Numerical Methods with Minimal Memory Requirements for Solving the Cauchy Problem for Integro-Differential Equations with a Difference Kernel

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V Всероссийская научная конференция «Осенние математические чтения в Адыгее»
(October 9-14, 2025, Maykop)

Outline

Consider the Cauchy problem for an evolutionary equation with memory which satisfies an integro-differential equation with a difference kernel

$$\frac{\partial u(\boldsymbol{x},t)}{\partial t} + \int_0^t k(t-\xi)\mathcal{A}u(\boldsymbol{x},\xi)d\xi = g(\boldsymbol{x},t), \qquad (\boldsymbol{x},t) \in \Omega \times (0,T], \tag{1}$$

$$u(\boldsymbol{x},t) = 0, \qquad (\boldsymbol{x},t) \in \partial\Omega \times (0,T], \tag{2}$$

$$u(\boldsymbol{x},0) = u_0, \qquad \boldsymbol{x} \in \Omega. \tag{3}$$

The domain $\Omega \subset \mathbf{R}^d$, $d = 1,2,3$, is a bounded convex polygonal domain with the Lipschitz continuous boundary $\partial\Omega$.

- The model inherits properties of BOTH a first-order evolutionary equation and a second-order evolutionary equation. for $\kappa > 0$:

$$k(t) = \kappa\delta(t): \quad \frac{\partial u}{\partial t} + \kappa\mathcal{A}u = g(t), \qquad \text{Classical local heat equation}$$

$$k(t) = \kappa: \quad \frac{\partial^2 u}{\partial t^2} + \kappa\mathcal{A}u = \frac{\partial g}{\partial t}(t), \qquad \text{Classical local wave equation}$$

$\frac{\partial u}{\partial t} + \int_0^t k(t-\xi)\mathcal{A}u(\xi)d\xi = g(t)$

- The kernel $k(t)$ is called convolution kernels of positive type.
- It is assumed to be real-valued and positive-definite.
  This implies that the kernel $k(t)$ belongs to $L_1(0,T)$, and also satisfies:

$$\int\limits_0^T u(t) \int\limits_0^t k(t-\eta)u(\eta)d\eta dt \geq 0, \quad u \in \mathcal{C}^1[0,T], \quad T > 0. \tag{4}$$

- The sufficient conditions for the kernel $k(t)$ to be a positive-definite kernel are:

$$k(t) \geq 0, \quad \frac{d}{dt}k(t) \leq 0, \quad \frac{d^2}{dt^2}k(t) \geq 0, \quad t > 0. \tag{5}$$

$\frac{\partial u}{\partial t} + \int_0^t k(t-\xi)\mathcal{A}u(\xi)d\xi = g(t)$

In the Hilbert space $\mathcal{H} = L_2(\Omega)$ the operator $\mathcal{A} : \mathcal{H} \to \mathcal{H}$ is self-adjoint and positive definite, that is

$$\mathcal{A} = \mathcal{A}^* \geq c_{\mathcal{A}}\mathcal{I},$$

where $c_{\mathcal{A}} > 0$ and $\mathcal{I}$ is the identity operator in the Hilbert space $\mathcal{H}$.
We introduce the elliptic operator $\mathcal{A}$ in the presented Cauchy problem as

$$\mathcal{A}u(\boldsymbol{x}, t) = -\mathrm{div}(\psi(\boldsymbol{x}) \operatorname{grad} u(\boldsymbol{x}, t)) + \phi(\boldsymbol{x})u(\boldsymbol{x}, t), \tag{6}$$

with coefficients $0 < c_1 \leq \psi(\boldsymbol{x}) \leq c_2$, and $\phi(\boldsymbol{x}) \geq 0$.

A practical example: The heat conduction equation with memory

1. The heat flow $q(\boldsymbol{x},t)$ with memory is determined by the temperature gradient $\nabla T(\boldsymbol{x},t)$:

$$\text{Nonlocal Fourier law: } q(\boldsymbol{x},t) = -\int_0^t k(t-\xi)\nabla T(\boldsymbol{x},\xi)d\xi, \quad (q \text{ is the heat flux}) \tag{7}$$

   The kernel $k(t)$ is a positive, decreasing relaxation function of the heat flux.

2. The internal energy conservation equation $e(\boldsymbol{x},t)$ for a stiff conductor is:

$$\frac{\partial e}{\partial t} + \text{div } q = r, \qquad (r \text{ is the distributed heat absorption}) \tag{8}$$

3. The local energy density $e(\boldsymbol{x},t)$ is due to changes in temperature, thus,

$$e = cT + c_1, \qquad (c \text{ is the heat capacity and } c_1 \text{ is a constant}) \tag{9}$$

Substituting (7) and (9) into (8) leads to the heat conduction equation with memory

$$c\frac{\partial T}{\partial t} - \int_0^t k(t-\xi)\text{div}\nabla T(\boldsymbol{x},\xi)d\xi = r. \tag{10}$$

Note: The classical Fourier law $(q(\boldsymbol{x},t) = -\kappa\ \nabla T(\boldsymbol{x},t))$ is valid when $k(t) = \kappa\delta(t)$, which converts this model to the classical heat conduction equation $c\frac{\partial T}{\partial t} - \kappa\ \text{div}\nabla T = r$.

A practical example: Viscoelastic aspects of glass relaxation models

When exposed to shaping temperatures, glass deforms with viscoelastic behavior. Researchers adopt a viscoelastic approach to study this phenomenon (Loreti, (2019) *Physica A* 526, 120768.):

$$\frac{\partial^2 u}{\partial t^2}(\boldsymbol{x},t) = \mathcal{A}u(\boldsymbol{x},t) - \alpha \int\limits_0^t \frac{e^{-(t-\xi)^\alpha}}{(t-\xi)^{1-\alpha}} \mathcal{A}u(\boldsymbol{x},\xi)d\xi, \tag{11}$$

Where $0 < \alpha < 1$, and the operator $\mathcal{A}$ denotes the Laplace operator.
Equation (11) is equivalent to the following system:

$$\frac{\partial v}{\partial t} - \int\limits_0^t k(t-\xi)\mathcal{A}v(\xi)d\xi = f(t), \tag{12}$$

$$\frac{\partial u}{\partial t} - v = 0. \tag{13}$$

with $k(t) = e^{-t^\alpha}$, and $f(t) = E(t)\mathcal{A}u(0)$.

