Implementation of high-order, discontinuous Galerkin time stepping for fractional diffusion problems

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Abstract

The discontinuous Galerkin (dG) method provides a robust and flexible technique for the time integration of fractional diffusion problems. However, a practical implementation uses coefficients defined by integrals that are not easily evaluated. We describe specialised quadrature techniques that efficiently maintain the overall accuracy of the dG method. In addition, we observe in numerical experiments that known superconvergence properties of dG time stepping for classical diffusion problems carry over in a modified form to the fractional-order setting.

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1 Introduction

The discontinuous Galerkin (dG) method provides an effective numerical procedure for the time integration of diffusion problems. In the mid-1980s, Eriksson, Johnson and Thomée [2] provided the first detailed error analysis, which has been subsequently extended and refined by numerous authors [6, 13, 14, and references therein]. The dG method has also proved effective for time stepping of fractional diffusion problems [9, 12] of the form

\[ \partial_t u + \partial_t^{1-\alpha} Au = f(t) \text{ for } 0 < t \leq T, \text{ with } u(0) = u_0. \]  

\[ \text{(1)} \]

Here, \( A \) is a linear, second-order, elliptic partial differential operator over a spatial domain \( \Omega \), subject to a homogeneous Dirichlet boundary condition \( u = 0 \) on \( \partial\Omega \). (Our notation suppresses the dependence of \( u \) and \( f \) on the spatial variables.) The fractional diffusion exponent is assumed to satisfy \( 0 < \alpha < 1 \) (the sub-diffusive case), and the fractional time derivative is understood in the Riemann–Liouville sense: for \( t > 0 \) and \( \mu > 0 \),

\[ \partial_t^\mu v = \frac{\partial}{\partial t} \int_0^t \omega_\mu(t-s)v(s)\,ds \quad \text{where} \quad \omega_\mu(t) = \frac{t^{\mu-1}}{\Gamma(\mu)}. \]

The partial integro-differential equation (1) arises in a variety of physical models [3, 11] of diffusing particles whose behaviour is described by a continuous-time random walk for which the waiting-time distribution is a power law that decays like \( 1/t^{1+\alpha} \). The expected waiting time is therefore infinite, and the mean-square displacement is proportional to \( t^\alpha \). Standard Brownian motion is recovered in the limit as \( \alpha \to 1 \), when (1) reduces to the classical diffusion equation.

Our main concern in the present work is with the practical implementation of dG time stepping for (1), and in particular with the accurate evaluation of certain coefficients \( H_{ij}^{n-\ell} \) used during the \( n \)th step. Section 2 introduces the dG method for the fractional ODE case of (1), in which the operator \( A \) is replaced by a scalar \( \lambda > 0 \). We will see in the simplest, lowest-order scheme, when the dG solution is piecewise-constant in time, that

\[ H_{11}^{n,0} = \int_{t_{n-1}}^{t_n} \frac{d}{dt} \left( \int_{t_{n-1}}^t \omega_\alpha(t-s)\,ds \right) dt \]

and

\[ H_{11}^{n,\ell} = \int_{t_{n-1}}^{t_n} \frac{d}{dt} \left( \int_{t_{\ell-1}}^{t_\ell} \omega_\alpha(t-s)\,ds \right) dt \quad \text{for } 1 \leq \ell \leq n-1, \]
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where $0 = t_0 < t_1 < t_2 < \cdots$ are the discrete time levels. We easily verify that $H_{11}^{n,0} = \omega_{\alpha+1}(k_n) = k_n^\alpha / \Gamma(\alpha + 1)$, for a step-size $k_n = t_n - t_{n-1}$, and

$$H_{11}^{n,n-\ell} = \omega_{\alpha+1}(t_n - t_{\ell-1}) - \omega_{\alpha+1}(t_n - t_{\ell}) - \omega_{\alpha+1}(t_{n-1} - t_{\ell-1}) + \omega_{\alpha+1}(t_{n-1} - t_{\ell}),$$

but for higher-order schemes the coefficients become progressively more complicated. Although the $H_{ij}^{n,n-\ell}$ can always be evaluated via repeated integration by parts, the resulting expressions are likely to suffer from roundoff when evaluated in floating-point arithmetic if $n - \ell$ is large. Consider just the lowest order case \[2\] with uniform time steps $t_n = nk$, so that

$$H_{11}^{n,n-\ell} = k^\alpha \left[ \omega_{\alpha+1}(n - \ell + 1) - 2\omega_{\alpha+1}(n - \ell) + \omega_{\alpha+1}(n - \ell - 1) \right].$$

Since the factor in square brackets is a second-difference of $\omega_{\alpha+1}$, its magnitude decays like $(n - \ell)^{\alpha - 2}$ as $n - \ell$ increases, but the individual terms grow like $(n - \ell)^\alpha$.

We are therefore led to evaluate the coefficients $H_{ij}^{n,n-\ell}$ via quadratures with positive weights. No special techniques are needed for $\ell \leq n - 2$, but when $\ell = n$ or $n - 1$ we must deal with weakly singular integrands. In Section 3, we show how certain substitutions reduce the problem to dealing with integrands that are either smooth, or are products of smooth functions and standard Jacobi weight functions. Similar substitutions, known as Duffy transformations \[1\], have long been used to compute singular integrals arising in the boundary element method.

Section 4 introduces a spatial discretisation for the fractional PDE \[1\] and describes the structure of the linear system that must be solved at each time step. In Section 5, we specialise the expressions for the coefficients by choosing Legendre polynomials as the shape functions employed in the dG time stepping.

Section 6 describes a post-processing technique that, when applied to the dG solution $U$, produces a more accurate approximate solution $\hat{U}$, known as the reconstruction \[6\] of $U$. If $U$ is a piecewise polynomial of degree at most $r - 1$, then $\hat{U}$ is a piecewise polynomial of degree at most $r$. For a classical diffusion problem, both $U$ and $\hat{U}$ are known to be quasi-optimal, that is, accurate of order $k^r$ and $k^{r+1}$, respectively. Thus, it is natural to ask what happens in the fractional-order case, and we investigate this question in numerical experiments reported in Section 7.
2 A fractional ODE

Our central concern is present already in the zero-dimensional case when we replace the elliptic operator $A$ with a scalar $\lambda \geq 0$, so that the solution $u(t)$ is a real-valued function satisfying the fractional ODE

$$u' + \lambda \partial_t^{1-\alpha} u = f(t) \quad \text{for } 0 < t \leq T, \text{ with } u(0) = u_0. \quad (3)$$

For the time discretisation, we introduce a grid

$$0 = t_0 < t_1 < t_2 < \cdots < t_N = T,$$

and form the vector $t = (t_0, t_1, \ldots, t_N)$. Let $k_n = t_n - t_{n-1}$ denote the length of the $n$th (open) subinterval $I_n = (t_{n-1}, t_n)$. We form the disjoint union

$$I = I_1 \cup I_2 \cup \cdots \cup I_N,$$

and for any function $v : I \rightarrow \mathbb{R}$ write

$$v^+_n = \lim_{\epsilon \downarrow 0} v(t + \epsilon), \quad v^-_n = \lim_{\epsilon \downarrow 0} v(t - \epsilon), \quad [v]^n = v^+_n - v^-_n,$$

provided the one-sided limits exist.

Given a vector $r = (r_1, r_2, \ldots, r_N)$ of integers $r_n \geq 0$, the trial space $X = X(t, r)$ consists of the functions $X : I \rightarrow \mathbb{R}$ such that $X|_{I_n} \in \mathbb{P}_{r_n-1}$ for $1 \leq n \leq N$. Here, $\mathbb{P}_m$ denotes the space of polynomials of degree at most $m \geq 0$, with real coefficients. The dG solution $U \in X$ of (3) is then defined by \[9, 12\]

$$[U]^{n-1}X^+_n + \int_{I_n} (U' + \lambda \partial_t^{1-\alpha} U)X dt = \int_{I_n} fX dt \quad (4)$$

for $X \in \mathbb{P}_{r_n-1}$ and $1 \leq n \leq N$, where, in the case $n = 1$, we set $U^0 = u_0$ so that $[U]^0 = U^+_n - U^-_n = U^+_n - u_0$. (The monograph of Thomée \[15, Chapter 12\] is a standard reference providing a general introduction to dG time stepping for classical diffusion problems.)

