A bilateral preconditioning for an L2-type all-at-once system arising from time-space fractional PDEs

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Outline

Why fractional models?

- Recently, fractional models, due to their ability to model anomalous transport phenomena, have attracted considerable interest in the fields of science and engineering[1];

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- Anomalous diffusion is a phenomenon connected with the interactions within complex and non-homogeneous backgrounds;

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- Traditional PDEs may not be adequate to describe the underlying phenomena;
- Anomalous diffusion is a phenomenon connected with the interactions within complex and non-homogeneous backgrounds;
- Time-space fractional diffusion equations can model the anomalous diffusion, that is, the suddiffusion in time and the super-diffusion in space simultaneously.

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Outline

The Caputo fractional derivatives

Definition

Consider $u(t)$ as an integrable function defined on $(0, T)$, (T is finite or ∞), $0 < \alpha < 1$. Define

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u'(\xi)}{(t-\xi)^\alpha} d\xi, \tag{1}$$

is the Caputo fractional derivative and where $\Gamma(\cdot)$ is the Gamma function. When $\alpha \to 1$, then $\partial_t^\alpha \to \partial_t$.

✓ M. Caputo, Linear Models of Dissipation whose Q is almost Frequency Independent-II, Geophys. J. Int., 13(5) (1967): 529-539.

The Riesz fractional derivative

Definition

Consider the function $u(x,\cdot)$ defined in $\mathbb{R}$, we define

$$\frac{\partial^\beta}{\partial|x|^\beta}u(x,\cdot) = -\frac{1}{2\cos\left(\frac{\beta\pi}{2}\right)\Gamma(2-\beta)}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{\infty}|x-\zeta|^{1-\beta}u(\zeta,\cdot)d\zeta, \quad (2)$$

where $1 < \beta < 2$. This is the so-called Riesz fractional derivative and if $\beta \to 2$, then $\frac{\partial^\beta}{\partial|x|^\beta} \to \frac{\partial^2}{\partial x^2}$.

✓ V.J. Ervin, J.P. Roop, Variational solution of fractional advection dispersion equations on bounded domains in $\mathbb{R}^d$, Numer. Methods Partial Differ. Equ., 23(2) (2007): 256-281.

The time-space fractional Bloch-Torrey equation

In this talk, we consider the following initial-boundary value problem of the time-space fractional Bloch-Torrey equation:

$$\begin{cases} \partial_t^{\alpha} u(x,t) = \kappa \frac{\partial^{\beta} u(x,t)}{\partial |x|^{\beta}} + f(x,t), & x \in \Omega,\ t > 0, \\ u(x,0) = \phi(x), & x \in \Omega \cup \partial\Omega, \\ u(x,t) = 0, & x \in \Omega^c,\ t \geq 0, \end{cases} \tag{3}$$

where $0 < \alpha \leq 1$ and $1 < \beta \leq 2$ are the orders of the fractional derivatives appeared in Eq. (3) and $\kappa > 0$ is the diffusion coefficient. We set $\Omega = (a, b)$, $\Omega^c = \mathbb{R} \setminus \Omega$. $f(x,t)$ is the known source term and $\phi(x)$ is a known function.

Review the previous work

The framework of establishing the numerical methods for Eq. (3):

Temporal discretization + Spatial discretization

- Temporal discretization:
  - L1 formula (Oldham & Spanier, Book74; Lin & Xu JCP07; Sun & Wu, ANM06);
  - L1-2 formula (Gao et al. JCP14, Lv & Xu, SISC16); L2-1_σ formula (Alikhanov, JCP15); L2-type formula (Alikhanov and Huang, AMC21).
  - Grünwald-Letnikov scheme (BDF1) and Lubich's convolution quadrature (i.e., BDFk, Lubich, SIMA86)
- Spatial discretization:
  - Finite difference method: fractional central difference formula, WSGD formula and related work.
  - Finite element method;
  - Finite volume method;
  - Spectral/collaction method.

Our research objective

We want to make the current work consider the following characteristics:

- We present a second-order implicit numerical methods for (3) and prove our scheme is unconditional stable and convergent;
- Set up the parallel-in-space formulation of the proposed difference scheme and solve it iteratively and quickly;
- Analyze the preconditioned PinS iterative algorithm for solving the model (3).

Outline

The high-order discretization of Caputo derivative (1)

Partition the time domain by $t_m = m\tau_t$ ($\tau_t = \frac{T}{M}$, $m = 0, 1, \cdots, M$). Let $u^m = u(x, t_m)$, then we discretize $\partial_t^\alpha u$ at $t = t_{m+1}$ for $1 \le m \le M-1$ by using the L2-type formula [Alikhanov & Huang, AMC21]:

$$\partial_t^\alpha u(x, t_{m+1}) \approx \mathbb{D}_t^\alpha u(x, t_{m+1}) + \mathcal{O}(\tau_t^{3-\alpha}) \triangleq \frac{\tau_t^{-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{m} c_{m-s}^{(\alpha)} [u^{s+1} - u^s] + \mathcal{O}(\tau_t^{3-\alpha}), \quad (4)$$

