Anomalous Diffusion, Fractional Differential Equations, High Order Discretization Schemes

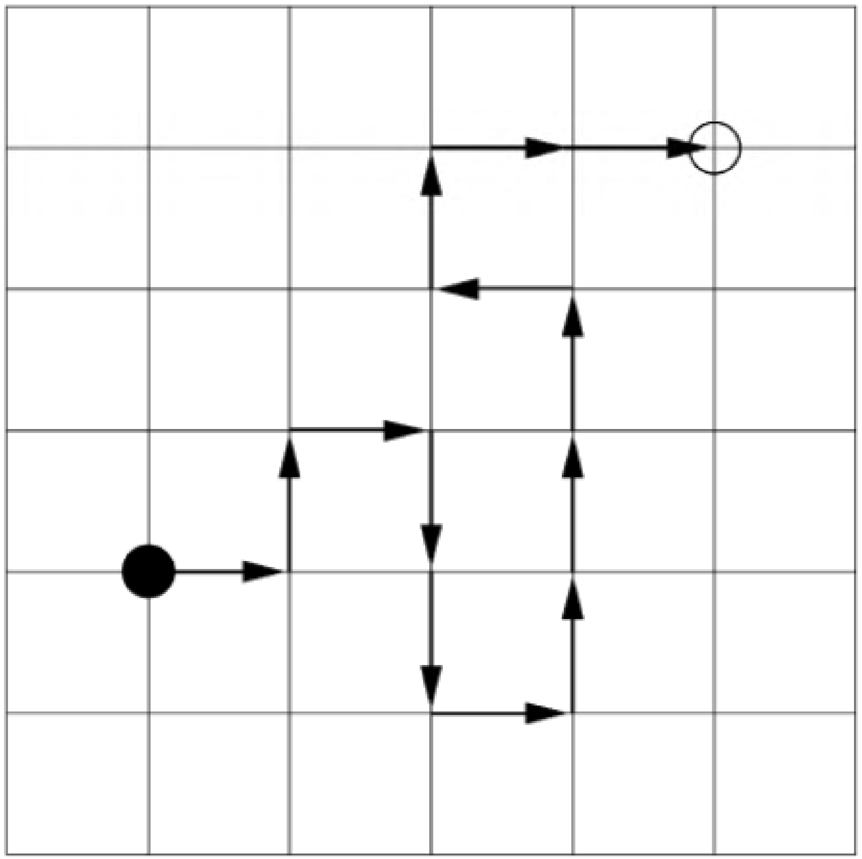
Weihua Deng

Lanzhou University

Email: dengwh@lzu.edu.cn

DTRW Model, Diffusion Equation

Albert Einstein, 1905



$$W_j(t+\Delta t) = \tfrac{1}{2}W_{j-1}(t) + \tfrac{1}{2}W_{j+1}(t)$$

$$W_j(t+\Delta t) = W_j(t) + \Delta t\frac{\partial W_j}{\partial t} + O([\Delta t]^2)$$

$$W_{j\pm1}(t) = W(x,t) \pm \Delta x\frac{\partial W}{\partial x} + \frac{(\Delta x)^2}{2}\frac{\partial^2 W}{\partial x^2} + O([\Delta x]^3)$$

$$\frac{\partial W}{\partial t} = K_1\frac{\partial^2}{\partial x^2}W(x,t)$$

Fick's Laws hold here!

