Fast numerical methods and mathematical analysis for space-fractional PDEs

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Fickian and anomalous diffusion processes

- Diffusion processes
  - describe the spreading of particles due to their random movements
  - are ubiquitous in nature, natural and social sciences, and engineering
- Since it was proposed in 1855, the classical diffusion equation
  - has been widely used in different disciplines
  - has generated satisfactory results in various applications
- However, certain diffusion processes cannot be described by the Fickian diffusion equation. They exhibit anomalous diffusion behavior
  - Photocopiers and laser printers played an important role in the study
  - In groundwater contaminant transport, remediation
    - is often not as effective as predicted by the classical diffusion equation
    - may take decades or centuries longer than previously thought
  - Increasingly more diffusion processes have been found to be non-Fickian (Metzler & Klafter, Phys. Rep., 339:1-77, 2000)
    - signaling of biological cells, anomalous electrodiffusion in nerve cells
    - foraging behavior of animals, electrochemistry, physics, finance
    - fluid and continuum mechanics, viscoelastic and viscoplastic flow

$$\frac{\partial u}{\partial t} - d_+(x,t)\frac{\partial^\alpha u}{\partial_+ x^\alpha} - d_-(x,t)\frac{\partial^\alpha u}{\partial_- x^\alpha} = f, \quad x \in (x_l, x_r), \ t \in (0,T], \tag{1}$$
$$u(x_l,t) = u(x_r,t) = 0, \ t \in [0,T], \quad u(x,0) = u_0(x), \ x \in [x_l, x_r].$$

- $1 < \alpha < 2$ is the order of the anomalous diffusion
- d_+ and d_- are the left- and right-sided diffusivity coefficients
- The left- and right-sided fractional derivatives are defined by

$$\begin{aligned} \frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} &:= \lim_{h\to 0^+} \frac{1}{h^\alpha} \sum_{k=0}^{\lfloor (x-x_l)/h \rfloor} g_k^{(\alpha)} u(x-kh,t), \\ \frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} &:= \lim_{h\to 0^+} \frac{1}{h^\alpha} \sum_{k=0}^{\lfloor (x_r-x)/h \rfloor} g_k^{(\alpha)} u(x+kh,t) \end{aligned} \tag{2}$$

- $g_k^{(\alpha)} := (-1)^k \binom{\alpha}{k}$ with $\binom{\alpha}{k}$ being the fractional binomial coefficients.

- The fully implicit finite difference method with a direct truncation of the series in (2) is unconditionally unstable (Meerschaert & Tadjeran, J. Comput. Appl. Math., 2004)!
- They utilized a shifted Grünwald approximation to derive an unconditionally stable finite difference method

$$\frac{u_i^m - u_i^{m-1}}{\Delta t} - \frac{d_i^{+,m}}{h^\alpha}\sum_{k=0}^{i+1} g_k^{(\alpha)} u_{i-k+1}^m - \frac{d_i^{-,m}}{h^\alpha}\sum_{k=0}^{N-i+1} g_k^{(\alpha)} u_{i+k-1}^m = f_i^m \quad (3)$$

- The finite difference method can be written in the matrix form

$$(I + \Delta t A^m) u^m = u^{m-1} + \Delta t f^m. \quad (4)$$

- A^m is a full (or dense) diagonally dominant M-matrix.
- The scheme is only of first-order accuracy in space and time!

Computational and memory cost of fractional numerical methods

- The stiffness matrix A^m is a dense or full matrix, traditionally
  - The scheme was inverted in $O(N^3)$ of operations per time step
  - The scheme was stored in $O(N^2)$ of memory
- Each time the mesh size and time step are refined by half
  - The total number of unknowns increases 2 times for 1D problems
    - The computational work increases $2^3 \times 2 = 16$ times
    - The memory increases by 4 times.
  - The total number of unknowns increases 4 times for 2D problems
    - The computational work increases $4^3 \times 2 = 128$ times
    - The memory increases by 16 times.
  - The total number of unknowns increases 8 times for 3D problems
    - The computational work increases $8^3 \times 2 = 1024$ times
    - The memory increases by 64 times.
- The significantly increased computational and memory cost of the numerical methods calls for the development of fast and faithful numerical methods with efficient memory storage.