where for $m = 1$

$$c_s^{(\alpha)} = \begin{cases} a_0^{(\alpha)} + b_0^{(\alpha)} + b_1^{(\alpha)}, & s = 0, \\ a_1^{(\alpha)} - b_1^{(\alpha)} - b_0^{(\alpha)}, & s = 1, \end{cases}$$

for $m = 2$

$$c_s^{(\alpha)} = \begin{cases} a_0^{(\alpha)} + b_0^{(\alpha)}, & s = 0, \\ a_1^{(\alpha)} + b_1^{(\alpha)} + b_2^{(\alpha)} - b_0^{(\alpha)}, & s = 1, \\ a_2^{(\alpha)} - b_2^{(\alpha)} - b_1^{(\alpha)}, & s = 2, \end{cases}$$

The high-order discretization of Caputo derivative (2)

for $m \geq 3$,

$$c_s^{(\alpha)} = \begin{cases} a_0^{(\alpha)} + b_0^{(\alpha)}, & s = 0, \\ a_s^{(\alpha)} + b_s^{(\alpha)} - b_{s-1}^{(\alpha)}, & 1 \leq s \leq m-2, \\ a_{m-1}^{(\alpha)} + b_{m-1}^{(\alpha)} + b_m^{(\alpha)} - b_{m-2}^{(\alpha)}, & s = m-1, \\ a_m^{(\alpha)} - b_m^{(\alpha)} - b_{m-1}^{(\alpha)}, & s = m, \end{cases}$$

with $a_\ell^{(\alpha)} = (\ell+1)^{1-\alpha} - \ell^{1-\alpha}$ $(\ell \geq 0)$ and

$$b_\ell^{(\alpha)} = \frac{1}{2-\alpha}\left[(\ell+1)^{2-\alpha} - \ell^{2-\alpha}\right] - \frac{1}{2}\left[(\ell+1)^{1-\alpha} + \ell^{1-\alpha}\right], \quad \ell \geq 0.$$

The fractional central difference approximation (1)

Denote

$$\Psi^{2+\alpha}(\mathbb{R}) = \left\{ y \,\middle|\, \int_{-\infty}^{+\infty} (1+|\omega|)^{2+\alpha} |\hat{y}(\omega)| d\omega < \infty,\ y \in L^1(\mathbb{R}) \right\},$$

where $\hat{y}(\omega) = \int_{-\infty}^{+\infty} e^{\boldsymbol{i}\omega t} y(t)dt$ is the Fourier transform of $y(t)$ and $\boldsymbol{i} = \sqrt{-1}$. The Riesz fractional derivative at $x = x_i$ can be approximated by the 2nd fractional centered difference approximation [Çelik & Duman, JCP12], that is, for $u(x,\cdot) \in \Psi^{2+\alpha}(\mathbb{R})$,

$$\begin{aligned} \frac{\partial^\beta u(x_i,t)}{\partial |x|^\beta} &= -h^\beta \sum_{k=-N+i}^{i} g_k^{(\beta)} u(x_{i-k},t) + \mathcal{O}(h^2) \\ &= \delta_x^\beta u(x_i,t) + \mathcal{O}(h^2), \end{aligned} \quad (5)$$

where

$$g_k^{(\beta)} = \frac{(-1)^k \Gamma(1+\beta)}{\Gamma(\beta/2 - k + 1)\Gamma(\beta/2 + k + 1)}, \quad k \in \mathbb{Z}.$$

Discretized mesh information

Discretize the space domain by $x_i = a + ih$ $(h = (b-a)/N,\ i = 0, 1, \cdots, N)$ and denote $x_{i+1/2} = (x_{i+1} + x_i)/2$ as the midpoint of the neighboring nodes x_{i+1} and x_i. We also consider the sets

$$\Omega_h = \{x_i | 0 \le i \le N\},\ \ \Omega_\tau = \{t_m | 0 \le m \le M\},$$

$$\Omega_{h,\tau} = \{(x_i, t_m) | 0 \le i \le N,\ 0 \le m \le M\}$$

and let $v = \{v_i^m | 0 \le i \le N,\ 0 \le m \le M\}$ be a grid function on $\Omega_{h\tau}$. We also consider the set $\mathcal{V}_h = \{v | v = (v_0, v_1, \cdots, v_{N-1}, v_N)\}$ of grid functions on Ω_h and provide it with the norm

$$\|v\|_\infty = \max_{0 \le i \le N} |v_i|.$$

Implicit difference schemes (1)

We define $u_i^m \approx u(x_i, t_m)$ and $f_i^m = f(x_i, t_m)$, the second-order implicit difference scheme for Eq. (3) reads

$$\begin{cases} \mathbb{D}_t^{\alpha} u_i^{m+1} = \kappa \delta_x^{\beta} u_i^{m+1} + f_i^{m+1}, & 1 \le i \le N-1,\ 1 \le m \le M-1, \\ u_i^0 = \phi(x_i), & 1 \le i \le N-1, \\ u_0^m = u_N^m = 0, & 0 \le m \le M, \end{cases} \tag{6}$$

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Notice that the above scheme is not a self-starting scheme because u_i^1 is unknown.

