# Fast numerical methods and mathematical analysis of fractional PDEs 

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## The initial-boundary value problem of space-fractional PDEs on a bounded domain

$$
\begin{gather*}
\partial_{t} u-d_{+}(x, t)_{a}^{G} D_{x}^{\alpha} u-d_{-}(x, t)_{x}^{G} D_{b}^{\alpha} u=f, \quad x \in(a, b), t \in(0, T]  \tag{1}\\
u(a, t)=u(b, t)=0, t \in[0, T], \quad u(x, 0)=u_{0}(x), x \in[a, b]
\end{gather*}
$$

- $d_{+}$and $d_{-}$are the left and right variable diffusivity coefficients (so analytical techniques do not apply, in general).
- The left- and right-sided Grünwald-Letnikov fractional derivatives of order $1<\alpha<2$ are defined by

$$
\begin{align*}
{ }_{a}^{G} D_{x}^{\alpha} u(x, t) & :=\lim _{\varepsilon \rightarrow 0^{+}} \frac{1}{\varepsilon^{\alpha}} \sum_{k=0}^{\lfloor(x-a) / \varepsilon\rfloor} g_{k}^{(\alpha)} u(x-k \varepsilon, t),  \tag{2}\\
{ }_{x}^{G} D_{b}^{\alpha} u(x, t) & :=\lim _{\varepsilon \rightarrow 0^{+}} \frac{1}{\varepsilon^{\alpha}} \sum_{k=0}^{\lfloor(b-x) / \varepsilon\rfloor} g_{k}^{(\alpha)} u(x+k \varepsilon, t)
\end{align*}
$$

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

A finite difference method (Lynch et al 2003, del-Castillo-Negrete et al 2004, Liu et al 2004, Meerschaert \& Tadjeran 2004)

- FPDEs have significantly different features from integer-order PDEs.
- Let $x_{i}:=a+i h$ and $t_{m}:=m \Delta t$. The fully implicit finite difference scheme obtained by truncating (2) is unconditionally unstable!
- An unconditionally stable scheme is (Meerschaert \& Tadjeran 2004) is

$$
\begin{equation*}
\frac{u_{i}^{m}-u_{i}^{m-1}}{\Delta t}-\frac{d_{i}^{+, m}}{h^{\alpha}} \sum_{k=0}^{i} g_{k}^{(\alpha)} u_{i-k+1}^{m}-\frac{d_{i}^{-, m}}{h^{\alpha}} \sum_{k=0}^{N-i+1} g_{k}^{(\alpha)} u_{i+k-1}^{m}=f_{i}^{m} \tag{3}
\end{equation*}
$$

- The stiffness matrix $A^{m}=\left[a_{i, j}^{m}\right]_{i, j=1}^{N}$

$$
a_{i, j}^{m}=\frac{1}{h^{\alpha}} \begin{cases}-\left(d_{i}^{+, m}+d_{i}^{-, m}\right) g_{1}^{(\alpha)}>0, & j=i  \tag{4}\\ -\left(d_{i}^{+, m} g_{2}^{(\alpha)}+d_{i}^{-, m} g_{0}^{(\alpha)}\right)<0, & j=i-1 \\ -\left(d_{i}^{+, m} g_{0}^{(\alpha)}+d_{i}^{-, m} g_{2}^{(\alpha)}\right)<0, & j=i+1 \\ -d_{i}^{+, m} g_{i-j+1}^{(\alpha)}<0, & j<i-1 \\ -d_{i}^{-, m} g_{j-i+1}^{(\alpha)}<0, & j>i+1\end{cases}
$$

- In the matrix form of the finite difference scheme (3)

$$
\begin{equation*}
\left(I+\Delta t A^{m}\right) u^{m}=u^{m-1}+\Delta t f^{m} \tag{5}
\end{equation*}
$$

- $A^{m}$ is full and has to be assembled in any traditional scheme.
- We utilize the following properties of $g_{k}^{(\alpha)}:=(-1)^{k}\binom{\alpha}{k}$ to conclude

$$
\begin{align*}
& g_{1}^{(\alpha)}=-\alpha<0, \quad 1=g_{0}^{(\alpha)}>g_{2}^{(\alpha)}>g_{3}^{(\alpha)}>\cdots>0 \\
& \sum_{k=0}^{\infty} g_{k}^{(\alpha)}=0, \quad \sum_{k=0}^{m} g_{k}^{(\alpha)}<0 \quad(m \geq 1)  \tag{6}\\
& g_{k}^{(\alpha)}=\frac{\Gamma(k-\alpha)}{\Gamma(-\alpha) \Gamma(k+1)}=\frac{1}{\Gamma(-\alpha) k^{\alpha+1}}\left(1+O\left(\frac{1}{k}\right)\right)
\end{align*}
$$

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

$$
\begin{align*}
& a_{i, i}^{m}-\sum_{\substack{j=1, j \neq i}}^{N}\left|a_{i, j}^{m}\right| \\
& \quad=-\left(r_{i}^{+, m}+r_{i}^{-, m}\right) g_{1}^{(\alpha)}-r_{i}^{+, m} \sum_{k=0, k \neq 1}^{i} g_{k}^{(\alpha)}-r_{i}^{-, m} \sum_{k=0, k \neq 1}^{N-i} g_{k}^{(\alpha)}  \tag{7}\\
& \quad>-\left(r_{i}^{+, m}+r_{i}^{-, m}\right) g_{1}^{(\alpha)}-\left(r_{i}^{+, m}+r_{i}^{-, m}\right) \sum_{k=0, k \neq 1}^{\infty} g_{k}^{(\alpha)}=0 .
\end{align*}
$$

- $A^{m}$ is a strictly diagonally dominant M-matrix, the scheme is monotone


## Exploring the structure of the stiffness matrix $A^{m}=\left[a_{i, j}^{m}\right]_{i, j=1}^{N}$ (W. et al 2010)

## Theorem

$$
\begin{equation*}
A^{m}=\left(\operatorname{diag}\left(d_{i}^{+, m}\right)_{i=1}^{N} T^{\alpha, N}+\operatorname{diag}\left(d_{i}^{-, m}\right)_{i=1}^{N}\left(T^{\alpha, N}\right)^{T}\right) / h^{\alpha} \tag{8}
\end{equation*}
$$

$$
T^{\alpha, N}:=-\left[\begin{array}{cccccc}
g_{1}^{(\alpha)} & g_{0}^{(\alpha)} & 0 & \cdots & 0 & 0 \\
g_{2}^{(\alpha)} & g_{1}^{(\alpha)} & g_{0}^{(\alpha)} & \ddots & \ddots & 0 \\
\vdots & g_{2}^{(\alpha)} & g_{1}^{(\alpha)} & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & 0 \\
g_{N-1}^{(\alpha)} & \ddots & \ddots & \ddots & g_{1}^{(\alpha)} & g_{0}^{(\alpha)} \\
g_{N}^{(\alpha)} & g_{N-1}^{(\alpha)} & \cdots & \cdots & g_{2}^{(\alpha)} & g_{1}^{(\alpha)}
\end{array}\right]
$$

## A fast evaluation of $A v$

## Theorem

$A^{m} v$ can be evaluated in $O(N \log N)$ operations for any vector $v$.
The matrix $T^{\alpha, N}$ is embedded into a $2 N \times 2 N$ circulant matrix $C^{\alpha, 2 N}$

$$
C^{\alpha, 2 N}:=\left[\begin{array}{cc}
T^{\alpha, N} & S^{\alpha, N} \\
S^{\alpha, N} & T^{\alpha, N}
\end{array}\right], \quad S^{\alpha, N}:=\left[\begin{array}{cccccc}
0 & g_{N}^{(\alpha)} & \cdots & \cdots & g_{3}^{(\alpha)} & g_{2}^{(\alpha)} \\
0 & 0 & g_{N}^{(\alpha)} & \cdots & \ddots & g_{3}^{(\alpha)} \\
0 & 0 & 0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & \ddots & 0 & g_{N}^{(\alpha)} \\
g_{0}^{(\alpha)} & 0 & \cdots & 0 & 0 & 0
\end{array}\right]
$$