- The development of a fast methods replies on the stiffness matrix $A^m = [a^m_{i,j}/h^\alpha]_{i,j=1}^N$

$$a^m_{i,j} = \begin{cases} -(d_i^{+,m} + d_i^{-,m}) g_1^{(\alpha)} > 0, & j = i, \\ -(d_i^{+,m} g_2^{(\alpha)} + d_{-,i}^{m+1} g_0^{(\alpha)}) < 0, & j = i-1, \\ -(d_i^{+,m} g_0^{(\alpha)} + d_i^{-,m} g_2^{(\alpha)}) < 0, & j = i+1, \\ -d_i^{+,m} g_{i-j+1}^{(\alpha)} < 0, & j < i-1, \\ -d_i^{-,m} g_{j-i+1}^{(\alpha)} < 0, & j > i+1. \end{cases} \tag{5}$$

1. A^m is a full matrix
2. A^m has a special structure
3. The information A^m is sparse ($\approx 3N$).

- We utilize the following properties of $g_k^{(\alpha)} := (-1)^k \binom{\alpha}{k}$ to conclude

$$
\begin{aligned}
& g_1^{(\alpha)} = -\alpha < 0, \quad 1 = g_0^{(\alpha)} > g_2^{(\alpha)} > g_3^{(\alpha)} > \cdots > 0, \\
& \sum_{k=0}^{\infty} g_k^{(\alpha)} = 0, \quad \sum_{k=0}^{m} g_k^{(\alpha)} < 0 \quad (m \geq 1), \\
& g_k^{(\alpha)} = \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} = \frac{1}{\Gamma(-\alpha)k^{\alpha+1}}\Big(1 + O\Big(\frac{1}{k}\Big)\Big)
\end{aligned}
\tag{6}
$$

- $a_{i,i\pm k}/a_{i,i}$ decay at a rate of $1/k^{\alpha+1}$ as $k \to \infty$.

$$
\begin{aligned}
& a_{i,i}^m - \sum_{j=1, j\neq i}^{N} |a_{i,j}^m| \\
& = -(d_{+,i}^m + d_{-,i}^m) g_1^{(\alpha)} - d_{i,+}^m \sum_{k=0,k\neq 1}^{i} g_k^{(\alpha)} - d_{-,i}^m \sum_{k=0,k\neq 1}^{N-i} g_k^{(\alpha)} \\
& > -(r_{+,i}^{m+1} + r_{-,i}^{m+1}) g_1^{(\alpha)} - (r_{i,+}^{m+1} + r_{-,i}^{m+1}) \sum_{k=0,k\neq 1}^{\infty} g_k^{(\alpha)} = 0.
\end{aligned}
\tag{7}
$$

- A^m is a strictly diagonally dominant M-matrix, so the scheme is monotone.

Based on the properties of the stiffness matrix A^m of the difference method

$$(I + \Delta t A^m) u^m = u^{m-1} + \Delta t f^m,$$

- Split the stiffness matrix A^m as $A^m = A_k^m + A_o^m$ with the properties
  - A_k^m contains the $2k+1$ diagonals of A^m and is zero elsewhere
  - A_k^m approximates A^m asymptotically as $N \to \infty$
  - $A_o^m v$ can be computed efficiently for any vector v
- Derivation of a fast operator-splitting finite difference method
  - Substitute the decomposition $A^m = A_k^m + A_o^m$ into (4).
  - Move $A_o^m u^m$ to the right-hand side and approximate the u^m by a linear extrapolation of u^{m-2} and u^{m-1}.

$$\begin{aligned} (I + \Delta t A_k^m) u^m &= (I - 2\Delta t A_o^m) u^{m-1} + \Delta t A_o^m u^{m-2} + \Delta t f^m, \ m \geq 1, \\ (I + \Delta t A_k^1) u^1 &= (I - \Delta t A_o^1) u^0 + \Delta t f^1. \end{aligned} \tag{8}$$

Lemma

Scheme (5) with $k = \log N$ has the approximation property

$$\frac{\|A_o^m\|_\infty}{\|A^m\|_\infty} = \frac{\|A^m - A_k^m\|_\infty}{\|A^m\|_\infty} = O(\log^{-\alpha} N) \to 0 \qquad \textit{as } N \to \infty. \tag{9}$$

$$\begin{aligned}
\|A_o^m\|_\infty &= h^{-\alpha} \max_{i=1,\ldots,N} \big(d_i^{-,m} + d_i^{+,m}\big) \sum_{l>k=\log N} g_{l+1}^{(\alpha)} \\
&= h^{-\alpha} \max_{i=1,\ldots,N} \big(d_i^{-,m} + d_i^{+,m}\big) \sum_{l>k} \frac{1}{\Gamma(-\alpha)k^{\alpha+1}} \Big(1 + O\Big(\frac{1}{k}\Big)\Big) \\
&= h^{-\alpha} \max_{i=1,\ldots,N} \big(d_i^{-,m} + d_i^{+,m}\big) O\Big(\frac{1}{k^\alpha}\Big),
\end{aligned} \tag{10}$$

$$\|A^m\|_\infty > \alpha h^{-\alpha} \max_{i=1,\ldots,N} \big(d_i^{-,m} + d_i^{+,m}\big).$$

The ratio of the two preceding estimates gives the desired result.