Superdiffusion

The pdf of jump length: $\eta(x) \sim x^{-(1+\beta)}, \;\; 0 < \beta < 2$

$$\frac{\partial W}{\partial t} = K_1 \frac{\partial^\beta W}{\partial x^\beta}$$

$$\langle x^2(t) \rangle \sim K_\beta t^{\frac{2}{\beta}}$$

Competition between Subdiffusion and Superdiffusion

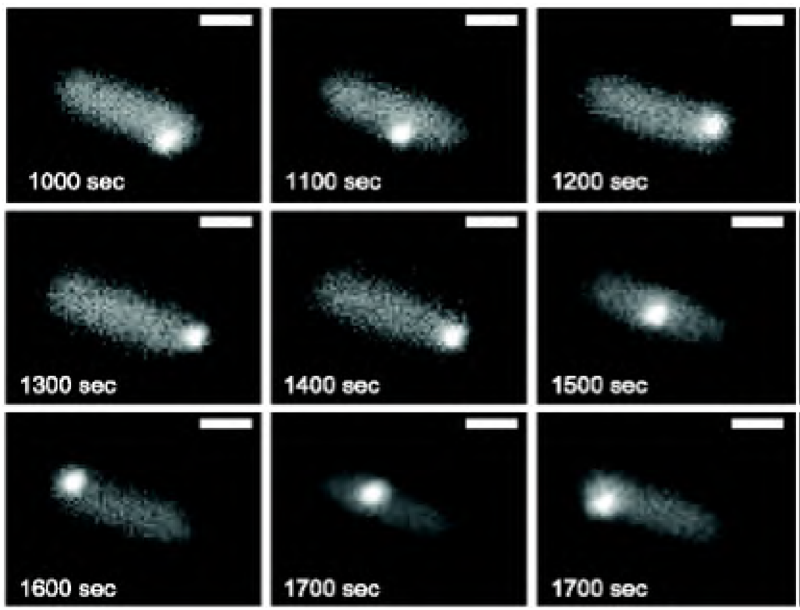
The pdf of waiting time: $\psi(t) \sim t^{-(1+\alpha)},\ \ 0 < \alpha < 1$

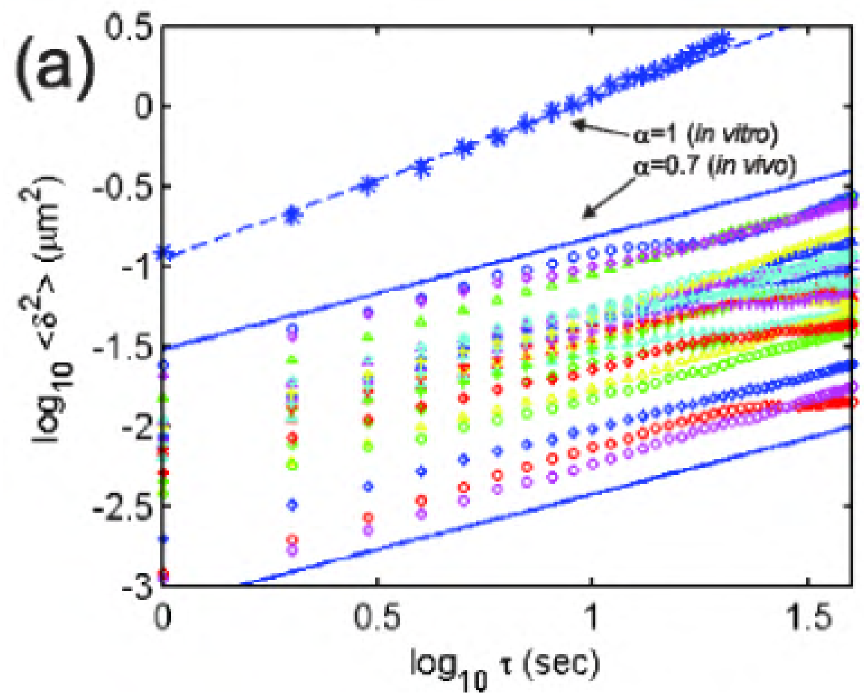
The pdf of jump length: $\eta(x) \sim x^{-(1+\beta)},\ \ 0 < \beta < 2$

$$\frac{\partial^{\alpha} W}{\partial t^{\alpha}} = K_1 \frac{\partial^{\beta} W}{\partial x^{\beta}} \qquad \left\langle x^2(t) \right\rangle \sim K_{\beta} t^{\frac{2\alpha}{\beta}}$$