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Notice that the above scheme is not a self-starting scheme because u_i^1 is unknown.

- Other numerical methods for u_i^1 is required;
- To ensure the global error such that $\mathcal{O}(\tau_t^{3-\alpha})$, the temporal step size of the method for u_i^1 is specially chosen;
- Reduce the computational cost of getting u_i^1 is still important.

Implicit difference schemes (2)

In order to fast calculation of u_i^1, the fast L1 scheme [Jiang, et al. CiCP17] is exploited as follow.

$$\begin{cases} \hat{\mathbb{D}}_t^{\alpha} \tilde{u}_i^j = \kappa \delta_x^{\beta} \tilde{u}_i^j + f_i^j, & 1 \le i \le N-1,\ 1 \le j \le \hat{M} = \lfloor t_1/\hat{\tau} \rfloor, \\ \tilde{u}_i^0 = \phi(x_i), & 1 \le i \le N-1, \\ \tilde{u}_0^j = \tilde{u}_N^j = 0, & 0 \le j \le M, \end{cases} \tag{7}$$

where $\hat{\tau} = \tau_t^{\frac{3-\alpha}{2-\alpha}}$, $u_i^1 = \tilde{u}_i^{\hat{M}}$ and

$$\hat{\mathbb{D}}_t^{\alpha} u_i^j = \frac{1}{\Gamma(1-\alpha)} \left[\check{b}_j^{(\alpha)} \tilde{u}_i^j - \sum_{k=1}^{j-1} \left(\check{b}_{k+1}^{(\alpha)} - \check{b}_k^{(\alpha)} \right) \tilde{u}_i^k - \check{b}_1^{(\alpha)} \tilde{u}_i^0 \right] \tag{8}$$

with

$$\check{b}_k^{(\alpha)} = \begin{cases} \sum_{\ell}^{\hat{M}_{exp}} \omega_\ell \int_{k-1}^{k} e^{-\hat{\tau} s_\ell (j-s)} ds, & k = 1, 2, \cdots, j-1, \\ \frac{\hat{\tau}^{-\alpha}}{1-\alpha}, & k = j, \end{cases} \tag{9}$$

and $\hat{M}_{exp} \in \mathbb{N}^+$ and $\omega_\ell, s_\ell \ge 0$ $(\ell = 1, 2, \cdots, \hat{M}_{exp})$.

Implicit difference schemes (3)

In order to implement the above difference scheme, we note that:

- In each time level, we need to solve a symmetric Toeplitz linear system where the coefficient matrix is strictly diagonally dominant; (PCG + τ preconditioner)
- Due to the historical effect, we must repeatedly compute the linear combination of numerical solutions from the time level t_0 to t_{m-1}; (About the $\mathcal{O}(M^2)$ complexity)
- Fast and parallel numerical schemes are not easy but very meaningful especially when the number of time levels is fairly large.

Outline

Stability and convergence of IDS (1)

For $\forall \boldsymbol{v},\ \boldsymbol{w} \in \mathcal{S} = \{\boldsymbol{v} | \boldsymbol{v} = (v_0, v_1, \ldots, v_N),\ v_0 = v_N = 0\}$, we define an inner product and the corresponding norm:

$$(\boldsymbol{v}, \boldsymbol{w}) = h \sum_{i=1}^{N-1} v_i w_i, \qquad \|\boldsymbol{v}\| = \sqrt{(\boldsymbol{v}, \boldsymbol{v})}.$$

Let $\boldsymbol{u}^m = [u_1^m, u_2^m, \ldots, u_{N-1}^m]^\top$ and $\boldsymbol{f}^m = [f_1^m, f_2^m, \ldots, f_{N-1}^m]^\top$. With these at hand, we have the following priori estimate.

Theorem

Suppose u_i^m $(0 \le i \le N, 1 \le m \le M-1)$ be a solution of the scheme (6). Then, we have

$$\tau_t \sum_{m=1}^{M-1} \left(\|\boldsymbol{u}^{m+1}\|^2 + \|\Xi^\beta \boldsymbol{u}^{m+1}\|^2\right) \le C_1 \left(\|\boldsymbol{u}^1\|^2 + \|\boldsymbol{u}^0\|^2 + \tau_t \sum_{m=1}^{M-1} \|\boldsymbol{f}^{m+1}\|^2\right),$$

where Ξ^β is the square root of $-\delta_x^\beta$, and C_1 is a positive constant independent of τ_t and h.

Stability and convergence of IDS (2)

This proof is similar to the proof of Theorem 3.1 in [Alikhanov & Huang, AMC21]. Thus, we omit it here. It is worth mentioning that in this proof, the property given as follows is used:

$$(-\delta_x^\beta \boldsymbol{u}^m, \boldsymbol{u}^m) = \|\Xi^\beta \boldsymbol{u}^m\|^2 \geq c_*^\beta (x_R - x_L)^{-\beta} \|\boldsymbol{u}^m\|^2,$$

where $c_*^\beta = 2e^{-2}\frac{(4-\beta)(2-\beta)\Gamma(\beta+1)}{(6+\beta)(4+\beta)(2+\beta)\Gamma^2(\beta/2+1)}(3/2+\beta/4)^{\beta+1}$, see [Sun et al. AMC16] for details.