Lemma

The stiffness matrix A^m can be stored in $3N+2$ of memory.

A^m can be decomposed as

$$A^m = h^{-\alpha}\left(\operatorname{diag}(d_i^{+,m})_{i=1}^N A_L^{\alpha,N} + \operatorname{diag}(d_i^{-,m})_{i=1}^N A_R^{\alpha,N}\right) \tag{11}$$

with $A_L^{\alpha,N}$ being defined below and $A_R^{\alpha,N} = (A_L^{\alpha,N})^T$

$$A_L^{\alpha,N} := -\begin{bmatrix} g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \dots & 0 & 0 \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & \ddots & \ddots & 0 \\ \vdots & g_2^{(\alpha)} & g_1^{(\alpha)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ g_{N-1}^{(\alpha)} & \ddots & \ddots & \ddots & g_1^{(\alpha)} & g_0^{(\alpha)} \\ g_N^{(\alpha)} & g_{N-1}^{(\alpha)} & \dots & \dots & g_2^{(\alpha)} & g_1^{(\alpha)} \end{bmatrix}.$$

- h, $(d_i^{+,m})_{i=1}^N$, $(d_i^{-,m})_{i=1}^N$, and $A_L^{\alpha,N}$ contain $3N+2$ parameters.

Lemma

$A^m v$ can be evaluated in $O(N \log N)$ operations for any vector v.

The matrix $A_L^{\alpha,N}$ is embedded into a $2N \times 2N$ circulant matrix $C_{2N,L}$

$$C_{2N,L} := \begin{bmatrix} A_L^{\alpha,N} & C_L^{\alpha,N} \\ C_L^{\alpha,N} & A_L^{\alpha,N} \end{bmatrix}, \qquad u_{2N} = \begin{bmatrix} v \\ 0 \end{bmatrix},$$

$$C_L^{\alpha,N} := -\begin{bmatrix} 0 & g_N^{(\alpha)} & \dots & \dots & g_3^{(\alpha)} & g_2^{(\alpha)} \\ 0 & 0 & g_N^{(\alpha)} & \dots & \ddots & g_3^{(\alpha)} \\ 0 & 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \ddots & 0 & g_N^{(\alpha)} \\ g_0^{(\alpha)} & 0 & \dots & 0 & 0 & 0 \end{bmatrix}. \tag{12}$$

- We can similarly define another $2N \times 2N$ circulant matrix $C_{2N,R}$
- A circulant matrix C_{2N} can be decomposed as

$$C_{2N} = F_{2N}^{-1} \operatorname{diag}(F_{2N} \mathsf{c}_{2N}) \; F_{2N} \tag{13}$$

where F_{2N} is the $2N \times 2N$ discrete Fourier transform matrix and c_{2N} is the first column vector of C_{2N}.

- $F_{2N} \mathsf{u}_{2N}$ can be carried out in $O(N \log N)$ operations via FFT.
- $C_{2N} \mathsf{u}_{2N}$ can be evaluated in $O(N \log N)$ operations.
- $A_L^{\alpha,N} \mathsf{u}$ and $A_R^{\alpha,N} \mathsf{u}$ can be evaluated in $O(N \log N)$ operations.
- $A^m \mathsf{u}$ can be evaluated in $O(N \log N)$ operations.
- The right-hand side of the finite difference method (5) can be evaluated in $O(N \log N)$ operations!

Theorem

The fast finite difference method (5) can be inverted in $O(N \log^2 N)$ of operations per time step using $O(N \log N)$ of memory.