Discretisation in space of $\frac{\partial u}{\partial t} + \int_0^t k(t-\xi)\mathcal{A}u(\xi)d\xi = g(t)$:

For an approximate solution $v(t)$ of $u(t)$, the Cauchy problem is equivalent to:

$$\frac{\partial v}{\partial t} + \int_0^t k(t-\xi)\mathcal{A}_h v(\xi)d\xi = f(t), \qquad (\boldsymbol{x}, t) \in \bar{\Omega} \times (0, T], \tag{14}$$

$$v(0) = u_0, \qquad \boldsymbol{x} \in \Omega, \tag{15}$$

The discrete operator $\mathcal{A}_h$ approximates the operator $\mathcal{A}$ and has the same properties (self-adjoint and positive-definite). Some common methods to approaches of $\mathcal{A}_h$ are:

- Finite volume method
- Finite element method, or the Galerkin finite-element method
- Finite difference operator
- Space spectral scheme

Convergence: The solution v of the Cauchy problem (14)–(15) satisfies:

$$\|v(t)\| \leq \|v_0\| + \int_0^t \|f(s)\|ds. \tag{16}$$

Standard discretisation in time for $\frac{\partial v}{\partial t} + \int_0^t k(t-\xi)\mathcal{A}_h v(\xi)d\xi = f(t)$:
Consider a uniform temporal grid: $\{t_j = j\tau,\, j = 0, 1, \ldots, N,\, \tau = T/N\}$.

1. Utilize a specific finite difference approximation for the derivative in first term ($\frac{\partial v}{\partial t}$)
2. Approximate $\int_0^t k(t-\xi)\mathcal{A}_h v(\xi)d\xi$ by replacing the integrand $v(\xi)$ with its piecewise interpolating polynomials (Rectangular quadrature formula, Trapezoidal quadrature formula, Mid-point quadrature formula, etc.)

A leading research of such studies: (W. McLean, and V. Thomée, (1993), *The ANZIAM Journal*, 35 (1) 23–70)

- First-order backward Euler method: $\frac{u^{j+1}-u^j}{\tau} + \sum_{s=0}^{j} a_{j-s}\mathcal{A}_h u^{s+1} = f^{j+1}$,
- Second-order Crank-Nicolson method: $\frac{u^{j+1}-u^j}{\tau} + \sum_{s=0}^{j} a_{j-s}\mathcal{A}_h \frac{u^{s+1}+u^s}{2} = f^{j+1/2}$.

The memory term is main disadvantage of such methods; When numerically approximating a problem at a certain time layer, information about all the previous time layers is required. This cause great demands for processing time and storage of the data.

The idea of converting a nonlocal equation to a local model: Consider our practical example:

The heat flow:
$$q(\boldsymbol{x},t) = -\int_0^t k(t-\xi)\nabla T(\boldsymbol{x},\xi)d\xi, \tag{17}$$

The heat conduction equation:
$$c\frac{\partial T}{\partial t} - \int_0^t k(t-\xi)\text{div}\nabla T(\boldsymbol{x},\xi)d\xi = r. \tag{18}$$

Let's assume: $k(t) = \frac{\kappa}{\tau_q}\exp(-\frac{t}{\tau_q})$, ($\tau_q$ is the relaxation time), from (17) for the fluxes we have

$$\tau_q\frac{\partial q}{\partial t} + q = -\kappa\nabla T, \qquad \text{(The Maxwell-Cattaneo law)} \tag{19}$$

This leads us to the hyperbolic heat conduction equation

$$c\ \tau_q\frac{\partial^2 T}{\partial t^2} + c\frac{\partial T}{\partial t} - \kappa\ \text{div}\nabla T = r + \tau_q\frac{\partial r}{\partial t} \tag{20}$$

The fundamental point is that by choosing $k(t) = \frac{\kappa}{\tau_q}\exp(-\frac{t}{\tau_q})$:

1. Instead of a nonlocal model (17), we have a local model as a differential relation (19) for the dependence of heat flux on temperature gradient.
2. Instead of the nonlocal integro-differential equation (18), we have a second-order local evolution equation (20) for the heat conduction equation.

Similar to our example, a transition of nonlocal integro-differential equation to a local system of differential equations can be expected when the kernel in the Cauchy problem is expressed by a function $\bar{k}(t)$, using the sum of exponentials (SoE) approach:

$$\bar{k}(t) = \sum_{r=1}^{N_{exp}} a_r \exp(-b_r t), \quad t \geq 0. \tag{21}$$

- The coefficients a_r and b_r satisfy:

$$a_r > 0, \quad b_r > 0, \quad r = 1, 2, \ldots, N_{exp}.$$

- The kernel $\bar{k}(t)$ is positive definite.
- The utilization of kernel approximations through the SoE enables the transition from a nonlocal equation to a system of local equations (NO NEED for information about all the previous times anymore).

Denote $w(t)$ as the approximate solution of the problem $\frac{\partial v}{\partial t} + \int_0^t k(t-\xi)\mathcal{A}_h v(\xi)d\xi$, which is defined as a solution to the Cauchy problem

$$\frac{\partial w}{\partial t} + \int_0^t \bar{k}(t-\xi)\mathcal{A}_h w(\xi)d\xi = f(t), \quad t > 0, \tag{22}$$

$$w(0) = v_0, \tag{23}$$

Theorem (The accuracy of the approximate solution $w(t)$ of $v(t)$)

Let the error of approximation of the kernel by the SoE approach satisfies

$$\left|k(t) - \bar{k}(t)\right| \leq \varepsilon_1, \quad t > 0.$$

Then, for the error of the approximate solution $e = w - v$, the following estimate holds true.

$$\|e(t)\| \leq \varepsilon_1 \int_0^t \xi \left(\|\mathcal{A}_h v_0\| + \int_0^\xi \|\mathcal{A}_h f(s)\| ds \right) d\xi.$$

- Consider the problem $\frac{dw}{dt} + \int_0^t \bar{k}(t-\xi)\mathcal{A}_h w(\xi)d\xi = f(t)$, with $\bar{k}(t) = \sum_{r=1}^{N_{exp}} a_r \exp(-b_r t)$.
- Define $w_r(t) = \int_0^t \exp\left(-b_r(t-\xi)\right) w(\xi)d\xi, \quad r = 1, 2, \ldots, N_{exp}$.

