

Numerical solution of the space-time fractional diffusion equation: Alternatives to finite differences

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Which numerical method is best suited to solve the space-time tempered fractional diffusion equation?

$$\partial_t^{\gamma,\beta,s} f(x, t) = d(x) \partial_x^{\alpha,\theta,\lambda} f(x, t) + q(x, t),$$

where the tempered time and space fractional derivatives of order γ and α are defined as:

$$\begin{aligned} \partial_t^{\gamma,\beta,s} f(x, t) &= \frac{\partial f}{\partial t}(x, t) + \beta e^{-st} {}_0 D_t^\gamma (e^{st} f(x, t)) - \beta s^\gamma f(x, t), \\ \partial_x^{\alpha,\theta,\lambda} f(x, t) &= \frac{1-\theta}{2} e^{-\lambda x} {}_0 D_x^\alpha (e^{\lambda x} f(x, t)) + \frac{1+\theta}{2} e^{\lambda x} {}_x D_L^\alpha (e^{-\lambda x} f(x, t)) \\ &\quad - \lambda^\alpha f(x, t) + \alpha \theta \lambda^{\alpha-1} \frac{\partial f}{\partial x}(x, t), \end{aligned}$$

where β is a capacity coefficient, $s \geq 0$ is the time truncation parameter, $\lambda \geq 0$ is the space truncation parameter and $\theta \in [-1, 1]$ is a skewness parameter. That equation is defined for $0 \leq x \leq L$ and $0 \leq t \leq T$.

OK, that's quite complicate. Let's start with something easier...

We are first going to consider the space-fractional diffusion equation without tempering :

$$\partial_t f(x, t) = d(x) \partial_x^{\alpha, \theta} f(x, t) + q(x, t),$$

where

$$\partial_x^{\alpha, \theta} f(x, t) = \frac{1 - \theta}{2} {}_0D_x^\alpha f(x, t) + \frac{1 + \theta}{2} {}_xD_L^\alpha f(x, t).$$

The fractional derivatives ${}_0D_x^\alpha$ and ${}_xD_L^\alpha$ can be defined either in the Riemann-Liouville or Caputo sense.

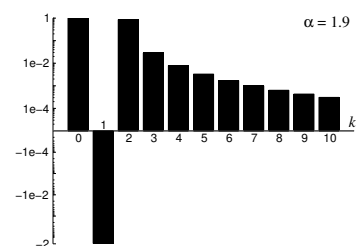
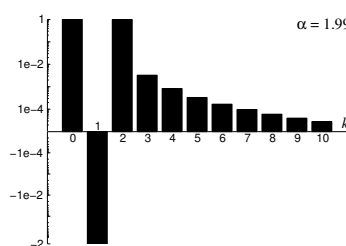
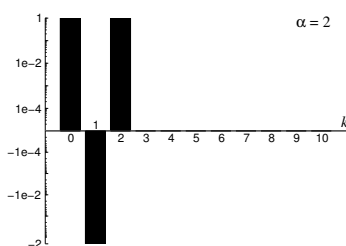
A finite difference (FD) discretization of the diffusion term leads to a full diffusion matrix

FD schemes are based on the Grünwald approximation:

$${}_0D_x^\alpha f(x_i, t) \approx \frac{\sum_{j=0}^i w_j f_{i-j+1}}{\Delta x^\alpha}$$

$${}_xD_L^\alpha f(x_i, t) \approx \frac{\sum_{j=0}^{N-i} w_j f_{i+j-1}}{\Delta x^\alpha}$$

where the domain has been divided in N segments of finite size $\Delta x = \frac{L}{N}$ and $w_k = \frac{\Gamma(k-\alpha)}{\Gamma(k+1)\Gamma(-\alpha)}$ for $k = 0, 1, 2, \dots$



The FD stencil covers the entire domain as soon as $\alpha < 2$

$$D_2 \propto \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix}$$

$$D_{1.99} \propto \begin{pmatrix} -1.9900 & 0.9850 & 0.0033 & 0.0008 & 0.0003 & 0.0002 \\ 0.9850 & -1.9900 & 0.9850 & 0.0033 & 0.0008 & 0.0003 \\ 0.0033 & 0.9850 & -1.9900 & 0.9850 & 0.0033 & 0.0008 \\ 0.0008 & 0.0033 & 0.9850 & -1.9900 & 0.9850 & 0.0033 \\ 0.0003 & 0.0008 & 0.0033 & 0.9850 & -1.9900 & 0.9850 \\ 0.0002 & 0.0003 & 0.0008 & 0.0033 & 0.9850 & -1.9900 \end{pmatrix}$$

The computational cost of the method is thus $\mathcal{O}(N^3)$ and storage is $\mathcal{O}(N^2)$ (unless something clever is done...)

The finite element (FE) method is a bit more flexible than the FD method but not more efficient

The exact solution is approximated by an expansion in terms of low-order compact-support basis functions ϕ_j :