Examples of Subiffusion

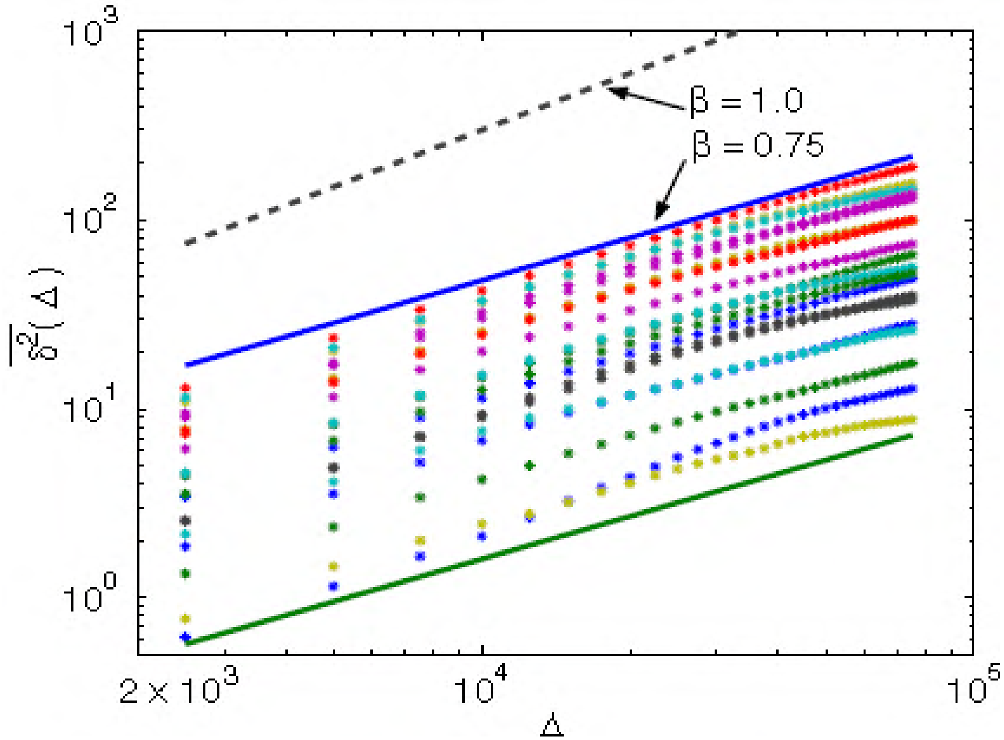
Trajectories of the motion of individual fluorescently labeled mRNA molecules inside live E. coli cells:





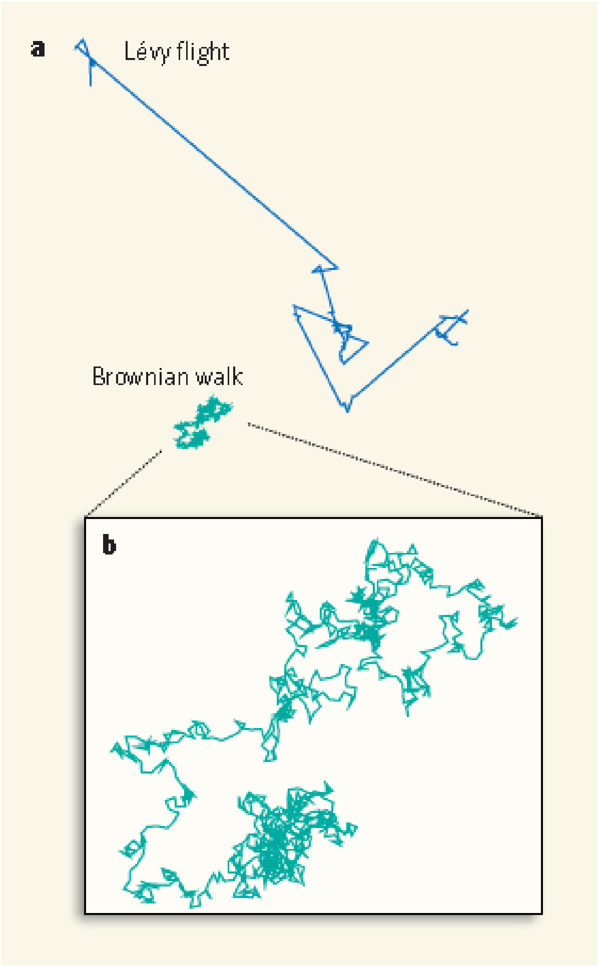
I. Golding and E.C. Cox,, Phys. Rev. Lett., 96, 098102, 2006.

