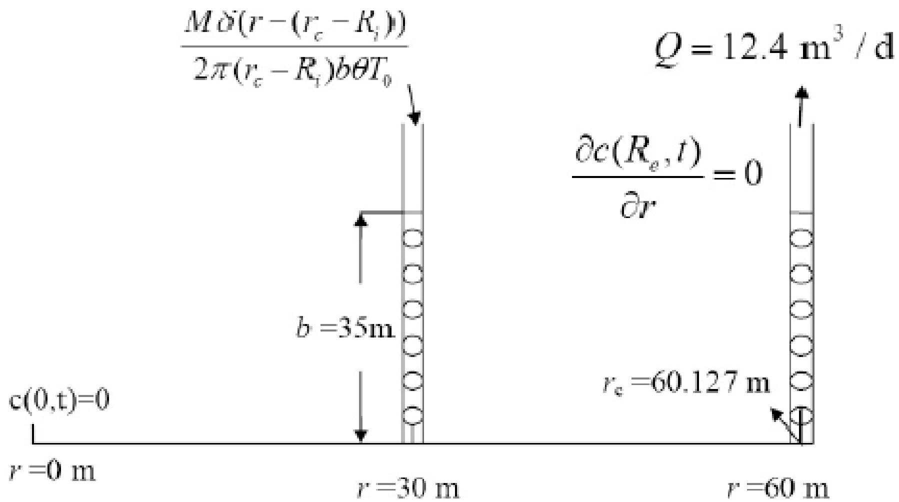


LTBPM
($\Delta h = 0.2$)
results
(x_1=0
section)

Left endpoint has dramatic changes with different α

Contaminant transport（I）

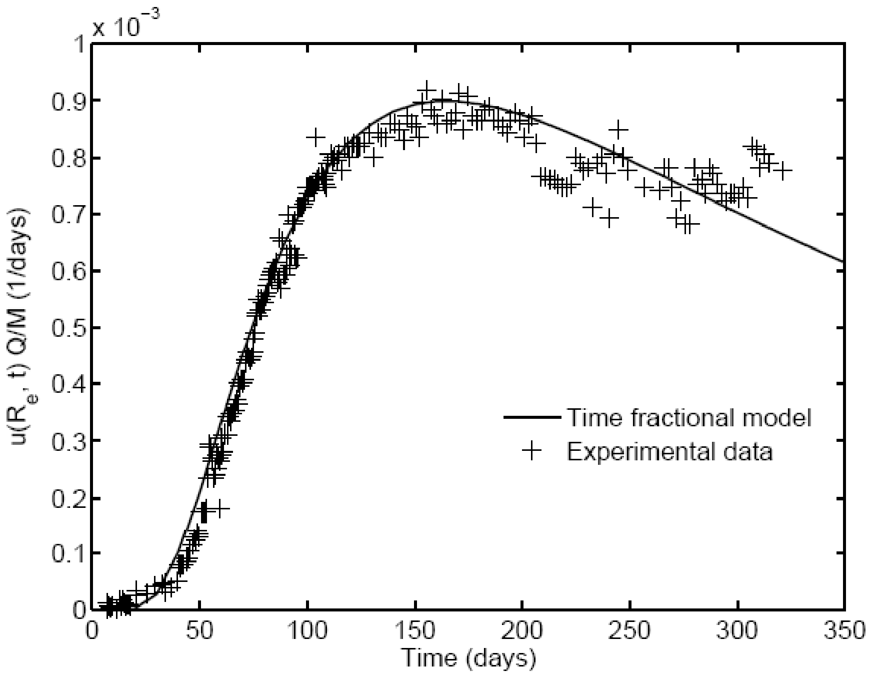
Transport process of Bromide ion in underground aquifers（Nevada, US）



Mathematical model

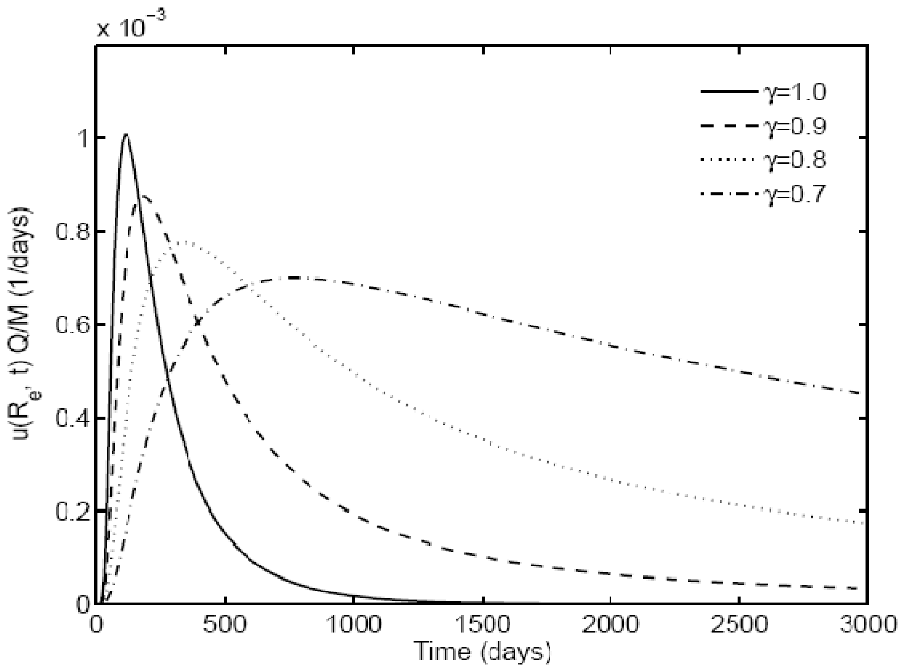
$$
\begin{cases}
\dfrac{d^\gamma u(r,t)}{dt^\gamma} = -\dfrac{v_0}{r_c - r}\dfrac{\partial u(r,t)}{\partial r} + \dfrac{1}{r_c - r}\dfrac{\partial}{\partial r}\left(d_0 \dfrac{\partial u(r,t)}{\partial r}\right), \ r \in (0, R_e), \\
u(0,t) = 0, \quad \dfrac{\partial u(R_e,t)}{\partial r} = 0, \ t > 0, \\
u(r,0) = f(r), \ r \in [0, R_e]
\end{cases}
$$

Contaminant transport（I）



$\gamma = 0.92$

Experiment and numerical results



Long-time history evolution for solute concentration

Sun HG, et al. *Philosophical Transactions of Royal Society A* (In press)

Contaminant transport（II）

Transport process of Hydrogen isotopes (Tritium) in Natural Media （(Mississippi , US)）