To compute $U$, we choose for each $n$ a basis $\psi_{n1}, \psi_{n2}, \ldots, \psi_{nr_n}$ for $\mathbb{P}_{r_n-1}$ and write

$$U(t) = \sum_{j=1}^{r_n} U^{nj} \psi_{nj}(t) \quad \text{for } t \in I_n. \quad (5)$$

When $X = \psi_{ni}$, we find that

$$U^+_{n-1}X^+_n + \int_{I_n} U'X dt = \sum_{j=1}^{r_n} G^{nj}_{ij} U^{nj} \quad \text{and} \quad U^-_{n-1}X^+_n = \sum_{j=1}^{r_n-1} K^{n,n-1}_{ij} U^{n-1,j},$$
with coefficients given by

\[ G^n_{ij} = \psi_{nj}(t_{n-1})\psi_{ni}(t_{n-1}) + \int_{I_n} \psi'_{nj}\psi_{ni} \, dt \]

and

\[ K^{n,n-1}_{ij} = \psi_{n-1,j}(t_{n-1})\psi_{ni}(t_{n-1}). \]

Owing to the convolutional structure of the fractional derivative, it is convenient to introduce the notation

\[ \bar{\ell} = n - \ell \]

and define, if \( t \in I_n \),

\[ \rho^n_{\bar{\ell}}(t) = \rho^{n,n-\ell}_j(t) = \int_{I_{n-1}} \omega_\alpha(t-s)\psi_{ij}(s) \, ds \quad \text{for } 1 \leq \ell \leq n - 1, \]

with \( \rho^n_0(t) = \rho^n_j(t) = \int_{I_{n-1}} \omega_\alpha(t-s)\psi_{nj}(s) \, ds. \)

We find that

\[ \partial^{1-\alpha}t U = \sum_{\ell=1}^{n} \sum_{j=1}^{r_\ell} U^{\bar{\ell}j}(\rho^{n\bar{\ell}}_j)'(t) \quad \text{for } t \in I_n, \]

and thus

\[ \int_{I_n} (\partial^{1-\alpha}t U)X \, dt = \sum_{\ell=1}^{n} \sum_{j=1}^{r_\ell} H^{n\bar{\ell}}_{ij} U^{\bar{\ell}j} \quad \text{where } H^{n\bar{\ell}}_{ij} = H^{n,n-\bar{\ell}}_{ij} = \int_{I_n} (\rho^{n\bar{\ell}}_j)'\psi_{ni} \, dt. \]

Hence, putting

\[ F_{ni} = \int_{I_n} f\psi_{ni} \, dt, \]

the dG method requires

\[ \sum_{j=1}^{r_n} (G^n_{ij} + \lambda H^{00}_{ij}) U^{nj} = F_{ni} - \sum_{\ell=1}^{n-1} \sum_{j=1}^{r_\ell} \lambda H^{n,n-\ell}_{ij} U^{\bar{\ell}j} \]

\[ + \left\{ \begin{aligned} &\psi_{1i}(0)u_0, \quad n = 1, \\ &\sum_{j=1}^{r_{n-1}} K^{n,n-1}_{ij} U^{n-1,j}, \quad 2 \leq n \leq N. \end{aligned} \right. \]

At the \( n \)th time step, this \( r_n \times r_n \) linear system must be solved to determine \( U^{n1}, U^{n2}, \ldots, U^{nr_n} \) and hence \( U(t) \) for \( t \in I_n \).
Remark 1. If we send $\alpha \to 1$, so that the fractional ODE in (3) reduces to the classical ODE $u' + \lambda u = f(t)$, then $H^\ell_{ij} = 0$ for $1 \leq \ell \leq n - 1$. Indeed, since $\omega_1(t) = 1$, we see that $\rho_n^{\ell j}(t) = \int_t^1 \psi_{ij}(s) ds$ is constant and so $(\rho_n^{\ell j})'(t) = 0$ for $t \in I_n$. Moreover, $(\rho_n^{0 j})'(t) = \psi_{nj}(t)$ so $H^{00}_{ij} = \int_{I_n} \psi_{nj} \psi_{ni} dt$.

Remark 2. Later we will show certain symmetry properties of $H^{00}_{ij}$ using the identity

$$\int_a^b \left( \frac{\partial}{\partial t} \int_a^t \omega_{\alpha}(t-s)u(s) \, ds \right) v(t) \, dt = -\int_a^b u(s) \left( \frac{\partial}{\partial s} \int_s^b \omega_{\alpha}(t-s)v(t) \, dt \right) ds. \quad (7)$$

In fact, the substitution $x = t - s$ gives

$$\frac{\partial}{\partial t} \int_a^t \omega_{\alpha}(t-s)u(s) \, ds = \frac{\partial}{\partial t} \int_0^{t-a} \omega_{\alpha}(x)u(t-x) \, dx$$

$$= \omega_{\alpha}(t-a)u(a) + \int_0^{t-a} \omega_{\alpha}(x)u'(t-x) \, dx$$

$$= \omega_{\alpha}(t-a)u(t_{n-1}) + \int_a^t \omega_{\alpha}(t-s)u'(s) \, ds,$$

and (7) follows after reversing the order of integration and then integrating by parts. Similarly, for $\ell \leq n - 1$,

$$\int_a^b \left( \frac{\partial}{\partial \tau} \int_a^t \omega_{\alpha}(t-s)u(s) \, ds \right) v(t) \, dt = -\int_a^b u(s) \left( \frac{\partial}{\partial \tau} \int_s^b \omega_{\alpha}(t-s)v(t) \, dt \right) ds. \quad (8)$$

3 Evaluation of the coefficients

To compute $G^n_{ij}$, $H^{\ell t}_{ij}$ and $K^{n,n-1}_{ij}$ it is convenient to map each closed subinterval $I_n = [t_{n-1}, t_n]$ to the reference element $[-1, 1]$. We therefore define the affine function $t_n : [-1, 1] \to I_n$ by

$$t_n(\tau) = \frac{1}{2} \left[ (1 - \tau)t_{n-1} + (1 + \tau)t_n \right] \quad \text{for } -1 \leq \tau \leq 1,$$

and let

$$\Psi_{nj}(\tau) = \psi_{nj}(t) \quad \text{for } t = t_n(\tau) \text{ and } -1 \leq \tau \leq 1.$$

In this way,

$$G^n_{ij} = \Psi_{nj}(-1)\Psi_{ni}(-1) + \int_{-1}^1 \Psi'_{nj}(\tau)\Psi_{ni}(\tau) \, d\tau \quad (9)$$
and

\[ K^{n,n-1}_{ij} = \Psi_{n-1,i} (+1) \Psi_{n,m} (-1). \]  

Both of these coefficients are readily computed; the remainder of this section is devoted to \( H_{ij}^{00} \). The formulae in the next lemma allow us to compute \( H_{ij}^{00} \) to machine precision via Gauss–Legendre and Gauss–Jacobi quadrature.