- Let $c^{\alpha, 2 N}$ be the first column of $C^{\alpha, 2 N}$. Then $C^{\alpha, 2 N}$ can be decomposed as

$$
\begin{equation*}
C^{\alpha, 2 N}=F_{2 N}^{-1} \operatorname{diag}\left(F_{2 N} c^{\alpha, 2 N}\right) F_{2 N} \tag{9}
\end{equation*}
$$

- A fast matrix-vector multiplication $A^{m} v$ is formulated as follows
- For any $v \in \mathbb{R}^{N}$, define $v_{2 N}$ by

$$
v_{2 N}=\left[\begin{array}{l}
v  \tag{10}\\
0
\end{array}\right], \quad C^{\alpha, 2 N} v_{2 N}=\left[\begin{array}{ll}
T^{\alpha, N} & S^{\alpha, N} \\
S^{\alpha, N} & T^{\alpha, N}
\end{array}\right]\left[\begin{array}{l}
v \\
0
\end{array}\right]=\left[\begin{array}{c}
T^{\alpha, N} v \\
S^{\alpha, N} v
\end{array}\right] .
$$

- $F_{2 N} v_{2 N}$ can be carried out in $O(N \log N)$ operations via FFT, so $C^{\alpha, 2 N} v_{2 N}$ can be evaluated in $O(N \log N)$ operations.
- The first $N$ entries of $C^{\alpha, 2 N} v_{2 N}$ yields $T^{\alpha, N} v$.
- Similarly, $\left(T^{\alpha, N}\right)^{T} v$ can be evaluated in $O(N \log N)$ operations.
- $A^{m} v$ can be evaluated in $O(N \log N)$ operations.


## Summary of the fast numerical method

- The fast algorithm
- is not lossy, since no compression used in evaluating $A^{m} v$;
- retains the conservation, stability, and convergence of the underlying scheme;
- is nonintrusive, only the matrix-vector multiplication module needs to be modified.
- By (8)-(10), the fast algorithm is matrix-free.
- The evaluatation of $A^{m} \vee$ requires only formulating the vectors $\left\{d_{i}^{ \pm, m}\right\}_{i=1}^{N}$ and $c^{\alpha, 2 N}$;
- The storage of $A^{m}$ requires only storing the $(3 N+1)$ parameters $\left\{d_{i}^{ \pm, m}\right\}_{i=1}^{N}$ and $\left\{g_{i}^{(\alpha)}\right)_{i=0}^{N}$.
- In contrast, any traditional method requires the assembly of the full stiffness matrix $A^{m}$.


## A two-dimensional space-fractional PDE

$$
\begin{gather*}
\partial_{t} u(x, y, t)-d_{+}(x, y, t){ }_{a}^{G} D_{x}^{\alpha} u(x, y, t)-d_{-}(x, y, t)_{x}^{G} D_{b}^{\alpha} u(x, y, t) \\
-e_{+}(x, y, t)_{c}^{G} D_{y}^{\beta} u(x, y, t)-e_{-}(x, y, t)_{y}^{G} D_{d}^{\beta} u(x, y, t)=f(x, y, t), \\
(x, y) \in \Omega:=(a, b) \times(c, d), \quad t \in(0, T], \quad 1<\alpha, \beta<2  \tag{11}\\
u(x, y, t)=0, \quad(x, y) \in \partial \Omega, \quad t \in[0, T] \\
u(x, y, 0)=u_{o}(x, y), \quad(x, y) \in \bar{\Omega} .
\end{gather*}
$$

- The fractional spatial derivatives are only in the coordinate directions.


## A two-dimensional finite difference scheme

- A two-dimensional shifted finite difference scheme is

$$
\begin{align*}
& \frac{u_{i, j}^{m}-u_{i, j}^{m-1}}{\Delta t}-\frac{d_{i, j}^{+, m}}{h_{1}^{\alpha}} \sum_{k=0}^{i} g_{k}^{(\alpha)} u_{i-k+1, j}^{m}-\frac{d_{i, j}^{-, m}}{h_{1}^{\alpha}} \sum_{k=0}^{N_{1}-i+1} g_{k}^{(\alpha)} u_{i+k-1, j}^{m} \\
& -\frac{e_{i, j}^{+, m}}{h_{2}^{\beta}} \sum_{l=0}^{j} g_{j}^{(\beta)} u_{i, j-l+1}^{m}-\frac{e_{i, j}^{-, m}}{h_{2}^{\beta}} \sum_{k=0}^{N_{2}-i+1} g_{l}^{(\beta)} u_{i, j+l-1}^{m}=f_{i, j}^{m}  \tag{12}\\
& 1 \leq i \leq N_{1}, \quad 1 \leq j \leq N_{2}, \quad m=1,2, \ldots, M
\end{align*}
$$

Let $N=N_{1} N_{2}$. Introduce $N$-dimensional vectors $u^{m}$ and $f^{m}$ defined by

$$
\begin{align*}
u^{m} & :=\left[u_{1,1}^{m}, \cdots, u_{N_{1}, 1}^{m}, u_{1,2}^{m}, \cdots, u_{N_{1}, 2}^{m}, \cdots, u_{1, N_{2}}^{m}, \cdots, u_{N_{1}, N_{2}}^{m}\right]^{T}, \\
f^{m} & :=\left[f_{1,1}^{m}, \cdots, f_{N_{1}, 1}^{m}, f_{1,2}^{m}, \cdots, f_{N_{1}, 2}^{m}, \cdots, f_{1, N_{2}}^{m}, \cdots, f_{N_{1}, N_{2}}^{m}\right]^{T} . \tag{13}
\end{align*}
$$

The finite difference scheme (12) can be expressed in the matrix form

$$
\begin{equation*}
\left(I+\Delta t A^{m}\right) u^{m}=u^{m-1}+\Delta t f^{m} . \tag{14}
\end{equation*}
$$

## Structure of the stiffness matrix $A^{m}=A^{m, x}+A^{m, y}$ (W. \& Basu 2012)

- $A^{m, x}$ accounts for the coupling of all the nodes in the $x$ direction
- $A^{m, x}$ is block-diagonal with full diagonal blocks.
- Each diagonal block $A_{j}^{m, x}$ is identical to that for a 1D problem

$$
\begin{equation*}
A_{j}^{m, x}=-\operatorname{diag}\left(r_{j}^{+, m}\right) T^{\alpha, N_{1}}-\operatorname{diag}\left(r_{j}^{-, m}\right)\left(T^{\alpha, N_{1}}\right)^{T} . \tag{15}
\end{equation*}
$$

- $A^{m, x} v$ can be evaluated in $N_{2} O\left(N_{1} \log N_{1}\right)=O(N \log N)$ operations.
- $A^{m, x}$ can be stored in $N_{2} O\left(N_{1}\right)=O(N)$ memory.
- $A^{m, y}$ accounts for the coupling of all the nodes in the $y$ direction.
- As the labelling runs $x$ first, $A^{m, y}$ is a full block matrix but with sparse matrix blocks.
- We prove that $A^{m, y}$ is block-Toeplitz-circulant-block

$$
\begin{equation*}
A^{m, y}=-\operatorname{diag}\left(s_{j}^{+, m}\right)_{j=1}^{N_{2}}\left(T^{\beta, N_{2}} \otimes \boldsymbol{I}_{N_{1}}\right)-\operatorname{diag}\left(s_{j}^{-, m}\right)_{j=1}^{N_{2}}\left(\left(T^{\beta, N_{2}}\right)^{T} \otimes \boldsymbol{I}_{N_{1}}\right) . \tag{16}
\end{equation*}
$$

## A numerical simulation of a 3D space-fractional FPDE (W. \& Du 2013c)

- In the numerical experiments the data are given as follows
- $a_{+}(x, y, z, t)=a_{-}(x, y, z, t)=b_{+}(x, y, z, t)=b_{-}(x, y, z, t)=$ $c_{+}(x, y, z, t)=c_{-}(x, y, z, t)=D=0.005$
- $f=0, \alpha=\beta=\gamma=1.8, \Omega=(-1,1)^{3},[0, T]=[0,1]$.
- The true solution is expressed via the inverse Fourier transform

$$
\begin{align*}
u(x, y, z, t)= & \frac{1}{\pi} \int_{0}^{\infty} e^{-2 D\left|\cos \left(\frac{\pi \alpha}{2}\right)\right|(t+0.5) \xi^{\alpha}} \cos (\xi x) d \xi \\
& \times \frac{1}{\pi} \int_{0}^{\infty} e^{-2 D\left|\cos \left(\frac{\pi \beta}{2}\right)\right|(t+0.5) \eta^{\beta}} \cos (\eta y) d \eta  \tag{17}\\
& \times \frac{1}{\pi} \int_{0}^{\infty} e^{-2 D\left|\cos \left(\frac{\pi \gamma}{2}\right)\right|(t+0.5) \zeta^{\gamma}} \cos (\zeta z) d \zeta .
\end{align*}
$$

- The initial condition $u_{o}(x, y, z)$ is chosen to be $u(x, y, z, 0)$.
- The Meerschaert \& Tadjeran FDM and the fast FDM implemented in Fortran 90 on a workstation of 120 GB of memory.