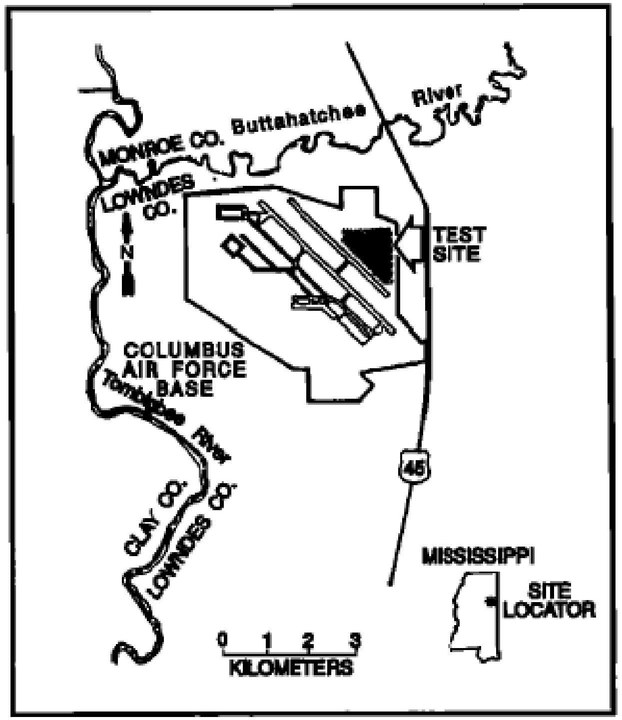
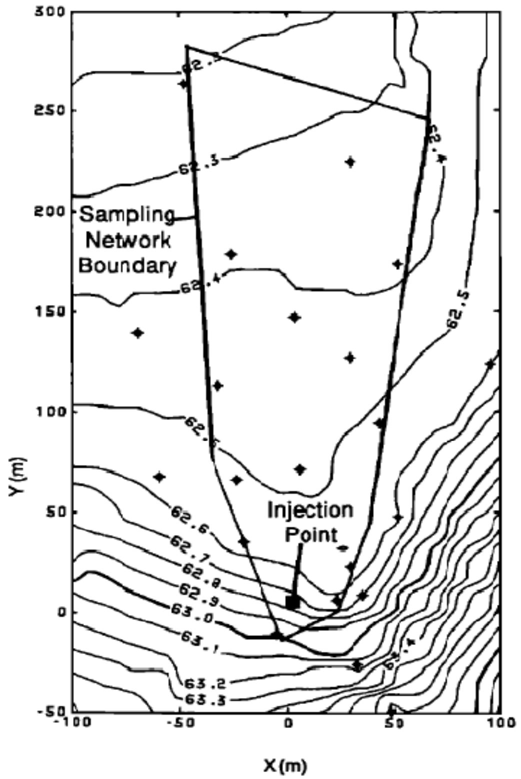
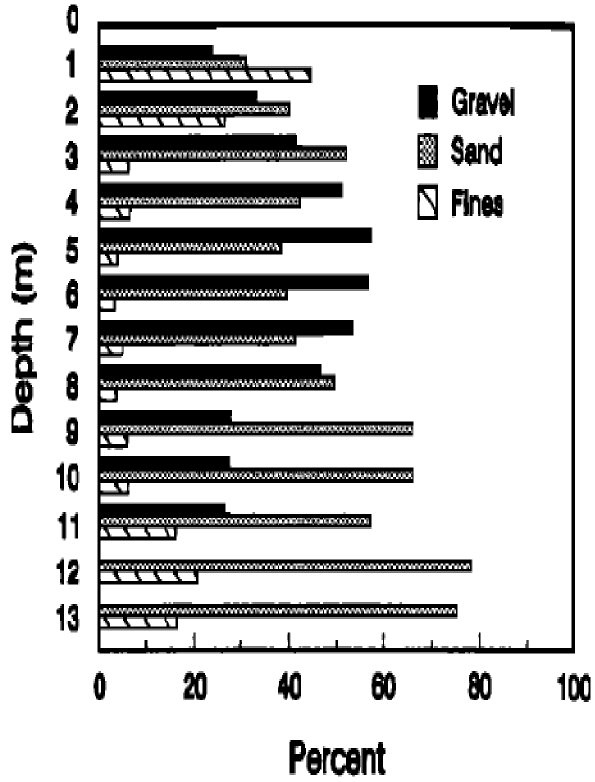


Fig. 1. Site location map.