**Lemma 3.** If we define the polynomial

\[ \Phi_{ij}^n(y) = \frac{1}{2} \int_{-1}^{1} \Psi_{nj}(\frac{1}{2}(1-y)(1+z) - 1) \Psi_{ni}'(1 - \frac{1}{2}(1-y)(1-z)) \, dz, \]

then

\[ H_{ij}^{00} = \frac{(kn/2)^\alpha}{\Gamma(\alpha)} \left( \Psi_{ni}(1) \int_{-1}^{1} (1 - \sigma)^{\alpha} \Psi_{nj}(\sigma) \, d\sigma \right) - \int_{-1}^{1} (1 + y)^{\alpha-1} (1 - y) \Phi_{ij}^n(y) \, dy. \]

**Proof:** Since \( \rho_{ji}^{00}(t_{n-1}) = 0 \), integration by parts gives

\[ H_{ij}^{00} = \rho_{ji}^{00}(t_{n}) \psi_{mi}(t_{n}) - \int_{t_{n}} \rho_{ji}^{00}(t) \psi_{mi}'(t) \, dt \]

\[ = \rho_{ji}^{00}(t_{n}) \Psi_{mi}(1) - \int_{-1}^{1} \rho_{ji}^{00}(t_{n}(\tau)) \Psi_{mi}'(\tau) \, d\tau, \]

and since \( t_{n}(\tau) - t_{n}(\sigma) = (\tau - \sigma)kn/2 \), the substitution \( s = t_{n}(\sigma) \) yields

\[ \rho_{ji}^{00}(t_{n}(\tau)) = \frac{k_n}{2} \int_{-1}^{\tau} \omega_{\alpha}(t_{n}(\tau) - t_{n}(\sigma)) \Psi_{nj}(\sigma) \, d\sigma \]

\[ = \frac{(kn/2)^\alpha}{\Gamma(\alpha)} \int_{-1}^{\tau} (\tau - \sigma)^{\alpha-1} \Psi_{nj}(\sigma) \, d\sigma. \]

Thus,

\[ H_{ij}^{00} = \frac{(kn/2)^\alpha}{\Gamma(\alpha)} \left( \Psi_{ni}(1) \int_{-1}^{1} (1 - \sigma)^{\alpha-1} \Psi_{nj}(\sigma) \, d\sigma - B_{ij}^n \right), \]

where

\[ B_{ij}^n = \int_{-1}^{1} \int_{-1}^{\tau} (\tau - \sigma)^{\alpha-1} \Psi_{nj}(\sigma) \, d\sigma \Psi_{ni}'(\tau) \, d\tau. \]

We make the substitution \( 1 + y = \tau - \sigma \), which results in a fixed singularity at \( y = -1 \), and then reverse the order of integration:

\[ B_{ij}^n = \int_{-1}^{1} \int_{-1}^{\tau} (1 + y)^{\alpha-1} \Psi_{nj}(\tau - y - 1) \, dy \Psi_{ni}'(\tau) \, d\tau \]
3 Evaluation of the coefficients

\[ = \int_{-1}^{1} (1 + y)^{\alpha - 1} \int_{y}^{1} \psi_{nj}(\tau - y - 1) \psi_{ni}(\tau) d\tau dy. \]

The substitution \( \tau = \frac{1}{2} [(1 - z)y + (1 + z)] \) then yields

\[ \int_{y}^{1} \psi_{nj}(\tau - y - 1) \psi_{ni}(\tau) d\tau dy = (1 - y) \Phi_{ij}^{n}(y), \]

implying the desired formula for \( H_{ij}^{n0} \).

To deal with \( H_{ij}^{n-n-\ell} \) for \( \ell \leq n - 1 \), we introduce the notation

\[ t_{n-1/2} = t_n(0) = \frac{1}{2}(t_{n-1} + t_n) \quad \text{and} \quad D_{n\ell} = D_{n,n-\ell} = t_{n-1/2} - t_{\ell-1/2}, \]

with

\[ \Delta_{n\ell}(\tau, \sigma) = \Delta_{n,n-\ell}(\tau, \sigma) = \frac{\tau k_n - \sigma k_\ell}{2 D_{n\ell}}, \]

so that

\[ t_n(\tau) - t_\ell(\sigma) = D_{n\ell}(1 + \Delta_{n\ell}(\tau, \sigma)). \]

**Lemma 4.** If \( 1 \leq \ell \leq n - 1 \), then

\[ H_{ij}^{n\ell} = \frac{D_{n\ell}^{\alpha-1}}{\Gamma(\alpha)} \frac{k_\ell}{2} (\Psi_{ni}(1) \mathcal{A}_{ij}^{n\ell} - \Psi_{ni}(-1) \mathcal{B}_{ij}^{n\ell} - \mathcal{C}_{ij}^{n\ell}), \]

where

\[ \mathcal{A}_{ij}^{n\ell} = \int_{-1}^{1} (1 + \Delta_{n\ell}(1, \sigma))^{\alpha-1} \psi_{ij}(\sigma) d\sigma, \]

\[ \mathcal{B}_{ij}^{n\ell} = \int_{-1}^{1} (1 + \Delta_{n\ell}(-1, \sigma))^{\alpha-1} \psi_{ij}(\sigma) d\sigma, \]

\[ \mathcal{C}_{ij}^{n\ell} = \int_{-1}^{1} \psi_{ij}'(\tau) \int_{-1}^{1} (1 + \Delta_{n\ell}(\tau, \sigma))^{\alpha-1} \psi_{ij}(\sigma) d\sigma d\tau. \]

**Proof:** Integrating by parts, we find that

\[ H_{ij}^{n\ell} = \rho_{ij}^{n\ell}(t_n) \psi_{ni}(t_n) - \rho_{ij}^{n\ell}(t_{n-1}) \psi_{ni}(t_{n-1}) - \int_{t_n}^{t_{n-1}} \rho_{ij}^{n\ell}(t) \psi_{ni}'(t) dt \]

\[ = \rho_{ij}^{n\ell}(t_n) \psi_{ni}(1) - \rho_{ij}^{n\ell}(t_{n-1}) \psi_{ni}(-1) - \int_{-1}^{1} \rho_{ij}^{n\ell}(t_n(\tau)) \psi_{ni}'(\tau) d\tau. \]

The substitution \( s = t_\ell(\sigma) \) gives

\[ \rho_{ij}^{n\ell}(t_n(\tau)) = \frac{D_{n\ell}^{\alpha-1}}{\Gamma(\alpha)} \frac{k_\ell}{2} \int_{-1}^{1} (1 + \Delta_{n\ell}(\tau, \sigma))^{\alpha-1} \psi_{ij}(\sigma) d\sigma, \]
and the formula for $H_{ij}^n$ follows at once.

Notice that

$$1 + \Delta_n(x, \sigma) = \frac{2(t_n - t_{\ell}) + (1 - \sigma)k_{\ell}}{k_n + 2(t_{n-1} - t_{\ell}) + k_{\ell}} > 0$$

for $1 \leq \ell \leq n - 1$, so the integrand of $A_{ij}^n$ is always smooth. However,

$$1 + \Delta_n(-1, \sigma) = \frac{2(t_{n-1} - t_{\ell}) + (1 - \sigma)k_{\ell}}{k_n + 2(t_{n-1} - t_{\ell}) + k_{\ell}},$$

so the integrands of $B_j^n$ and $C_j^n$ are weakly singular if $\ell = 1$ (i.e., if $\ell = n - 1$). The next lemma provides alternative expressions that are amenable to Gauss–Jacobi and Gauss–Legendre quadrature.

**Lemma 5.** Let $\rho_n = k_n/k_{n-1}$. Then,

$$A_{j}^{n,1} = (1 + \rho_n)^{1-\alpha} \int_{-1}^{1} (2\rho_n + 1 - \sigma)^{\alpha-1} \Psi_{n-1,j}(\sigma) d\sigma,$$

$$B_{j}^{n,1} = (1 + \rho_n)^{1-\alpha} \int_{-1}^{1} (1 - \sigma)^{\alpha-1} \Psi_{n-1,j}(\sigma) d\sigma$$

and

$$C_{ij}^{n,1} = (1 + \rho_n)^{1-\alpha} \left( \int_{-1}^{1} (1 + \tau)^{\alpha} \Psi_{n,j}(\tau) \int_{0}^{1} (\rho_n + z)^{\alpha-1} \Psi_{n-1,j}(1 - z(1 + \tau)) dz d\tau \
+ \int_{-1}^{1} (1 - \sigma)^{\alpha} \Psi_{n-1,j}(\sigma) \int_{0}^{1} (\rho_n z + 1)^{\alpha-1} \Psi_{n,j}'(z(1 - \sigma) - 1) dz d\sigma \right).$$

**Proof:** Since $1 + \Delta_{n,1}(-1, \sigma) = k_{n-1}(1 - \sigma)/(k_n + k_{n-1})$, the formula for $B_{ij}^{n,1}$ follows at once. To deal with $C_{ij}^{n,1}$ we begin by mapping $[-1,1]^2$ onto $[0,2]^2$ with the substitution $(\tau, \sigma) = (x - 1, y)$. In this way, the singularity at $(\tau, \sigma) = (-1, 1)$ moves to $(x, y) = (0, 0)$, and

$$C_{ij}^{n,1} = \int_{0}^{2} \int_{0}^{2} \left(1 + \Delta_{n,1}(x - 1, 1 - y)\right)^{\alpha-1} \Psi_{n-1,j}(1 - y) \Psi_{n,j}'(x - 1) dx dy$$

with

$$1 + \Delta_{n,1}(x - 1, 1 - y) = \frac{xk_n + yk_{n-1}}{k_n + k_{n-1}}.$$
3 Evaluation of the coefficients