$$f(x, t) \approx \sum_{j=1}^N f_j(t) \phi_j(x).$$

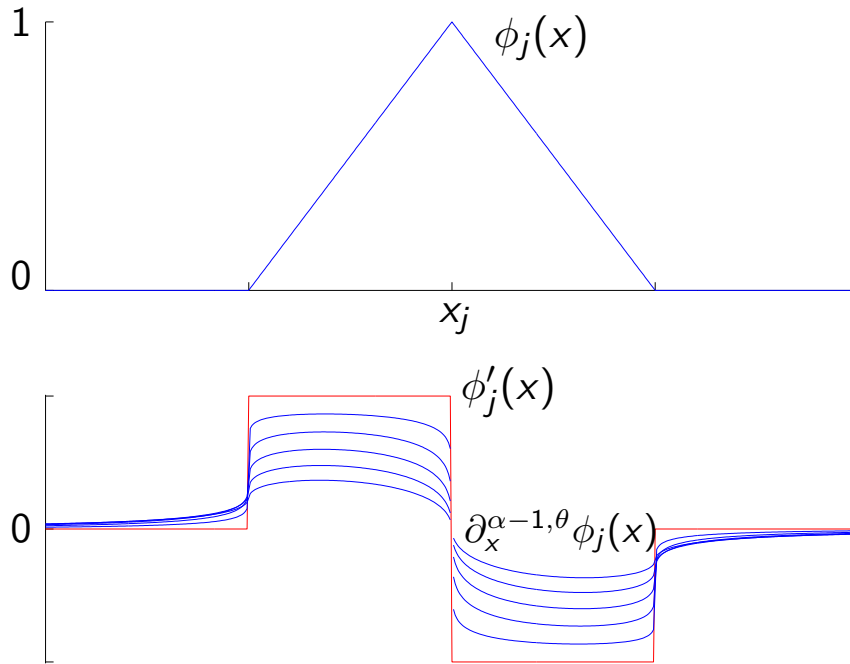
The discrete equations are obtained by using a Galerkin formulation, which amounts to multiply the model equation by ϕ_i ($i = 1, \dots, N$) and integrate by parts on $[0, L]$. The diffusion term is then discretized as follows:

$$d(x) \partial_x^{\alpha, \theta} f(x, t) \approx D_{ij} f_j(t),$$

where the elements of the diffusion matrix D read:

$$D_{ij} = - \int_0^L \frac{d}{dx} (d \phi_i) \partial_x^{\alpha-1, \theta} \phi_j \, dx.$$

The fractional derivative of a compact-support FE basis function does not have a compact support anymore



The diffusion matrix is thus again a full matrix.

The FE diffusion matrix can be obtained quite easily with piecewise linear basis functions

Assuming that the support of the basis function ϕ_i corresponds to $[x_{i-1}, x_i] \cup [x_i, x_{i+1}]$, we see that

$$D_{ij} = -d \frac{d\phi_i}{dx} \Big|_{[x_{i-1}, x_i]} \int_{x_{i-1}}^{x_i} \partial_x^{\alpha-1, \theta} \phi_j \, dx - d \frac{d\phi_i^x}{dx} \Big|_{[x_i, x_{i+1}]} \int_{x_i}^{x_{i+1}} \partial_x^{\alpha-1, \theta} \phi_j \, dx,$$

$$= \frac{d}{\Gamma(2-\alpha)} \left(- \frac{\left[\int_0^x \frac{\phi_j(y)}{(x-y)^{\alpha-1}} \, dy \right]_{x_{i-1}}^{x_i}}{x_i - x_{i-1}} + \frac{\left[\int_x^L \frac{\phi_j^x(y)}{(y-x)^{\alpha-1}} \, dy \right]_{x_i}^{x_{i+1}}}{x_{i+1} - x_i} \right),$$

where we assumed that the diffusivity d is constant.

On a uniform grid, the FE diffusion matrix could be interpreted as a FD matrix. This suggests a way to obtain a second-order FD scheme without having recourse to Grünwald approximation.

The pseudo-spectral (PS) method seems better suited to global differential operators

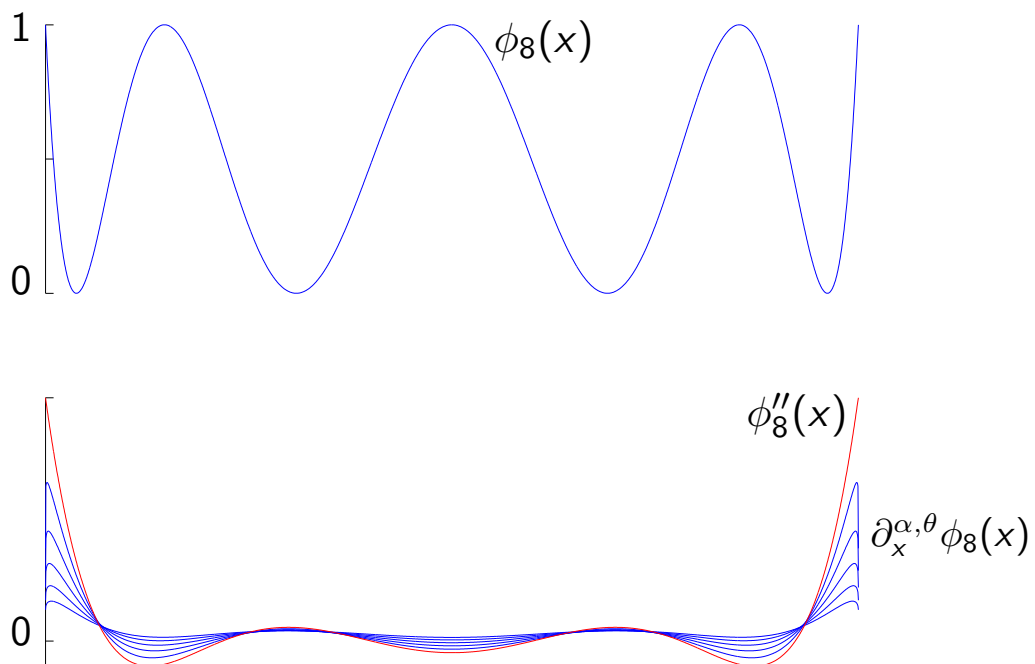
The PS method is quite similar to the FE method with the exception that basis functions $\phi_j(x)$ are now global high-order functions, like Chebyshev polynomials. As a result, less degrees of freedom are required to achieve the same accuracy as with the FE method and the discrete operators are always represented by full matrices whatever the value of α .