Location



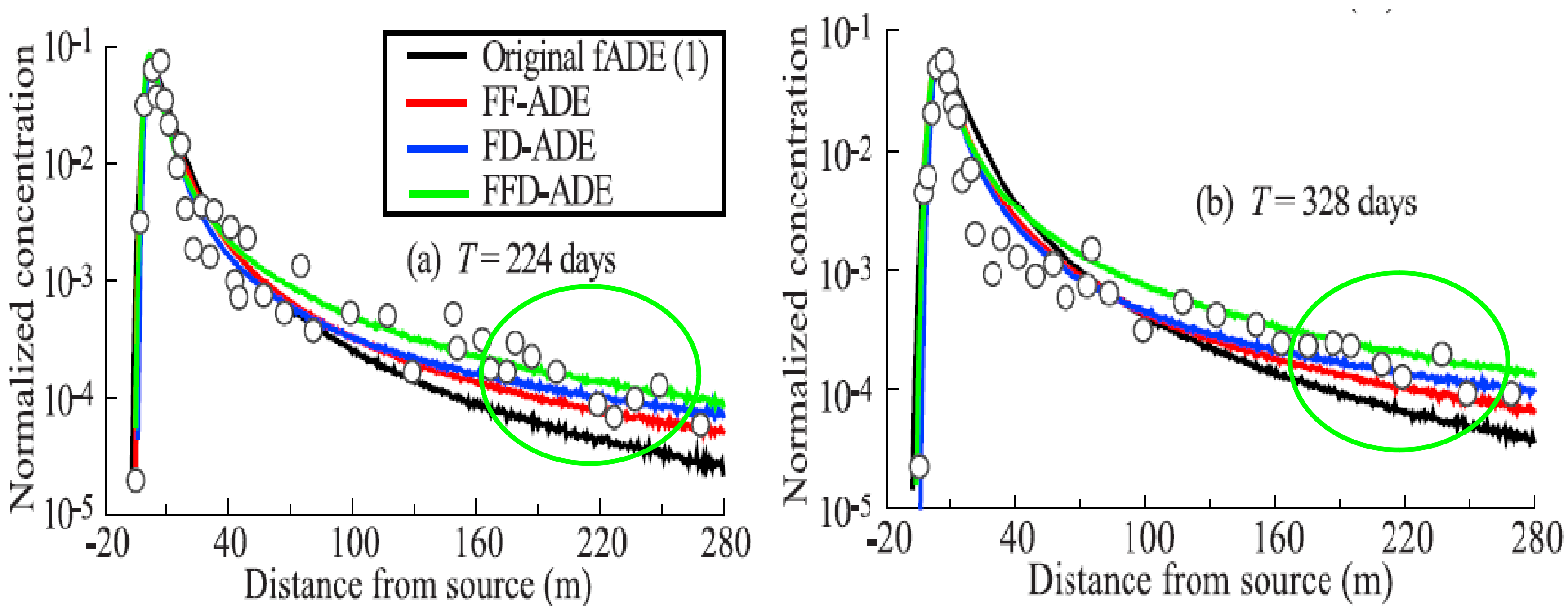
Measurement points



Aquifer ingredients

Boggs, J. M., et al., *Water Resour. Res.*, 28(12), 243 3281-3291, 1992

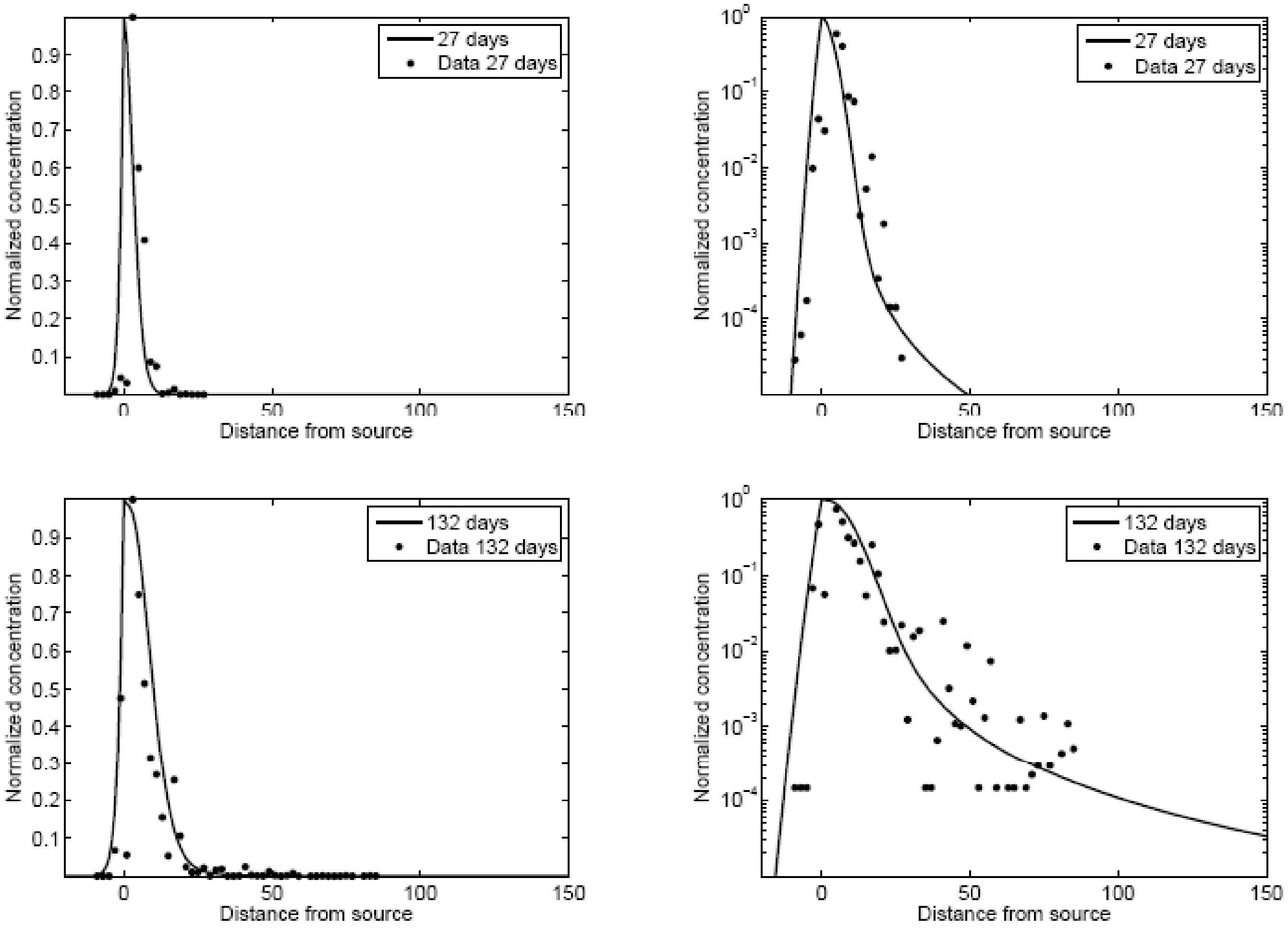
Contaminant transport（II）



$$\beta = 1.1$$

Y. Zhang , et al. *Water Resour. Res.*, 43 (2009): W05439

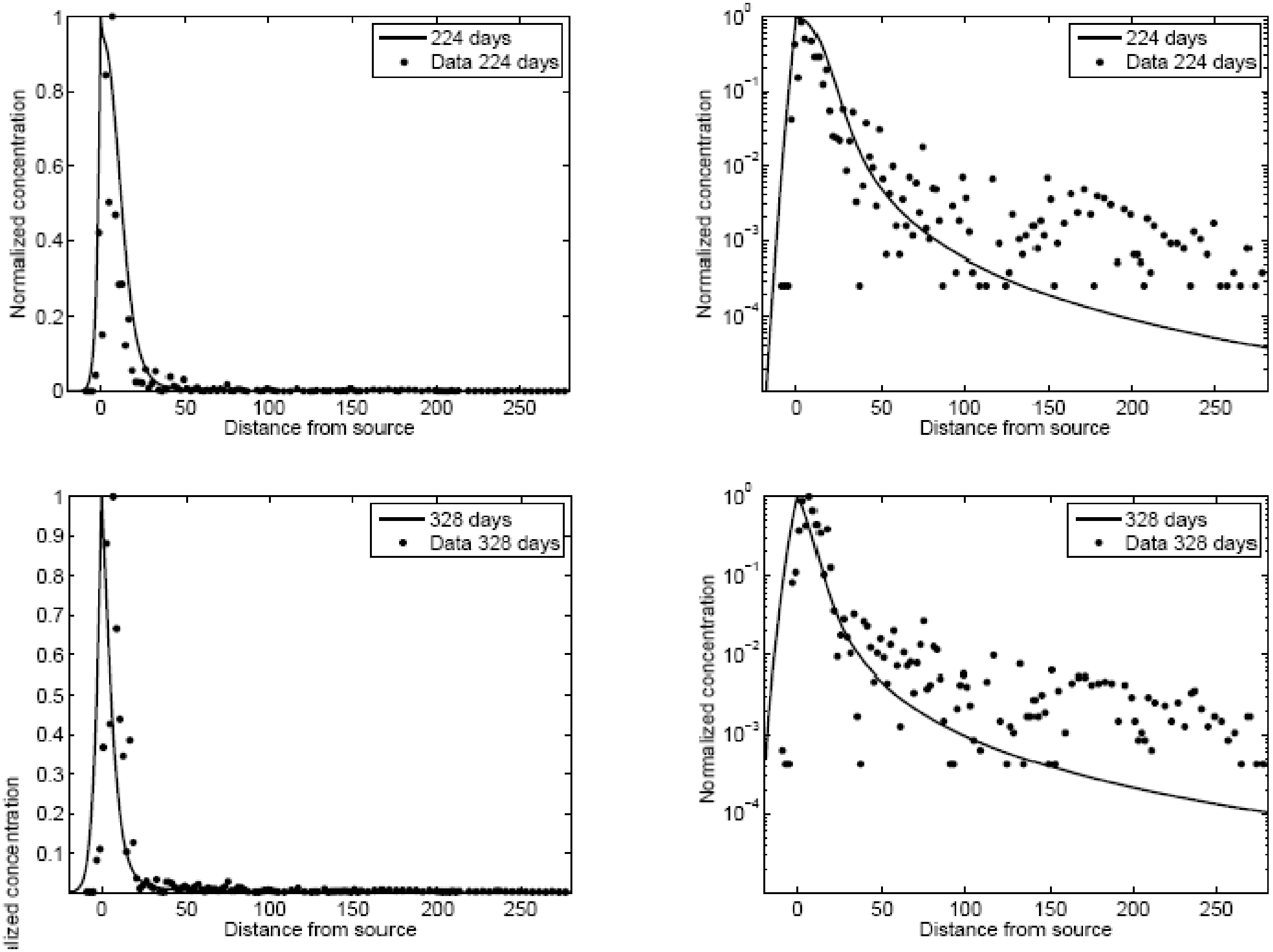
Contaminant transport（II）



Variable order FPDE model

$$D_t^{\alpha[f(x,t)]}c(x,t) = K\frac{\partial^2 c(x,t)}{\partial x^2}, \quad 0 < \alpha[f(x,t)] < 1.$$