## Table: The CPU of the FDM and fast FDM

| $h=\Delta t$ | \# of nodes | The FDM | The fast FDM |
| :---: | :---: | :---: | :---: |
| $2^{-3}$ | 4,096 | 1h 4m 26s | 0.58 s |
| $2^{-4}$ | 32,768 | 2 month 25d 9h 12m | 5.74 s |
| $2^{-5}$ | 262,144 | N/A | 1 m 6 s |
| $2^{-6}$ | $2,097,152$ | N/A | 14 m 22 s |
| $2^{-7}$ | $16,777,216$ | N/A | $3 \mathrm{~h} \mathrm{49m56s}$ |
| $2^{-8}$ | $134,217,728$ | N/A | 3days 3 h 18 m 52 s |

- It would take the regular FDM about 1,000 years of CPU times on state of the art supercomputers (10 petaflops, Nov 2011) to finish the simulation, provided that the computer has enough memory.
- Parallelization was used in measuring the peak performance of supercomputers. The nonlocal nature of FPDEs makes the communications in the numerical simulations global, which further increases the CPU times of the FDM simulations.

$$
\begin{gather*}
-D\left(K(x)\left(\theta_{0}^{C, l} D_{x}^{1-\beta} u-(1-\theta){ }_{x}^{C, r} D_{1}^{1-\beta} u\right)\right)=f(x), \quad x \in(0,1)  \tag{18}\\
u(0)=u_{l}, \quad u(1)=u_{r}, \quad 0<\beta<1, \quad 0 \leq \theta \leq 1
\end{gather*}
$$

- derived from a local mass balance + a fractional Fick's law.
- $\theta$ is the weight of forward versus backward transition probability.
- The left- and right-fractional integrals, Caputo and Riemann-Liouville fractional derivatives are defined by

$$
\begin{align*}
&{ }_{0} I_{x}^{\beta} u(x)={ }_{0} D_{x}^{-\beta} u(x):= \\
&{ }_{x} I_{1}^{\beta} u(x)={ }_{x} D_{1}^{-\beta} u(x):=\int_{x}^{1} \frac{(x-s)^{\beta-1} u(s)}{\Gamma(\beta)} d s,  \tag{19}\\
& \Gamma(\beta) \\
&{ }_{0}^{C, l} D_{x}^{1-\beta} u:={ }_{0} I_{x}^{\beta} D u, \quad{ }_{x}^{C, r} D_{1}^{1-\beta} u:=-{ }_{x} I_{1}^{\beta} D u, \\
&{ }_{0}^{R, l} D_{x}^{1-\beta} u:=D_{0} I_{x}^{\beta} u, \quad{ }_{x}^{C, r} D_{1}^{1-\beta} u:=-D{ }_{x} I_{1}^{\beta} u .
\end{align*}
$$

## Analysis for (18) with constant $K \& u_{l}=u_{r}=0$ (Ervin \& Roop 2005)

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

$$
\begin{equation*}
B(u, v)=\langle f, v\rangle, \quad \forall v \in H_{0}^{1-\frac{\beta}{2}}(0,1) . \tag{20}
\end{equation*}
$$

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

$$
\begin{aligned}
B(u, v):= & \theta\left\langle K{ }_{0} D_{x}^{-\beta} D u, D v\right\rangle+(1-\theta)\left\langle K_{x} D_{1}^{-\beta} D u, D v\right\rangle \\
= & \theta\left(K_{0} D_{x}^{-\beta / 2} D u,{ }_{x} D_{1}^{-\beta / 2} D v\right)_{L^{2}(0,1)} \\
& +(1-\theta)\left(K_{x} D_{1}^{-\beta / 2} D u,{ }_{0} D_{x}^{-\beta / 2} D v\right)_{L^{2}(0,1)}
\end{aligned}
$$

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

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

$$
\begin{aligned}
B(u, u) & =K\left({ }_{0} D_{x}^{-\beta / 2} D u,{ }_{x} D_{1}^{-\beta / 2} D u\right)_{L^{2}(0,1)} \\
& =-\cos ((1-\beta / 2) \pi) K|u|_{H^{1-\beta / 2}(0,1)}^{2} \\
& =\cos (\beta \pi / 2) K|u|_{H^{1-\beta / 2}(0,1)}^{2}
\end{aligned}
$$

## 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 (20) has a unique solution. Moreover,

$$
\|u\|_{H^{1-\frac{\beta}{2}}(0,1)} \leq C\|f\|_{H^{-\left(1-\frac{\beta}{2}\right)}(0,1)} .
$$

## Galerkin finite element methods and their error estimates

- 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

$$
B\left(u_{h}, v_{h}\right)=\left\langle f, v_{h}\right\rangle, \quad \forall v_{h} \in S_{h}(0,1) .
$$

- Assume that the true solution $u \in H^{m}(0,1) \cap H_{0}^{1-\frac{\beta}{2}}(0,1)$. Then the optimal-order error estimate in the energy norm holds

$$
\left\|u_{h}-u\right\|_{H^{1-\frac{\beta}{2}}(0,1)} \leq C h^{m-1+\beta / 2}\|u\|_{H^{m}(0,1)}
$$

- Assume that the dual problem has the full regularity for each $g \in L^{2}$. Then the optimal-order error estimate in the $L^{2}$ norm holds for $u \in H^{m}(0,1) \cap H_{0}^{1-\frac{\beta}{2}}(0,1)$
- Extensions to spectral Galerkin methods and other methods were proved under the same assumptions.


## A finite volume method (FVM) for conservative FDE (18) with $u_{l}=u_{r}=0$

- Conservative and non-conservative FDEs are not equivalent.
- Finite element/volume methods are suited for conservative FDEs.
- Finite difference methods are suited for nonconservative FDEs.
- In many applications, local mass conservation is crucial.
- A finite-volume scheme naturally has second-order accuracy in space, without a Richardson extrapolation as in finite difference methods.
- Let $u=\sum_{j=1}^{N} u_{j} \phi_{j}, u:=\left[u_{1}, u_{2}, \ldots, u_{N}\right]^{T}, f:=\left[f_{1}, f_{2}, \ldots, f_{N}\right]^{T}$, $A:=\left[A_{i, j}\right]_{i, j=1}^{N}$. Integrating (18) over $\left(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right)$ yields

$$
\begin{align*}
& A u=f, \quad f_{i}:=\int_{x_{i-1 / 2}}^{x_{i+1 / 2}} f(x) d x, \quad 1 \leq i, j \leq N .  \tag{21}\\
& A_{i, j}:=\left[K(x)\left(\theta{ }_{0}^{C, l} D_{x}^{1-\beta} u-(1-\theta){ }_{x}^{C, r} D_{1}^{1-\beta} u\right)\right]_{x=x_{i+1 / 2}}^{x=x_{i-1 / 2}} .
\end{align*}
$$

## Structure of $A$ (Cheng et al, 2015; W. et al, 2015)

## Theorem

$$
\begin{equation*}
A=\gamma(\beta)\left(K_{-} T_{L}^{\beta, N}+K_{+} T_{R}^{\beta, N}\right), \quad K_{ \pm}:=\operatorname{diag}\left(\left\{K\left(x_{i \pm \frac{1}{2}}\right)\right\}_{i=1}^{N}\right) \tag{22}
\end{equation*}
$$

where $T_{L}^{\beta, N}$ and $T_{R}^{\beta, N}$ are full Toeplitz matrices. So $A$ can be stored in $O(N)$ memory and $A v$ can be evaluated in $O(N \log N)$ operations for any $v \in \mathbb{R}^{N}$.