Here we use the Galerkin formulation to discretize the model equations. The diffusion matrix then reads:

$$D_{ij} = \int_0^L \phi_i(x) d(x) \partial_x^{\alpha, \theta} \phi_j(x) w(x) dx.$$

where $w(x)$ is a weight function with respect to which the polynomial basis functions are orthogonal.

Integer- and fractional-order derivatives of a PS basis function are global functions



Going from an integer-order to a fractional-order diffusion operator does not significantly change the computational cost.

The radial basis function (RBF) method can be seen as a compromise between the FE and PS methods

With the RBF method, the model solution is generally expressed as follows:

$$f(x, t) \approx \sum_{j=1}^N f_j(t) \phi(|x - x_j|),$$

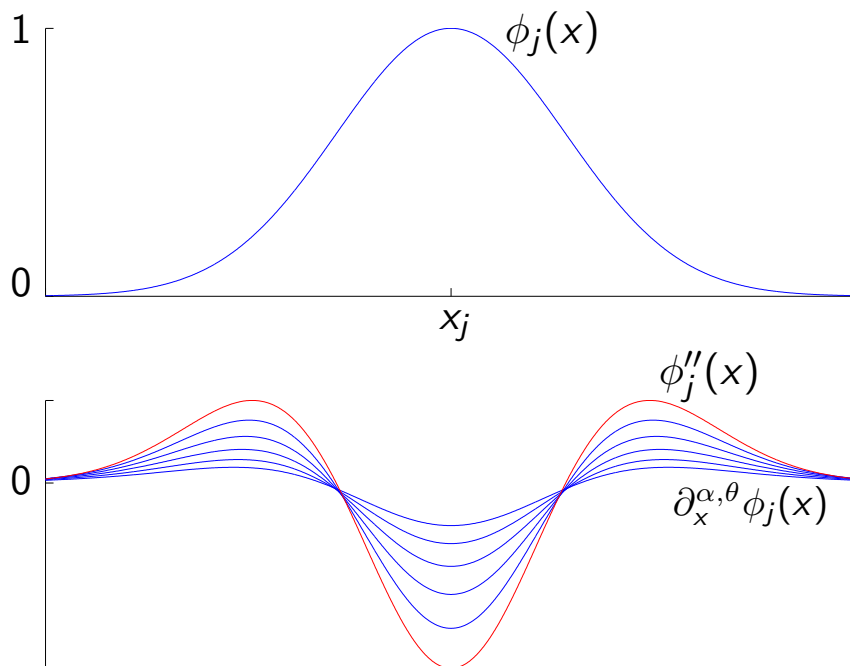
where $\phi(r)$ is a radial function and x_j its center. Here we consider the Gaussian radial functions $\phi(r) = e^{-(\varepsilon r)^2}$, where the shape parameter ε controls the flatness of the function.

A collocation method is usually used to derive the discrete equations. The diffusion matrix then reads:

$$D_{ij} = d(x_i) \partial_x^{\alpha, \theta} \phi_j(x_i).$$

It is a full matrix whatever the value of α .

The RBF's are global functions that have a spatial location



They can be clustered in the region where the solution is steep (like with the FE method) while preserving high-order accuracy (like with the PS method).

The fractional derivatives of RBF's can be computed analytically

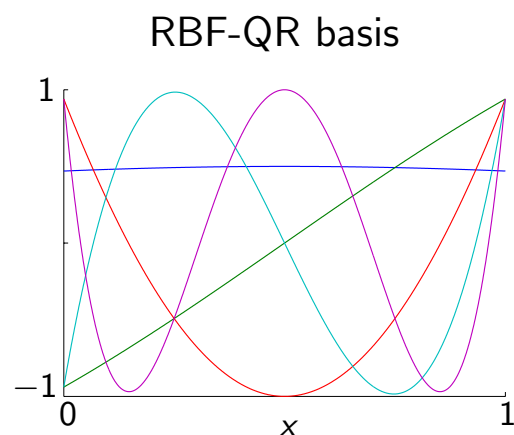
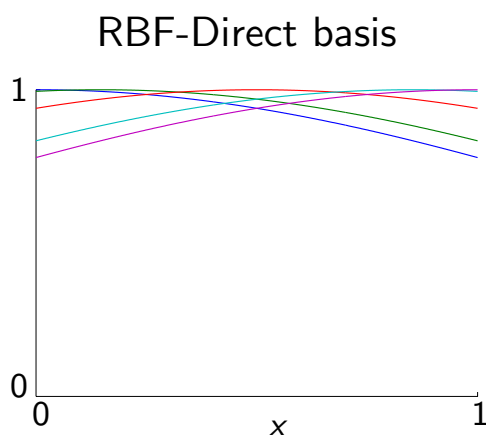
This can be done by expanding the Gaussian radial function in a MacLaurin series:

$$\partial_x^{\alpha,\theta} e^{-\varepsilon^2|x-x_i|^2} = \sum_{j=0}^{\infty} \frac{(-1)^j \varepsilon^{2j}}{j!} \left(\sum_{k=0}^{2j} \frac{(2j)!(-1)^k x_i^{2j-k}}{k!(2j-k)!} \partial_x^{\alpha,\theta} x^k \right),$$

and truncating the infinite sum once the terms are smaller in magnitude than machine precision.

How to avoid ill conditionning? Try RBF-QR...

The standard implementation of the RBF method exhibits an increasing ill conditioning when N increases and when ε decreases. This is due to the RBF basis that becomes increasingly lousy. The RBF-QR algorithm avoids this issue by constructing a new basis spanning exactly the same function space but much better conditioned. The RBF-QR converges towards Chebyshev polynomials when $\varepsilon \rightarrow 0$.