Based on Theorem 3, both the stability and the convergence of the scheme (6) can be proved without difficulty. (Hint: $\mathcal{O}(\tau_t^{3-\alpha} + h^2)$)

Outline

The L2-type all-at-once system (1)

We can rewrite the scheme (6) into the matrix-vector product form for $1 \leq m \leq M-1$.

$$\frac{h^{\beta}\tau_t^{-\alpha}}{\Gamma(2-\alpha)}\sum_{s=0}^{m} c_{m-s}^{(\alpha)}\left(\boldsymbol{u}^{s+1}-\boldsymbol{u}^{s}\right)+\kappa\, G_{\beta}\boldsymbol{u}^{m+1}=h^{\beta}\boldsymbol{f}^{m+1}, \qquad (10)$$

where

$$G_{\beta}=\begin{bmatrix} g_0^{\beta} & g_{-1}^{\beta} & g_{-2}^{\beta} & \cdots & g_{3-N}^{\beta} & g_{2-N}^{\beta} \\ g_1^{\beta} & g_0^{\beta} & g_{-1}^{\beta} & g_{-2}^{\beta} & \cdots & g_{3-N}^{\beta} \\ \vdots & g_1^{\beta} & g_0^{\beta} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & g_{-2}^{\beta} \\ g_{N-3}^{\beta} & \ddots & \ddots & \ddots & g_0^{\beta} & g_{-1}^{\beta} \\ g_{N-2}^{\beta} & g_{N-3}^{\beta} & \cdots & \cdots & g_1^{\beta} & g_0^{\beta} \end{bmatrix}$$

is a symmetric positive definite Toeplitz matrix.

The L2-type all-at-once system (2)

Suppose that O is a zero matrix with suitable size, I_t and I_x are two identity matrices with orders $M-1$ and $N-1$, respectively. Denote

$$\boldsymbol{u} = \left[\left(\boldsymbol{u}^2\right)^T, \cdots, \left(\boldsymbol{u}^M\right)^T\right]^T \text{ and } \boldsymbol{f} = \left[\left(\boldsymbol{f}^2\right)^T, \cdots, \left(\boldsymbol{f}^M\right)^T\right]^T.$$

To avoid the misunderstanding, let $\tilde{c}_0^{(\alpha)} = a_0^{(\alpha)} + b_0^{(\alpha)} + b_1^{(\alpha)}$, $\tilde{c}_k^{(\alpha)} = a_k^{(\alpha)} + b_k^{(\alpha)} + b_{k+1}^{(\alpha)} - b_{k-1}^{(\alpha)}$, $\hat{c}_k^{(\alpha)} = a_k^{(\alpha)} - b_k^{(\alpha)} - b_{k-1}^{(\alpha)}$, $k = 1, 2, \ldots, M-1$. Then, let $A_{11} = \frac{h^\beta \tau_t^{-\alpha}}{\Gamma(2-\alpha)} \tilde{c}_0^{(\alpha)}$,

$$A_{12} = \frac{h^\beta \tau_t^{-\alpha}}{\Gamma(2-\alpha)} \left[\tilde{c}_1^{(\alpha)} - c_0^{(\alpha)}, \tilde{c}_2^{(\alpha)} - c_1^{(\alpha)}, \ldots, \tilde{c}_{M-2}^{(\alpha)} - c_{M-3}^{(\alpha)}\right]^T$$

and

The L2-type all-at-once system (3)

$$A_{22} = \frac{h^{\beta}\tau_t^{-\alpha}}{\Gamma(2-\alpha)} \begin{bmatrix} c_0^{(\alpha)} & 0 & \cdots & \cdots & 0 \\ c_1^{(\alpha)} - c_0^{(\alpha)} & c_0^{(\alpha)} & \ddots & \ddots & \vdots \\ \ddots & \ddots & \ddots & \ddots & 0 \\ \ddots & \ddots & \ddots & c_0^{(\alpha)} & 0 \\ c_{M-3}^{(\alpha)} - c_{M-4}^{(\alpha)} & \cdots & \cdots & c_1^{(\alpha)} - c_0^{(\alpha)} & c_0^{(\alpha)} \end{bmatrix}.$$