Substituting the value of $w_r(t)$ in the main problem and differentiating of $w_r(t)$, the Cauchy problem converts to the following local system of evolutionary equations

$$\frac{dw}{dt} + \sum_{r=1}^{N_{exp}} a_r \mathcal{A}_h w_r = f(t), \tag{24}$$

$$\frac{dw_r}{dt} + b_r w_r - w = 0, \qquad r = 1, 2, \ldots, N_{exp}. \tag{25}$$

with the initial conditions

$$w(0) = u_0,$$
$$w_r(0) = 0, \quad r = 1, 2, \ldots, N_{exp}.$$

In (Petr N. Vabishchevich, (2022) *Applied Numerical Mathematics* 174, 177-190.) for approximating this local system of equations, an IMPLICIT numerical scheme constructed and analysed.

For the presented Cauchy problem, there are some issues and open problems that we aim to address:

1. What about an explicit method for the Cauchy problem?
2. What if there is a singularity in the kernel $k(t)$, such as when fractional operators are involved?

- Consider the problem $\frac{dw}{dt} + \int_0^t \bar{k}(t-\xi)\mathcal{A}_h w(\xi)d\xi = f(t)$, in the special case $(N_{exp} = 1)$:

$$\bar{k}(t) = \sum_{r=1}^{N_{exp}} a_r \exp(-b_r t) = a_1 \exp(-b_1 t), \quad t \geq 0.$$

- Define $w_1(t) = \int_0^t \exp\left(-b_1(t-\xi)\right) w(\xi)d\xi$.

The Cauchy problem converts to the the following system of evolutionary equations

$$\frac{dw}{dt} + a_1\mathcal{A}_h w_1 = f(t),$$
$$\frac{dw_1}{dt} + b_1 w_1 - w = 0.$$

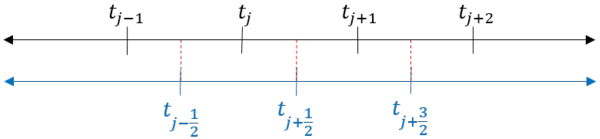
with the initial conditions

$$w(0) = u_0,$$
$$w_1(0) = 0.$$

To achieve a second-order explicit numerical method:

$$\int_{t_j}^{t_{j+1}} \left(\frac{dw}{dt} + a_1\mathcal{A}_h w_1 = f(t)\right) dt, \quad \text{(Midpoint integration rule)}$$

$$\frac{w(t_{j+1}) - w(t_j)}{\tau} + a_1\mathcal{A}_h w_1(t_{j+\frac{1}{2}}) = f(t_{j+\frac{1}{2}}) + \mathcal{O}\left(\tau^2\right),$$



$$\int_{t_{j+\frac{1}{2}}}^{t_{j+\frac{3}{2}}} \left(\frac{dw_1}{dt} + b_1 w_1 - w = 0\right) dt, \quad \text{(Trapezoidal and Midpoint integration rules)}$$

$$\frac{w_1(t_{j+\frac{3}{2}}) - w_1(t_{j+\frac{1}{2}})}{\tau} + b_1\frac{w_1(t_{j+\frac{3}{2}}) + w_1(t_{j+\frac{1}{2}})}{2} - w(t_{j+1}) = 0 + \mathcal{O}\left(\tau^2\right).$$

- Replace $w(t_j)$ and $w_1(t_{j+\frac{1}{2}})$ by their numerical approximations y^j and y_1^j, respectively.

The following form of the second-order explicit two-level system of local equations to approximate the Cauchy problem is reached

$$\frac{y^{j+1} - y^j}{\tau} + a_1 \mathcal{A}_h y_1^j = \varphi^j, \tag{26}$$

$$\frac{y_1^{j+1} - y_1^j}{\tau} + b_1 \frac{y_1^{j+1} + y_1^j}{2} - y^{j+1} = \varphi_1^j, \tag{27}$$

- We denoted $f(t_{j+\frac{1}{2}}) = \varphi^j$.
- The right-hand side of the above equation may not be exactly 0. Thus, to analyze the convergence of the numerical scheme, we considered a more general form.
- NO NEED to remember the solution at previous points in time.

For this system of equations we impose initial conditions of the form

$$\begin{aligned} y^0 &= u_0, \\ y_1^0 &= \frac{\tau}{2} u_0. \end{aligned}$$

Theorem

For the solution to the problem (26)–(27)*, under the condition*

$$1 - \frac{\tau^2}{4}\bar{k}(0)\|\mathcal{A}_h\| \geq \epsilon_2 > 0,$$

with $\bar{k}(0) = a_1$*,the following stability estimate of the solution with respect to the initial data and the right-hand side is valid.*

$$\|y^{j+1}\| \leq \frac{1}{\epsilon_2}\sum_{s=0}^{j}\|\varphi^s\|\tau + \sqrt{\frac{1}{\epsilon_2}\left(\|y^0\|^2 + \frac{a_1}{2b_1}\sum_{s=0}^{N}\|\varphi_r^s\|^2_{\mathcal{A}_h}\tau\right)}.$$

Sketch of the proof:

In the space H denote: $(\mathcal{A}_h u, v) = (u, v)_{\mathcal{A}_h}$, $\|u\|^2_{\mathcal{A}_h} = (u, u)_{\mathcal{A}_h}$.

$$\left(y^j_t + a_1 \mathcal{A}_h y^j_1 = \varphi^j\right) \cdot \frac{y^{j+1} + y^j}{2}$$

$$\left((y_1)^j_t + b_1 \frac{y^{j+1}_1 + y^j_1}{2} - y^{j+1} = \varphi^j_1\right) \cdot a_1 \mathcal{A}_h \frac{y^{j+1}_1 + y^j_1}{2},$$

where $y^j_t = (y^{j+1} - y^j)/\tau$. Adding the resulting equations yields:

$$\left(\|y\|^2 + a_1\|y_1\|^2_{\mathcal{A}_h} - a_1\tau(y, \mathcal{A}_h y_1)\right)^j_t \le \left(\varphi^j, y^{j+1} + y^j\right) + \frac{a_1}{2b_1}\|\varphi^j_1\|^2. \tag{28}$$