Convergence analysis

Find $f(x, t)$ such that

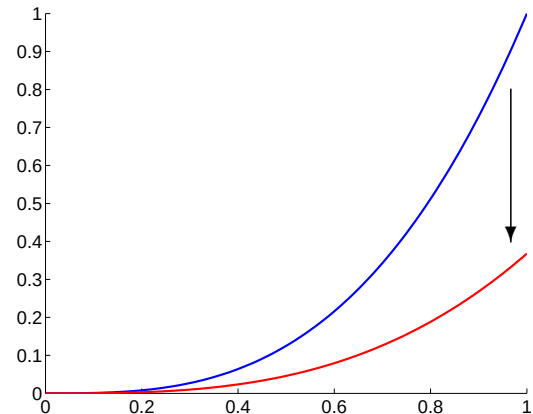
$$\frac{\partial f(x, t)}{\partial t} = d(x)_0 D_x^{1.2} f(x, t) + q(x, t) \quad \text{for } x \in [0, 1] \text{ and } t > 0,$$

with
$$\begin{cases} d(x) &= \Gamma(3.8)x^{1.2}/24, \\ q(x, t) &= -2e^{-t}x^4, \\ f(x, 0) &= x^4, \\ f(0, t) &= 0, \\ f(1, t) &= e^{-t}. \end{cases}$$

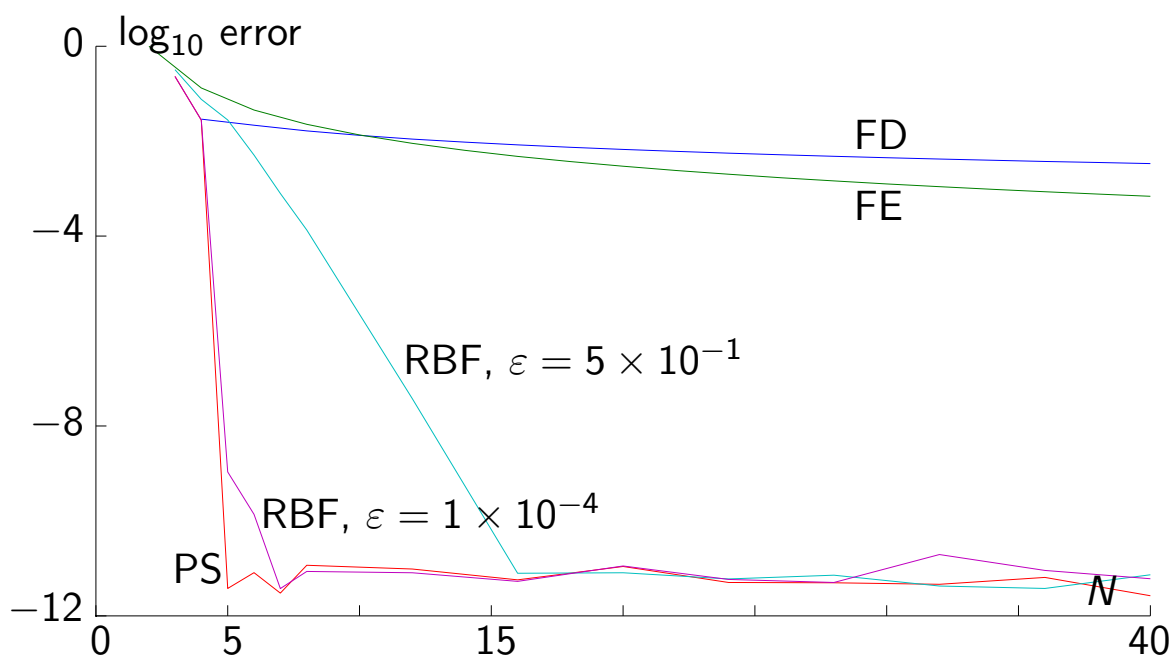
In that case, the exact solution is:

$$f(x, t) = e^{-t}x^4.$$

We solve that equation until $t = 1$ with the 4 numerical schemes and then compute the L_2 error between the discrete and exact solutions.

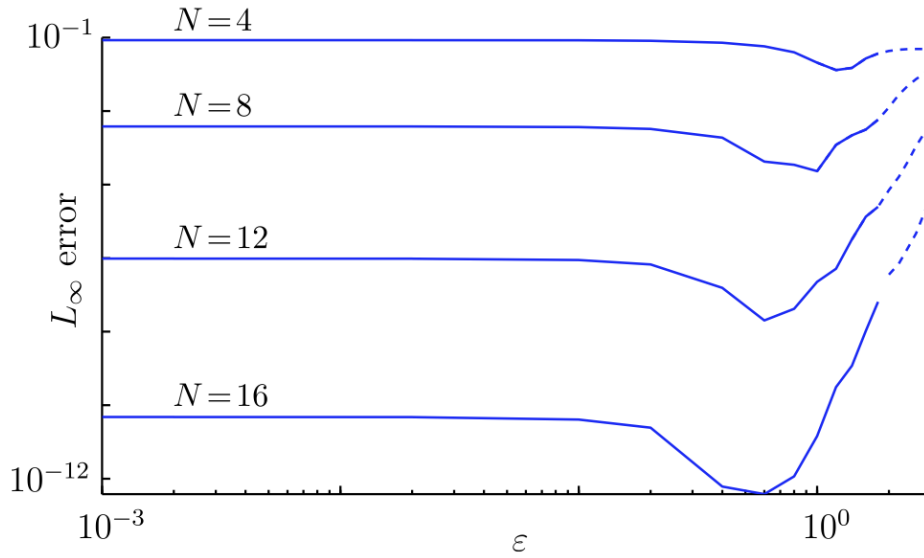


The expected convergence rates are achieved



The RBF solution converges towards the PS solution as $\varepsilon \rightarrow 0$.
The FD scheme is 1st-order accurate and the FE scheme is 2nd-order accurate.