Here $c_0^{(\alpha)} = a_0^{(\alpha)} + b_0^{(\alpha)}$ and $c_s^{(\alpha)} = a_s^{(\alpha)} + b_s^{(\alpha)} - b_{s-1}^{(\alpha)}$ $(s = 1, \ldots, M-3)$. With the help of Eq. (10) and the above notations, the all-at-once system is written as:

$$\mathcal{M}\boldsymbol{u} = -\boldsymbol{\eta} + h^{\beta}\boldsymbol{f}, \tag{11}$$

where $\mathcal{M} = A_t \otimes I_x + I_t \otimes (\kappa\ G_{\beta})$ with

$$A_t = \begin{bmatrix} A_{11} & O \\ A_{12} & A_{22} \end{bmatrix}$$

The L2-type all-at-once system (4)

$$\boldsymbol{\eta} = \frac{h^{\beta}\tau_t^{-\alpha}}{\Gamma(2-\alpha)} \begin{bmatrix} \hat{c}_1^{(\alpha)}\left(\boldsymbol{u}^1 - \boldsymbol{u}^0\right) - \tilde{c}_0^{(\alpha)}\boldsymbol{u}^1 \\ \hat{c}_2^{(\alpha)}\left(\boldsymbol{u}^1 - \boldsymbol{u}^0\right) - \tilde{c}_1^{(\alpha)}\boldsymbol{u}^1 \\ \vdots \\ \hat{c}_{M-1}^{(\alpha)}\left(\boldsymbol{u}^1 - \boldsymbol{u}^0\right) - \tilde{c}_{M-2}^{(\alpha)}\boldsymbol{u}^1 \end{bmatrix}.$$

Inspired by [Lin, et al. JCP21], in this work, we concentrate on another version of (11).

The L2-type all-at-once system (4)

$$\boldsymbol{\eta} = \frac{h^{\beta}\tau_t^{-\alpha}}{\Gamma(2-\alpha)} \begin{bmatrix} \hat{c}_1^{(\alpha)}\left(\boldsymbol{u}^1 - \boldsymbol{u}^0\right) - \tilde{c}_0^{(\alpha)}\boldsymbol{u}^1 \\ \hat{c}_2^{(\alpha)}\left(\boldsymbol{u}^1 - \boldsymbol{u}^0\right) - \tilde{c}_1^{(\alpha)}\boldsymbol{u}^1 \\ \vdots \\ \hat{c}_{M-1}^{(\alpha)}\left(\boldsymbol{u}^1 - \boldsymbol{u}^0\right) - \tilde{c}_{M-2}^{(\alpha)}\boldsymbol{u}^1 \end{bmatrix}.$$

Inspired by [Lin, et al. JCP21], in this work, we concentrate on another version of (11). More precisely, after doing a permutation transformation of $\boldsymbol{u}$, $\boldsymbol{\eta}$ and $\boldsymbol{f}$, we have

$$\tilde{\mathcal{M}}\tilde{\boldsymbol{u}} = -\tilde{\boldsymbol{\eta}} + h^{\beta}\tilde{\boldsymbol{f}}, \qquad (12)$$

where $\tilde{\mathcal{M}} = (\kappa\ G_{\beta}) \otimes I_t + I_x \otimes A_t$.

Outline

A bilateral preconditioning (1)

Following the idea of [Lin, et al. JCP21], our left and right preconditioners can be written as follows:

$$P_l = (\kappa\ G_h)^{-\frac{1}{2}} \otimes A_t + (\kappa\ G_h)^{\frac{1}{2}} \otimes I_t \tag{13}$$

and

$$P_r = (\kappa\ G_h)^{\frac{1}{2}} \otimes I_t, \tag{14}$$

respectively. Here, $G_h = G_\beta - H_\beta$ is a τ-matrix [Bini & Benedetto, SPAA'90], where H_β is a Hankel matrix and its antidiagonals are given by

$$\left[g_2^\beta, g_3^\beta, \ldots, g_{N-2}^\beta, 0, 0, 0, g_{N-2}^\beta, \ldots, g_3^\beta, g_2^\beta\right]^T.$$

A bilateral preconditioning (2)

The bilateral precondtioning is used to Eq. (12)

$$\begin{cases} P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}\hat{\boldsymbol{u}} = P_l^{-1}\left(-\tilde{\boldsymbol{\eta}} + h^{\beta}\tilde{\boldsymbol{f}}\right), \\ \tilde{\boldsymbol{u}} = P_r^{-1}\hat{\boldsymbol{u}}. \end{cases} \tag{15}$$

In a Krylov subspace method, we need to compute the matrix-vector product $P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}\boldsymbol{v}$ ($\boldsymbol{v}$ is a vector with suitable size) efficiently.

A bilateral preconditioning (2)

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In a Krylov subspace method, we need to compute the matrix-vector product $P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}\boldsymbol{v}$ ($\boldsymbol{v}$ is a vector with suitable size) efficiently. First, the product $\boldsymbol{z} = P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}\boldsymbol{v}$ can be split into the three sub-steps:

$$\begin{cases} \boldsymbol{v}_1 = P_r^{-1}\boldsymbol{v}, & \text{Step1}, \\ \boldsymbol{v}_2 = \tilde{\mathcal{M}}\boldsymbol{v}_1, & \text{Step2}, \\ \boldsymbol{z} = P_l^{-1}\boldsymbol{v}_2, & \text{Step3}. \end{cases} \tag{16}$$

✠ The property (e.g., matrix diagonalization) of the matrix G_h is a key to finishing the above computations.

A bilateral preconditioning (3)

According to [Bini & Benedetto, SPAA'90], the τ-matrix G_h can be diagonalized as

$$G_h = Q_x^\top D_h Q_x$$

where $D_h = \mathrm{diag}(\lambda_{h,1}, \lambda_{h,2}, \ldots, \lambda_{h,N-1})$ is a diagonal matrix containing all eigenvalues of G_τ, and

$$Q_x = \left[\sqrt{2/N}\sin\left(\frac{ij\pi}{N}\right)\right]_{1\le i,j\le N-1}$$

is the sine transform matrix.