By splitting the integration domain \([0,2]^2\) into the triangular halves where \(x > y\) and \(x < y\), we obtain

\[
C_{ij}^{n1} = \int_0^2 \Psi'_n(x-1) \int_0^x \left(\frac{xk_n + yk_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi_{n-1,j}(1-y) \, dy \, dx \\
+ \int_0^2 \Psi_{n-1,j}(1-y) \int_0^y \left(\frac{xk_n + yk_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi'_n(x-1) \, dx \, dy.
\]

The substitution \(y = zx\) transforms the inner integral in the first term to

\[
x^\alpha \int_0^1 \left(\frac{k_n + zk_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi_{n-1,j}(1-zx) \, dz,
\]

and the substitution \(x = zy\) transforms that in the second to

\[
y^\alpha \int_0^1 \left(\frac{zk_n + k_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi'_n(zy-1) \, dz.
\]

Thus,

\[
C_{ij}^{n1} = \int_0^2 x^\alpha \Psi'_n(x-1) \int_0^1 \left(\frac{k_n + zk_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi_{n-1,j}(1-zx) \, dz \, dx \\
+ \int_0^2 y^\alpha \Psi_{n-1,j}(1-y) \int_0^1 \left(\frac{zk_n + k_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi'_n(zy-1) \, dz \, dy.
\]

Now make the substitutions \(x = 1 + \tau\) and \(y = 1 - \sigma\). ♠

We also have the following alternative representation.

**Lemma 6.** If \(1 \leq \ell \leq n - 2\), then

\[
H_{ij}^{n\ell} = -\frac{1 - \alpha}{\Gamma(\alpha)} k_n k_{\ell}^2 D_n^{\alpha-2} \int_{-1}^1 \Psi_{\ell}(\tau) \int_{-1}^1 \left(1 + \Delta_n(\tau, \sigma)\right)^{\alpha-2} \Psi_{\ell}(\sigma) \, d\sigma \, d\tau.
\]

**Proof:** When \(\ell \leq n - 2\),

\[
(\rho_j^{n\ell})'(t) = \int_{I_t} \omega_{\alpha-1}(t-s) \psi_{\ell}(s) \, ds \quad \text{for } t > t_\ell,
\]

and so

\[
H_{ij}^{n\ell} = \int_{I_n} \psi_{\ell}(t) \int_{I_t} \omega_{\alpha-1}(t-s) \psi_{\ell}(s) \, ds.
\]

(11)

The result now follows via the substitutions \(t = t_n(\tau)\) and \(s = t_\ell(\sigma)\), noting that \(\Gamma(\alpha) = (\alpha - 1)\Gamma(\alpha - 1)\). ♠
Remark 7. If the time levels are uniformly spaced, and if the reference basis functions are the same for each subinterval, say
\[ k_\ell = k, \quad r_\ell = r \quad \text{and} \quad \Psi_{\ell j} = \Psi_j \quad \text{for} \quad 1 \leq \ell \leq n \quad \text{and} \quad 1 \leq j \leq r, \]
then
\[ D_{n\ell} = \bar{\ell}k \quad \text{and} \quad \Delta_{n\ell}(\tau, \sigma) = \frac{\tau - \sigma}{2\ell}, \]
so the formulae of Lemma 4 show that \( H_{ij}^{n\ell} \) depends on \( n \) and \( \ell \) only through the difference \( \bar{\ell} = n - \ell \); for further details, see Example 12 below.

4 Spatial discretisation

The initial-boundary value problem (1) is known to be well-posed [5, 8, 10]. Let \( \langle u, v \rangle = \int_{\Omega} uv \) denote the usual inner product in \( L^2(\Omega) \), and let \( a(u, v) \) denote the bilinear form associated with \( A \) via the first Green identity. For example, if \( A = -\nabla^2 \) then \( a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \). In this way, the weak solution \( u : (0, T] \rightarrow H^1_0(\Omega) \) satisfies
\[ \langle \partial_t u, v \rangle + a(\partial_t^{1-\alpha} u, v) = \langle f(t), v \rangle \quad \text{for} \quad v \in H^1_0(\Omega) \quad \text{and} \quad 0 < t \leq T. \]
We choose a finite dimensional subspace \( V_n \subseteq H^1_0(\Omega) \) for \( 0 \leq n \leq N \), and form the vector \( V = (V_1, \ldots, V_N) \). For example, \( V_n \) might be a (conforming) finite element space constructed using a triangulation of \( \Omega \). Our trial space \( X = X(t, r, V) \) then consists of the functions \( X : I \rightarrow H^1_0(\Omega) \) such that \( X|_{I_n} \in \mathbb{P}_{r_n-1}(I_n; V_n) \), that is, the restriction \( X|_{I_n} \) is a polynomial in \( t \) of degree at most \( r_n - 1 \), with coefficients from \( V_n \). Generalising (4), the DG solution \( U \in X \) of (1) satisfies
\[ \langle [U]^{n-1}, X^{n-1}_+ \rangle + \int_{I_n} \langle \partial_t U, X \rangle \, dt + \int_{I_n} a(\partial_t^{1-\alpha} U, X) \, dt = \int_{I_n} \langle f(t), X \rangle \, dt \quad (12) \]
for \( X \in \mathbb{P}_{r_n-1}(I_n; V_n) \) and \( 1 \leq n \leq N \), with \( U_0^0 = U_0 \) for a suitable \( U_0 \in V_0 \) such that \( U_0 \approx u_0 \).

We choose a basis \( \{ \phi_{np} \}_{p=1}^{P_n} \) for \( V_n \). In the expansion (5), the coefficient \( U_{nq} \) is now a function in \( V_n \), so there exist real numbers \( U_{nq}^{m} \) such that
\[ U_{nq}^{m}(x) = \sum_{q=1}^{P_n} U_{nq}^{m} \phi_{nq}(x) \quad \text{for} \quad x \in \Omega; \]
for example, \( U_{nq}^{m} = U_{nq}^{m}(x_{nq}) \) if \( x_{nq} \) is the \( q \)th free node of a finite element mesh and if \( \phi_{nq} \) is the corresponding nodal basis function. Similarly, for the
discrete initial data, there are real numbers \( U_{0q} \) such that

\[
U_0(x) = \sum_{q=1}^{P_0} U_{0q} \phi_{0q}(x) \quad \text{for } x \in \Omega.
\]

Choosing \( X(x,t) = \psi_{ni}(t) \phi_{nq}(x) \) in (12), we find that the equations (6) for time stepping the scalar problem generalise to

\[
\sum_{j=1}^{r_n} \sum_{q=1}^{P_n} \left( G_{ij}^n M_{pq}^n + H_{ij}^n A_{pq}^n \right) U_{nj}^n = F_{ni}^n - \sum_{\ell=1}^{r_\ell} \sum_{j=1}^{P_\ell} H_{ij}^{n,\ell} A_{pq}^{\ell} U_{\ell j}^q
\]

\[
+ \begin{cases} \psi_{1i}(0) \sum_{q=1}^{P_0} M_{pq}^{10} U_{0q}, & n = 1, \\ \sum_{j=1}^{r_n-1} \sum_{q=1}^{P_n-1} K_{ij}^{n,n-1} M_{pq}^{n,n-1} U_{n-1,j}^q, & 2 \leq n \leq N, \end{cases}
\]

where

\[
M_{pq}^{nt} = \langle \phi_{tq}, \phi_{np} \rangle, \quad A_{pq}^{nt} = a(\phi_{tq}, \phi_{np}), \quad F_{ni}^n = \int_{I_n} (f(t), \phi_{np}) \psi_{ni}(t) \, dt.
\]