By carefully selecting the shape parameter ε , RBF can yield better accuracy than PS



Relative max-norm error in computing ${}_0^C D_x^{1.8} \cos(6x)$ with respect to ε , for several Chebyshev distributions of N nodes.

Now, let's consider the fully fractional equation with space and time tempering...

Just to remind you, the model equation is:

$$\partial_t^{\gamma, \beta, s} f(x, t) = d(x) \partial_x^{\alpha, \theta, \lambda} f(x, t) + q(x, t),$$

where the time and space fractional derivatives are both tempered:

$$\begin{aligned} \partial_t^{\gamma, \beta, s} f(x, t) &= \frac{\partial f}{\partial t}(x, t) + \beta e^{-st} {}_0 D_t^\gamma (e^{st} f(x, t)) - \beta s^\gamma f(x, t), \\ \partial_x^{\alpha, \theta, \lambda} f(x, t) &= \frac{1-\theta}{2} e^{-\lambda x} {}_0 D_x^\alpha (e^{\lambda x} f(x, t)) + \frac{1+\theta}{2} e^{\lambda x} {}_x D_L^\alpha (e^{-\lambda x} f(x, t)) \\ &\quad - \lambda^\alpha f(x, t) + \alpha \theta \lambda^{\alpha-1} \frac{\partial f}{\partial x}(x, t). \end{aligned}$$

Since the PS method seems to work quite well, let's use that method for the time discretization as well...

For the space discretization, we leave it open...

The discrete solution is expressed in terms of a matrix of unknown nodal values F_{jk} as follows:

$$f(x, t) \approx \tilde{f}(x, t) = \sum_{j=0}^{N_x} \sum_{k=0}^{N_t} \phi_j^x(x) F_{jk} \phi_k^t(t),$$

where $\phi_k^t(t)$ is a Chebyshev polynomial of order k and $\phi_j^x(x)$ could be either a FE, PS or radial basis function.

We also introduce the following three intermediate variables and assume that they have the same discretization as the model solution:

$$g(x, t) \equiv e^{st} f(x, t) \approx \tilde{g}(x, t) = \sum_{j=0}^{N_x} \sum_{k=0}^{N_t} \phi_j^x(x) G_{jk} \phi_k^t(t),$$

$$h^l(x, t) \equiv e^{\lambda x} f(x, t) \approx \tilde{h}^l(x, t) = \sum_{j=0}^{N_x} \sum_{k=0}^{N_t} \phi_j^x(x) H_{jk}^l \phi_k^t(t),$$

$$h^r(x, t) \equiv e^{-\lambda x} f(x, t) \approx \tilde{h}^r(x, t) = \sum_{j=0}^{N_x} \sum_{k=0}^{N_t} \phi_j^x(x) H_{jk}^r \phi_k^t(t),$$

To derive the discrete equations, we use a Galerkin formulation in space and time

The discrete equations read:

$$\langle\langle \phi_i^x \partial_t^{\gamma, \beta, s} \tilde{f}(x, t) \phi_l^t \rangle\rangle = \langle\langle \phi_i^x d(x, t) \partial_x^{\alpha, \theta, \lambda} \tilde{f}(x, t) \phi_l^t \rangle\rangle + \langle\langle \phi_i^x q(x, t) \phi_l^t \rangle\rangle,$$

for $0 \leq i \leq N_x$ and $0 \leq l \leq N_t$.

The time derivative term can be expressed as follows:

$$\begin{aligned} \langle\langle \phi_i^x \partial_t^{\gamma, \beta, s} \tilde{f} \phi_l^t \rangle\rangle &= \langle\langle \phi_i^x \frac{\partial \tilde{f}}{\partial t} \phi_l^t \rangle\rangle + \beta \langle\langle \phi_i^x e^{-st} {}_0 D_t^\gamma \tilde{g} \phi_l^t \rangle\rangle - \beta s^\gamma \langle\langle \phi_i^x \tilde{f} \phi_l^t \rangle\rangle \\ &= \langle\langle \phi_i^x \phi_j^x \rangle_x F_{jk} \langle \frac{d \phi_k^t}{dt} \phi_l^t \rangle_t + \beta \langle\langle \phi_i^x \phi_j^x \rangle_x G_{jk} \langle e^{-st} {}_0 D_t^\gamma \phi_k^t \phi_l^t \rangle_t - \beta s^\gamma \langle\langle \phi_i^x \phi_j^x \rangle_x F_{jk} \langle \phi_k^t \phi_l^t \rangle_t \\ &= M_{ij} F_{jk} T_{kl}^1 + \beta M_{ij} G_{jk} T_{kl}^\gamma - \beta s^\gamma M_{ij} F_{jk} N_{kl}, \end{aligned}$$

That's almost OK but we still have to express G_{jk} in terms of F_{jk} ...

Tempering is easily handled with a L_2 projection

The following L_2 projection can be used to express G_{jk} in terms of F_{jk} :

$$\langle\langle \phi_i^x \tilde{g}(x, t) \phi_l^t \rangle\rangle = \langle\langle \phi_i^x e^{st} \tilde{f}(x, t) \phi_l^t \rangle\rangle,$$

or

$$\langle \phi_i^x \phi_j^x \rangle_x G_{jk} \langle \phi_k^t \phi_l^t \rangle_t = \langle \phi_i^x \phi_j^x \rangle_x F_{jk} \langle e^{st} \phi_k^t \phi_l^t \rangle_t,$$

which amounts to say that $G = FE^p N^{-1}$, where the matrix E^p is such that $E_{kl}^p = \langle e^{st} \phi_k^t \phi_l^t \rangle_t$.