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is the sine transform matrix. With this decomposition, **Step1** in Eq. (16) can be fast implemented in the following way:

$$\boldsymbol{v}_1 = P_r^{-1} \boldsymbol{v} = \left(Q_x^T \otimes I_t \right) \left[(\kappa\, D_h)^{-\frac{1}{2}} \otimes I_t \right] (Q_x \otimes I_t)\, \boldsymbol{v}.$$

A bilateral preconditioning (4)

As for **Step2** in Eq. (16), $\tilde{\mathcal{M}}\boldsymbol{z}_1 = [(\kappa G_\beta) \otimes I_t + I_x \otimes A_t]\boldsymbol{z}_1$ can be computed by using FFTs since A_{22} and G_β are two Toeplitz matrices.

A bilateral preconditioning (4)

As for **Step2** in Eq. (16), $\tilde{\mathcal{M}} \boldsymbol{z}_1 = [(\kappa G_\beta) \otimes I_t + I_x \otimes A_t] \boldsymbol{z}_1$ can be computed by using FFTs since A_{22} and G_β are two Toeplitz matrices. **Step3** is a little more complicated. Using the diagonalization of G_h, we can rewrite P_l as:

$$P_l = \left(Q_x^T \otimes I_t\right) \left[(\kappa\ D_h)^{\frac{1}{2}} \otimes I_t + (\kappa\ D_h)^{-\frac{1}{2}} \otimes A_t\right] (Q_x \otimes I_t)\,.$$

Denote

$$\Sigma_i = (\kappa\ \lambda_{h,i})^{\frac{1}{2}} I_t + (\kappa\ \lambda_{h,i})^{-\frac{1}{2}} A_t, \quad \text{for } i = 1, 2, \ldots, N-1.$$

The product $\boldsymbol{z} = P_l^{-1} \boldsymbol{v}_2$ can be calculated via the three steps:

$$\begin{cases} \boldsymbol{z}_1 = (Q_x \otimes I_t)\, \boldsymbol{v}, & \text{Step-(a)}, \\ \Sigma_n\ \boldsymbol{z}_{2,n} = \boldsymbol{z}_{1,n},\ 1 \leq n \leq N-1, & \text{Step-(b)}, \\ \boldsymbol{z} = \left(Q_x^T \otimes I_t\right) \boldsymbol{z}_2, & \text{Step-(c)}, \end{cases} \tag{17}$$

A bilateral preconditioning (5)

where $\boldsymbol{z}_j = \left[\boldsymbol{z}_{j,1}^T, \boldsymbol{z}_{j,2}^T, \cdots, \boldsymbol{z}_{j,N-1}^T\right]^T$ with $j = 1, 2$. Note that Σ_i $(1 \leq i \leq N-1)$ are 2-by-2 block matrices, i.e.,

$$\Sigma_i = \begin{bmatrix} \Sigma_{i,11} & \mathbf{0} \\ \Sigma_{i,12} & \Sigma_{i,22} \end{bmatrix},$$

where

$$\Sigma_{i,11} = (\kappa\, \lambda_{h,i})^{\frac{1}{2}}\, I_{t1} + (\kappa\, \lambda_{h,i})^{-\frac{1}{2}}\, A_{11},\ \ \Sigma_{i,12} = (\kappa\, \lambda_{h,i})^{-\frac{1}{2}}\, A_{12},$$
$$\Sigma_{i,22} = (\kappa\, \lambda_{h,i})^{\frac{1}{2}}\, I_{t2} + (\kappa\, \lambda_{h,i})^{-\frac{1}{2}}\, A_{22}$$

and $\mathrm{blkdiag}(I_{t1}, I_{t2}) = I_t$. Then, we have $\boldsymbol{z}_{2,n} = \Sigma_n^{-1}\, \boldsymbol{z}_{1,n}$ for $1 \leq n \leq N-1$, where

$$\Sigma_n^{-1} = \begin{bmatrix} \Sigma_{n,11}^{-1} & \mathbf{0} \\ -\Sigma_{n,22}^{-1}\Sigma_{n,12}\Sigma_{n,11}^{-1} & \Sigma_{n,22}^{-1} \end{bmatrix}. \qquad (18)$$

Outline

Condition number of preconditioned matrices (1)

For the calculation of (18), we note

- The inverse of an invertible lower triangular Toeplitz matrix is still a lower triangular Toeplitz matrix;
- The modified version of Bini's algorithm [Lin et al. TCS04] to compute $\Sigma_{n,22}^{-1}$ in $\mathcal{O}(M \log M)$ operations. (Not exactly)

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In order to analyze the condition number of the preconditioned matrix, we need to some conclusions:

- The preconditioners P_l and P_r are nonsingular when $\alpha \in (0,1)$ and $\beta \in (1,2)$;
- The matrix $A_t + A_t^\top$ should be positive; (Set $\alpha \in (0, 0.3624)$ and the monotonicity of $c_k^{(\alpha)}$ and $\tilde{c}_{k+1}^{(\alpha)}$);
- We have $\frac{1}{2} < \lambda(G_h^{-1} G_\beta) < \frac{3}{2}$, where $\lambda(\cdot)$ represents all the eigenvalues of $G_h^{-1} G_\beta$.