- Remarks on the fast finite difference method
  - It is not lossy, since no compression is involved.
  - Stability and convergence of the method yet to be proved
  - A fast conjugate gradient iterative solver can be used to solve the original (single-step) finite difference method, which has proved stability and convergence.
- Development of other fast methods
  - A fast Crank-Nicolson scheme of similar computational and storage cost (Basu & W., Int'l J. Numer. Anal. Modeling, 2012). Crank-Nicolson scheme with a Richardson extrapolation in space was originally developed by Tadjeran et al. to recover second-order accuracy in space and time (J. Comput. Phys., 2006).
  - A Eulerian-Lagrangian method for space-fractional advection-diffusion equation (K. Wang & W., Adv. Water Resources, 2011)
  - Finite and finite volume methods (W. & Du, J. Comput. Phys., 2013).

Multidimensional transient space-fractional diffusion equations

$$
\begin{aligned}
&\frac{\partial u(x,y,t)}{\partial t} - d_+(x,y,t)\frac{\partial^\alpha u(x,y,t)}{\partial_+ x^\alpha} - d_-(x,y,t)\frac{\partial^\alpha u(x,y,t)}{\partial_- x^\alpha} \\
&\quad -e_+(x,y,t)\frac{\partial^\beta u(x,y,t)}{\partial_+ y^\beta} - e_-(x,y,t)\frac{\partial^\beta u(x,y,t)}{\partial_- y^\beta} = f(x,y,t), \\
&\qquad (x,y)\in\Omega, \quad 0 < t \le T, \\
&u(x,y,t) = u_D(x,y,t), \qquad (x,y)\in\partial\Omega, \quad t\in[0,T], \\
&u(x,y,0) = u_o(x,y), \qquad (x,y)\in\overline{\Omega}.
\end{aligned}
\tag{14}
$$

Here $\Omega := (x_l, x_r) \times (y_l, y_r)$ is a rectangular domain. $1 < \alpha, \beta < 2$.

$$\begin{aligned}\frac{u_{i,j}^m - u_{i,j}^{m-1}}{\Delta t} - \frac{d_{i,j}^{+,m}}{h_1^\alpha}\sum_{k=0}^{i+1} g_k^{(\alpha)} u_{i-k+1,j}^m - \frac{d_{i,j}^{-,m}}{h_1^\alpha}\sum_{k=0}^{N_1-i+2} g_k^{(\alpha)} u_{i+k-1,j}^m \\ -\frac{e_{i,j}^{+,m}}{h_2^\beta}\sum_{l=0}^{j+1} g_j^{(\beta)} u_{i,j-l+1}^m - \frac{e_{i,j}^{-,m}}{h_2^\beta}\sum_{k=0}^{N_2-i+2} g_l^{(\beta)} u_{i,j+l-1}^m = f_{i,j}^m, \\ 1 \le i \le N_1, \quad 1 \le j \le N_2, \quad m = 1, 2, \ldots, M.\end{aligned} \tag{15}$$

Let $N = N_1 N_2$. Introduce N-dimensional vectors u^m and f^m defined by

$$\begin{aligned} u^m &:= \left[u_{1,1}^m, \cdots, u_{N_1,1}^m, u_{1,2}^m, \cdots, u_{N_1,2}^m, \cdots, u_{1,N_2}^m, \cdots, u_{N_1,N_2}^m\right]^T, \\ f^m &:= \left[f_{1,1}^m, \cdots, f_{N_1,1}^m, f_{1,2}^m, \cdots, f_{N_1,2}^m, \cdots, f_{1,N_2}^m, \cdots, f_{N_1,N_2}^m\right]^T. \end{aligned} \tag{16}$$

The finite difference method (15) can be expressed in the matrix form

$$(I + \Delta t A^m) u^m = u^{m-1} + \Delta t f^m. \tag{17}$$

For $m = 1, 2, \ldots, M$, at time step t^m:

1. solve the following equations in the x-direction (for each fixed y_j)

$$\begin{aligned} u^{m,*}_{i,j} - \frac{d^{+,m}_{i,j}\Delta t}{h_1^\alpha}\sum_{k=0}^{i+1} g_k^{(\alpha)} u^{m,*}_{i-k+1,j} - \frac{d^{-,m}_{i,j}}{h_1^\alpha}\sum_{k=0}^{N_1-i+2} g_k^{(\alpha)} u^{m,*}_{i+k-1,j} \\ = u^{m-1}_{i,j} + \Delta t f^m_{i,j}, \qquad 1 \le i \le N_1, \quad 1 \le j \le N_2, \end{aligned} \tag{18}$$