+ A fast Krylov subspace iterative method reduces the computational complexity of each iteration from $O\left(N^{2}\right)$ to $O(N \log N)$.
- For problem (18), the condition number $\kappa(A)=O\left(h^{-(2-\beta)}\right)$.
- The number of Krylov iterations is $O\left(h^{-(1-\beta / 2)}\right)=O\left(N^{1-\beta / 2}\right)$, leading to an overall computational complexity of $O\left(N^{2-\beta / 2} \log N\right)$.
- This calls for an effective and efficient preconditioner.


## A preconditioner for (18) with $\theta=1 / 2$ (W. \& Du 2013)

## Theorem

$M:=T_{L}^{\beta, N}+T_{R}^{\beta, N}$ is a full symmetric and positive-definite, Toeplitz matrix.

- Outline of (a perburbation-based) proof: Let $K_{0}:=\operatorname{diag}\left(\left\{K\left(x_{i}\right)\right\}_{i=1}^{N}\right)$.

$$
\begin{align*}
& \gamma(\beta)^{-1} K_{0}^{-1} A \\
& \quad=K_{0}^{-1} K_{-} T_{L}^{\beta, N}+K_{0}^{-1} K_{+} T_{R}^{\beta, N} \\
& \quad=K_{0}^{-1}\left[K_{0}+\left(K_{-}-K_{0}\right)\right] T_{L}^{\beta, N}+K_{0}^{-1}\left[K_{0}+\left(K_{+}-K_{0}\right)\right] T_{L}^{\beta, N}  \tag{23}\\
& \quad=M+K_{0}^{-1}\left[\left(K_{-}-K_{0}\right) T_{L}^{\beta, N}+\left(K_{+}-K_{0}\right) T_{R}^{\beta, N}\right] \\
& \quad=M+O(h)
\end{align*}
$$

- $M$ is a good preconditioner for the finite volume scheme (21).

$$
\begin{equation*}
\left(K_{0}^{-1} K_{-} T_{L}^{\beta, N}+K_{0}^{-1} K_{+} T_{R}^{\beta, N}\right) u=\gamma(\beta)^{-1} K_{0}^{-1} A u=\gamma(\beta)^{-1} K_{0}^{-1} f . \tag{24}
\end{equation*}
$$

- $M$ can be inverted via the superfast algorithm (Ammar \& Gragg, 1988) in $O\left(N \log ^{2} N\right)$ operations.


## An example run by a preconditioned fast FVM

- The data in (18): $\beta=0.2, \theta=0.5, K(x)=\Gamma(1.2)(1+x), u_{l}=u_{r}=0$.
- The true solution $u(x)=x^{2}(1-x)^{2}, f$ is computed accordingly

|  | Gauss |  |  | CGS |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| N | $\left\\|u-u_{G}\right\\|_{L}$ ( ${ }^{\infty}$ | CPU(s) |  | $\left\\|u-u_{C}\right\\|_{L}$ ( ${ }^{\text {a }}$ | CPU(s) | Itr. \# |
| $2^{5}$ | $2.018 \times 10^{-4}$ | 0.000 |  | $2.018 \times 10^{-4}$ | 0.000 | 32 |
| $2^{6}$ | $5.157 \times 10^{-5}$ | 0.000 |  | $5.157 \times 10^{-5}$ | 0.000 | 65 |
| $2^{7}$ | $1.294 \times 10^{-5}$ | 0.000 |  | $1.294 \times 10^{-5}$ | 0.016 | 128 |
| $2^{8}$ | $3.214 \times 10^{-6}$ | 0.047 |  | $3.214 \times 10^{-6}$ | 0.141 | 217 |
| $2^{9}$ | $7.893 \times 10^{-7}$ | 0.500 |  | $7.893 \times 10^{-7}$ | 3.359 | 599 |
| $2^{10}$ | $1.887 \times 10^{-7}$ | 7.797 |  | $1.886 \times 10^{-7}$ | 2 m 2 s | 1,110 |
| $2^{11}$ | $4.030 \times 10^{-8}$ | 2 m 38 s |  | $4.047 \times 10^{-8}$ | 21 ml 13 s | 2,624 |
| $2^{12}$ | $6.227 \times 10^{-9}$ | 24 m 29 s |  | $7.468 \times 10^{-8}$ | 4 h 19 m | 7,576 |
| $2^{13}$ | $5.783 \times 10^{-9}$ | 3 h 27 m |  | N/A | $>2$ days | > 20,000 |
|  |  | GS |  |  | FCGS |  |
|  | $\left\\|u-u_{F}\right\\|_{L}$ ( ${ }^{\text {a }}$ | CPU(s) | Itr. \# | $\left\\|u-u_{S}\right\\|_{L}{ }^{\infty}$ | CPU(s) | Itr. \# |
| $2^{5}$ | $2.018 \times 10^{-4}$ | 0.000 | 32 | $2.018 \times 10^{-4}$ | 0.000 | 6 |
| $2^{6}$ | $5.157 \times 10^{-5}$ | 0.016 | 63 | $5.157 \times 10^{-5}$ | 0.000 | 5 |
| $2^{7}$ | $1.294 \times 10^{-5}$ | 0.031 | 128 | $1.294 \times 10^{-5}$ | 0.000 | 5 |
| $2^{8}$ | $3.214 \times 10^{-6}$ | 0.125 | 248 | $3.214 \times 10^{-6}$ | 0.006 | 5 |
| $2^{9}$ | $7.893 \times 10^{-7}$ | 0.578 | 576 | $7.893 \times 10^{-7}$ | 0.016 | 5 |
| $2^{10}$ | $1.886 \times 10^{-7}$ | 2.281 | 1,078 | $1.887 \times 10^{-7}$ | 0.047 | 5 |
| $2^{11}$ | $4.037 \times 10^{-8}$ | 9.953 | 1,997 | $4.038 \times 10^{-8}$ | 0.078 | 5 |
| $2^{12}$ | $1.587 \times 10^{-8}$ | 57.27 | 5,130 | $6.194 \times 10^{-9}$ | 0.188 | 5 |
| $2^{13}$ | $2.372 \times 10^{-8}$ | 2 m 52 s | 7,410 | $4.345 \times 10^{-9}$ | 0.391 | 5 |

- Use the numerical solutions by Gaussian elimination as a benchmark:
- The conjugate gradient squared (CGS) method diverges, due to significant amount of round-off errors.
- The fast CGS (FCGS) reduced the CPU time significantly, as the operations for each iteration is reduced from $O\left(N^{2}\right)$ to $O(N \log N)$.
- The number of iterations is still $O\left(N^{1-\beta / 2}\right)$,
- It is less accurate than Gaussian at fine meshes due to round-off errors.
- The preconditioner $M$ is optimal, so the preconditioned FCGS (PFCGS) has an overall computational cost of $O\left(N \log ^{2} N\right)$.
- It significantly reduces round-off errors.
- It generates more accurate solutions than Gaussian elimination.
- It further reduces CPU time.


## W. \& Zhang 2015)

- Error estimates were proved for numerical methods for FDEs, under the assumption that the true solution is smooth.
- For integer-order elliptic or parabolic PDEs, smooth data (and domain for multi-D problem) $\Longrightarrow$ smooth solution.
- $u(x)=\left(x^{2-\beta}-x^{1-\beta}\right) / \Gamma(3-\beta) \notin W^{1,1 / \beta}(0,1)$ is the solution of

$$
\begin{equation*}
D\left({ }_{0} D_{x}^{-\beta} D u\right)=1, \quad x \in(0,1), \quad u(0)=u(1)=0 \tag{25}
\end{equation*}
$$

- In particular, $u \notin H^{1}(0,1)$ for $1 / 2 \leq \beta \leq 1$.
- For FDEs smooth data does not ensure smooth solutions
- No conditions in the literature to ensure smooth solutions to FDEs.
- The Nitsche-lifting based proof of optimal-order $L^{2}$ error estimates in the literature does not hold even for constant $K>0$.
- What conditions ensures that high-order methods $\Longrightarrow$ high-order convergence rates?
- Solutions may have boundary layers and other singularity, which need to be resolved numerically.