Contaminant transport（II）

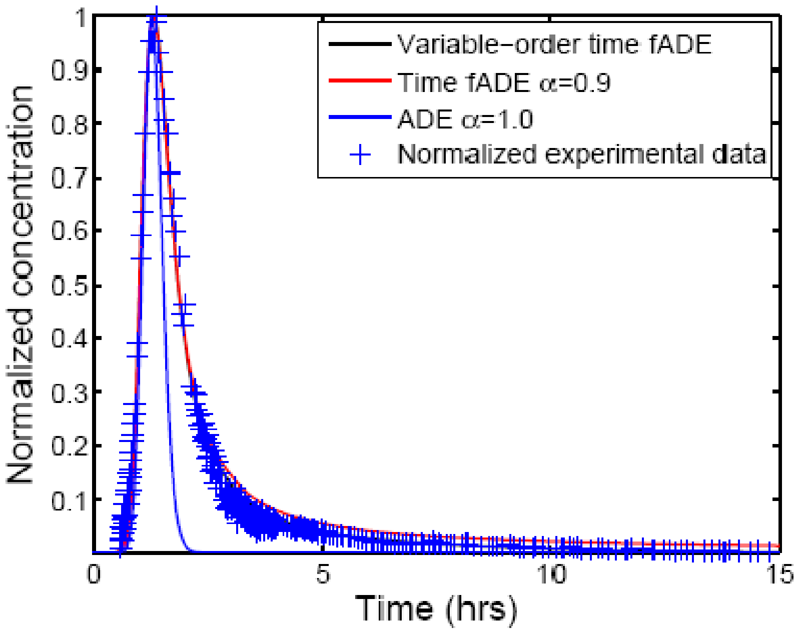


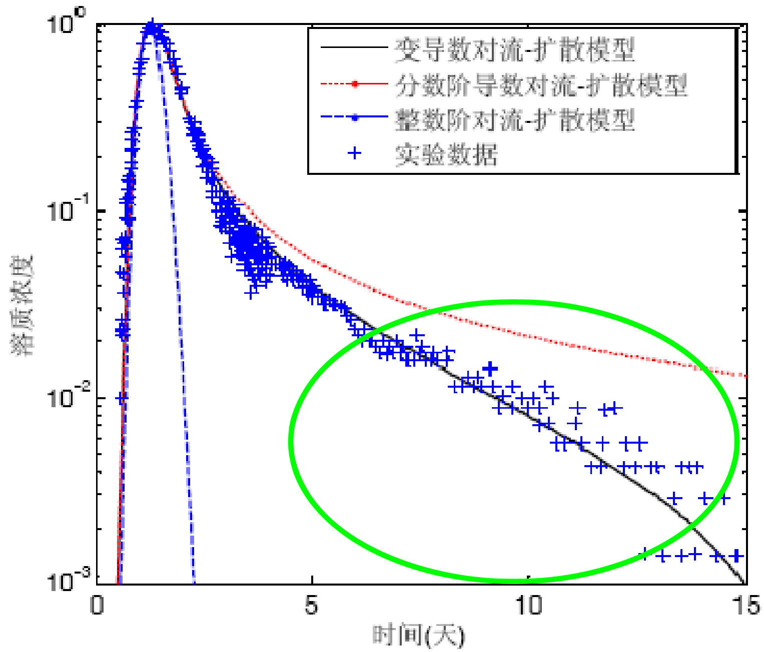
Variable order FPDE model

$$D_t^{\alpha[f(x,t)]}c(x,t) = K\frac{\partial^2 c(x,t)}{\partial x^2}, \quad 0 < \alpha[f(x,t)] < 1.$$

Contaminant transport（III）

Transport process of Sodium fluorescein in Natural fractured media (Grimsel , Switzerland)





Factors on diffusion behavior: Media structure, porosity, saturation

Kosakowski, G., et al., *PSI Rep. 05-03*, Paul Scherrer Inst., Switzerland, 2005.

Numerical methods for spatial fractional derivative equations

- **Finite difference methods** (FDM)

- **Random walker model (RWM) for anomalous diffusion**

- **Comparison between FDM and RWM**:

  1. The RWM is based on mechanics and physics of anomalous diffusion process

  2. The FDM is a type of numerical solution method for fractional derivative equations.

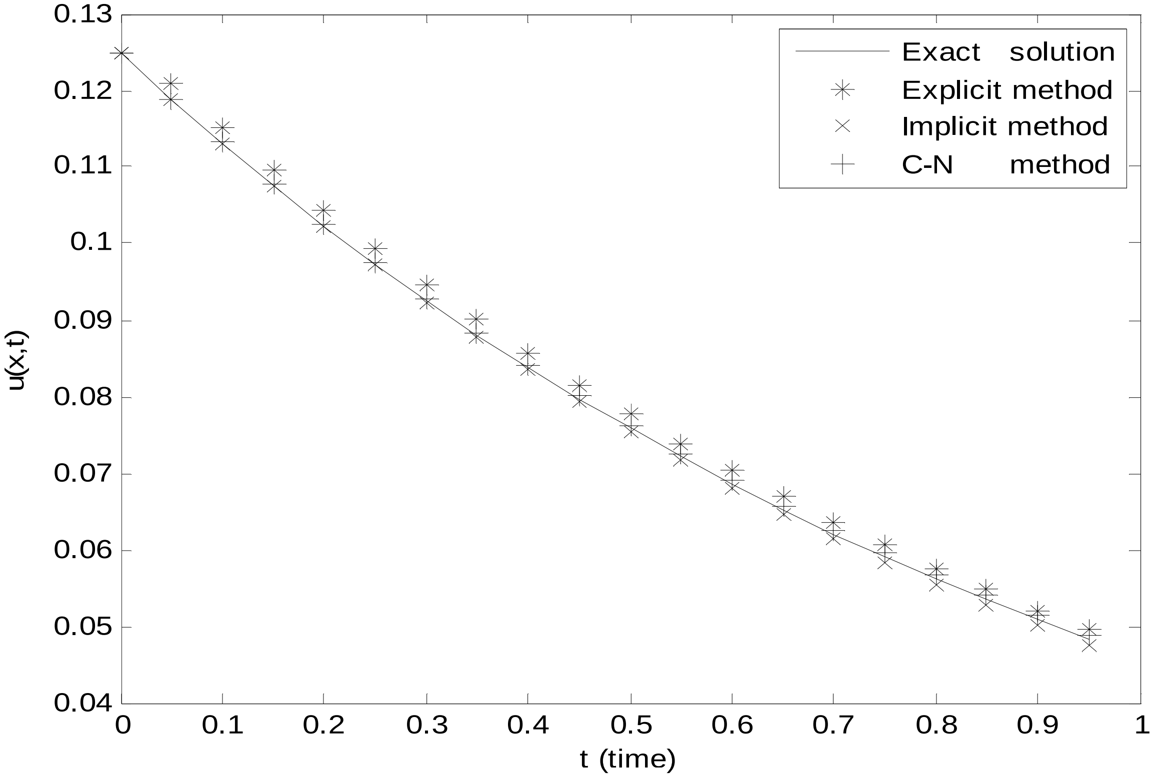
Numerical examples — Spatial fractional anomalous diffusion equation

$$\begin{cases} \dfrac{\partial u(x,t)}{\partial t} = d(x,t)\dfrac{\partial^{\alpha} u(x,t)}{\partial x^{\alpha}} + q(x,t), \quad 1 < \alpha \le 2 \\ u(x_L,t) = a(t); u(x_M,t) = b(t) \\ u(x,0) = c(x) \end{cases}$$

Master equation for various anomalous diffusions in porous media, complex fluids and turbulence.