2. solve the following equations in the y-direction (for each fixed x_i)

$$\begin{aligned} u^{m}_{i,j} - \frac{e^{+,m}_{i,j}\Delta t}{h_2^\beta}\sum_{l=0}^{j+1} g_j^{(\beta)} u^{m}_{i,j-l+1} - \frac{e^{-,m}_{i,j}\Delta t}{h_2^\beta}\sum_{k=0}^{N_2-i+2} g_l^{(\beta)} u^{m}_{i,j+l-1} \\ = u^{m,*}_{i,j}, \qquad 1 \le j \le N_2, \quad 1 \le i \le N_1. \end{aligned} \tag{19}$$

Let $u_j^m := [u_{1,j}^m, u_{2,j}^m, \cdots, u_{N_1,j}^m]^T$ and $f_j^m := [f_{1,j}^m, \cdots, f_{N_1,j}^m]^T$. Then (18) are written as fully decoupled one-dimensional systems

$$\left(I_{N_1} + \Delta t A_j^{m,x}\right) u_j^{m,*} = u_j^{m-1} + \Delta t f_j^m, \qquad 1 \le j \le N_2. \tag{20}$$

Let $v_i^m := [u_{i,1}^m, u_{i,2}^m, \cdots, u_{i,N_2}^m]^T$ and $v_i^{m,*} := [u_{i,1}^{m,*}, u_{i,2}^{m,*}, \cdots, u_{i,N_2}^{m,*}]^T$ for $i = 1, \ldots, N_1$ be the rearrangements of u_j^m and $u_j^{m,*}$ for $j = 1, \ldots, N_2$. Then (21) can be rewritten as fully decoupled one-dimensional systems

$$\left(I_{N_2} + \Delta t B_i^{m,y}\right) v_i^m = v_i^{m,*}, \qquad 1 \le i \le N_1. \tag{21}$$

- The ADI approach enables a direct application of the fast 1D solver to two- and three-dimensional space-fractional diffusion equations.
- The ADI approach does not need a direct decomposition of A^m.

A fast operator-splitting multistep ADI finite difference method (W. & K. Wang, J. Comput. Phys., 2011)

Theorem

The fast ADI method can be performed in $O(N \log^2 N)$ of operations per time step and requires $O(N \log N)$ of memory to store for two- and three-dimensional space-fractional diffusion equations.

An efficient storage of the fast ADI method requires the storage of the coefficient matrices $A_j^{m,x}$ for $j = 1, \ldots, N_2$ and $B_i^{m,y}$ for $i = 1, \ldots, N_1$. This requires $N_2 O(N_1) + N_1 O(N_2) = O(N)$ of memory.
All the systems (20) can be solved in $N_2 O(N_1 \log^2 N_1) = O(N \log^2 N)$ of operations, and those in (21) can be solved in $N_1 O(N_2 \log^2 N_2) = O(N \log^2 N)$ of operations.

- The same result holds true for 3D problems.
- No multiple substeps needed if a conjugate-gradient type of iterative solver is used to solve the one-dimensional systems.

- In the numerical experiments the data are given as follows
  - $d_+(x,y,t) = d_-(x,y,t) = e_+(x,y,t) = e_-(x,y,t) = D = 0.005$
  - $f = 0$, $\alpha = \beta = 1.8$, $\Omega = (-1,1) \times (-1,1)$, $[0,T] = [0,1]$.
  - The true solution is the fundamental solution to (14) expressed via the inverse Fourier transform

$$
\begin{aligned}
u(x,y,t) &= \frac{1}{\pi}\int_0^\infty e^{-2D|\cos(\frac{\pi\alpha}{2})|(t+0.5)\xi^\alpha}\cos(\xi x)d\xi \\
&\quad \times \frac{1}{\pi}\int_0^\infty e^{-2D|\cos(\frac{\pi\beta}{2})|(t+0.5)\eta^\beta}\cos(\eta y)d\eta.
\end{aligned} \tag{22}
$$

  - The initial condition $u_o(x,y)$ is chosen to be $u(x,y,0)$.
- In the numerical experiments the Meerschaert & Tadjeran scheme and the fast ADI method were implemented using Matlab.