Condition number of preconditioned matrices (2)

Conclusion [Zhao, et al. arXiv21]: For $\forall \alpha \in (0, 0.3624)$, the condition number of $P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}$ is bounded, i.e.,

$$\kappa_2(P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}) < 2\sqrt{3}.$$

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There are some remarks:

- The condition $\alpha \in (0, 0.3624)$ is assumed for our theoretical analysis;
- For $\alpha \in [0.3624, 1)$, numerical results show that the condition number of $P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}$ is no more than $2\sqrt{3}$;
- Maybe our theoretical tools for analyzing the condition number of $P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}$ can be further improved;
- The eigenvalue analysis of $P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}$ is not completed.

Outline

Example 1

We consider Eq. (3) with $x_L = 0$, $\kappa = x_R = T = 1$ and the source term reads

$$f(x,t) = \left(\frac{\Gamma(4+\alpha)}{\Gamma(4)} t^3 + \frac{\Gamma(3)}{\Gamma(3-\alpha)} t^{2-\alpha} \right) x^2(1-x)^2 + \frac{\kappa\left(t^{3+\alpha}+t^2+1\right)}{2\cos(\pi\beta/2)} \times \left\{ \frac{\Gamma(3)}{\Gamma(3-\beta)} \left[x^{2-\beta} + (1-x)^{2-\beta}\right] - \frac{2\Gamma(4)}{\Gamma(4-\beta)} \left[x^{3-\beta} + (1-x)^{3-\beta}\right] + \frac{\Gamma(5)}{\Gamma(5-\beta)} \left[x^{4-\beta} + (1-x)^{4-\beta}\right] \right\}.$$

The exact solution is $u(x,t) = \left(t^{3+\alpha} + t^2 + 1\right) x^2(1-x)^2$.

Example 1

Table: Numerical errors and the observed time convergence orders for Example 1 with $N = M^{(3-\alpha)/2}$.

(α, β)	M	$Err_\infty(h,\tau)$	$CO_{\infty,\tau}$	$Err_2(h,\tau)$	$CO_{2,\tau}$
(0.1, 1.5)	10	3.3558E-04	–	2.1958E-04	–
	20	4.2391E-05	2.9848	2.7415E-05	3.0017
	40	5.3517E-06	2.9857	3.5198E-06	2.9614
	80	6.7403E-07	2.9891	4.5958E-07	2.9371
(0.4, 1.7)	10	1.0146E-03	–	6.9999E-04	–
	20	1.5215E-04	2.7373	1.0266E-04	2.7695
	40	2.4455E-05	2.6373	1.6239E-05	2.6603
	80	3.8098E-06	2.6823	2.5054E-06	2.6963
(0.7, 1.4)	10	1.2174E-03	–	8.0414E-04	–
	20	2.4993E-04	2.2842	1.6106E-04	2.3198
	40	4.9078E-05	2.3484	3.1689E-05	2.3455
	80	9.5109E-06	2.3674	6.2572E-06	2.3404
(0.9, 1.9)	10	4.0154E-03	–	2.8992E-03	–
	20	9.8220E-04	2.0315	7.0490E-04	2.0402
	40	2.3079E-04	2.0894	1.6464E-04	2.0981
	80	5.4304E-05	2.0875	3.8477E-05	2.0972

Example 1

Table: Numerical errors and the observed space convergence orders for Example 1 with $M = 1024$.

(α, β)	N	$Err_\infty(h,\tau)$	$CO_{\infty,\tau}$	$Err_2(h,\tau)$	$CO_{2,\tau}$
(0.1, 1.5)	10	3.1533E-03	–	2.1393E-03	–
	20	7.3035E-04	2.1102	4.8195E-04	2.1502
	40	1.7021E-04	2.1013	1.1044E-04	2.1256
	80	3.9928E-05	2.0918	2.5825E-05	2.0964
(0.4, 1.7)	10	4.1944E-03	–	2.9495E-03	–
	20	9.9378E-04	2.0775	6.8541E-04	2.1054
	40	2.3585E-04	2.0751	1.5982E-04	2.1005
	80	5.6098E-05	2.0718	3.7467E-05	2.0928
(0.7, 1.4)	10	2.4866E-03	–	1.6468E-03	–
	20	5.7380E-04	2.1156	3.7013E-04	2.1536
	40	1.3363E-04	2.1023	8.5825E-05	2.1086
	80	3.1405E-05	2.0892	2.0534E-05	2.0634
(0.9, 1.9)	10	5.4166E-03	–	3.9271E-03	–
	20	1.3277E-03	2.0285	9.5644E-04	2.0377
	40	3.2529E-04	2.0291	2.3276E-04	2.0388
	80	7.9708E-05	2.0289	5.6655E-05	2.0386