Finite difference method for spatial anomalous diffusion equation

$\alpha = 1.8$

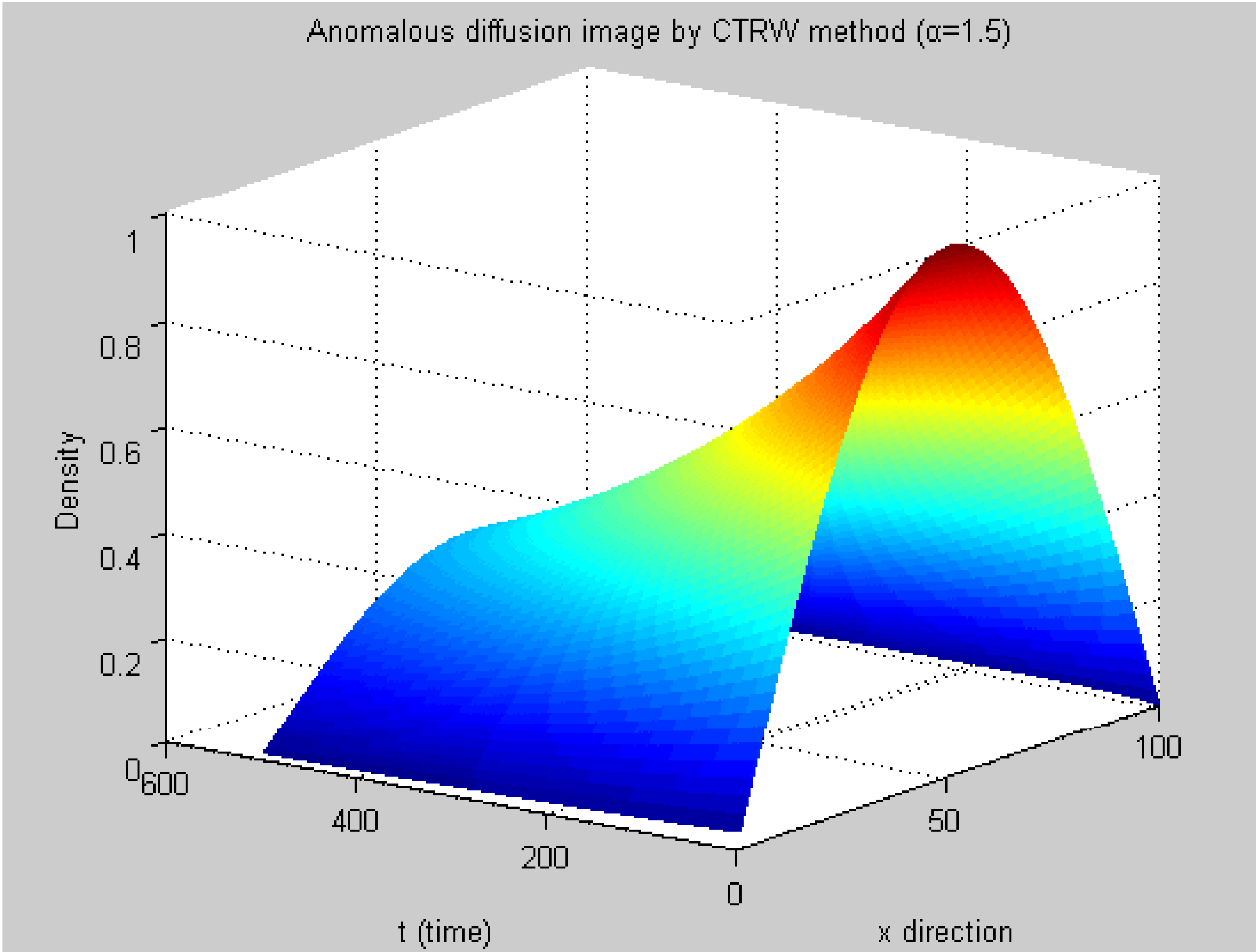


Comparison of numerical and analytical solutions at x=0.45

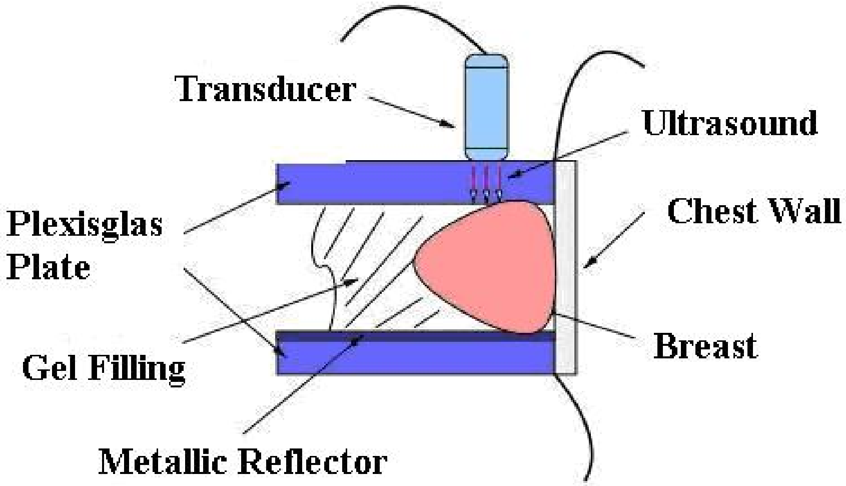
$$d(x,t) = \Gamma(2.2)x^{2.8}/6; q(x,t) = -(1+x)e^{-t}x^3$$