Denote the left-hand side of the Eq. as: $E = \|y\|^2 + a_1\|y_1\|^2_{\mathcal{A}_h} - a_1\tau(y, \mathcal{A}_h y_1)$, then

$$\begin{aligned} E =& \|y\|^2 + a_1\left(\|y_1\|^2_{\mathcal{A}_h} - \tau(y, \mathcal{A}_h y_1) + \frac{\tau^2}{4}\|y\|^2_{\mathcal{A}_h}\right) - a_1\frac{\tau^2}{4}\|y\|^2_{\mathcal{A}_h} \\ =& \|y\|^2 - a_1\frac{\tau^2}{4}\|y\|^2_{\mathcal{A}_h} + a_1\left(\|y_1 - \frac{\tau}{2}y\|^2_{\mathcal{A}_h}\right) \ge \underbrace{\left(1 - a_1\frac{\tau^2}{4}\|\mathcal{A}_h\|\right)}_{> \epsilon_1 > 0}\|y\|^2 + a_1\|y_1 - \frac{\tau}{2}y\|^2_{\mathcal{A}_h}, \end{aligned}$$

Sketch of the proof:

To proceed:

- Impose the stability condition $\left(1 - a_1\frac{\tau^2}{4}\|\mathcal{A}_h\|\right) \geq \epsilon_1 > 0$, and substitute estimation of E in the main inequality,
- Multiply the resulting equation by τ, then summing over s from 0 to j,
- Eliminate positive terms,

$$\|y^{j+1}\|^2 \leq \frac{1}{\epsilon_1}\|y^0\|^2 + \frac{1}{\epsilon_1}\sum_{s=0}^{j}\left(\varphi^s, y^{s+1} + y^s\right)\tau + \frac{1}{\epsilon_1}\sum_{s=0}^{j}\frac{a_1}{2b_1}\|\varphi_1^s\|^2_{\mathcal{A}_h}\tau.$$

One can complete the proof after estimating the second term in the right-hand side. $\square$

The typical case $(N_{exp} \geq 1)$ of the Cauchy problem $\frac{dw}{dt} + \int_0^t \bar{k}(t-\xi)\mathcal{A}_h w(\xi)d\xi = f(t)$ is approximated in a similar manner.

- Consider: $\bar{k}(t) = \sum\limits_{r=1}^{N_{exp}} a_r \exp(-b_r t), \quad t \geq 0.$
- Define: $w_r(t) = \int_0^t \exp\left(-b_r(t-\xi)\right) w(\xi)d\xi, \quad r = 1, 2, \ldots, N_{exp}.$

$$\frac{dw}{dt} + \sum_{r=1}^{N_{exp}} a_r \mathcal{A}_h w_r = f(t),$$

$$\frac{dw_r}{dt} + b_r w_r - w = 0, \qquad r = 1, 2, \ldots, N_{exp}.$$

To construct a second-order numerical scheme:

- Integrate in the same manner as the special case.
- Denote: $f(t_{j+\frac{1}{2}}) = \varphi^j$ and replace the functions $w(t_j)$ and $w_r(t_{j+\frac{1}{2}})$ by their numerical approximations y^j and y_r^j, respectively.

After numerically integration, the following final form of the second-order explicit two-level system of $(N_{exp}+1)$ local equations to approximate the Cauchy problem is reached

$$\frac{y^{j+1}-y^j}{\tau} + \sum_{r=1}^{N_{exp}} a_r \mathcal{A}_h y_r^j = \varphi^j, \tag{29}$$

$$\frac{y_r^{j+1}-y_r^j}{\tau} + b_r \frac{y_r^{j+1}+y_r^j}{2} - y^{j+1} = \varphi_r^j, \quad r = 1, 2, \ldots, N_{exp}. \tag{30}$$

Initial conditions:

$$y^0 = u_0,$$
$$y_r^0 = \frac{\tau}{2} u_0, \quad r = 1, 2, \ldots, N_{exp}.$$

Theorem

For the solution to the problem (29)–(30), *under the condition*

$$1-\frac{\tau^2}{4}\bar{k}(0)\|\mathcal{A}_h\|\geq\epsilon_2>0,$$

with $\bar{k}(0)=\sum_{r=1}^{N_{exp}}a_r$, *the following stability estimate of the solution with respect to the initial data and the right-hand side is valid.*

$$\|y^{j+1}\|\leq\frac{1}{\epsilon_2}\sum_{s=0}^{j}\|\varphi^s\|\tau+\sqrt{\frac{1}{\epsilon_2}\left(\|y^0\|^2+\sum_{r=1}^{N_{exp}}\frac{a_r}{2b_r}\sum_{s=0}^{N}\|\varphi_r^s\|_{\mathcal{A}_h}^2\tau\right)}.$$

Application for time-fractional diffusion-wave equations

Direct Numerical methods to approximate time-fractional PDEs

- Exact analytical solutions for time fractional PDEs is considerably more challenging to achieve. As a result, developing precise and stable numerical schemes is vital.
- The L1 formula is the most well-known direct method to approximate the Caputo derivative (using linear lagrange interpolation):

$$\partial_{0t_{j+1}}^{\alpha} u(t) = \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^{j} \int_{t_s}^{t_{s+1}} \frac{u'(\xi)}{(t_j-\xi)^{\alpha}} d\xi = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} a_{j-s}^{(\alpha)} u_{t,s} + \mathcal{O}(\tau^{2-\alpha}), \quad u(t) \in C^2[0,T],$$

with $0<\alpha<1$, and $u_{t,s} = (u^{s+1}-u^{s})/\tau$.

- A substantial question: what about a Crank–Nicolson type method for time-fractional PDEs?
- This improvement has been thoroughly accomplished by introducing L2-1_{σ} formula in A. Alikhanov (2015). Journal of Computational Physics, 280, 424-438.

$$\partial_{0t_{j+\sigma}}^{\alpha} u(t) = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} b_{j-s}^{(\alpha,\sigma)} u_{t,s} + \mathcal{O}(\tau^{3-\alpha}), \qquad u(t) \in C^3[0,T], 0<\alpha<1.$$

with $\sigma = 1-\frac{\alpha}{2}$.