The PS Galerkin discretization of the tempered fractional derivative can then be expressed as a product of 3 matrices:

$$\langle\langle \phi_i^x \partial_t^{\gamma, \beta, s} \tilde{f}(x, t) \phi_l^t \rangle\rangle = (\text{MFT})_{il},$$

where

$$\mathbf{T} \equiv \mathbf{T}^1 + \beta E^p N^{-1} \mathbf{T}^\gamma - \beta s^\gamma \mathbf{N}.$$

The same can be done for the tempered space derivative

$$\begin{aligned} & \langle\langle \phi_i^x d \partial_x^{\alpha, \theta, \lambda} \tilde{f} \phi_l^t \rangle\rangle \\ &= \frac{1-\theta}{2} \langle\langle \phi_i^x d e^{-\lambda x} {}_0 D_x^\alpha \tilde{h}^l \phi_l^t \rangle\rangle + \frac{1+\theta}{2} \langle\langle \phi_i^x d e^{\lambda x} {}_x D_L^\alpha \tilde{h}^r \phi_l^t \rangle\rangle \\ & \quad - \lambda^\alpha \langle\langle \phi_i^x d \tilde{f} \phi_l^t \rangle\rangle + \alpha \theta \lambda^{\alpha-1} \langle\langle \phi_i^x d \frac{\partial \tilde{f}}{\partial x} \phi_l^t \rangle\rangle, \\ &= \frac{1-\theta}{2} \langle \phi_i^x d e^{-\lambda x} {}_0 D_x^\alpha \phi_j^x \rangle_x \mathbf{H}_{jk}^l \langle \phi_k^t \phi_l^t \rangle_t + \frac{1+\theta}{2} \langle \phi_i^x d e^{\lambda x} {}_x D_L^\alpha \phi_j^x \rangle_x \mathbf{H}_{jk}^r \langle \phi_k^t \phi_l^t \rangle_t \\ & \quad - \lambda^\alpha \langle \phi_i^x d \phi_j^x \rangle_x F_{jk} \langle \phi_k^t \phi_l^t \rangle_t + \alpha \theta \lambda^{\alpha-1} \langle \phi_i^x \frac{d \phi_j^x}{dx} \rangle_x F_{jk} \langle \phi_k^t \phi_l^t \rangle_t \\ &= \mathbf{D}_{ij}^l \mathbf{H}_{jk}^l \mathbf{N}_{kl} + \mathbf{D}_{ij}^r \mathbf{H}_{jk}^r \mathbf{N}_{kl} - \mathbf{R}_{ij} F_{jk} \mathbf{N}_{kl} + \mathbf{A}_{ij} F_{jk} \mathbf{N}_{kl}, \end{aligned}$$

Spatial tempering can again be handled with a L_2 -projection

The L_2 projection leads to

$$\begin{aligned}\langle \phi_i^x \phi_j^x \rangle_x H_{jk}^l \langle \phi_k^t \phi_l^t \rangle_t &= \langle \phi_i^x e^{\lambda x} \phi_j^x \rangle_x F_{jk} \langle \phi_k^t \phi_l^t \rangle_t, \\ \langle \phi_i^x \phi_j^x \rangle_x H_{jk}^r \langle \phi_k^t \phi_l^t \rangle_t &= \langle \phi_i^x e^{-\lambda x} \phi_j^x \rangle_x F_{jk} \langle \phi_k^t \phi_l^t \rangle_t.\end{aligned}$$

and by introducing the matrices $E_{ij}^l = \langle \phi_i^x e^{\lambda x} \phi_j^x \rangle_x$ and $E_{ij}^r = \langle \phi_i^x e^{-\lambda x} \phi_j^x \rangle_x$, we can express $H^l = M^{-1}E^l F$ and $H^r = M^{-1}E^r F$.

The PS Galerkin discretization of the tempered fractional diffusion term can then be expressed as the product of 3 matrices:

$$\langle \langle \phi_i^x d(x, t) \partial_x^{\alpha, \theta, \lambda} \tilde{f}(x, t) \phi_l^t \rangle \rangle = (DFN)_{il},$$

where

$$D \equiv D^l M^{-1} E^l + D^r M^{-1} E^r - R + A.$$

Finally, the discrete equations have a very simple expression

By putting everything together, we can express the discrete equations in matrix form:

$$MFT = DFN + Q,$$

where F is the matrix of unknown coefficients and where Q is the reaction matrix whose entries are $Q_{il} = \langle \langle \phi_i^x q(x, t) \phi_l^t \rangle \rangle$.

That equation can be “vectorized” by using the Kronecker product (represented by “ $\otimes$ ”):

$$(T^t \otimes M - N^t \otimes D) \text{vec}(F) = \text{vec}(Q), \quad (1)$$

where $\text{vec}(F)$ is the vector obtained by stacking the columns of F on top of one another.