By introducing the \( P_n \times P_\ell \) mass matrix \( M_{pq}^{nt} = [M_{pq}^{nt}] \) and stiffness matrix \( A_{pq}^{nt} = [A_{pq}^{nt}] \), and forming the column vectors

\[
U^{nj} = \begin{bmatrix} U_{nj}^1 \\ U_{nj}^2 \\ \vdots \\ U_{nj}^{P_n} \end{bmatrix}, \quad F^{ni} = \begin{bmatrix} F_{ni1}^n \\ F_{ni2}^n \\ \vdots \\ F_{niP_n}^n \end{bmatrix}, \quad U_0 = \begin{bmatrix} U_{01} \\ U_{02} \\ \vdots \\ U_{0P_0} \end{bmatrix},
\]

we can rewrite the equations (13) as

\[
\sum_{j=1}^{r_n} \sum_{q=1}^{P_n} \left( G_{ij}^n M_{pq}^n + H_{ij}^n A_{pq}^n \right) U_{nj}^n = F_{ni}^n - \sum_{\ell=1}^{r_\ell} \sum_{j=1}^{P_\ell} H_{ij}^{n,\ell} A_{pq}^{\ell} U_{\ell j}^q
\]

\[
+ \begin{cases} \psi_{1i}(0) \sum_{q=1}^{P_0} M_{pq}^{10} U_{0q}, & n = 1, \\ \sum_{j=1}^{r_n-1} \sum_{q=1}^{P_n-1} K_{ij}^{n,n-1} M_{pq}^{n,n-1} U_{n-1,j}^q, & 2 \leq n \leq N. \end{cases}
\]

To write (14) even more compactly, define the \( r_n \times r_n \) matrix \( G^n = [G_{ij}^n] \) and the \( r_n \times r_\ell \) matrix \( H^{n,\ell} = [H_{ij}^{n,\ell}] \), together with the (block) column vectors

\[
U^n = \begin{bmatrix} U_{n1} \\ U_{n2} \\ \vdots \\ U_{nr_n} \end{bmatrix} \quad \text{and} \quad F^n = \begin{bmatrix} F_{n1} \\ F_{n2} \\ \vdots \\ F_{nr_n} \end{bmatrix}.
\]
We also form the \( r_n \times r_{n-1} \) matrix \( K^{n,n-1} = [K_{ij}^{n,n-1}] \) and the column vector
\[
\psi^0_n = \begin{bmatrix}
\psi_{11}(0) \\
\psi_{12}(0) \\
\vdots \\
\psi_{1r_n}(0)
\end{bmatrix}.
\]
Utilising the Kronecker product, the linear system (14) takes the form
\[
(G^n \otimes M^{nn} + H^{n0} \otimes A^{nn}) U^n = F^n - \sum_{\ell=1}^{n-1} (H^{n,n-\ell} \otimes A^{n\ell}) U^\ell
\]
\[
+ \begin{cases}
(\psi^0_n \otimes M^{10}) U_0, & n = 1, \\
(K^{n,n-1} \otimes M^{n,n-1}) U^{n-1,j}, & 2 \leq n \leq N.
\end{cases}
\]
\[(15)\]

5 Legendre polynomials

Let \( P_0, P_1, P_2, \ldots \) denote the Legendre polynomials with the standard normalisation \( P_j(1) = 1 \) for all \( j \geq 0 \). By choosing
\[
\Psi_{nj}(\tau) = P_{j-1}(\tau),
\]
we obtain a convenient and well-conditioned basis for \( \mathbb{P}_{r_n-1} \) with the properties
\[
\int_{-1}^{1} \Psi_{nj}(\tau) \Psi_{ni}(\tau) d\tau = \frac{2\delta_{ij}}{2j-1} \text{ and } \Psi_{nj}(-\tau) = (-1)^{j-1} \Psi_{nj}(\tau)
\]
for \( i, j \in \{1, 2, \ldots, r_n\} \).

Lemma 8. With the choice (16) of basis functions,
\[
\Psi_{nj}(1) = 1 \quad \text{and} \quad \Psi_{nj}(-1) = (-1)^{j-1},
\]
and the coefficients (9) and (10) are given by
\[
G_{ij}^n = \begin{cases}
(-1)^{i+j}, & \text{if } i \geq j, \\
1, & \text{if } i < j,
\end{cases}
\]
and
\[
K_{ij}^{n,n-1} = (-1)^{i-1}.
\]
Proof: The properties follow from $P_j(1) = 1$ and $P_j(-1) = (-1)^j$. Hence, the formula for $K_{ij}^{n,n-1}$ follows from (10), and by (9),

$$G_{ij}^n = (-1)^{i+j} + E_{ij}$$ where

$$E_{ij} = \int_{-1}^{1} P'_{j-1}(\tau) P_{i-1}(\tau) d\tau.$$

If $j \leq i$, then $E_{ij} = 0$ because $P'_{j-1}$ is orthogonal to $P_{i-1}$. Otherwise, if $j > i$, then $P_{j-1}$ is orthogonal to $P'_{i-1}$ so integration by parts gives

$$E_{ij} = \left[P_{j-1}(x) P_{i-1}(x)\right]_{-1}^{1} - \int_{-1}^{1} P_{j-1}(x) P'_{i-1}(x) dx = 1 - (-1)^{i+j}$$

and hence $G_{ij}^n = 1$.

Example 9. If $r_n = 4$ and $r_{n-1} = 3$, then the matrices $\mathbf{G}^n = [G_{ij}^n]$ and $\mathbf{K}^{n,n-1} = [K_{ij}^{n,n-1}]$ are

$$\mathbf{G}^n = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{K}^{n,n-1} = \begin{bmatrix} 1 & 1 & 1 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ -1 & -1 & -1 \end{bmatrix}. $$

We have no analogous, simple formula for the remaining coefficients $H_{ij}^{n,\ell}$. However, when $\ell = 0$ ($\ell = n$) the following parity property holds.

Lemma 10. With the choice of basis functions,

$$H_{ji}^{n,0} = (-1)^{i+j} H_{ij}^{n,0}. \tag{18}$$

Proof: Using (7), we find that

$$H_{ji}^{n,0} = \int_{-1}^{1} (BP_{j-1})'(\tau) P_{i-1}(\tau) d\tau = - \int_{-1}^{1} P_{i-1}(\sigma)(B^*P_j-1)'(\sigma) d\sigma,$$

where

$$(Bv)(\tau) = \int_{-1}^{\tau} \omega_\alpha(\tau - \sigma)v(\sigma) d\sigma \quad \text{and} \quad (B^*v)(\sigma) = \int_{\sigma}^{1} \omega_\alpha(\tau - \sigma)v(\tau) d\tau.$$

Let $(RV)(\tau) = V(-\tau)$. A short calculation shows that $RB^* = BR$, so

$$(B^*P_{j-1})'(-\sigma) = -\frac{d}{d\sigma}[(B^*P_{j-1})(-\sigma)] = -\frac{d}{d\sigma}(RB^*P_j-1)'(\sigma) = -(BRP_{j-1})'(\sigma) = (-1)^j(BP_{j-1})'(\sigma),$$
and therefore, using the substitution \( \sigma = -x \),

\[
H_{ji}^{0} = (-1)^{i+j} \int_{-1}^{1} P_{i-1}(-x)(BP_{j-1})'(x) \, dx
\]

\[
= (-1)^{i+j} \int_{-1}^{1} (BP_{j-1})'(x) P_{i-1}(x) \, dx = (-1)^{i+j} H_{ij}^{0},
\]
as claimed.

\[\♠\]

Remark 11. In the limit as \( \alpha \to 1 \), we see from Remark 1 that

\[
H_{ij}^{0} \to \int_{I} \psi_{nj}(t)\psi_{ni}(t) \, dt = \frac{k_n}{2} \int_{-1}^{1} \Psi_{j}(\tau)\Psi_{i}(\tau) \, d\tau = \frac{k_n\delta_{ij}}{2j-1}.
\]