$h = \Delta t$	$\|u_{FD} - u\|_{L^1}$	$\|u_{FD} - u\|_{L^2}$	$\|u_{FD} - u\|_{L^\infty}$
2^{-4}	3.0281×10^{-2}	7.0346×10^{-2}	5.7095×10^{-1}
2^{-5}	9.8231×10^{-3}	2.1051×10^{-2}	1.6409×10^{-1}
2^{-6}	3.9081×10^{-3}	7.3313×10^{-3}	5.5939×10^{-2}
2^{-7}	1.9647×10^{-3}	3.0910×10^{-3}	2.1663×10^{-2}
	$\|u_{FFD} - u\|_{L^1}$	$\|u_{FFD} - u\|_{L^2}$	$\|u_{FFD} - u\|_{L^\infty}$
2^{-4}	2.8115×10^{-2}	6.1891×10^{-2}	4.8644×10^{-1}
2^{-5}	8.4583×10^{-3}	1.6793×10^{-2}	1.2472×10^{-1}
2^{-6}	3.1232×10^{-3}	5.2155×10^{-3}	3.6594×10^{-2}
2^{-7}	1.5340×10^{-3}	2.1439×10^{-3}	1.2013×10^{-2}

Table : The (normalized) L^1, L^2, and L^∞ errors of the fast ADI (FFD) method and traditional finite difference (FD) method with Gaussian elimination

$h = \Delta t$	CPU of finite difference (FD) with Gaussian elimination
2^{-4}	49 s
2^{-5}	8.07×10^2 s = 13 m 27 s
2^{-6}	6.43×10^4 s = 17 h 51 m
2^{-7}	5.90×10^6 s = 1639 h 42 m = 2 month and 8 days
	CPU of the fast ADI finite difference method (FFD)
2^{-4}	7.4 s
2^{-5}	63.6 s = 1 m 4 s
2^{-6}	5.88×10^2 s = 9 m 48 s
2^{-7}	5.22×10^3 s = 1 h 27 m

Table : The consumed CPU of the fast ADI (FFD) method and the traditional finite difference (FD) method with Gaussian elimination.

- Strength: easy to implement
  - Numerical experiments show the utility of ADI methods.
  - ADI methods reduce the solution of multidimensional space-fractional diffusion equations to one-dimensional systems.
  - Avoid the relatively complex multidimensional coefficient matrix A^m.
- Weakness: restrictive
  - The ADI methods for space-fractional diffusion equations were proved to be unconditionally stable and convergent if the finite difference operators in the x- and y-directions commute.
  - This condition is satisfied if $d_{\pm}(x, y, t)$ are independent of y and $e_{\pm}(x, y, t)$ are independent of x.

A steady-state space-fractional diffusion equation in conservative form

$$-D\big(K(x)\big(\theta\ {}_0D_x^{-\beta} + (1-\theta)\ {}_xD_1^{-\beta}\big)Du\big) = f(x), \quad x \in (0,1), \qquad (23)$$
$$u(0) = u(1) = 0.$$

- $2-\beta$ with $0<\beta<1$ represents the order of anomalous diffusion
- K is the diffusivity coefficient, $0 \le \theta \le 1$ indicates the relative weight of forward versus backward transition probability of the particles
- f is the source and sink term
- ${}_0D_x^{-\beta}u(x)$ and ${}_xD_1^{-\beta}u(x)$ are the left- and right-fractional integrals

$$\begin{cases} {}_0D_x^{-\beta}u(x) := \dfrac{1}{\Gamma(\beta)} \displaystyle\int_0^x (x-s)^{\beta-1}u(s)ds, \\ {}_xD_1^{-\beta}u(x) := \dfrac{1}{\Gamma(\beta)} \displaystyle\int_x^1 (s-x)^{\beta-1}u(s)ds \end{cases} \qquad (24)$$

$\Gamma(\cdot)$ is the Gamma function

- Galerkin formulation: given $f \in H^{-(1-\frac{\beta}{2})}(0,1)$, seek $u \in H_0^{1-\frac{\beta}{2}}(0,1)$

$$B(u,v) = \langle f, v \rangle, \qquad \forall\, v \in H_0^{1-\frac{\beta}{2}}(0,1). \tag{25}$$

Here $B : H_0^{1-\frac{\beta}{2}}(0,1) \times H_0^{1-\frac{\beta}{2}}(0,1) \to \mathbb{R}$ is defined to be

$$\begin{aligned} B(u,v) \quad &:= \theta K \big\langle {}_0D_x^{-\beta} Du, Dv \big\rangle + (1-\theta) K \big\langle {}_xD_1^{-\beta} Du, Dv \big\rangle \\ &= \theta K \big({}_0D_x^{1-\beta/2} u, {}_xD_1^{1-\beta/2} Dv \big)_{L^2(0,1)} \\ &\quad + (1-\theta) K \big({}_xD_1^{1-\beta/2} u, {}_0D_x^{1-\beta/2} v \big)_{L^2(0,1)} \end{aligned}$$

$\langle \cdot, \cdot \rangle$ is the duality pair between $H^{-(1-\frac{\beta}{2})}(0,1)$ and $H_0^{1-\frac{\beta}{2}}(0,1)$.