## An FVM on a gridded mesh (Jia et al., 2014; Tian et al, 2013)

- Solutions to FDEs with smooth data and domain may have boundary layers, a uniform mesh is not effective.
- Finite-difference methods out of the question, as Grünwald-Letnikov derivatives are inherently defined on uniform meshes.
- Riemann-Liouville and Caputo derivatives offer such flexibilities.
- Bebause of the nonlocal nature of FDEs, a numerical scheme discretized on an arbitrarily adaptively refined mesh
- offers great flexbility and effective approximation property
- offers possible advantage on its theoretical analysis
- destroys the structure of its stiffness matrix and so efficiency.
- Motivation: balancing flexibility and efficiency.


## The structure of the stiffness matrix

- We assume a geometrically refined mesh towards the left endpoint.


## Theorem

The matrix $A$ can be decomposed as

$$
\begin{aligned}
A=\frac{1}{\Gamma(\beta+1)} & {\left[\operatorname{diag}\left(K^{-}\right)\left(\gamma Q_{l}+(1-\gamma) Q_{r}\right)\right.} \\
& \left.-\operatorname{diag}\left(K^{+}\right)\left(\gamma P_{l}+(1-\gamma) P_{r}\right)\right] \operatorname{diag}\left(\left\{h_{i}^{\beta-1}\right\}_{i=1}^{m}\right) .
\end{aligned}
$$

- $P_{l}, P_{r}, Q_{l}$ and $Q_{r}$ are Toeplitz.
- $A$ has an additional diagonal matrix (reflecting the impact of the mesh sizes) multiplier to that on the uniform mesh.


## Numerical experiments of a one-sided FDE on a gridded mesh

- Consider (18) with $K=1, f=0, \beta=0.98, \theta=1, u_{l}=0, u_{r}=1$, i.e.,

$$
\begin{aligned}
D\left({ }_{0} D_{x}^{-\beta} D u\right) & =0, \quad x \in(0,1), \\
u(0)=0, \quad u(1) & =1
\end{aligned}
$$

Its solution $u(x)=x^{1-\beta}$ for $x \in(0,1)$.

|  | N | CPU | \#of iterations |
| :---: | :---: | :---: | :---: |
| Gauss | 256 | 0.640 s |  |
|  | 512 | 5.567 s |  |
|  | 1024 | 59 s |  |
| CGS | 256 | 2.978 s | 256 |
|  | 512 | 29 s | 512 |
|  | 1024 | 403 s | 1024 |
| FCGS | 256 | 0.073 s | 256 |
|  | 512 | 0.139 s | 512 |
|  | 1024 | 0.391 s | 1024 |

Figure: First row: numerical solutions on a uniform mesh of $n=256,512,1024$; Second row: numerical solutions on a geometrically refined mesh $n=48,64,96$.







## An FVM on a locally refined composite mesh (Jia \& W. 2016)

- Solutions to FDEs with smooth data and domain may have boundary layers. Numerical solution of FDEs
- with a uniform mesh is not effective.
- with a gridded mesh may resolve the boundary layers, but does not necessarily provide an accurate global approximation.
- We propose to use a composite mesh that consists of
- a uniform mesh in most of the domain,
- a gridded mesh in the cells near the (left) boundary.
- The key issue is the structure of the stiffness matrix:

$$
A=\left[\begin{array}{ll}
A_{l, l} & A_{l, r}  \tag{26}\\
A_{r, l} & A_{r, r}
\end{array}\right] .
$$

- $A_{r, r}$, corresponding to the uniform mesh, has a Toeplitz-like structure.
- $A_{l, l}$, corresponding to the gridded mesh, has a Toeplitz-like structure with an extra right diagonal multiplier.


## The structure of the off-diagonal submatrices in the stiffness matrix

- The off-diagonal submatrices $A_{l, r}$ and $A_{r, l}$
- are full due to the nonlocal nature of FDEs,
- are not Toeplitz-like.


## Theorem

$$
\begin{aligned}
A_{l, r} & =\frac{(1-\gamma) h^{\beta-1}}{\Gamma(\beta+1)}\left(\operatorname{diag}\left(K_{l}^{-}\right) E-\operatorname{diag}\left(K_{l}^{+}\right) D\right) \\
A_{r, l} & =\frac{\gamma}{\Gamma(\beta+1)}\left(\operatorname{diag}\left(K_{r}^{-}\right) H-\operatorname{diag}\left(K_{r}^{+}\right) G\right) \operatorname{diag}\left(\left\{h_{i}^{\beta-1}\right\}_{i=1}^{m}\right)
\end{aligned}
$$

- The typical entries of $D$ and $E$ are of the form

$$
\begin{aligned}
d_{i, j} & =2\left(j+1-3 \cdot 2^{i-m-1}\right)^{\beta}-\left(j-3 \cdot 2^{i-m-1}\right)^{\beta}-\left(j+2-3 \cdot 2^{i-m-1}\right)^{\beta} \\
g_{i, j} & =\left[2^{m-j+1}\left(i+\frac{3}{2}\right)-1\right]^{\beta}-\frac{3}{2}\left[2^{m-j+1}\left(i+\frac{3}{2}\right)-2\right]^{\beta} \\
& +\frac{1}{2}\left[2^{m-j+1}\left(i+\frac{3}{2}\right)-4\right]^{\beta}
\end{aligned}
$$

- Use a fractional binomial expansion, we have

$$
\begin{aligned}
D \approx & -2\binom{\beta}{2}[1,1, \ldots, 1]^{T}\left[\frac{1}{2^{2-\beta}}, \frac{1}{3^{2-\beta}}, \ldots, \frac{1}{(n-1)^{2-\beta}}\right] \\
& -2\binom{\beta}{4}[1,1, \ldots, 1]^{T}\left[\frac{1}{2^{4-\beta}}, \frac{1}{3^{4-\beta}}, \ldots, \frac{1}{(n-1)^{4-\beta}}\right] \\
& +18\binom{\beta}{3}\left[2^{-m}, 2^{-m+1}, \ldots, 2^{-1}\right]^{T}\left[\frac{1}{2^{3-\beta}}, \frac{1}{3^{3-\beta}}, \ldots, \frac{1}{(n-1)^{3-\beta}}\right] \\
& -108\binom{\beta}{4}\left[2^{-2 m}, 2^{-2 m+2}, \ldots, 2^{-2}\right]^{T}\left[\frac{1}{2^{4-\beta}}, \frac{1}{3^{4-\beta}}, \ldots, \frac{1}{(n-1)^{4-\beta}}\right]
\end{aligned}
$$

- The matrices can be approximated by a finite sum of low-rank matrices.
- The matrix-vector multiplication can be performed in $O(N)$ operations.


## A block-diagonal preconditioner

- A preconditioner based on T. Chan's circulant preconditioner $C_{n}$, which minimizes $\left\|A-C_{n}\right\|_{F}$ over all circulant matrices.
- We define a block-diagonal-circulant-block preconditioner $M$ for $A$

$$
M:=\left[\begin{array}{cc}
M_{1} & 0  \tag{27}\\
0 & M_{2}
\end{array}\right]
$$

- $M_{1}$ is a preconditioner for $A_{l, l}$
- $M_{2}$ is a preconditioner for $A_{r, r}$


## Numerical experiments of a one-sided FDE on a composite mesh

- Consider (18) with $K=1, f=0, \theta=1, \beta=0.9, u_{l}=0, u_{r}=1$, i.e.,

$$
\begin{aligned}
D\left({ }_{0} D_{x}^{-\beta} D u\right) & =0, \quad x \in(0,1), \\
u(0)=0, \quad u(1) & =1
\end{aligned}
$$

Its solution $u(x)=x^{1-\beta}$ for $x \in(0,1)$.

| n | $\left\\|u_{n}-u\right\\|$ | $\left\\|u_{n, m}-u\right\\|$ | $\left\\|u_{n, m}-u\right\\|$ |
| ---: | :---: | :---: | :---: |
| 128 | $4.3546 \times 10^{-1}$ | $2.6805 \times 10^{-1}, m=7$ | $2.0315 \times 10^{-1}, m=11$ |
| 256 | $4.0630 \times 10^{-1}$ | $2.3336 \times 10^{-1}, m=8$ | $1.3403 \times 10^{-1}, m=16$ |
| 512 | $3.7909 \times 10^{-1}$ | $2.0315 \times 10^{-1}, m=9$ | $8.2504 \times 10^{-2}, m=22$ |
| 1024 | $3.5370 \times 10^{-1}$ | $1.7685 \times 10^{-1}, m=10$ | $3.8488 \times 10^{-2}, m=32$ |
| 8192 | $2.8730 \times 10^{-1}$ | $1.6668 \times 10^{-1}, m=13$ | $\mathrm{~N} / \mathrm{A}$ |

Figure: First row: numerical solutions on a uniform mesh of $n=256,8192$; Second row: numer. solns. on a composite mesh with $n=256$ and $m=8,16$.