Example 12. Consider the uniform case \( k_n = k \), \( r_n = r \) and \( \Psi_{nj} = \Psi_{j} \) for \( 1 \leq n \leq N \) (as in Remark 7), with \( \Psi_{j}(\tau) = P_{j-1}(\tau) \) as above. We then have

\[
H_{ij}^{\ell} = k^\alpha H_{ij}^{\ell} \quad \text{for } 1 \leq \ell \leq n \leq N \text{ and } i, j \in \{1, 2, \ldots, r\},
\]

where, by Lemma 3

\[
H_{ij}^{0} = \frac{1}{2\alpha \Gamma(\alpha)} \left( \int_{-1}^{1} (1 - \sigma)^{\alpha} P_{j-1}(\sigma) \, d\sigma \right.
\]

\[
- \left. \int_{-1}^{1} (1 + y)^{\alpha-1}(1 - y)\Phi_{ij}(y) \, dy \right),
\]

with

\[
\Phi_{ij}(y) = \frac{1}{2} \int_{-1}^{1} P_{j-1}(\frac{1}{2}(1 - y)(1 + z) - 1) P_{i-1}'(1 - \frac{1}{2}(1 - y)(1 - z)) \, dz,
\]

and by Lemma 4

\[
H_{ij}^{\ell} = \frac{\ell^{\alpha-1}}{2\Gamma(\alpha)} \left( A_{ij}^{\ell} + (-1)^{i}B_{ij}^{\ell} - C_{ij}^{\ell} \right) \quad \text{for } \ell \geq 1,
\]

with, letting \( \Delta_{\ell}(\tau) = \tau/(2\ell) \),

\[
A_{ij}^{\ell} = \int_{-1}^{1} (1 + \Delta_{\ell}(1 - \sigma))^{\alpha-1} P_{j-1}(\sigma) \, d\sigma,
\]

\[
B_{ij}^{\ell} = \int_{-1}^{1} (1 - \Delta_{\ell}(1 + \sigma))^{\alpha-1} P_{j-1}(\sigma) \, d\sigma,
\]

and

\[
C_{ij}^{\ell} = \int_{-1}^{1} (1 - \Delta_{\ell}(1 + \sigma))^{\alpha-1} P_{j-1}(\sigma) \, d\sigma.
\]
6 Reconstruction

\[ C_{ij}^\ell = \int_{-1}^{1} P'_{i-1}(\tau) \int_{-1}^{1} (1 + \Delta \ell(\tau - \sigma))^{\alpha - 1} P_{j-1}(\sigma) \, d\sigma \, d\tau. \]

Moreover, Lemma 5 provides alternative expressions when \( \ell = 1 \):

\[ A_{ij}^1 = 2^{1-\alpha} \int_{-1}^{1} (3 - \sigma)^{\alpha - 1} P_{j-1}(\sigma) \, d\sigma, \]

\[ B_{ij}^1 = 2^{1-\alpha} \int_{-1}^{1} (1 - \sigma)^{\alpha - 1} P_{j-1}(\sigma) \, d\sigma \]

and

\[ C_{ij}^1 = 2^{1-\alpha} \left( \int_{-1}^{1} (1 + \tau)^{\alpha} P'_{i-1}(\tau) \int_{0}^{1} (1 + z)^{\alpha - 1} P_{j-1}(1 - z(1 + \tau)) \, dz \, d\tau \right. \]
\[ + \left. \int_{-1}^{1} (1 - \sigma)^{\alpha} P_{j-1}(\sigma) \int_{0}^{1} (z + 1)^{\alpha - 1} P'_{i-1}(z(1 - \sigma) - 1) \, dz \, d\sigma \right). \]

Likewise, Lemma 6 provides an alternative expression for \( \ell \geq 2 \):

\[ H_{ij}^\ell = -\frac{1 - \alpha}{4\Gamma(\alpha)} \ell^{\alpha - 2} \int_{-1}^{1} P_{i-1}(\tau) \int_{-1}^{1} (1 + \Delta \ell(\tau - \sigma))^{\alpha - 2} P_{j-1}(\sigma) \, d\sigma \, d\tau. \] (21)

Finally, by arguing as in the proof of Lemma 10, we can show that

\[ H_{ji}^\ell = (-1)^{i+j} H_{ij}^\ell \quad \text{for all} \quad \ell \geq 0. \] (22)

6 Reconstruction

Throughout this section, we continue to use the Legendre basis (16). Some insight into the DG method can be had by considering the trivial case of (1) when \( A = 0 \), that is, \( \partial_t u = f(t) \) for \( 0 < t \leq T \), with \( u(0) = u_0 \). The DG scheme (12) then reduces to

\[ \langle [U]^n, X^n \rangle + \int_{I_n} \langle \partial_t U, X \rangle \, dt = \int_{I_n} \langle \partial_t u, X \rangle \, dt \] (23)

for \( X \in \mathbb{P}_{r-1}(I_n; V_n) \) and \( 1 \leq n \leq N \), with \( U_0^0 = U_0 \). To state our next result, let \( P_n \) denote the orthoprojector from \( L_2(\Omega) \) onto \( V_n \), and define

\[ Q_{n\ell} = P_n P_{n-1} \cdots P_{\ell+1}. \]
Lemma 13. If $A = 0$ and $U_0 = P_0u_0$, then for $1 \leq n \leq N$ the DG solution $U \in X$ satisfies

$$U^n_n = P_n u(t_n) + \sum_{\ell=0}^{n-1} Q_{n\ell} (P_\ell - I) u(t_\ell)$$

(24)

and

$$\int_{I_n} \langle U - u, \partial_t X \rangle \, dt = 0 \quad \text{for all } X \in P_n(I_n; V).$$

(25)

Proof: Integrating by parts in (23), we find that

$$\langle U^n_n - u(t_n), X^n_n \rangle = \langle U^{n-1}_n - u(t_{n-1}), X^n_+ \rangle + \int_{I_n} \langle U - u, \partial_t X \rangle \, dt.$$

Given $v \in V_n$, by choosing the constant function $X(t) = v$ for $t \in I_n$ we deduce that $\langle U^n_n - u(t_n), v \rangle = \langle U^{n-1}_n - u(t_{n-1}), v \rangle$ and so (25) is satisfied. Moreover,

$$P_n(U^n_n - u(t_n)) = P_n(U^{n-1}_n - u(t_{n-1})),$$

and, by the choice of initial condition, we see that (24) is satisfied for $n = 1$:

$$U^1_+ - P_1 u(t_1) = P_1(U^1_+ - u(t_1)) = P_1(I - P_0 + P_0)(U^0_+ - u(t_0))$$

$$= P_1(P_0 - I)u(t_0) + P_1(U_0 - P_0 u_0) = Q_{11}(P_0 - I)u(t_0).$$

Letting $n \geq 2$, we make the induction hypothesis

$$U^{n-1}_+ = P_{n-1} u(t_{n-1}) + \sum_{\ell=0}^{n-1} Q_{n-1,\ell}(P_\ell - I) u(t_\ell),$$

and observe that

$$U^n_n - P_n u(t_n) = P_n(U^n_n - u(t_n)) = P_n(I - P_{n-1} + P_{n-1})(U^{n-1}_+ - u(t_{n-1}))$$

$$= P_n(P_{n-1} - I)u(t_{n-1}) + P_n \sum_{\ell=0}^{n-1} Q_{n-1,\ell}(P_\ell - I) u(t_\ell),$$

which gives the desired formula (24).

For the remainder of this section, we will assume that the subspaces $V_n$ are nested, as follows:

$$V_0 \supseteq V_1 \supseteq V_2 \supseteq \cdots \supseteq V_N.$$  

(26)

It follows that $P_{\ell+1}(P_\ell - I) = 0$ for $0 \leq \ell \leq N - 1$ and so

$$U^n_n = P_n u(t_n).$$

(27)

The following explicit representation for $U$ holds.
Lemma 14. If $A = 0$, $U_0 = \mathcal{P}_0u_0$ and the subspaces satisfy (26), then

$$U(t) = \sum_{j=1}^{r_n-1} a_{nj} \psi_{nj}(t) + \tilde{a}_n \psi_{nr_n}(t) \quad \text{for } t \in I_n,$$

where

$$a_{nj} = \frac{2j - 1}{k_n} \int_{I_n} \mathcal{P}_n u(t) \psi_{nj}(t) \, dt$$

are the local Fourier–Legendre coefficients of $\mathcal{P}_n u$, but

$$\tilde{a}_n = \mathcal{P}_n u(t_n) - \sum_{j=1}^{r_n-1} a_{nj}.$$

**Proof:** By definition, $U|_{I_n} \in \mathbb{P}_{r_n-1}(I_n; V_n)$ so there exist coefficients $a_{nj}$ and $\tilde{a}_n$ in $V_n$ such that $U$ has the desired expansion. The formula for $a_{nj}$ follows at once from the orthogonality property of the $\psi_{nj}$ (see Remark 11). The formula for $\tilde{a}_n$ follows from (27) because $\psi_{nj}(t_n) = P_{j-1}(1) = 1$ for all $j$. ♠