Convergence analysis

Let's consider a PS discretization in both space and time and evaluate the convergence rate. We take $\alpha = 1.8$, $\gamma = 0.8$, $\beta = 1$, $\theta = -1$, and the following diffusivity and reaction functions :

$$d(x, t) = x^\alpha \frac{\Gamma(p+1-\alpha)}{\Gamma(p+1)},$$

$$q(x, t) = x^p e^{-\lambda x} e^{-st} (q_{\gamma, \beta, s}(t) - t^q q_{\alpha, \lambda}(x)),$$

where p and $q \in \mathbb{R}$, and

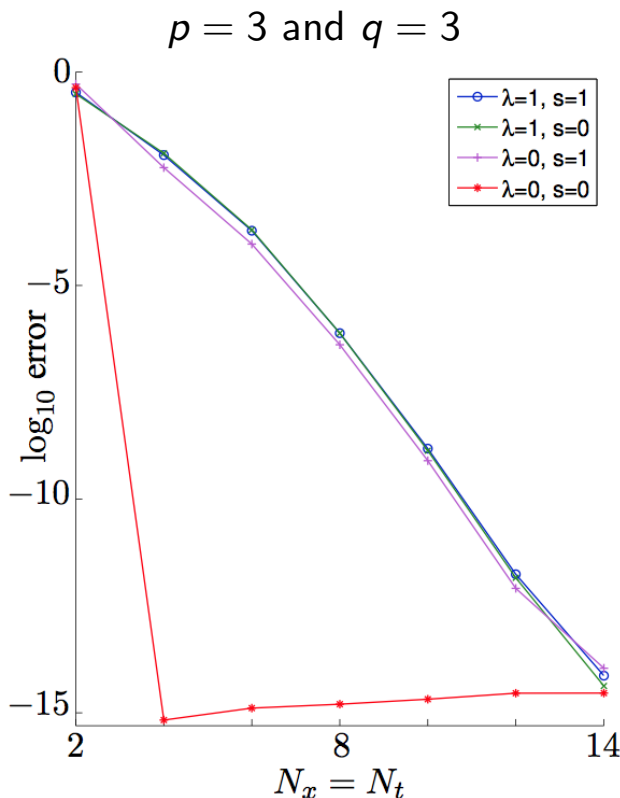
$$q_{\gamma, \beta, s}(t) = qt^{q-1} - st^q + \beta \frac{\Gamma(q+1)}{\Gamma(q+1-\gamma)} t^{q-\gamma} - \beta s^\gamma t^q,$$

$$q_{\alpha, \lambda}(x) = 1 - \frac{\Gamma(p+1-\alpha)}{\Gamma(p+1)} (\lambda^\alpha x^\alpha + \alpha \lambda^{\alpha-1} (px^{\alpha-1} - \lambda x^\alpha)).$$

In that case, the exact solution is

$$f(x, t) = x^p t^q e^{-\lambda x} e^{-st}.$$

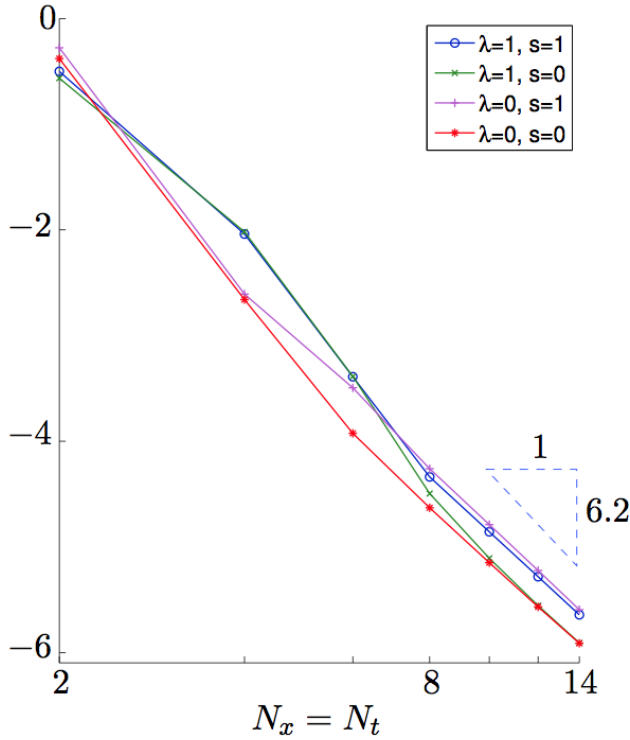
When p and q take integer values, the error convergence is exponential



When the polynomial powers p and q take integer values, the exact solution is $\mathcal{C}^\infty$ and convergence is exponential. When there is no truncation (*i.e.* when $\lambda = s = 0$), only 4 modes in space and time are necessary to exactly represent the solution.

When p and/or q take non-integer values, the error convergence is algebraic

$$p = 2.8 \text{ and } q = 2.6$$



Convergence is only algebraic since the exact solution has a singularity $t = 0$ and $x = 0$. According to Darboux's principle, the algebraic rate of convergence is controlled by the gravest singularity, which here is due to t^q since $q < p$. Numerical results are in agreement with a theoretical convergence rate of $2q + 1 = 6.2$.

Diffusion of a Gaussian hill

This more qualitative test case just looks at the diffusion of a Gaussian hills. The initial and boundary conditions are:

$$f^0(x) = f(x, 0) = \exp(-10(x - L/2)^2),$$

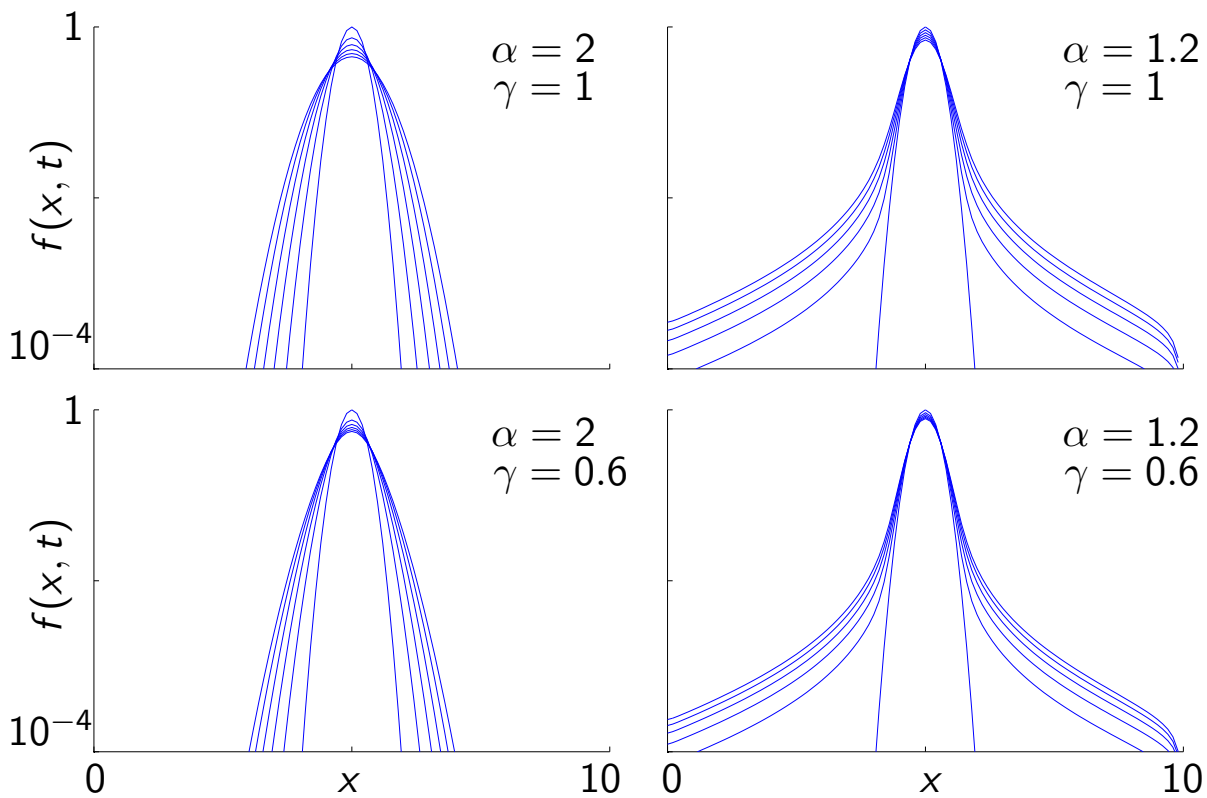
$$f^l(t) = \frac{\partial f}{\partial x}(0, t) = 0,$$

$$f^r(t) = f(L, t) = 0,$$

for $L = 10$ and $T = 2$. To account for the change of dimension of the diffusivity and capacity coefficients when changing the values of α and γ , we define them as $d(x) = \mathcal{D}\mathcal{L}^\alpha\mathcal{T}^{-1}$ and $\beta = \mathcal{T}^{\gamma-1}$, where $\mathcal{L}$ and $\mathcal{T}$ are characteristic length and time scale, respectively, and where $\mathcal{D}$ is a dimensionless constant.

We still consider a PS expansion in both space and time. Because of the steepness of the initial solution, we had to use a Chebyshev polynomial expansion with 190 modes in space and 10 modes in time.

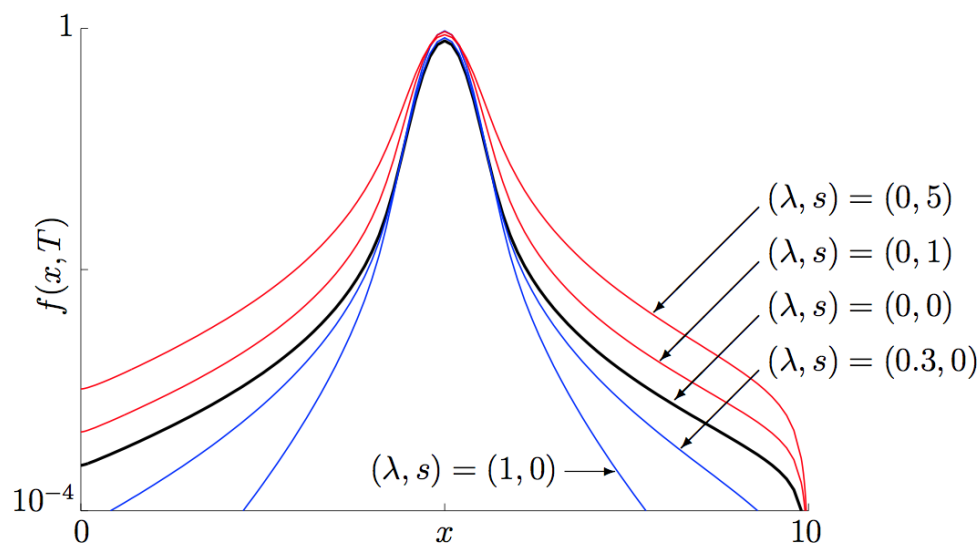
Diffusion patterns for different values of α and γ without truncation



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Final solution for different values of the truncation parameters and for $\alpha = 1.2$ and $\gamma = 0.6$



As the value of λ increases, the truncation length decreases and the diffusion process becomes subdiffusive. As the value of s increases, the truncation time decreases and the diffusion process becomes superdiffusive.

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Conclusions

Different strokes for different folks

- Non-local differential operators are best discretized with non-local numerical methods that naturally take the global behavior of the solution into account.
- Unlike the FD and FE methods, the PS and RBF methods do not result in an extra computational cost when going from integer-order to fractional-order differential operators.
- The PS and RBF methods achieve exponential convergence rates and thus require a much less degrees of freedom than the FD and FE methods when the solution is smooth enough.
- Numerical methods based on a “functional approximation” of the model solution can easily handle tempered fractional derivatives.

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