## Numerical experiments of a two-sided FDE on a locally refined composite mesh

- Consider (18) with $K=1, \theta=0.5, \beta=0.95, u_{l}=0, u_{r}=1$,

$$
f(x)=\frac{(1-\gamma)(1-\beta)}{\Gamma(\beta) x(1-x)^{1-\beta}}, \quad u(x)=x^{1-\beta}, \quad x \in(0,1)
$$

|  | m | n | Error | Iterations |
| :---: | :---: | :---: | :---: | :---: |
| Gauss | $2^{3}$ | $2^{8}$ | $1.4379 \times 10^{-1}$ |  |
|  | $2^{4}$ | $2^{9}$ | $1.0491 \times 10^{-1}$ |  |
|  | $2^{5}$ | $2^{10}$ | $5.8194 \times 10^{-2}$ |  |
| CGS | $2^{3}$ | $2^{8}$ | $1.4379 \times 10^{-2}$ | 48 |
|  | $2^{4}$ | $2^{9}$ | $1.0491 \times 10^{-1}$ | 77 |
|  | $2^{5}$ | $2^{10}$ | $5.8194 \times 10^{-2}$ | 142 |
| FCGS | $2^{3}$ | $2^{8}$ | $1.4379 \times 10^{-1}$ | 48 |
|  | $2^{4}$ | $2^{9}$ | $1.0491 \times 10^{-1}$ | 78 |
|  | $2^{5}$ | $2^{10}$ | $5.8194 \times 10^{-2}$ | 150 |
| PFCGS | $2^{3}$ | $2^{8}$ | $1.4379 \times 10^{-1}$ | 9 |
|  | $2^{4}$ | $2^{9}$ | $1.0491 \times 10^{-1}$ | 13 |
|  | $2^{5}$ | $2^{10}$ | $5.8194 \times 10^{-2}$ | 16 |

Table: Numerical results on a uniform mesh

|  | n | Error | Iterations | CPUs |
| :---: | :---: | :---: | :---: | :---: |
| Gauss | $2^{8}$ | $1.8827 \times 10^{-1}$ |  | 0.01 s |
|  | $2^{9}$ | $1.8206 \times 10^{-1}$ |  | 0.01 s |
|  | $2^{10}$ | $1.7596 \times 10^{-1}$ |  | 0.05 s |
|  | $2^{11}$ | $1.7002 \times 10^{-1}$ |  | 0.25 s |
|  | $2^{12}$ | $1.6425 \times 10^{-1}$ |  | 1.25 s |
|  | $2^{13}$ | $1.5867 \times 10^{-1}$ |  | 9.76 s |
|  | $2^{14}$ | $1.5327 \times 10^{-1}$ |  | 97 s |
| CGS | $2^{8}$ | $1.8827 \times 10^{-1}$ | 46 | 0.01 s |
|  | $2^{9}$ | $1.8206 \times 10^{-1}$ | 66 | 0.01 s |
|  | $2^{10}$ | $1.7596 \times 10^{-1}$ | 94 | 0.18 s |
|  | $2^{11}$ | $1.7002 \times 10^{-1}$ | 133 | 0.86 s |
|  | $2^{12}$ | $1.6425 \times 10^{-1}$ | 188 | 4.94 s |
|  | $2^{13}$ | $1.5867 \times 10^{-1}$ | 266 | 30.78 s |
|  | $2^{14}$ | $1.5327 \times 10^{-1}$ | 379 | 187 s |
|  | $2^{8}$ | $1.8827 \times 10^{-1}$ | 46 | 0.05 s |
|  | $2^{9}$ | $1.8206 \times 10^{-1}$ | 66 | 0.16 s |
|  | $2^{10}$ | $1.7596 \times 10^{-1}$ | 94 | 0.29 s |
|  | $2^{11}$ | $1.7002 \times 10^{-1}$ | 133 | 1.16 s |
|  | $2^{12}$ | $1.6425 \times 10^{-1}$ | 188 | 2.00 s |
|  | $2^{13}$ | $1.5867 \times 10^{-1}$ | 266 | 12 s |
|  | $2^{14}$ | $1.5327 \times 10^{-1}$ | 379 | 27 s |
|  | $2^{8}$ | $1.8827 \times 10^{-1}$ | 8 | 0.02 s |
| PFCGS | $2^{9}$ | $1.8206 \times 10^{-1}$ | 8 | 0.02 s |
|  | $2^{10}$ | $1.7596 \times 10^{-1}$ | 9 | 0.05 s |
|  | $2^{11}$ | $1.7002 \times 10^{-1}$ | 10 | 0.09 s |
|  | $2^{12}$ | $1.6425 \times 10^{-1}$ | 10 | 0.14 s |
| $2^{13}$ | $1.5867 \times 10^{-1}$ | 10 | 0.66 s |  |
| $2^{14}$ | $1.5327 \times 10^{-1}$ | 11 | 1.00 s |  |

- FPDEs have significantly different mathematical and numerical properties from their integer-order analogues. For instance,
- For $u_{l}=u_{r}=0,(18)$ and its Riemann-Liouville analogue coincide. They are well posed if $K$ is a positive constant.
- When $u_{l}, u_{r}$ do not vanish, then (18) is well posed for a postive constant $K$. But its Riemann-Liouville analogue does not admit a solution.


## Extensions to variable-coefficient problems: A counterexample (W. \& Yang 2013)

## Lemma

$B(w, w)<0$ for some $K(x)$ of two positive constants and $w \in H_{0}^{1-\frac{\beta}{2}}(0,1)$
Let $K(x)$ and $w \in H_{0}^{1}(0,1) \subset H_{0}^{1-\frac{\beta}{2}}(0,1)$ be defined by

$$
\begin{gathered}
K(x):=\left\{\begin{array}{ll}
K_{l}, & x \in(0,1 / 2), \\
1, & x \in(1 / 2,1) .
\end{array} \quad w(x):= \begin{cases}2 x, & x \in(0,1 / 2], \\
2(1-x), & x \in[1 / 2,1) .\end{cases} \right. \\
C_{0}^{C, l} D_{x}^{1-\beta} w(x)= \begin{cases}2 x^{\beta} / \Gamma(\beta+1), \\
2\left(x^{\beta}-2(x-1 / 2)^{\beta}\right) / \Gamma(\beta+1), & x \in(0,1 / 2),\end{cases} \\
B(w, w)=2^{1-\beta}\left(K_{l}-\left(2^{\beta+1}-3\right)\right) / \Gamma(\beta+2) .
\end{gathered}
$$

As $0<\log _{2} 3-1<1$, choose $\log _{2} 3-1<\beta<1$ so that $2^{\beta+1}-3>0$. Select $K_{l}>0$ such that $K_{l}-\left(2^{\beta+1}-3\right)<0$. For such $K$ and $w, B(w, w)<0$.