Simulation Results



Y. He, S. Burov, R. Metzler, and E. Barkai, Phys. Rev. Lett., 101, 058101, 2008.

Applications of Superdiffusion



N.E. Humphries et al, Nature, 465, 1066-1069, 2010;
M. Viswanathan, Nature, 1018-1019, 2010;
Viswanathan, G. M. et al. Nature, 401, 911-914, 1999.

Where to locate N radar stations to optimize the search for M targets?

1. Lévy walkers can outperform Brownian walkers by revisiting sites far less often.
2. The number of new visited sites is much larger for N Levy walkers than for N brownian walkers.

Definitions of Fractional Calculus

Fractional Integral

$$\int_a^x d\xi_n \int_a^{\xi_n} d\xi_{n-1} \cdots \int_a^{\xi_2} v(\xi_1) d\xi_1 = \frac{1}{(n-1)!} \int_a^x (x-\xi)^{n-1} v(\xi) d\xi, \quad x > a,$$

$$_aD_x^{-n} v(x) = \frac{1}{\Gamma(n)} \int_a^x (x-\xi)^{n-1} v(\xi) d\xi, \quad x > a.$$

$$_aD_x^{-\alpha} v(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-\xi)^{\alpha-1} v(\xi) d\xi, \quad x > a, \quad \alpha \in \mathbb{R}^+$$

Fractional Derivatives

Riemann-Liouville Derivative

$$_{\mathrm{RL}}D_{0,t}^{\alpha} x(t) = \frac{\mathrm{d}^m}{\mathrm{d}t^m} D_{0,t}^{-(m-\alpha)} x(t) = \frac{1}{\Gamma(m-\alpha)} \frac{\mathrm{d}^m}{\mathrm{d}t^m} \int_0^t (t-\tau)^{m-\alpha-1} x(\tau)\, \mathrm{d}\tau$$

Caputo Derivative

$$_{\mathrm{C}}D_{0,t}^{\alpha} x(t) = D_{0,t}^{-(m-\alpha)} \frac{\mathrm{d}^m}{\mathrm{d}t^m} x(t) = \frac{1}{\Gamma(m-\alpha)} \int_0^t (t-\tau)^{m-\alpha-1} x^{(m)}(\tau)\, \mathrm{d}\tau$$

Grunwald Letnikov Derivative

$$_{\mathrm{GL}}D_{0,t}^{\alpha} x(t) = \lim_{h \to 0, nh = t} h^{-\alpha} \sum_{k=0}^{n} (-1)^k \binom{p}{k} x(t-kh)$$

$$= \sum_{k=0}^{m-1} \frac{x^{(k)}(0) t^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{\Gamma(m-\alpha)} \int_0^t (t-\tau)^{m-\alpha-1} x^{(m)}(\tau)\, \mathrm{d}\tau$$

Hadamard Integral

$$\int_a^b (x-a)^{-\mu}\, \mathrm{d}x = \frac{1}{1-\mu}(b-a)^{1-\mu} \qquad (\mu > 1)$$

$$\frac{1}{\Gamma(1-\mu)} \int_a^b (b-x)^{-\mu} f(x)\, \mathrm{d}x = \sum_{k=0}^{m-1} \frac{(b-a)^{k-\mu+1}}{\Gamma(k-\mu+2)} f^{(k)}(a) + J_a^{m-\mu+1} f^{(m)}(b)$$