We have a Peano kernel $G_r$ for the Fourier–Legendre expansion of degree $r$,

$$f(\tau) = \sum_{j=1}^{r+1} b_j \Psi_j(\tau) + \int_{-1}^{1} G_r(\tau, \sigma) f(\sigma) \, d\sigma \quad \text{for } -1 \leq \tau \leq 1,$$

assuming $f : [-1, 1] \to \mathbb{R}$ is $C^{r+1}$, and also a Peano kernel $M_j(\tau)$ for the $j$th coefficient:

$$b_j = \frac{2j - 1}{2} \int_{-1}^{1} f(\tau) \Psi_j(\tau) \, d\tau = \int_{-1}^{1} M_j(\tau) f(j-1)(\tau) \, d\tau.$$

Thus, if $t = t_n(\tau)$ and $s = t_n(\sigma)$, and if we define the local Peano kernels

$$g_{nr}(t, s) = (k_n/2)^r G_r(\tau, \sigma) \quad \text{and} \quad m_{nj}(t) = (k_n/2)^{j-2} M_j(\tau),$$

then

$$\mathcal{P}_n u(t) = \sum_{j=1}^{r_n+1} a_{nj} \psi_{nj}(t) + \int_{I_n} g_{nr}(t, s) \mathcal{P}_n u^{(r_n+1)}(s) \, ds \quad \text{for } t \in I_n,$$

and

$$a_{nj} = \int_{I_n} m_{nj}(s) \mathcal{P}_n u^{(j-1)}(s) \, ds.$$

It follows that $a_{nj} = O(k_n^{j-1})$ provided $u$ is $C^{j-1}$ on $I_n$.

**Theorem 15.** Assume that $A = 0$, $U_0 = \mathcal{P}_0u_0$ and the subspaces satisfy (26). If $u : I_n \to L^2(\Omega)$ is $C^{r_n+r_n+1}$, then $a_{n,r_n+1} = O(k_n^{r_n})$ and

$$\mathcal{P}_n u(t) - U(t) = a_{n,r_n+1} [\psi_{n,r_n+1}(t) - \psi_{n,r_n}(t)] + O(k_n^{r_n+1}) \quad \text{for } t \in I_n.$$
Proof: Subtracting (28) from (29), we have
\[ P_n u(t) - U(t) = (a_{n,r} - \tilde{a}_n) \psi_{n,r}(t) + a_{n,r+1} \psi_{n,r+1}(t) + O(k_n^{r+1}) \]
for \( t \in I_n \). Since \( U_n = P_n u(t_n) \) and \( \psi_{n,r}(t_n) = \psi_{n,r+1}(t_n) = 1 \), taking the limit as \( t \to t_n \) yields \( a_{n,r} - \tilde{a}_n = -a_{n,r+1} + O(k_n^{r+1}) \). ♠

Corollary 16. \( P_n [U]^{n-1} = 2(-1)^{r+1} a_{n,r+1} + O(k_n^{r+1}) \).

Proof: As \( t \to t_{n-1}^+ \), the left-hand side of (30) tends to
\[
\begin{align*}
\mathcal{P}_n u(t_{n-1}) - U_{n-1}^{n-1} &= \mathcal{P}_n (I - \mathcal{P}_{n-1} + \mathcal{P}_{n-1}) U_{n-1}^{n-1} - U_{n-1}^{n-1} = \mathcal{P}_n U_{n-1}^{n-1} - U_{n-1}^{n-1} \\
&= -\mathcal{P}_n (U_+^{n-1} - U_-^{n-1}) = -\mathcal{P}_n [U]^{n-1},
\end{align*}
\]
and on the right-hand side, \( \psi_{n,r+1}(t) - \psi_{n,r}(t) \) tends to \( P_n (-1) - P_{n-1} (-1) = (-1)^{r_n} - (-1)^{r_{n-1}} = 2(-1)^{r_n} \). ♠

In light of Theorem 15, we consider the polynomials
\[ \psi_{n,r+1}(t) - \psi_{n,r}(t) = \Psi_{r+1}(\tau) - \Psi_r(\tau) = P_r(\tau) - P_{r-1}(\tau). \]
As illustrated in Figure 1, there are \( r + 1 \) points

\[-1 = \tau_{r_0} < \tau_{r_1} < \cdots < \tau_{rr} = 1\]

such that

\[(P_r - P_{r-1})(\tau_{rj}) = 0 \quad \text{for} \quad 1 \leq j \leq r.\]

In fact, the \( r \) zeros \( \tau_{r_1}, \tau_{r_2}, \ldots, \tau_{rr} \) are the points of a right-Radau quadrature rule [4, Chapter 9] on the interval \([-1, 1]\). We put

\[t^*_{nj} = t_n(\tau_{nj}) \quad \text{for} \quad 0 \leq j \leq r_n,\]

so that \( t^*_{n-1} = t^*_0 < t_n1 < \cdots < t^*_{nr_n} = t_n \) and

\[\psi_{n,r+n+1}(t^*_nj) - \psi_{n,r}(t^*_nj) = 0 \quad \text{for} \quad 1 \leq j \leq r_n.\]

From Theorem 15 we see that \( P_n u(t) - U(t) = O(k_r^n) \) for general \( t \in I_n \), but \( P_n u(t^*_nj) - U(t^*_nj) = O(k_r^{r-1}) \) for \( 1 \leq j \leq r_n \). Let \( \hat{\mathcal{X}} \) denote the space obtained from \( \mathcal{X} \) by increasing the maximum allowed polynomial degree over the subinterval \( I_n \) from \( r_n \) to \( \hat{r}_n = r_n + 1 \), for \( 1 \leq n \leq N \). The reconstruction \( \hat{U} \in \hat{\mathcal{X}} \) of \( U \in \mathcal{X} \) is then defined by requiring that

\[\hat{U}(t^*_nj) = U(t^*_nj) \quad \text{for} \quad 1 \leq j \leq r_n - 1,\]

and that the one-sided limits at the end points are

\[\hat{U}^{-1}_+ = P_n U^{-1}_- \quad \text{and} \quad \hat{U}^n_+ = U^n_.\]

Since \( \hat{U}|_{I_n} \) is a polynomial of degree at most \( \hat{r}_n - 1 = r_n \), it is uniquely determined by these \( r_n + 1 \) interpolation conditions. Notice also that \( \hat{U} \) is continuous at \( t_{n-1} \) if \( V_{n-1} = V_n \) because \( P_n U^{-1}_- = U^{-1}_n \).

Makridakis and Nochetto [6] introduced the reconstruction in their analysis of a posteriori error bounds for parabolic PDEs. Since the polynomial \( (U - \hat{U})|_{I_n} \) has degree at most \( r_n \) and vanishes at \( t^*_nj \) for \( 1 \leq n \leq r_n \), it must be a multiple of \( \psi_{n,e+n-1} - \psi_{n,e} \). In fact, by taking limits as \( t \to t^+_n \), we see that

\[U(t) - \hat{U}(t) = \frac{1}{2}(-1)^r P_n \|U\|^{n-1} [\psi_{n,e+n+1}(t) - \psi_{n,e}(t)] \quad \text{for} \quad t \in I_n. \]

At the same time, by Theorem 15 and Corollary 16

\[U(t) - P_n u(t) = \frac{1}{2}(-1)^r P_n \|U\|^{n-1} [\psi_{n,e+n+1}(t) - \psi_{n,e}(t)] + O(k_r^{r-1}) \quad \text{for} \quad t \in I_n, \]
implying that $\hat{U} - \mathcal{P}_n u$ is $O(k_n^{r_n+1})$ on $I_n$. One of our principal aims in the next section is to investigate numerically the error in the dG solution $U$ and its reconstruction $\hat{U}$ in non-trivial cases where $A \neq 0$. We can hope that something like (33) still holds, because the time derivative in the term $\partial_t^{1-\alpha} Au$ is of lower order than in $\partial_t u$. Notice that (5) and (32) imply

$$\hat{U}(t) = \sum_{j=1}^{r_n} \hat{U}^{nj} \psi_{nj}(t) \quad \text{for } t \in I_n,$$

where

$$\hat{U}^{nj} = \begin{cases} U^{nj}, & 1 \leq j \leq r_n - 1, \\ U^{nr_n} + \frac{1}{2} \left( -1 \right)^{r_n} \mathcal{P}_n [U]^{n-1}, & j = r_n, \\ \frac{1}{2} \left( -1 \right)^{r_n+1} \mathcal{P}_n [U]^{n-1}, & j = r_n + 1 = \hat{r}_n. \end{cases}$$

7 Numerical experiments

A Julia package [7] provides functions to evaluate the coefficients $G_{ij}^n$, $K_{ij}^{n,n-1}$ and $H_{ij}^\ell$ based on the results of Sections 3 and 5. This package also includes (in the examples directory) the scripts used for the examples below.