- For $\theta = 1/2$, $B(\cdot,\cdot)$ is symmetric. This problem reduces to fractional Laplacian which is well studied in harmonic analysis.

- The coercivity of $B(\cdot,\cdot)$ is derived as follows

$$\begin{aligned} B(u,u) &= K\big({}_0D_x^{1-\beta/2}u, {}_xD_1^{1-\beta/2}u\big)_{L^2(0,1)} \\ &= -\cos\big((1-\beta/2)\pi\big)K|u|^2_{H^{1-\beta/2}(0,1)} \\ &= \cos\big(\beta\pi/2\big)K|u|^2_{H^{1-\beta/2}(0,1)}. \end{aligned}$$

Theorem

$B(\cdot,\cdot)$ is coercive and continuous on $H_0^{1-\frac{\beta}{2}}(0,1) \times H_0^{1-\frac{\beta}{2}}(0,1)$. Hence, the Galerkin weak formulation (25) has a unique solution. Moreover,

$$\|u\|_{H^{1-\frac{\beta}{2}}(0,1)} \le (1/\alpha)\|f\|_{H^{-(1-\frac{\beta}{2})}(0,1)}.$$

- Let $S_h(0,1) \subset H_0^{1-\frac{\beta}{2}}(0,1)$ be the finite element space of piecewise polynomials of degree $m-1$. Find $u_h \in S_h(0,1)$ such that

$$B(u_h, v_h) = \langle f, v_h \rangle, \qquad \forall v_h \in S_h(0,1).$$

- The optimal-order error estimate holds for $u \in H^m(0,1) \cap H_0^{1-\frac{\beta}{2}}(0,1)$

$$\|u_h - u\|_{L^2(0,1)} + h^{1-\frac{\beta}{2}} \|u_h - u\|_{H^{1-\frac{\beta}{2}}(0,1)} \leq C h^m \|u\|_{H^m(0,1)}.$$

- The analysis was extended to DG and spectral methods.
- All of the analysis requires K to be positive constant.

- Variable-coefficient models were derived in applications. Can the previous analysis be extended to cover these problems?
- In the context of variable diffusivity K

$$\begin{aligned} B(u,v) &= \theta\big\langle K\,{}_0D_x^{-\beta}Du, Dv\big\rangle + (1-\theta)\big\langle K\,{}_xD_1^{-\beta}Du, Dv\big\rangle \\ &\neq \theta\big\langle KDu, {}_xD_1^{-\beta}Dv\big\rangle + (1-\theta)\big\langle KDu, {}_0D_x^{-\beta}Dv\big\rangle \\ &\neq \big(K\,{}_0D_x^{-\beta/2}Du, {}_xD_1^{-\beta/2}Dv\big)_{L^2(0,1)} \end{aligned}$$

- Each corresponds to a fractional equation of a different form

$$-D(KD^{1-\beta}u) \neq -D^{1-\beta}(KDu) \neq -D^{1-\beta/2}(KD^{1-\beta/2}u).$$

- The last form seems to be mathematically preferred, but still cannot guarantee its coercivity

$$\begin{aligned}&\left(K\,{}_0D_x^{-\beta/2}Du, {}_xD_1^{-\beta/2}Du\right)_{L^2(0,1)}\\ &\quad \ngeq K_{min}\left({}_0D_x^{-\beta/2}Du, {}_xD_1^{-\beta/2}Du\right)_{L^2(0,1)}\\ &\quad = \cos\left(\beta\pi/2\right)K_{min}|u|^2_{H^{1-\beta/2}(0,1)}.\end{aligned}$$

Lemma

There exist a $K(x)$ consisting of two positive constants and a function $w \in H_0^{1-\frac{\beta}{2}}(0,1)$ such that $B(w,w) < 0$.