Direct Numerical methods to approximate time-fractional PDEs

- Due to dependence of σ and α ($\sigma = 1 - \frac{\alpha}{2}$), the L2-$1_\sigma$ formula is not applicable for Sobolev-type equations and some classes of fractional variable, and distributed order PDEs.
- To overcome this challenge, the L2 method is presented in

  A. Alikhanov, & C. Huang, (2021) Applied Mathematics and Computation, 411, 126545.

$$\partial_{0t_{j+1}}^{\alpha} u(t) = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} c_{j-s}^{(\alpha)} u_{t,s} + \mathcal{O}(\tau^{3-\alpha}), \qquad u(t) \in C^3[0,T], 0 < \alpha < 1.$$

What are the Disadvantages of the direct methods?:

$$\text{L1:} \qquad \partial_{0t_{j+1}}^{\alpha} u(t) \approx \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} a_{j-s}^{(\alpha)} u_{t,s}$$

$$\text{L2-1}_\sigma\text{:} \qquad \partial_{0t_{j+\sigma}}^{\alpha} u(t) \approx \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} b_{j-s}^{(\alpha,\sigma)} u_{t,s},$$

$$\text{L2:} \qquad \partial_{0t_{j+1}}^{\alpha} u(t) \approx \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} c_{j-s}^{(\alpha)} u_{t,s}.$$

Fast IMPLICIT variants of these formulas have been investigated in the literature; however, constructing and analyzing an EXPLICIT fast numerical method for solving time-fractional diffusion-wave equation remains an open problem, with no reports available.

Consider the following time-fractional diffusion-wave equation (TFDWE)

$$
\begin{aligned}
&\partial_{0t}^{\alpha+1} u(\boldsymbol{x},t) + \mathcal{A}u(\boldsymbol{x},t) = g(\boldsymbol{x},t), && (\boldsymbol{x},t) \in \Omega \times (0,T], \\
&u(\boldsymbol{x},t) = 0, && (\boldsymbol{x},t) \in \partial\Omega \times (0,T], \\
&u(\boldsymbol{x},0) = u_0(\boldsymbol{x}), \quad u_t(\boldsymbol{x},0) = u_1(\boldsymbol{x}), && \boldsymbol{x} \in \Omega,
\end{aligned}
$$

- The operator $\mathcal{A}$ is defined as in the Cauchy problem.
- The Caputo time-fractional derivative is represented in the form

$$
\partial_{0t}^{\alpha+1} u(\boldsymbol{x},t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\eta)^{-\alpha} \frac{\partial^2 u(\boldsymbol{x},\eta)}{\partial \eta^2} d\eta, \quad 0 < \alpha < 1.
$$

- First, we transform the TFDWE model into an equivalent problem.

$$D_{0t}^{-\alpha}\left(\partial_{0t}^{\alpha+1}u(t)+\mathcal{A}u(t)=g(t)\right)$$

where $D_{0t}^{-\alpha}u(t)=\frac{1}{\Gamma(\alpha)}\int\limits_0^t(t-\xi)^{\alpha-1}u(\xi)d\xi$, (the Riemann-Liouville fractional integral)

$$\frac{du}{dt}+\int\limits_0^t\frac{(t-\xi)^{\alpha-1}}{\Gamma(\alpha)}\mathcal{A}u(\xi)d\xi=f(t), \tag{31}$$

$$u(\boldsymbol{x})=0, \qquad \boldsymbol{x}\in\partial\Omega, \tag{32}$$

$$u(\boldsymbol{x},0)=u_0(\boldsymbol{x}), \quad \boldsymbol{x}\in\Omega. \tag{33}$$

where $f(t)=\mathcal{D}_{0t}^{-\alpha}g(t)+u_1(\boldsymbol{x})$ is a known function.
Note: This methodology converts TFDWE to the format of the Cauchy problem
$\frac{du}{dt}+\int\limits_0^t k(t-\xi)\mathcal{A}u(\xi)d\xi=f(t)$, which we have already investigated.

- Next, we approximate the kernel $k(t)=t^{\alpha-1}/\Gamma(\alpha)$ in (31) by the SoE approach

$$D_{0t}^{-\alpha}u(t) = \frac{1}{\Gamma(\alpha)}\int_0^t (t-\xi)^{\alpha-1}u(\xi)d\xi$$

Theorem (Beylkin and Monzón, 2010)

For a given prescribed error ε_2, using SoE approach the kernel function $k(t) = t^{-\nu}(0 < \nu < 1)$ can be approximated by a function $\bar{k}(t)$ in the interval $[\delta, T]$, where $\delta > 0$ is a given small parameter and T is the final time. That is, there exist positive real numbers $\bar{a}_r$ and b_r $(r = 1, 2, \ldots, N_{exp})$, such that

$$\left| t^{-\nu} - \sum_{r=1}^{N_{exp}} \bar{a}_r \exp(-b_r t) \right| \leq \varepsilon_2, \quad t \in [\delta, T],$$

where

$$N_{exp} = \mathcal{O}\left(\log\frac{1}{\varepsilon_2}\left(\log\log\frac{1}{\varepsilon_2} + \log\frac{T}{\delta}\right) + \log\frac{1}{\delta}\left(\log\log\frac{1}{\varepsilon_2} + \log\frac{T}{\delta}\right)\right).$$

$$t^{-\nu} \approx \sum_{r=1}^{N_{exp}} \bar{a}_r \exp(-b_r t):$$

To make a conceptional understanding of the actual number (N_{exp}) needed:
The Table shows when $T = 1$, how many exponentials (N_{exp}) are required to approximate $t^{\alpha-1}$ with different α, δ and ε_2.

	$\alpha = 0.3$			$\alpha = 0.5$			$\alpha = 0.7$		
δ \ ε_2	10^{-4}	10^{-8}	10^{-12}	10^{-4}	10^{-8}	10^{-12}	10^{-4}	10^{-8}	10^{-12}
10^{-4}	27	48	69	27	48	68	27	48	68
10^{-6}	35	63	90	35	62	90	34	62	89
10^{-8}	43	77	111	42	77	111	42	76	111