$$u(0,t) = 0; u(x_M,t) = e^{-t} \quad u(x,0) - x^3.$$

Continuous Time Random Walk

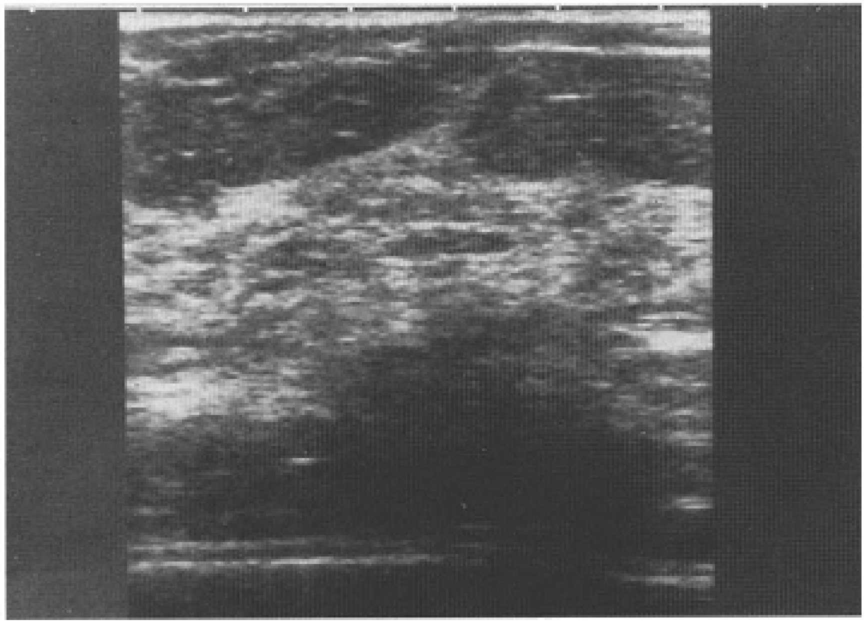


Ultrasonic Medical Imaging



Configuration of the CARI imaging of breast tumor

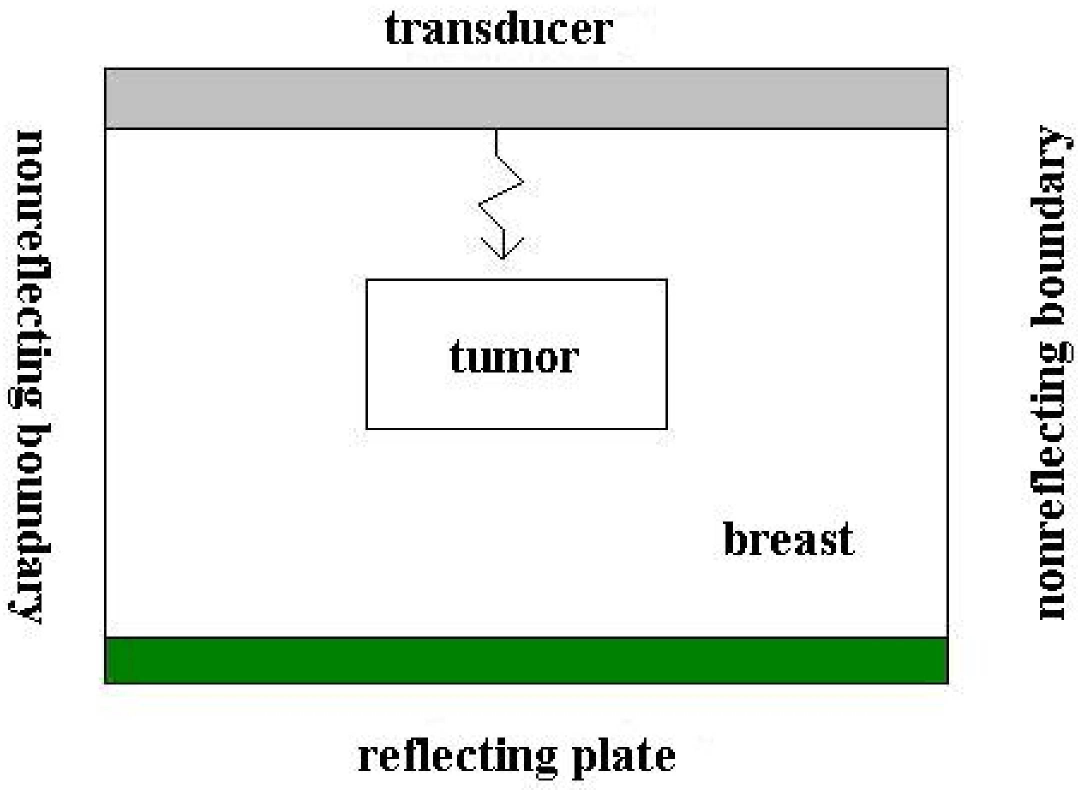
Ultrasonics, 42, 919-925, 2004



Imaging figure of breast tumors by CARI

Retrieved from http://www.ncbi.nlm.nih.gov/pubmed/7591649

Fractional Laplacian wave equation



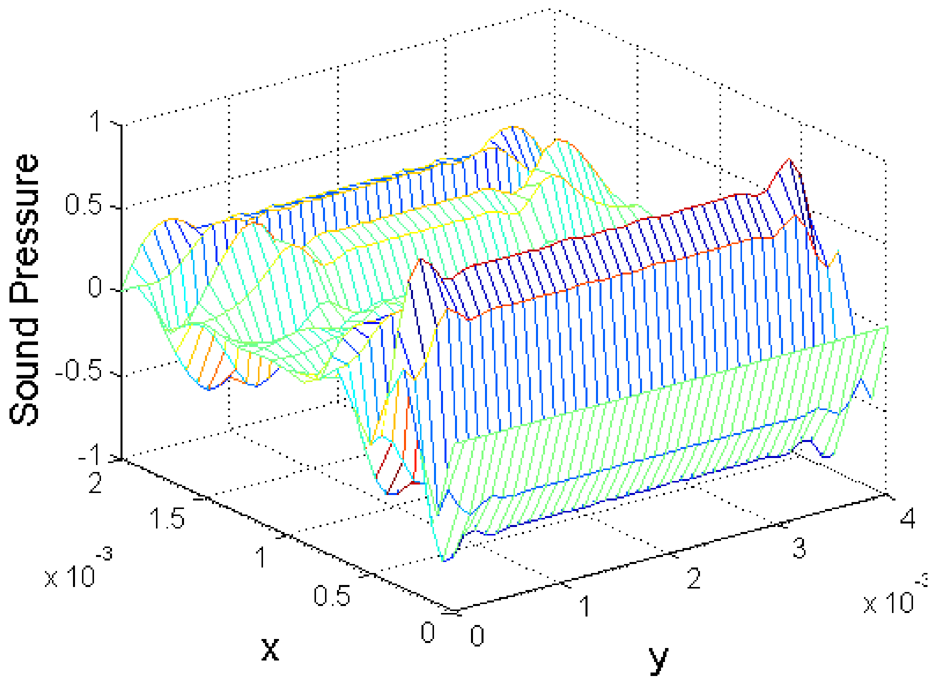
2D configuration of the CARI technique of breast tumors

$$\Delta p = \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + \frac{2\alpha_0}{c_0^{1-\eta}}\frac{\partial}{\partial t}(-\Delta)^{\eta/2} p$$

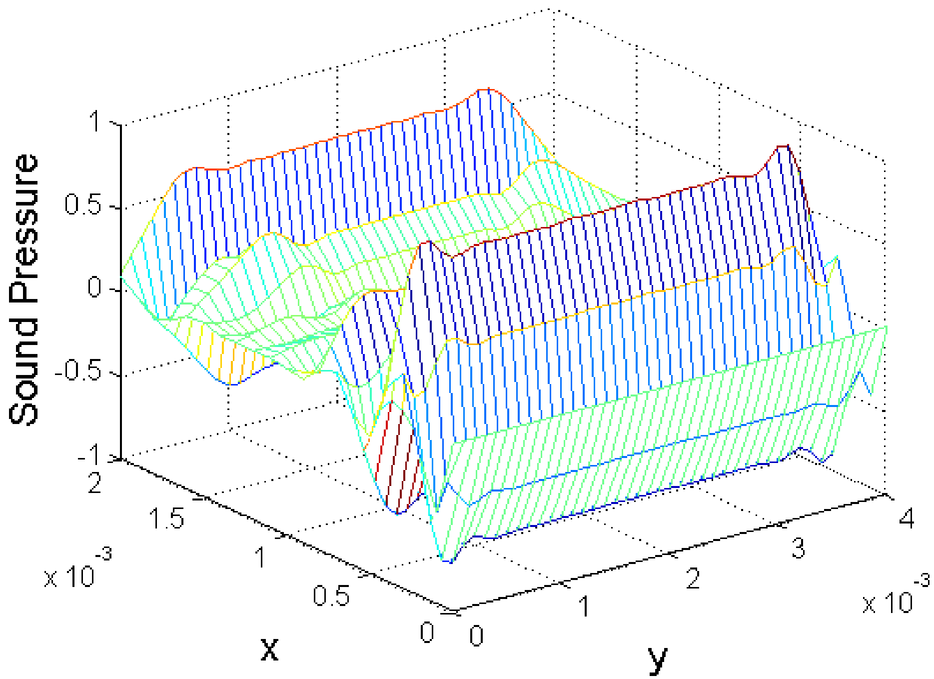
α_{0fat}=15.8/(2π)$^{1.7}$dB/m/MHz$^{1.7}$, c_{0fat}=1475m/s, η_{fat} =1.7