Let $K(x)$ and $w \in H_0^1(0,1) \subset H_0^{1-\frac{\beta}{2}}(0,1)$ be defined by

$$K(x) := \begin{cases} K_l, & x \in (0,1/2), \\ 1, & x \in (1/2,1). \end{cases}$$

$$w(x) := \begin{cases} 2x, & x \in (0,1/2], \\ 2(1-x), & x \in [1/2,1). \end{cases}$$

Direct calculation gives

$$
{}_0D_x^{1-\beta} w(x) = \begin{cases} \dfrac{2x^\beta}{\Gamma(\beta+1)}, & x \in (0, 1/2), \\ \dfrac{2\big(x^\beta - 2(x-1/2)^\beta\big)}{\Gamma(\beta+1)}, & x \in (1/2, 1). \end{cases}
$$

Then we have

$$
B(w,w) = \frac{2^{1-\beta}}{\Gamma(\beta+2)} \Big(K_l - \big(2^{\beta+1} - 3\big) \Big).
$$

Since $0 < \log_2 3 - 1 < 1$, choose $\log_2 3 - 1 < \beta < 1$ so that $2^{\beta+1} - 3 > 0$. Then we select $K_l > 0$ sufficiently small such that $K_l - \big(2^{\beta+1} - 3\big) < 0$. For such K and w, we have $B(w,w) < 0$.

- Consider a one-sided problem (problem (23) with $\theta = 1$)

$$-D\big(K(x)\ {}_0D_x^{-\beta} Du\big) = f(x), \quad x \in (0,1), \quad u(0) = u(1) = 0. \quad (26)$$

- mass balance of a fractional Darcy's law, physically reasonable

Theorem

Assume that $K \in C^{1,\alpha}[0,1]$ and $f \in C^{\alpha}[0,1]$. Then u is the unique solution to (26) if and only if it can be expressed as

$$u = {}_0D_x^{\beta} w_f - {}_0D_1^{\beta} w_f \big({}_0D_1^{\beta} w_b\big)^{-1} {}_0D_x^{\beta} w_b, \quad (27)$$

where w_f and w_b are the solutions to the following problems

$$\begin{aligned} -D\big(K(x)Dw_f\big) &= f, \quad x \in (0,1); \qquad w_f(0) = w_f(1) = 0, \\ -D\big(K(x)Dw_b\big) &= 0, \quad x \in (0,1); \qquad w_b(0) = 0,\ w_b(1) = 1. \end{aligned} \quad (28)$$

- For a constant diffusivity coefficient K, the Galerkin formulation is coercive on the product space $H_0^{1-\beta/2}(0,1) \times H_0^{1-\beta/2}(0,1)$.
- In the context of a variable diffusivity coefficient K
  - The Galerkin formulation is *not* coercive on any product space $H \times H$.
  - A physically reasonable equation is expressed as the divergence of a fractional diffusive flux of order $1-\beta$.
  - We propose a Petrov-Galerkin formulation imposed on $H_0^{1-\beta}(0,1) \times H_0^1(0,1)$: Seek $u \in H_0^{1-\beta}(0,1)$ such that

$$A(u,v) := \int_0^1 K(x)\ {}_0D_x^{1-\beta} u Dv dx = \langle f, v \rangle, \quad \forall v \in H_0^1(0,1) \tag{29}$$

- Even for constant K, the Petrov-Galerkin formulation is different from the Galerkin formulation
  - The latter is defined on $H_0^{1-\beta/2}(0,1) \times H_0^{1-\beta/2}(0,1)$ for any given $f \in H^{-(1-\beta/2)}(0,1)$
  - The former is defined on $H_0^{1-\beta}(0,1) \times H_0^1(0,1)$ for any given $f \in H^{-1}(0,1)$.

Theorem

Assume $0 \le \beta < 1/2$ and $0 < K_{min} \le K \le K_{max} < \infty$. The bilinear form $A(w,v)$ is weakly coercive

$$\begin{aligned} &\inf_{w \in H_0^{1-\beta}(0,1)} \sup_{v \in H_0^1(0,1)} \frac{A(w,v)}{\|w\|_{H^{1-\beta}(0,1)} \|v\|_{H^1(0,1)}} \ge \gamma(\beta) > 0, \\ &\sup_{w \in H_0^{1-\beta}(0,1)} A(w,v) > 0 \quad \forall\, v \in H_0^1(0,1) \setminus \{0\}. \end{aligned} \tag{30}$$

Thus, the Petrov-Galerkin formulation (29) has a unique weak solution $u \in H_0^{1-\beta}(0,1)$. Furthermore,

$$\|u\|_{H^{1-\beta}(0,1)} \le \frac{K_{max}}{\gamma} \|f\|_{H^{-1}(0,1)}. \tag{31}$$

Thank You!