1. Define: $u_r(t) = \int_0^t \exp\left(-b_r(t-\xi)\right) u(\xi)d\xi,\ r = 1, 2, \dots, N_{exp}$,
2. Employ the SoE approach for the kernel in the Riemann-Liouville fractional integral,
3. Replace the operator $\mathcal{A}$ with its approximation $\mathcal{A}_h$,

$$D_{0t}^{-\alpha}\mathcal{A}_h u(t) = \int\limits_{t-\delta}^{t} \frac{(t-\xi)^{\alpha-1}}{\Gamma(\alpha)}\mathcal{A}_h u(\xi)d\xi + \int\limits_{0}^{t-\delta} \frac{(t-\xi)^{\alpha-1}}{\Gamma(\alpha)}\mathcal{A}_h u(\xi)d\xi$$

$$\approx \int\limits_{t-\delta}^{t} \left(\frac{(t-\xi)^{\alpha-1}}{\Gamma(\alpha)} - \sum_{r=1}^{N_{exp}} a_r \exp(-b_r(t-\xi)) \right) \mathcal{A}_h u(\xi)d\xi + \sum_{r=1}^{N_{exp}} a_r \int\limits_{0}^{t} \exp(-b_r(t-\xi))\mathcal{A}_h u(\xi)d\xi$$

$$= \int\limits_{t-\delta}^{t} \varkappa(t-\xi)\mathcal{A}_h u(\xi)d\xi + \sum_{r=1}^{N_{exp}} a_r \mathcal{A}_h u_r(t), \quad t \geq \delta$$

where $a_r = \bar{a}_r/\Gamma(\alpha)$, and $\varkappa(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)} - \sum_{r=1}^{N_{exp}} a_r \exp(-b_r t)$.

$\frac{du}{dt} + \mathcal{D}_{0t}^{-\alpha}\mathcal{A}u = f(t)$

We reach the following system of evolutionary equations for approximating the TFDWE model

$$\frac{du}{dt} + \int\limits_{t-\delta}^{t} \varkappa(t-\xi)\mathcal{A}_h u(\xi)d\xi + \sum_{r=1}^{N_{exp}} a_r \mathcal{A}_h u_r(t) = f(t), \quad t \geq \delta, \tag{34}$$

$$\frac{du_r}{dt} + b_r u_r - u = 0, \quad r = 1, 2, \ldots, N_{exp}. \tag{35}$$

To develop a fast method for approximating this system, for a function $u(t) \in C^3[0,T]$, we evaluate this equation at the fixed point $t_{j+\frac{1}{2}}$, $(j = 0, 1, \ldots, N-1)$.

$$\frac{u^{j+1}-u^j}{\tau}+\int\limits_{t_{j+\frac{1}{2}}-\delta}^{t_{j+\frac{1}{2}}}\varkappa(t_{j+\frac{1}{2}}-\xi)\mathcal{A}_h u(\xi)d\xi+\sum_{r=1}^{N_{exp}}a_r\mathcal{A}_h u_r(t_{j+\frac{1}{2}})=\varphi^j+\mathcal{O}\left(\tau^2\right),$$

$$\frac{u_r(t_{j+\frac{3}{2}})-u_r(t_{j+\frac{1}{2}})}{\tau}+b_1\frac{u_r(t_{j+\frac{3}{2}})+u_r(t_{j+\frac{1}{2}})}{2}-u(t_{j+1})=0+\mathcal{O}\left(\tau^2\right).$$

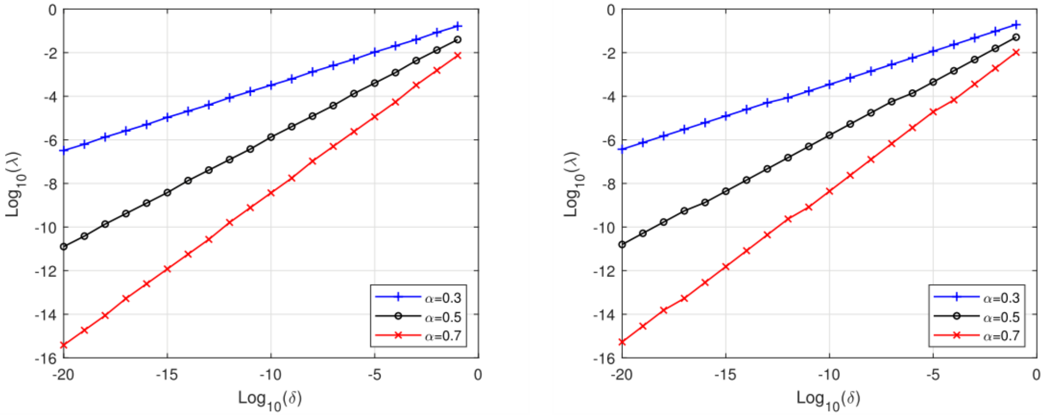
where $f(t_{j+\frac{1}{2}})=\varphi^j$, and the integral in the first equation is approximated as follows

$$\int\limits_{t_{j+\frac{1}{2}}-\delta}^{t_{j+\frac{1}{2}}}\varkappa(t_{j+\frac{1}{2}}-\xi)\mathcal{A}_h u(\xi)d\xi=\lambda\mathcal{A}_h u(t_j)+\mathcal{O}\left(\tau\lambda+\tau^2\right).$$

In which

$$\lambda=\frac{\delta^\alpha}{\Gamma(\alpha+1)}-\sum_{r=1}^{N_{exp}}\frac{a_r}{b_r}(1-\exp(-b_r\delta))\geq 0.$$

$$\lambda = \frac{\delta^\alpha}{\Gamma(\alpha+1)} - \sum_{r=1}^{N_{exp}} \frac{a_r}{b_r}(1-\exp(-b_r\delta)).$$



(a) $\varepsilon_2 = 10^{-8}$ (b) $\varepsilon_2 = 10^{-4}$

Figure : Variation of λ in the $\log_{10}$ scale, for different values of δ and α with $\varepsilon_2 = 10^{-8}, 10^{-4}$.

By replacing the functions $v(t_j)$ and $v_r(t_{j+\frac{1}{2}})$ by their numerical approximations y^j and y_r^j, respectively, we reach the following final form of the explicit fast system of local equations to approximate TFDWE.

$$\frac{y^{j+1}-y^j}{\tau}+\lambda\mathcal{A}_h y^j+\sum_{r=1}^{N_{exp}} a_r\mathcal{A}_h y_r^j=\varphi^j, \tag{36}$$

$$\frac{y_r^{j+1}-y_r^j}{\tau}+b_r\frac{y_r^{j+1}+y_r^j}{2}-y^{j+1}=\varphi_r^j, \quad r=1,2,\ldots,N_{exp}. \tag{37}$$

Initial conditions:

$$\begin{aligned} y^0 &= u_0, \\ y_r^0 &= \frac{\tau}{2}u_0. \quad r=1,2,\ldots,N_{exp}, \end{aligned}$$