- Consider the one-sided problem ((18) with $\theta=1)$

$$
\begin{equation*}
-D\left(K_{0} D_{x}^{-\beta} D u\right)=f(x), \quad x \in(0,1), \quad u(0)=u(1)=0 . \tag{28}
\end{equation*}
$$

- For a variable $K$

$$
\begin{aligned}
B(u, v) & =\theta\left\langle K_{0} I_{x}^{\beta} D u, D v\right\rangle+(1-\theta)\left\langle K{ }_{x} I_{1}^{\beta} D u, D v\right\rangle \\
& \neq \theta\left\langle K D u,{ }_{x} I_{1}^{\beta} D v\right\rangle+(1-\theta)\left\langle K D u,{ }_{0} I_{x}^{\beta} D v\right\rangle \\
& \neq\left(K_{0} I_{x}^{\beta / 2} D u,{ }_{x} I_{1}^{\beta / 2} D v\right)_{L^{2}(0,1)}
\end{aligned}
$$

- Even the best possible (last) form cannot guarantee the coercivity of $B$

$$
\begin{aligned}
& \left(K_{0} I_{x}^{\beta / 2} D u,{ }_{x} I_{1}^{\beta / 2} D u\right)_{L^{2}(0,1)} \\
& \quad \nsupseteq K_{\min }\left({ }_{0} I_{x}^{\beta / 2} D u,_{x} I_{1}^{\beta / 2} D u\right)_{L^{2}(0,1)} \\
& \quad=\cos (\beta \pi / 2) K_{\text {min }}|u|_{H^{1-\beta / 2}(0,1)}^{2} .
\end{aligned}
$$

- ${ }_{0} I_{x}^{\beta / 2} D u$ and ${ }_{x} I_{1}^{\beta / 2} D u$ do not always have the same sign on $(0,1)$.
- One can choose a smooth $K$ such that the left-hand side negative.


## A Petrov-Galerkin formulation (W. \& Yang 2013)

- For a variable $K$, the Galerkin formulation is not coercive on any product space $H \times H$ so $H_{0}^{1-\frac{\beta}{2}}(0,1) \times H_{0}^{1-\frac{\beta}{2}}(0,1)$ is not a feasible choice.
- That the FDE is a local mass balance incorporated with a fractional Fick's law motivates a Petrov-Galerkin formulation: Seek $u \in H_{0}^{1-\beta}(0,1)$ such that

$$
\begin{equation*}
A(u, v):=\int_{0}^{1} K(x)\left({ }_{0} D_{x}^{-\beta} D u\right) D v d x=\langle f, v\rangle, \quad \forall v \in H_{0}^{1}(0,1) \tag{29}
\end{equation*}
$$

## Theorem

Assume $0<\beta<1 / 2$ and $0<K_{\text {min }} \leq K \leq K_{\max }<\infty$. Then

$$
\begin{align*}
& \inf _{w \in H_{0}^{1-\beta}(0,1)} \sup _{v \in H_{0}^{1}(0,1)} \frac{A(w, v)}{\|w\|_{H^{1-\beta}(0,1)}\|v\|_{H^{1}(0,1)}} \geq \gamma(\beta)>0,  \tag{30}\\
& \sup _{w \in H_{0}^{1-\beta}(0,1)} A(w, v)>0 \quad \forall v \in H_{0}^{1}(0,1) \backslash\{0\} .
\end{align*}
$$

Hence, (29) has a unique solution $u \in H_{0}^{1-\beta}(0,1)$ with the estimate

$$
\begin{equation*}
\|u\|_{H^{1-\beta}(0,1)} \leq\left(K_{\max } / \gamma\right)\|f\|_{H^{-1}(0,1)} . \tag{31}
\end{equation*}
$$

## A spectral Galerkin method

- $P_{N}[-1,1]$ : the space of polynomials of degree $\leq N$ on $[-1,1]$
- $L_{n}(x)$ : the $n$th degree Legendre polynomial on $[-1,1]$

$$
\begin{gathered}
L_{0}(x)=1, \quad L_{1}(x)=x, \quad L_{n+1}(x)=\frac{2 n+1}{n+1} x L_{n}(x)-\frac{n}{n+1} L_{n-1}(x), n \geq 1 \\
\int_{-1}^{1} L_{n}(x) L_{m}(x) d x=\frac{2}{2 n+1} \delta_{m, n}, \quad L_{n}( \pm 1)=( \pm 1)^{n}
\end{gathered}
$$

- $\phi_{n}(x):=L_{n}(x)-L_{n+2}(x)$ are linearly independent with $\phi( \pm 1)=0$.

$$
S_{N}[-1,1]:=\left\{v \in P_{N}[-1,1]: v(-1)=v(1)=0\right\}=\operatorname{span}\left\{\phi_{n}\right\}_{n=0}^{N-2}
$$

- A spectral-Galerkin method: Seek $u_{N} \in S_{N}[-1,1]$ such that

$$
B\left(u_{N}, v_{N}\right)=\left\langle f, v_{N}\right\rangle, \quad \forall v_{N} \in S_{N}[-1,1]
$$

## Theorem

(Huang et al. 2013; Zeng et al. 2014) If $u \in H^{r} \cap H_{0}^{1-\beta / 2}$ and $1-\beta / 2 \leq s \leq r$, then

$$
\begin{equation*}
\left\|u_{N}-u\right\|_{H^{s}} \leq C N^{-(r-s)}\|u\|_{H^{r}}, \quad 1-\beta / 2 \leq s \leq r . \tag{32}
\end{equation*}
$$

Assume full regularity of the dual problem for each right-hand side, then the estimate holds for $0 \leq s \leq r$.

## Theorem

(W. \& Zhang 2015) The solution $u$ to problem (18) with $0<\beta<1 / 2$, constant $K$ and $f$ and $u_{l}=u_{r}=0$ is not in $H^{\frac{3}{2}-\beta}$ but in $B_{\infty}^{\frac{3}{2}-\beta}\left(L^{2}\right)$. The best provable convergence rate in (32) is $r=\frac{3}{2}-\beta$.

- In particular, the convergence rate in $\|\cdot\|_{H^{1-\beta / 2}}$ is $O\left(N^{-(1-\beta) / 2}\right)$.


## An indirect spectral Galerkin (ISPG) method (W. \& Zhang 2015)

## Theorem

For $0<\beta<1 / 2$ the true solution $u$ to a one-dimensional, one-sided FDE can be decomposed as

$$
\begin{array}{ll}
u=u_{l}+\left(u_{r}-u_{l}-{ }_{-1}^{C} D_{1}^{\beta} w_{f}\right)\left({ }_{-1}^{C} D_{1}^{\beta} w_{b}\right)^{-1}{ }_{-1}^{C} D_{x}^{\beta} w_{b}+{ }_{-1}^{C} D_{x}^{\beta} w_{f} . \\
-D\left(K(x) D w_{f}\right)=f, \quad x \in(-1,1) ; & w_{f}(-1)=w_{f}(1)=0 \\
-D\left(K(x) D w_{b}\right)=0, \quad x \in(-1,1) ; & w_{b}(-1)=0, w_{b}(1)=1 . \tag{34}
\end{array}
$$

- Use SPG to solve the second-order DE (34) (Canuto et al 2006, Shen et al 2011): Find $w_{N} \in S_{N}[-1,1]$ such that

$$
\left(K(x) D w_{N}, D v_{N}\right)_{L^{2}(-1,1)}=\left(f, v_{N}\right)_{L^{2}(-1,1)}, \quad \forall v_{N} \in S_{N}[-1,1]
$$

- Use (33) to postprocess $w_{N}$ to obtain $u_{N}$


## Numerical issues

- Properties of $\left({ }_{-1}^{C} D_{1}^{\beta} w_{b}\right)^{-1}$ and ${ }_{-1}^{C} D_{x}^{\beta} w_{b}$
- ${ }_{-1}^{C} D_{x}^{\beta} w_{b}$ can be evaluated as follows

$$
\begin{aligned}
{ }_{-1}^{C} D_{x}^{\beta} w_{b} & ={ }_{-1} D_{x}^{-(1-\beta)} D w_{b} \\
& =\left(\int_{-1}^{1} \frac{1}{K(s)} d s\right)^{-1}{ }_{-1} D_{x}^{-(1-\beta)} \frac{1}{K(x)} \\
& =\left(\int_{-1}^{1} \frac{1}{K(s)} d s\right)^{-1} \frac{1}{\Gamma(1-\beta)} \int_{-1}^{x} \frac{1}{K(s)(x-s)^{\beta}} d s>0 .
\end{aligned}
$$

- $\left({ }_{-1}^{C} D_{1}^{\beta} w_{b}\right)^{-1}$ is well defined and ${ }_{-1}^{C} D_{x}^{\beta} w_{b}$ is bounded in $L^{\infty}(-1,1)$.
- Spetral method offers additional computational benefit
- Evaluating ${ }_{-1}^{C} D_{x}^{\beta} w_{N}$ requires numerical integration of a weakly singular integral of $D w_{N}$.
- Spectral method can carry out the calculation analytically in a systematic manner.