α_{0tum}=57.0/(2π)$^{1.3}$dB/m/MHz$^{1.3}$, c_{0tum}=1527m/s, η_{tum} =1.3

Numerical solution-1



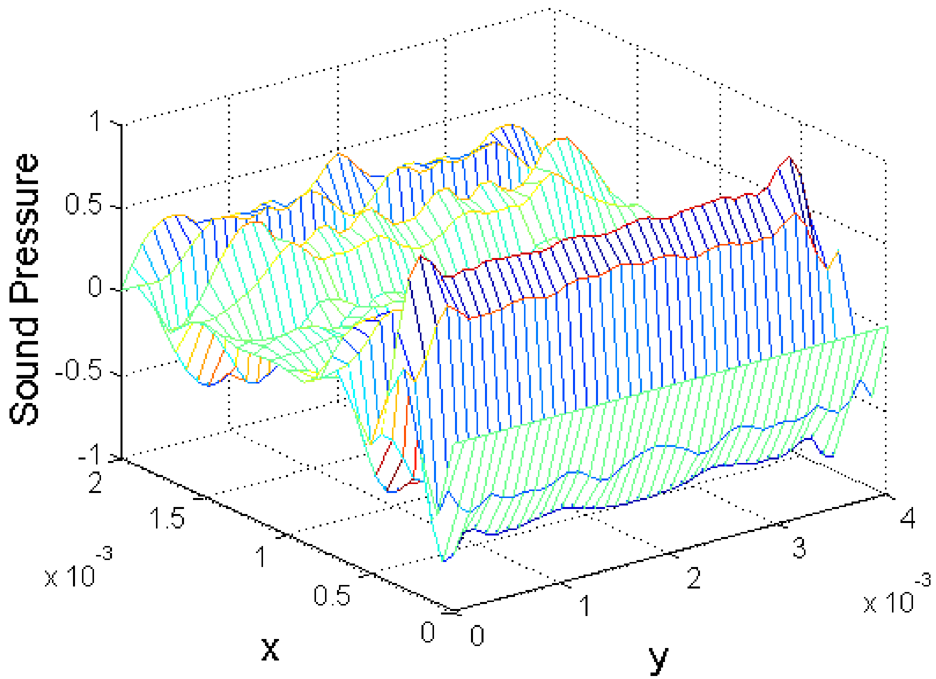
Human fatty tissue



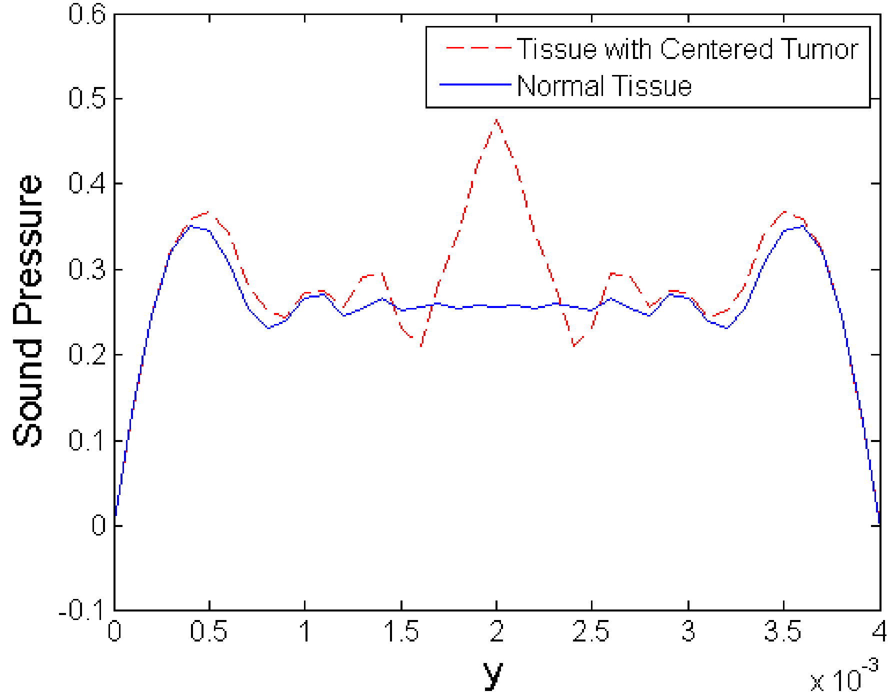
Human tumor tissue

Figure 3.75MHz ultrasound propagation at t=1.3μs

Numerical solution-2

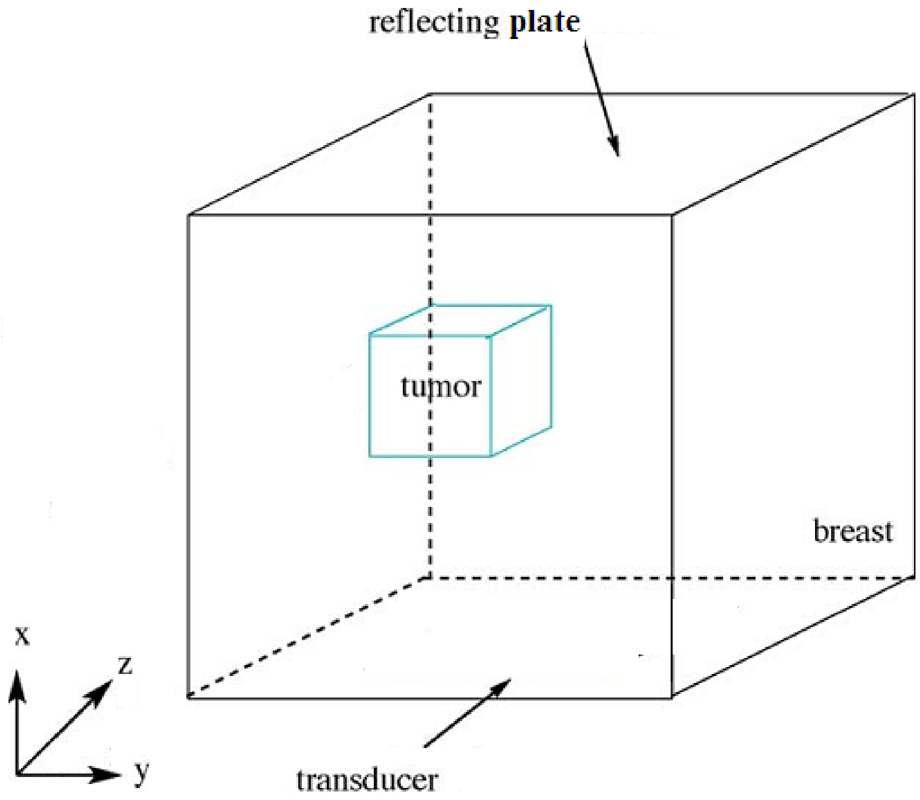


Tissue with a 0.4mm×0.4mm centered tumor under 3.75MHz ultrasound propagation at t=1.3μs



Normalized sound pressure along the reflecting line (*x*=2mm) when *t*=1.3μs.

Modified Szabo's wave equation



3D configuration of the CARI technique of breast tumors

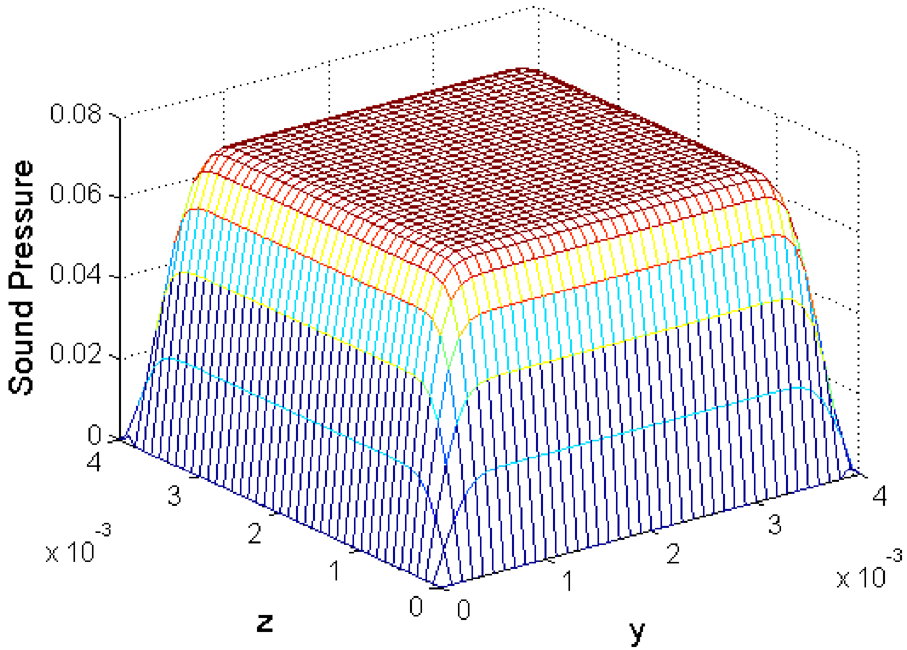
$$\Delta p = \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + \frac{2\alpha_0}{c_0 \cos\frac{\eta\pi}{2}}\frac{\partial^{\eta+1} p}{\partial t^{\eta+1}}$$