Existing Discretization Schemes

Shifted Grunwald Letnikov Discretization (Meerschaert and Tadjeran, 2004, JCAM), most widely used

Transforming into Caputo Derivative

Centralinzed Finite Difference Scheme with Piecewise Linear Approximation

Hadamard Integral

A Class of Second Order Schemes

(Lanzhou group)

Based on the Analysis in Frequency Domain by Combining the Different Shifted Grunwald Letnikov Discretizations

The shifted Grunwald Letnikov Discretization

$$A_{h,p}^{\alpha}u(x) = \frac{1}{h^{\alpha}}\sum_{k=0}^{\infty} g_k^{(\alpha)} u(x-(k-p)h)$$

which has first order accuracy, i.e.,

$$A_{h,p}^{\alpha}u(x) = {}_{-\infty}D_x^{\alpha}u(x) + O(h)$$

What happens if

$${}_L\mathcal{D}_{h,p,q}^{\alpha}u(x) = \frac{\lambda_1}{h^{\alpha}}\sum_{k=0}^{\infty} g_k^{(\alpha)} u(x-(k-p)h) + \frac{\lambda_2}{h^{\alpha}}\sum_{k=0}^{\infty} g_k^{(\alpha)} u(x-(k-q)h)$$

Taking Fourier Transform on both Sides of above Equation, there exists

$$
\begin{aligned}
\mathscr{F}[{}_L\mathcal{D}^{\alpha}_{h,p,q}u](\omega) &= \frac{1}{h^{\alpha}}\sum_{k=0}^{\infty} g_k^{(\alpha)}\Big(\lambda_1 \mathrm{e}^{-i\omega(k-p)h} + \lambda_2 \mathrm{e}^{-i\omega(k-q)h}\Big)\hat{u}(\omega) \\
&= \frac{1}{h^{\alpha}}\Big(\lambda_1(1-\mathrm{e}^{-i\omega h})^{\alpha}\mathrm{e}^{i\omega hp} + \lambda_2(1-\mathrm{e}^{-i\omega h})^{\alpha}\mathrm{e}^{i\omega hq}\Big)\hat{u}(\omega) \\
&= (i\omega)^{\alpha}\Big(\lambda_1 W_p(i\omega h) + \lambda_2 W_q(i\omega h)\Big)\hat{u}(\omega),
\end{aligned} \tag{2.9}
$$

where

$$
W_r(z) = \Big(\frac{1-\mathrm{e}^{-z}}{z}\Big)^{\alpha}\mathrm{e}^{rz} = 1 + (r-\frac{\alpha}{2})z + O(z^2),\ \ r = p, q. \tag{2.10}
$$

In order to have second order accuracy, coefficients λ_1 and λ_2 satisfy

$$
\begin{cases}
\lambda_1 + \lambda_2 = 1, \\
(p-\dfrac{\alpha}{2})\lambda_1 + (q-\dfrac{\alpha}{2})\lambda_2 = 0,
\end{cases}
$$

which indicates that $\lambda_1 = \frac{\alpha-2q}{2(p-q)}$ and $\lambda_2 = \frac{2p-\alpha}{2(p-q)}$.

Denoting $\hat{\phi}(\omega,h) = \mathscr{F}[{}_L\mathcal{D}^{\alpha}_{h,p,q}u](\omega) - \mathscr{F}[{}_{-\infty}D^{\alpha}_x u](\omega)$, then from (2.9) and (2.10) there exists

$$
|\hat{\phi}(\omega,h)| \le Ch^2|i\omega|^{\alpha+2}|\hat{u}(\omega)|. \tag{2.11}
$$

With the condition $\mathscr{F}[{}_{-\infty}D^{\alpha+2}_x u](\omega) \in L^1(\mathbb{R})$, it yields

$$
|{}_L\mathcal{D}^{\alpha}_{h,p,q}u - {}_{-\infty}D^{\alpha}_x u| = |\phi| \le \frac{1}{2\pi}\int_{\mathbb{R}} |\hat{\phi}(\omega,h)| \le C\|\mathscr{F}[{}_{-\infty}D^{\alpha+2}_x u](\omega)\|_{L^1}h^2 = O(h^2). \tag{2.12}
$$