## Using Jacobi polynomials to handle singularity

- $J_{n}^{\mu, \nu}(x)$ - the $n$th order Jacobi polynomials that are orthogonal with respect to the Jacobi weight function $\omega^{\mu, \nu}:=(1-x)^{\mu}(1+x)^{\nu}$

$$
\begin{aligned}
J_{0}^{\mu, \nu}= & 1, \quad J_{1}^{\mu, \nu}=\frac{1}{2}(\mu+\nu+2) x+\frac{1}{2}(\mu-\nu) \\
J_{n+1}^{\mu, \nu}= & \left(a_{n}^{\mu, \nu} x-b_{n}^{\mu, \nu}\right) J_{n}^{\mu, \nu}-c_{n}^{\mu, \nu} J_{n-1}^{\mu, \nu} \\
= & \frac{n+\mu+1}{n!\Gamma(n+\mu+\nu+1)} \sum_{k=0}^{n}\binom{n}{k} \frac{\Gamma(n+k+\mu+\nu+1)}{\Gamma(k+\mu+1)}\left(\frac{x-1}{2}\right)^{k} \\
& n \geq 1
\end{aligned}
$$

where $a_{n}^{\mu, \nu}, b_{n}^{\mu, \nu}$, and $c_{n}^{\mu, \nu}$ are constants having explicit expressions.

## Theorem

(Huang et al 2011; Shen et al 2011) For $\mu>0$,

$$
\begin{aligned}
& { }_{-1}^{R} D_{x}^{\mu} L_{n}(x)=\frac{\Gamma(n+1)}{\Gamma(n-\mu+1)}(1+x)^{-\mu} J_{n}^{\mu,-\mu}(x), \quad x \in[-1,1], \\
& { }_{x}^{R} D_{1}^{\mu} L_{n}(x)=\frac{\Gamma(n+1)}{\Gamma(n-\mu+1)}(1-x)^{-\mu} J_{n}^{-\mu, \mu}(x), \quad x \in[-1,1] .
\end{aligned}
$$

- The SPG solution $w_{N} \in S_{N}[-1,1]$ can be expressed as

$$
\begin{gathered}
w_{N}(x)=\sum_{n=0}^{N-2} d_{n} \phi_{n}(x)=\sum_{n=0}^{N-2} d_{n}\left(L_{n}(x)-L_{n+2}(x)\right) \\
{ }_{-1}^{C} D_{x}^{\beta} w_{N}={ }_{-1}^{R} D_{x}^{\beta} w_{N}= \\
\\
\left.-\frac{\sum_{n=0}^{N-2} d_{n}(1+x)^{-\beta}\left(\frac{\Gamma(n+1)}{\Gamma(n+1-\beta)} J_{n}^{\beta,-\beta}(x)\right.}{\Gamma(n+3-\beta)} J_{n+2}^{\beta,-\beta}(x)\right)
\end{gathered}
$$

## Error estimates requiring only the smoothness of the data

## Theorem

(W. \& Zhang 2015) Let $0<\beta<1 / 2, K \in C^{m}[-1,1]$, and $f \in H^{m-1}(-1,1)$ for any $m \geq 1$. Then,

$$
\left\|u_{N}-u\right\|_{L^{2}(-1,1)} \leq C N^{-m}
$$

where $C=C\left(\beta, m,\|K\|_{C^{m}[-1,1]},\|f\|_{H^{m-1}(-1,1)}\right)$.

## Numerical comparison between the SPG and the ISPG

- $K=1, u_{l}=0, u_{r}=2$, and

$$
f(x)=-\frac{\Gamma(7)}{2^{2-\beta} \Gamma(5+\beta)}\left(\frac{x+1}{2}\right)^{4+\beta} .
$$

- This gives the true solution $u(x)=\left(\frac{x+1}{2}\right)^{1-\beta}+\left(\frac{x+1}{2}\right)^{6}$.
- For SPG, $\left\|u_{N}-u\right\|_{L^{2}(-1,1)} \leq C_{\kappa} N^{-\kappa}$.
- For our improvements, $\left\|u_{N}-u\right\|_{L^{2}(-1,1)} \leq C_{\kappa} e^{-\kappa N}$.

Table: The comparison of the SPG and ISPG methods (W. \& Zhang 2015)

|  | $\left\\|u_{S P G, N}-u\right\\|_{L^{2}(0,1)}$ |  |  | $\left\\|u_{I S P G, N}-u\right\\|_{L^{2}(0,1)}$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $N$ | $\beta=0.1$ | $\beta=0.5$ | $\beta=0.9$ | $\beta=0.1$ | $\beta=0.5$ | $\beta=0.9$ |
| 4 | $2.139 \mathrm{e}-03$ | $5.104 \mathrm{e}-02$ | 1.677 | $9.377 \mathrm{e}-03$ | $2.319 \mathrm{e}-02$ | $7.737 \mathrm{e}-02$ |
| 5 | $1.334 \mathrm{e}-03$ | $4.195 \mathrm{e}-02$ | 0.472 | $8.451 \mathrm{e}-04$ | $2.823 \mathrm{e}-03$ | $1.283 \mathrm{e}-02$ |
| 6 | $9.014 \mathrm{e}-04$ | $3.431 \mathrm{e}-02$ | 1.331 | $6.482 \mathrm{e}-06$ | $1.087 \mathrm{e}-04$ | $9.541 \mathrm{e}-04$ |
| 7 | $6.738 \mathrm{e}-04$ | $2.676 \mathrm{e}-02$ | 0.439 | $4.185 \mathrm{e}-07$ | $3.892 \mathrm{e}-06$ | $7.135 \mathrm{e}-06$ |
| 8 | $5.204 \mathrm{e}-04$ | $2.308 \mathrm{e}-02$ | 1.119 | $5.348 \mathrm{e}-08$ | $3.943 \mathrm{e}-07$ | $5.563 \mathrm{e}-07$ |
| 9 | $4.126 \mathrm{e}-04$ | $1.913 \mathrm{e}-02$ | 0.415 | $9.807 \mathrm{e}-09$ | $6.239 \mathrm{e}-08$ | $7.625 \mathrm{e}-08$ |
| 10 | $3.342 \mathrm{e}-04$ | $1.691 \mathrm{e}-02$ | 0.986 | $2.280 \mathrm{e}-09$ | $1.307 \mathrm{e}-08$ | $1.468 \mathrm{e}-08$ |
| 11 | $2.755 \mathrm{e}-04$ | $1.454 \mathrm{e}-02$ | 0.395 | $6.296 \mathrm{e}-10$ | $3.324 \mathrm{e}-09$ | $3.481 \mathrm{e}-09$ |
| 12 | $2.306 \mathrm{e}-04$ | $1.309 \mathrm{e}-02$ | 0.893 | $1.984 \mathrm{e}-10$ | $9.811 \mathrm{e}-10$ | $9.807 \mathrm{e}-10$ |
| 13 | $1.955 \mathrm{e}-04$ | $1.154 \mathrm{e}-02$ | 0.380 | $6.952 \mathrm{e}-11$ | $3.248 \mathrm{e}-10$ | $3.105 \mathrm{e}-10$ |
| 14 | $1.676 \mathrm{e}-04$ | $1.052 \mathrm{e}-02$ | 0.824 | $2.656 \mathrm{e}-11$ | $1.183 \mathrm{e}-10$ | $1.097 \mathrm{e}-10$ |
| 15 | $1.450 \mathrm{e}-04$ | $9.439 \mathrm{e}-03$ | 0.366 | $1.091 \mathrm{e}-11$ | $4.659 \mathrm{e}-11$ | $4.182 \mathrm{e}-11$ |
| $C_{\kappa}$ | 0.034 | 0.342 | 2.479 | 0.675 | 4.343 | 35.521 |
| $\kappa$ | 2.016 | 1.315 | 0.600 | 1.800 | 1.817 | 1.985 |

## Thank You

## for Your Attention!