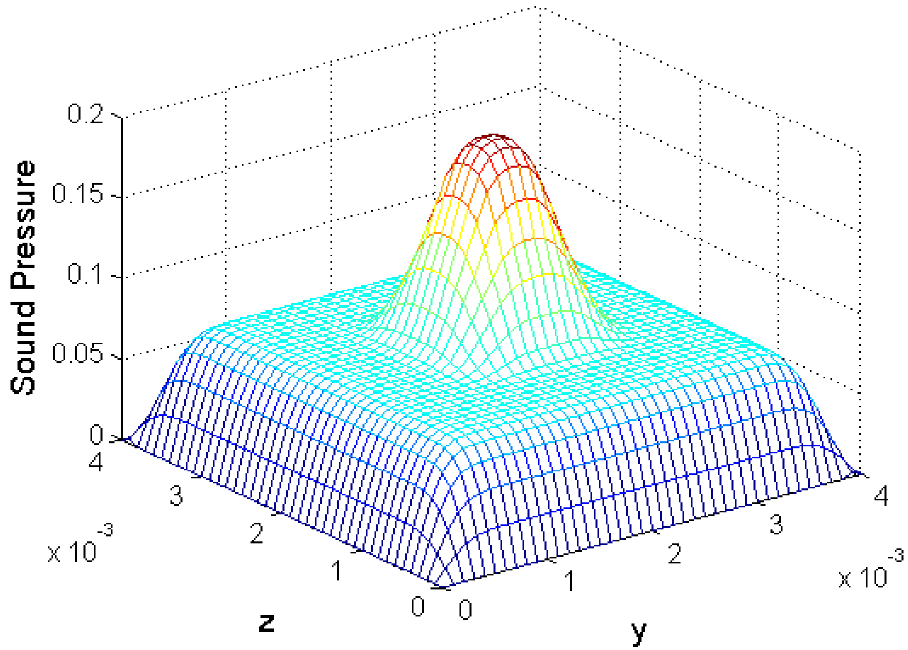
$(0 < \eta < 2,\ \eta \neq 1)$

α_{0F} =15.8/(2π)$^{1.7}$dB/m/MHz$^{1.7}$,
c_{0F}=1475m/s, η_F=1.7

α_{0T}=57.0/(2π)$^{1.3}$dB/m/MHz$^{1.3}$,
c_{0T} =1527m/s, η_T =1.3

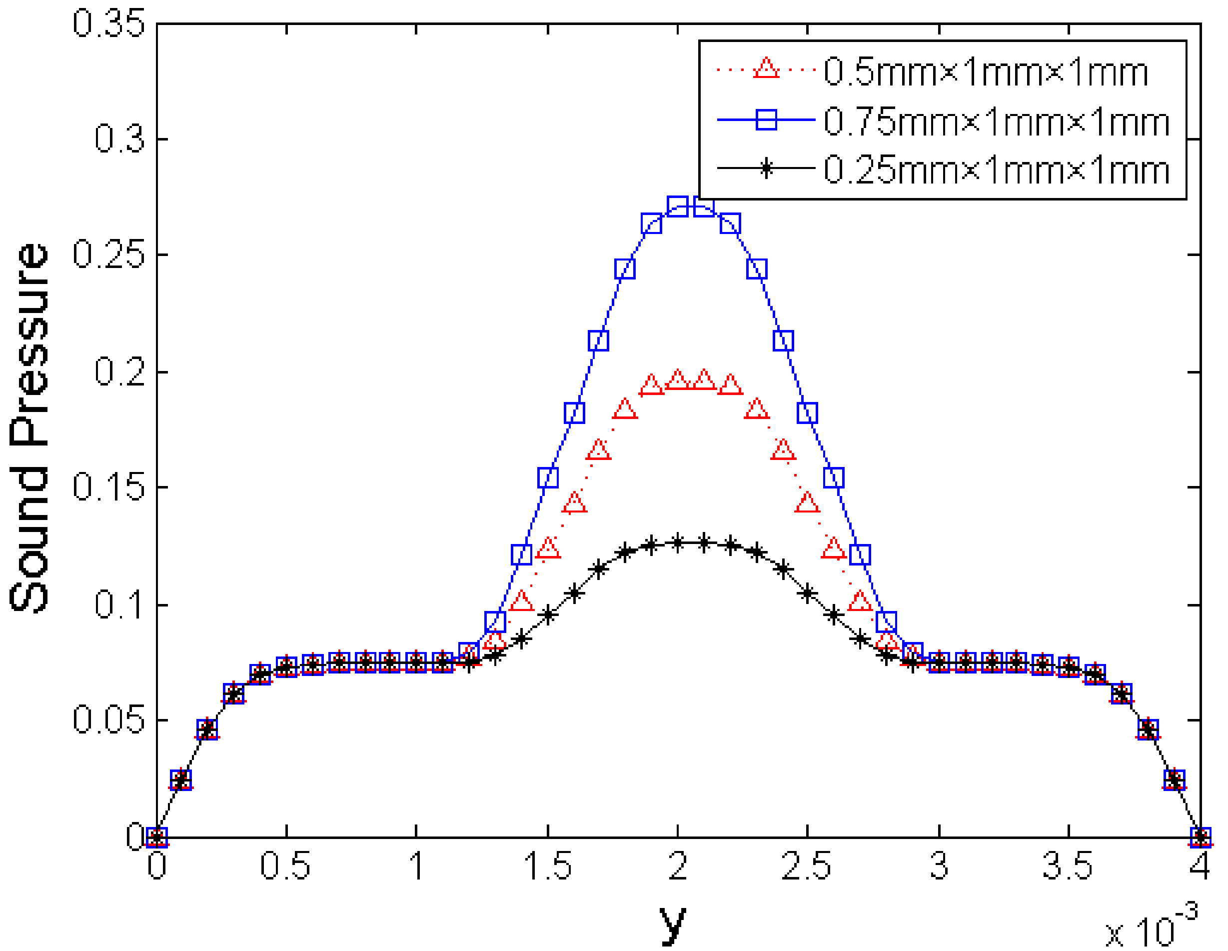
Numerical solution-1





Normalized sound pressure on the reflecting plate (x=2mm) at time t=1.3μs of normal (fatty) tissue and tissue with a centered 0.5mm×1mm×1mm tumor

Numerical solution-2



Normalized sound pressure along the reflecting line (x=2mm, z=2mm) at time t=1.3μs versus axial sizes of tumors

Summary of numerical methods

- The Caputo definition of fractional derivative is suitable for time fractional derivative equation discretization.
- The Grunwald-Letnikov and the Riesz–Feller definitions can be used to the discretization of spatial fractional derivative equations.
- Variable order FPDE model may be a choice to describe the contaminant transport in natural media
- Random walk model has more explicit mechanics significance but is feasible only for a particular use, anomalous diffusion.
- Laplace transformed Meshless method may be a competitive method to save the computing cost for long-range time simulation

Opening issues

- The solution of large-scale fractional models is still a challenging issue thanks to the exponential increase of CPU time and storage requirements with expanding space domain；
- The solution of multidimensional fractional space derivative equation has not been reported in literature；
- Implementation of boundary conditions in fractional space derivative models；
- No commercial codes available for fractional derivative models.

Comments

- Finite difference methods are of a dominant numerical scheme for fractional derivative models；
- Numerical methods for fractional time derivative equations are much more mature than those for fractional spatial derivative equations;
- Very little research on stability, convergence, accuracy of meshless methods for fractional derivative equations.
- Variable order FPDE model or Constant order FPDE model

Outlook: A challenge, an opportunity

- Fast computational methods；
- Basic computational mathematics issues of fractional derivative equations;
- Related computational mechanics software；
- Inherent relationship between fractional derivative equations and statistical mechanics approaches.

More information

- **Website for fractional dynamics and power law phenomena**：
  http://www.ismm.ac.cn/ismmlink/PLFD/index_c.html

- **Conferences**： ASME Workshop on "Fractional calculus modeling", each odd year (e.g. Sept. 4-7, 2007, Las Vegas)， IFA Workshop on "Fractional calculus and its Applications", France 2004, Portugal 2006, Turkey 2008, Spain 2010, China 2012, Some physicist conferences about "anomalous diffusion", e.g., Denmark 2003, New Zealand 2005.

Search Indices:

- Geophysics, bioinformatics, soft matter, porous media
- frequency dependency, power law, non-gradient law
- History- and path-dependent process, memory
- Levy stable distribution, fractional Brownian motion
- Fractal, microstructures, self-similarity
- Fractional calculus, fractional derivative
- Entropy, irreversibility

Thanks!

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http://www.ismm.ac.cn/ismmlink/PLFD/index_c.html