We introduce the WSGD operator

$$ {}_{L}\mathcal{D}^{\alpha}_{h,p,q}u(x) = \frac{\alpha - 2q}{2(p-q)} A^{\alpha}_{h,p}u(x) + \frac{2p-\alpha}{2(p-q)} A^{\alpha}_{h,q}u(x), $$

and there exists

$$ {}_{L}\mathcal{D}^{\alpha}_{h,p,q}u(x) = {}_{-\infty}D^{\alpha}_{x}u(x) + O(h^2) $$

Similarly, for the right Riemann-Liouville derivative

$$ {}_{R}\mathcal{D}^{\alpha}_{h,p,q}u(x) = \frac{\alpha - 2q}{2(p-q)} B^{\alpha}_{h,p}u(x) + \frac{2p-\alpha}{2(p-q)} B^{\alpha}_{h,q}u(x) = {}_{x}D^{\alpha}_{\infty}u(x) + O(h^2) $$

uniformly for $x \in \mathbb{R}$ under the conditions that $u \in L^1(\mathbb{R})$, ${}_{x}D^{\alpha+2}_{\infty}u$ and its Fourier transform belong to $L^1(\mathbb{R})$, where p, q are integers and

$$ B^{\alpha}_{h,r}u(x) = \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} g^{(\alpha)}_{k} u(x + (k-r)h). $$

The simplified forms of the discreted approximations (2.15) for Riemann-Liouville fractional derivatives on grid points $\{x_i = a + ih, h = (b-a)/n, i = 1, \ldots, n-1\}$ with $(p,q) = (1,0)$, $(1,-1)$ are

$$\begin{aligned} {}_aD_x^\alpha u(x_i) &= \frac{1}{h^\alpha}\sum_{k=0}^{i+1} w_k^{(\alpha)} u(x_{i-k+1}) + O(h^2), \\ {}_xD_b^\alpha u(x_i) &= \frac{1}{h^\alpha}\sum_{k=0}^{N-i+1} w_k^{(\alpha)} u(x_{i+k-1}) + O(h^2), \end{aligned} \tag{2.16}$$

where

$$\begin{cases} (p,q) = (1,0), & w_0^{(\alpha)} = \dfrac{\alpha}{2} g_0^{(\alpha)}, \ w_k^{(\alpha)} = \dfrac{\alpha}{2} g_k^{(\alpha)} + \dfrac{2-\alpha}{2} g_{k-1}^{(\alpha)}, \ k \geq 1; \\ (p,q) = (1,-1), & w_0^{(\alpha)} = \dfrac{2+\alpha}{4} g_0^{(\alpha)}, \ w_1^{(\alpha)} = \dfrac{2+\alpha}{4} g_1^{(\alpha)}, \\ & w_k^{(\alpha)} = \dfrac{2+\alpha}{4} g_k^{(\alpha)} + \dfrac{2-\alpha}{4} g_{k-2}^{(\alpha)}, \ k \geq 2. \end{cases} \tag{2.17}$$

Theorem 2.13. *Let matrix A be of the following form,*

$$A = \begin{pmatrix} w_1^{(\alpha)} & w_0^{(\alpha)} & & & \\ w_2^{(\alpha)} & w_1^{(\alpha)} & w_0^{(\alpha)} & & \\ \vdots & w_2^{(\alpha)} & w_1^{(\alpha)} & \ddots & \\ w_{n-2}^{(\alpha)} & \cdots & \ddots & \ddots & w_0^{(\alpha)} \\ w_{n-1}^{(\alpha)} & w_{n-2}^{(\alpha)} & \cdots & w_2^{(\alpha)} & w_1^{(\alpha)} \end{pmatrix}, \tag{2.20}$$

where the diagonals $\{w_k^{(\alpha)}\}_{k=0}^{n-1}$ are the coefficients given in (2.16) corresponding to $(p,q) = (1,0)$ or $(1,-1)$. Then we have that any eigenvalue λ of A satisfies