Outline

Example 2

Consider Eq. (3) with $\kappa = T = 1$, $x_L = -1$, $x_R = 1$ and the source term

$$f(x,t) = \frac{\Gamma(4+\alpha)}{\Gamma(4)} t^3 (1+x)^2 (1-x)^2 + \frac{\kappa\left(t^{3+\alpha}+1\right)}{2\cos(\pi\beta/2)} \left\{ \frac{4\,\Gamma(3)}{\Gamma(3-\beta)} \left[(1+x)^{2-\beta} + (1-x)^{2-\beta}\right] - \frac{4\,\Gamma(4)}{\Gamma(4-\beta)} \left[(1+x)^{3-\beta} + (1-x)^{3-\beta}\right] + \frac{\Gamma(5)}{\Gamma(5-\beta)} \left[(1+x)^{4-\beta} + (1-x)^{4-\beta}\right] \right\}.$$

The exact solution is $u(x,t) = \left(t^{3+\alpha}+1\right)(1+x)^2(1-x)^2$.

Example 2

Table: Results of various methods for $M = N$ for Example 2.

(α, β)	N	BS Time	BFSM Time	$\mathcal{I}$ (Iter1, Iter2)	$\mathcal{I}$ Time	$\mathcal{P}$ (Iter1, Iter2)	$\mathcal{P}$ Time
(0.1, 1.1)	128	6.268	0.111	(56.0, 61.0)	1.021	(7.0, 5.0)	0.537
	256	1160.576	0.524	(80.0, 89.0)	5.141	(7.0, 5.0)	1.831
	512	$>$ 5 hours	5.097	(114.0, 137.0)	29.161	(8.0, 5.0)	5.985
	1024	OoM	50.948	(162.0, 191.0)	261.795	(8.0, 5.0)	20.847
	2048	OoM	537.730	(228.0, 283.0)	1605.622	(8.0, 6.0)	89.736
(0.2, 1.7)	128	6.220	0.116	(113.0, 233.0)	7.692	(6.0, 4.0)	0.447
	256	1092.552	0.534	(202.0, 438.0)	48.579	(6.0, 5.0)	1.873
	512	$>$ 5 hours	5.057	(360.0, 829.0)	307.938	(6.0, 5.0)	5.786
	1024	OoM	48.755	†	†	(6.0, 5.0)	20.128
	2048	OoM	537.980	†	†	(7.0, 6.0)	86.305
(0.35, 1.5)	128	6.210	0.110	(78.0, 189.0)	6.426	(6.0, 5.0)	0.539
	256	1277.143	0.526	(116.0, 310.0)	34.513	(6.0, 5.0)	1.835
	512	$>$ 5 hours	4.963	(163.0, 569.0)	212.494	(6.0, 5.0)	5.789
	1024	OoM	51.936	†	†	(6.0, 5.0)	20.159
	2048	OoM	582.579	†	†	(6.0, 6.0)	86.159
(0.9, 1.9)	128	6.211	0.127	†	†	(3.0, 4.0)	0.459
	256	1805.931	0.604	†	†	(3.0, 4.0)	1.534
	512	$>$ 5 hours	5.588	†	†	(3.0, 4.0)	4.831
	1024	OoM	52.250	†	†	(3.0, 4.0)	16.527
	2048	OoM	599.093	†	†	(3.0, 4.0)	60.787

Example 2

Table: The condition numbers of $\tilde{\mathcal{M}}$ and $P_l^{-1}\tilde{\mathcal{M}}P_r^{-1}$ for $M = N$ for Example 2.

(α, β)	N	$\kappa_2(\tilde{\mathcal{M}})$	$\kappa_2(P_l^{-1}\tilde{\mathcal{M}}P_r^{-1})$
(0.1, 1.1)	16	9.86	1.23
	32	20.63	1.30
	64	43.64	1.36
	128	92.89	1.42
(0.2, 1.7)	16	38.04	1.12
	32	123.25	1.15
	64	400.27	1.18
	128	1300.85	1.21
(0.35, 1.5)	16	25.02	1.17
	32	68.98	1.22
	64	192.69	1.27
	128	541.93	1.31
(0.9, 1.9)	16	70.45	1.04
	32	243.78	1.06
	64	870.27	1.07
	128	3171.08	1.08

Conclusion and remarks

- An implicit with the accuracy of $\mathcal{O}(\tau_t^{3-\alpha} + h^2)$ has been developed for TSFBTEs;
- Convergence and stability of the IDS have been investigated;
- A bilateral parallel preconditioning is established for the L2-type all-at-once linar systems;
- Efficient implementaion of preconditioned Krylov subspace solver and the condition number of the preconditioned matrix are investigated in details.

Future work

- Extend the efficient implicit numerical schemes with preconditioned iterative solvers for high-dimensional nonlinear problems;
- Eigenvalue analysis of the preconditioned matrix is still open but meaningful;
- How to design the bilateral parallel preconditioning for (nonlinear) high-dimensional VO time-fractional PDEs, especially fractional wave equations.

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Thank you for your attention!

Any questions or comments?