Theorem

For the solution to the problem (36)–(37)*, under the condition*

$$1 - \left(\lambda\frac{\tau}{2} + \frac{\tau^2}{4}\bar{k}(0)\right)\|\mathcal{A}_h\| \geq \epsilon_3 > 0,$$

with $\bar{k}(0) = \sum\limits_{r=1}^{N_{exp}} a_r$, *the following stability estimate of the solution with respect to the initial data and the right-hand side is valid.*

$$\|y^{j+1}\| \leq \frac{1}{\epsilon_3}\sum_{s=0}^{j}\|\varphi^s\|\tau + \sqrt{\frac{1}{\epsilon_3}\|y^0\|^2 + \sum_{s=0}^{N}\sum_{r=1}^{N_{exp}}\frac{a_r}{2b_r}\|\varphi_r^s\|^2_{\mathcal{A}_h}\tau}.$$

Example 1. Consider the two-dimensional Cauchy problem $\frac{du}{dt} + \int_0^t k(t-\xi)\mathcal{A}u(\xi)d\xi = f$ with

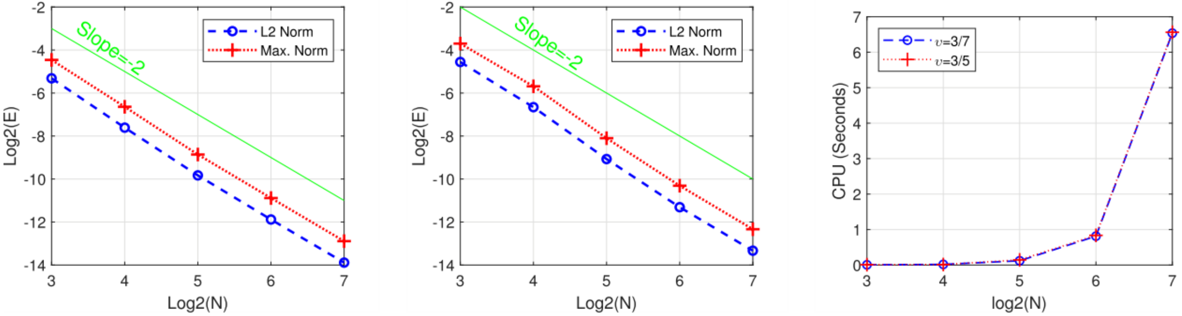
$$f(\boldsymbol{x}, t) = 0, \quad u(\boldsymbol{x}) = \sin(2\pi x_1)\sin(2\pi x_2).$$

We select the stretching exponential function as the kernel in the following form:

$$k(t) = \exp(-t^{\upsilon}), \quad 0 < \upsilon < 1.$$

- We choose the elliptic operator $\mathcal{A} = -\Delta$ and consider the uniform spatial domain.
- In the spatial direction, we choose $\mathcal{A}_h$ as the standard second order central finite difference formula, where $\|\mathcal{A}_h\| \leq \frac{4}{h_1^2} + \frac{4}{h_2^2}$.
- In (Mauro, 2018), using SoE approach the kernel function $k(t)$, is approximated by a function $\bar{k}(t) = \sum_{r=1}^{N_{exp}} a_r \exp(-b_r t)$, under an additional requirement: $\sum_{r=1}^{N_{exp}} a_r = 1$ for $N_{exp} = 12$ in the context of three different values of $\upsilon = 3/7, 1/2$, and $3/5$.
- Due to the absence of an exact solution, the two-mesh principle is applied to determine the errors:

$$E_2 = \max_{0\leq j\leq N} \|e^j\|, \quad E_c = \max_{0\leq j\leq N} \|e^j\|_{C(\bar{\Omega}_{h\tau})},$$

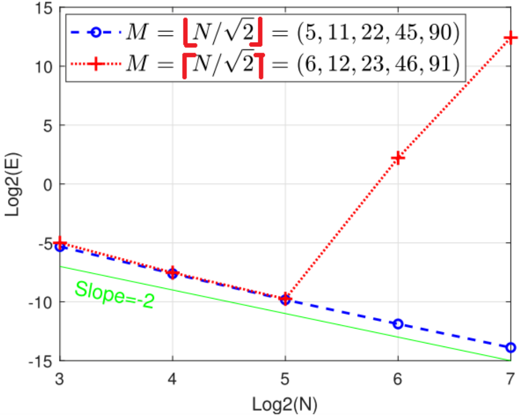


(a) $\upsilon = 3/7$ (b) $\upsilon = 3/5$ (c) CPU time in seconds

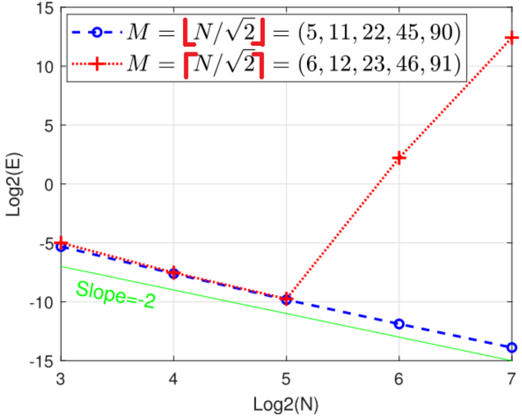
Fig: Error and temporal convergence order of the 2D Cauchy problem with decreasing temporal and spatial step sizes $\tau = T/N$, $h = 1/M$, for $M = (5, 11, 22, 45, 90)$ at $T = 1$.

Our aim is to highlight the significance of the stability condition: $1 - \frac{\tau^2}{4}\bar{k}(0)\|\mathcal{A}_h\| > 0.$

From data for this example $\left(\bar{k}(0) = \sum_{r=1}^{N_{exp}} a_r = 1,\ \|\mathcal{A}_h\| \leq \frac{8}{h^2}\right)$ we have $M < \frac{N}{\sqrt{2}}$.



(a) $\upsilon = 3/7$



(b) $\upsilon = 3/7$

Fig: Error and temporal convergence order of the 2D Cauchy problem with decreasing temporal and spatial step sizes $\tau = T/N$, $h = 1/M$, at $T = 1$.