(1) $\mathrm{Re}(\lambda) \equiv 0$, *for* $(p,q) = (1,0)$, $\alpha = 1$,
(2) $\mathrm{Re}(\lambda) < 0$, *for* $(p,q) = (1,0)$, $1 < \alpha \le 2$,
(3) $\mathrm{Re}(\lambda) < 0$, *for* $(p,q) = (1,-1)$, $1 \le \alpha \le 2$.

Moreover, when $1 < \alpha \le 2$, matrix A is negative definite, and the real parts of the eigenvalues of matrix $c_1 A + c_2 A^{\mathrm{T}}$ are less than 0, where $c_1, c_2 \ge 0, c_1^2 + c_2^2 \ne 0$.

Third Order Approximation

$$ {}_L\mathcal{G}^{\alpha}_{h,p,q,r}u(x) = \lambda_1 A^{\alpha}_{h,p}u(x) + \lambda_2 A^{\alpha}_{h,q}u(x) + \lambda_3 A^{\alpha}_{h,r}u(x) $$

where p, q, r are integers and mutually non-equal, and

$$ \lambda_1 = \frac{12qr - (6q + 6r + 1)\alpha + 3\alpha^2}{12(qr - pq - pr + p^2)}, \quad \lambda_2 = \frac{12pr - (6p + 6r + 1)\alpha + 3\alpha^2}{12(pr - pq - qr + q^2)}, \quad \lambda_3 = \frac{12pq - (6p + 6q + 1)\alpha + 3\alpha^2}{12(pq - pr - qr + r^2)}. \tag{2.24} $$

Assuming $u \in L^1(\mathbb{R})$, and taking Fourier transform on (2.23), we get

$$ \begin{aligned} \mathscr{F}[{}_L\mathcal{G}^{\alpha}_{h,p,q,r}u](\omega) &= (i\omega)^{\alpha}\Big(\lambda_1 W_p(i\omega h) + \lambda_2 W_q(i\omega h) + \lambda_3 W_r(i\omega h)\Big)\hat{u}(\omega) \\ &= (i\omega)^{\alpha}\Big(1 + C(i\omega h)^3\Big)\hat{u}(\omega), \end{aligned} \tag{2.25} $$

where $W_s(z)$ is defined in (2.10). If ${}_{-\infty}D^{\alpha+3}_x u$ and its Fourier transform belong to $L^1(\mathbb{R})$, then we have

$$ \begin{aligned} \left|{}_L\mathcal{G}^{\alpha}_{h,p,q,r}u - {}_{-\infty}D^{\alpha}_x u\right| &\le \frac{1}{2\pi}\int_{\mathbb{R}} \left|\mathscr{F}[{}_L\mathcal{G}^{\alpha}_{h,p,q,r}u - {}_{-\infty}D^{\alpha}_x u]\right| \\ &\le C\|\mathscr{F}[{}_{-\infty}D^{\alpha+3}_x u](\omega)\|_{L^1} h^3 = O(h^3). \end{aligned} \tag{2.26} $$

Compact Difference Operator with 3rd Order Accuracy

Substituting

$$\frac{1}{h^\alpha}\sum_{k=0}^{\infty} g_k^{(\alpha)} u\big(x-(k-p)h\big) = {}_{-\infty}D_x^\alpha u(x) + \sum_{l=1}^{n-1}\big(a_{p,l}^\alpha\ {}_{-\infty}D_x^{\alpha+l}u(x)\big)h^l + O\big(h^n\big)$$

into

$${}_L\mathcal{D}_{h,p,q}^\alpha u(x) = \frac{1}{h^\alpha}\sum_{k=0}^{\infty} g_k^{(\alpha)}\left(\frac{\alpha-2q}{2(p-q)}u\big(x-(k-p)h\big) + \frac{2p-\alpha}{2(p-q)}u\big(x-(k-q)h\big)\right)$$

leads to

$${}_L\mathcal{D}_{h,p,q}^\alpha u(x) = \left(1 + c_{p,q,2}^\alpha h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\big({}_{-\infty}D_x^\alpha u(x)\big) + c_{p,q,3}^\alpha\ {}_{-\infty}D_x^{\alpha+3}u(x)h^3 + O\big(h^4\big)$$

Further combining $\delta_x^2 u = \frac{\mathrm{d}^2}{\mathrm{d}x^2}u + O(h^2)$, there exists

$$\mathcal{C}_x u = (1 + c_{p,q,2}^\alpha h^2 \delta_x^2)u = \left(1 + c_{p,q,2}^\alpha h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)u + O\big(h^4\big)$$

We call $\mathcal{C}_x = 1 + c^{\alpha}_{p,q,2} h^2 \delta_x^2$ Compact WSGD operator (CWSGD)

$$ {}_L\mathcal{D}^{\alpha}_{h,p,q} u(x) = \mathcal{C}_x \left({}_a D_x^{\alpha} u(x) \right) + c^{\alpha}_{p,q,3} \, {}_a D_x^{\alpha+3} u(x) h^3 + O\left(h^4\right) $$

$$ {}_R\mathcal{D}^{\alpha}_{h,p,q} u(x) = \mathcal{C}_x \left({}_x D_b^{\alpha} u(x) \right) + c^{\alpha}_{p,q,3} \, {}_x D_b^{\alpha+3} u(x) h^3 + O\left(h^4\right) $$

$$ \frac{\partial u(x,t)}{\partial t} = K_1 \, {}_a D_x^{\alpha} u(x,t) + K_2 \, {}_x D_b^{\alpha} u(x,t) + f(x,t), \quad (x,t) \in (a,b) \times (0,T] $$

In time discretization, using the Crank-Nicolson technique, we obtain

$$ \delta_t u_i^n - \frac{1}{2}\left(K_1 \left({}_a D_x^{\alpha} u \right)_i^n + K_1 \left({}_a D_x^{\alpha} u \right)_i^{n+1} + K_2 \left({}_x D_b^{\alpha} u \right)_i^n + K_2 \left({}_x D_b^{\alpha} u \right)_i^{n+1} \right) = f_i^{n+1/2} + O\left(\tau^2\right) $$

Acting the operator $\tau \mathcal{C}_x$ on both sides of above equation leads to

$$ \begin{aligned} & \mathcal{C}_x u_i^{n+1} - \frac{K_1 \tau}{2} {}_L\mathcal{D}^{\alpha}_{h,p,q} u_i^{n+1} - \frac{K_2 \tau}{2} {}_R\mathcal{D}^{\alpha}_{h,p,q} u_i^{n+1} \\ & \quad = \mathcal{C}_x u_i^n + \frac{K_1 \tau}{2} {}_L\mathcal{D}^{\alpha}_{h,p,q} u_i^n + \frac{K_2 \tau}{2} {}_R\mathcal{D}^{\alpha}_{h,p,q} u_i^n + \tau \mathcal{C}_x f_i^{n+1/2} + \tau \varepsilon_i^{n+1/2} \end{aligned} $$

References:

MATHEMATICS OF COMPUTATION
Volume 00, Number 0, Pages 000–000
S 0025-5718(XX)0000-0

A CLASS OF SECOND ORDER DIFFERENCE APPROXIMATIONS FOR SOLVING SPACE FRACTIONAL DIFFUSION EQUATIONS

WENYI TIAN, HAN ZHOU, AND WEIHUA DENG

J Sci Comput
DOI 10.1007/s10915-012-9661-0

Quasi-Compact Finite Difference Schemes for Space Fractional Diffusion Equations

Han Zhou · WenYi Tian · Weihua Deng