Example 2. Consider the TFDWE model $\frac{du}{dt} + \mathcal{D}_{0t}^{-\alpha}\mathcal{A}u = f$ with the exact analytical solution

$$u(x,t) = t^2 \sin(\pi x).$$

- we choose the elliptic operator $\mathcal{A}$ as

$$\mathcal{A}u(x,t) = -\frac{\partial}{\partial x}\left(\psi(x)\frac{\partial u}{\partial x}\right) + \phi(x)u,$$

  with the coefficients

$$\psi(x) = 2 - \cos(x), \quad \phi(x) = 1 - \sin(x).$$

- The operator $\mathcal{A}$ is discretized by $\mathcal{A}_h$ as

$$\mathcal{A}u = \mathcal{A}_h u + \mathcal{O}(h^2), \tag{38}$$

  in which, for $i = 1, \ldots, M-1$, the difference operator $\mathcal{A}_h$ takes the form of

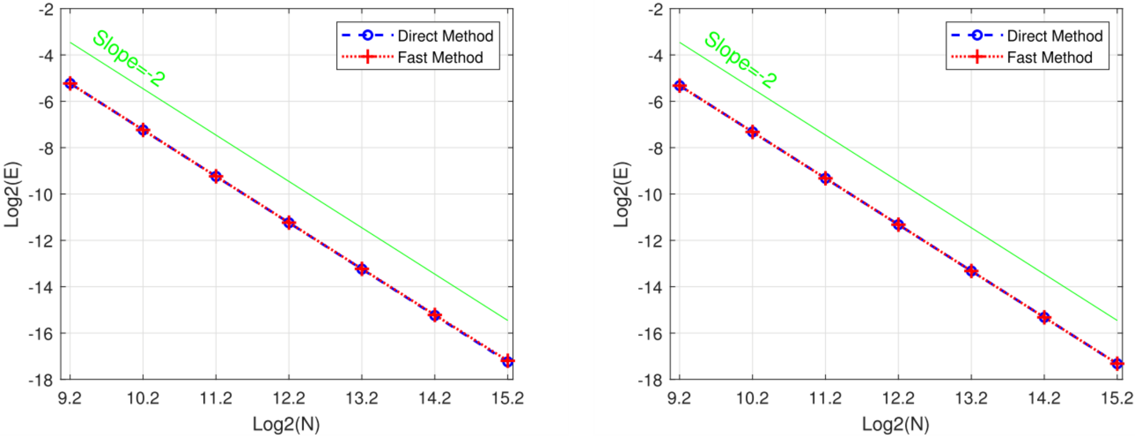
$$\mathcal{A}_h u_i = -\frac{\psi(x_{i+0.5})u_{i+1} - \left(\psi(x_{i+0.5}) + \psi(x_{i-0.5})\right)u_i + \psi(x_{i-0.5})u_{i-1}}{h^2} + \phi(x_i)u_i. \tag{39}$$

- For this operator with the considered coefficients, we have $\|\mathcal{A}_h\| \leq \frac{12}{h^2} + 2$.

- In (Beylkin and Monzón, 2010), using SoE approach the kernel function $k(t) = t^{\alpha-1}$ is approximated by a function $\bar{k}(t) = \sum_{r=1}^{N_{exp}} a_r \exp(-b_r t)$, in the interval $[\delta, T]$.
- We set prescribed error $\varepsilon_2 = 10^{-8}$ and $\delta = 10^{-5}$, which are small enough for our purpose. This results in:
  - $N_{exp} \approx 55$
  - For $\alpha = 0.3$, we have $\bar{k}(0) = 10398.11$
  - For $\alpha = 0.7$, we have $\bar{k}(0) = 73.35$
- By choosing $N = (6, 12, 24, 48, 96, 192, 384) \times 100$, and $M = (4, 8, 16, 32, 64, 128, 256)$ We compare our results with the results of

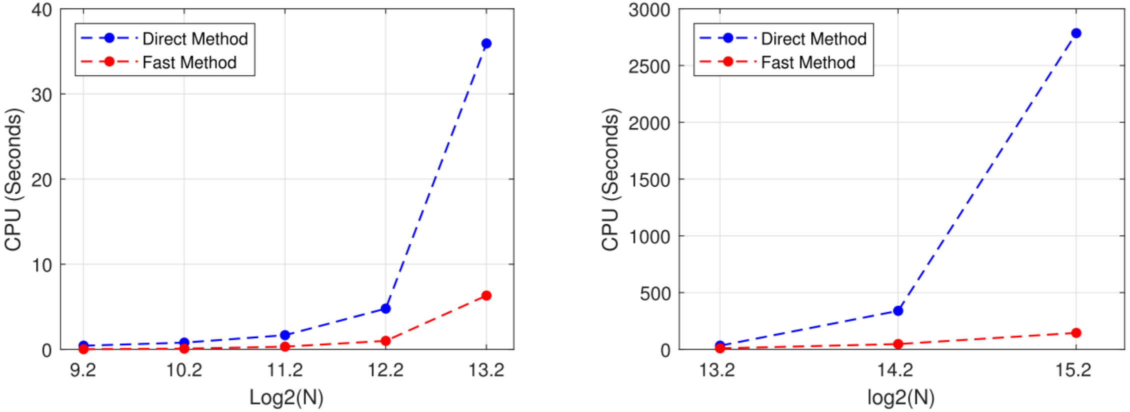
  A. Alikhanov, et al. (2024). Journal of Computational and Applied Mathematics, 438, 115515.

  where the authors presented an implicit second-order difference scheme for the time-fractional diffusion-wave equation with generalized memory kernel.



(a) $\alpha = 0.3$ (b) $\alpha = 0.7$

Fig: Error of the direct and fast difference schemes with varying temporal and spatial step sizes $\tau = T/N$, $h = 1/M$ for $\varepsilon_2 = 10^{-8}$, and $\delta = 10^{-5}$, and $M = (4, 8, 16, 32, 64, 128, 256)$ at $T = 1$.



(a) $\alpha = 0.3,\ M = (4, 8, 16, 32, 64)$ (b) $\alpha = 0.7,\ M = (64, 128, 2564)$

Fig: The CPU time in seconds with varying temporal and spatial step sizes.

Future direction

For the investigated Cauchy problem, there is one open problem:

- What about a general case when the kernel is positive-definite but not representable as a sum of exponentials?

we aim to construct an explicit scheme of the form:

$$\frac{u^{j+1}-u^j}{\tau}+\sum_{s=0}^{j} a_{j-s}\mathcal{A}_h u^s=\phi^j. \tag{40}$$

Investigating stability properties of such methods requires deeper study.

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Thank you for your attention!