7.1 The matrix $H^\ell$

Let $\alpha = 3/4$, and consider for simplicity the case when $k_n = k$ and $r_n = r$ are constant for all $n$, so that the formulae of Example 12 apply. To get a sense of how the matrix entries $H_{ij}^\ell$ behave, we computed

$$H^0 = \begin{bmatrix} 1.08807 & 0.15544 & 0.07065 & 0.04239 \\ -0.15544 & 0.49458 & 0.09326 & 0.04834 \\ 0.07065 & -0.09326 & 0.33839 & 0.06893 \\ -0.04239 & 0.04834 & -0.06893 & 0.26319 \end{bmatrix},$$

and

$$H^1 = \begin{bmatrix} -0.34623 & -0.13428 & -0.06884 & -0.04219 \\ 0.13428 & 0.08414 & 0.05405 & 0.03690 \\ -0.06884 & -0.05405 & -0.04050 & -0.03048 \\ 0.04219 & 0.03690 & 0.03048 & 0.02472 \end{bmatrix},$$

which illustrate the property (22). The factor $(1 + \Delta \tau (\tau - \sigma))^{\alpha-2}$ in (21) becomes very smooth as $\ell$ increases, with the result that $H_{ij}^\ell$ decays rapidly.
Figure 2: Decay of $\max_{i+j=m} |H_{ij}^\ell|$ for increasing $m$ and $\bar{\ell}$, when $\alpha = 3/4$.

to zero as $i + j$ increases. Even for $\bar{\ell} = 2$, we have

$$H^2 = 10^{-1} \times \begin{bmatrix}
-0.91483 & -0.10220 & -0.01261 & -0.00164 \\
0.10220 & 0.02027 & 0.00355 & 0.00059 \\
-0.01261 & -0.00355 & -0.00080 & -0.00016 \\
0.00164 & 0.00059 & 0.00016 & 0.00004
\end{bmatrix} ,$$

and Figure 2 shows this behaviour for larger values of $\bar{\ell}$, with entries in the lower right corner of the matrix reaching the order of the machine epsilon $(2^{-52} \approx 2.22 \times 10^{-16})$ once $\bar{\ell}$ is of order 100.

The value of $H^0_{ij}$ can be computed to machine precision using Gauss quadrature with $M_\sigma = [j/2]$ and $M_y = [(i+j)/2] - 1$ points for the integrals with respect to $\sigma$ and $y$ in (19), and using $M_z = [(i+j)/2] - 1$ points for the integral with respect to $z$ in (20). When $\ell \geq 1$, let $H^\ell_{ij}(M)$ denote the value of $H^\ell_{ij}$ computed by applying $M$-point Gauss rules to (21), that is, $M^2$ points for the double integral. For a given absolute tolerance $\texttt{atol}$, let $M^\ell_{ij}(\texttt{atol})$ denote the smallest $M$ for which

$$|H^\ell_{ij}(M) - H^\ell_{ij}(12)| < \texttt{atol} \quad \text{for all } i, j \in \{1, 2, \ldots, r\} .$$
Table 1: Numbers of Gauss points $M_r^{\ell}(\text{atol})$ required for $\text{atol} = 10^{-14}$, when $\alpha = 3/4$.

| $r$ | $\ell = 1$ | $\ell = 2$ | $\ell = 10$ | $\ell = 100$ | $\ell = 1000$ |
|-----|------------|------------|------------|-------------|-------------|
| 1   | 9          | 9          | 5          | 3           | 2           |
| 2   | 9          | 9          | 5          | 3           | 2           |
| 3   | 9          | 9          | 5          | 4           | 3           |
| 4   | 10         | 10         | 6          | 4           | 3           |
| 5   | 10         | 10         | 6          | 5           | 4           |
| 6   | 11         | 11         | 7          | 5           | 4           |

Figure 3: The exact solution $u$ of (3) in the case (34), together with the piecewise-quadratic ($r = 3$) dG solution with $N = 3$ subintervals.

Table 1 lists some values of $M_r^{\ell}(\text{atol})$ for $\text{atol} = 10^{-14}$. Unsurprisingly, fewer quadrature points are needed as $\ell$ increases.

### 7.2 A fractional ODE

We consider the initial-value problem (3) in the case

\[ \alpha = 1/2, \quad \lambda = 1/2, \quad f(t) = \cos \pi t, \quad u_0 = 1, \quad T = 2, \quad (34) \]
Table 2: Maximum weighted errors (36) at the points $t_{nj}^*$ using piecewise quadratics ($r = 3$) on a uniform grid.

| $N$  | $E_{0}^{\text{max}}$ | $E_{1}^{\text{max}}$ | $E_{2}^{\text{max}}$ | $E_{3}^{\text{max}}$ |
|------|----------------------|----------------------|----------------------|----------------------|
| 8    | 8.0e-03              | 8.8e-05              | 1.3e-04              | 1.0e-04              |
| 16   | 1.2e-03 2.69         | 1.4e-05 2.62         | 1.4e-05 3.15         | 9.3e-06 3.46         |
| 32   | 1.7e-04 2.87         | 1.5e-06 3.25         | 1.3e-06 3.40         | 8.2e-07 3.50         |
| 64   | 2.2e-05 2.94         | 1.4e-07 3.42         | 1.2e-07 3.47         | 7.2e-08 3.51         |
| 128  | 2.8e-06 2.97         | 1.3e-08 3.47         | 1.1e-08 3.49         | 6.3e-09 3.51         |
| 256  | 3.6e-07 2.98         | 1.1e-09 3.49         | 9.5e-10 3.50         | 5.5e-10 3.51         |

for which the solution is

$$u(t) = u_0 E_{1/2}(-\lambda \sqrt{t}) + \int_0^t E_{1/2}(-\lambda \sqrt{t-s}) f(s) \, ds,$$

where $E_{\alpha}(x) = \sum_{n=0}^{\infty} t^n / \Gamma(1+n\alpha)$ denotes the Mittag–Leffler function. The substitution $s = (1-y^2) t$ yields a smooth integrand, allowing $u(t)$ to be computed accurately via Gauss quadrature on the unit interval $[0, 1]$. Note that $E_{1/2}(-x) = \text{erfcx}(x) = e^{x^2} \text{erfc}(x)$ is just the scaled complementary error function.

Figure 3 shows $u$, together with the DG solution $U$ using piecewise quadratics ($r = 3$) and only $N = 3$ subintervals. In Figure 4 we plot the absolute errors,

$$\hat{E}(t) = |\hat{u}(t) - u(t)| \quad \text{and} \quad E_j^n = \begin{cases} |U(t_{n0}^* + 0) - u(t_{n0}^*)|, & j = 0, \\ |U(t_{nj}^* - u(t_{nj}^*)|, & 1 \leq j \leq r - 1, \\ |U(t_{nr}^* - u(t_{nr}^*)|, & j = r, \end{cases}$$

again using piecewise quadratics but now with $N = 5$ subintervals of uniform size $k_n = k = T/N$. Two features are immediately apparent. First, the accuracy is poor near $t = 0$, reflecting the singular behaviour of the solution: for $m \geq 1$, the $m$th derivative $u^{(m)}(t)$ blows up like $t^{-(m-1)/2}$ as $t \to 0$. Second, on intervals $I_n$ away from 0, the error is notably smaller at the right-Radau points ($t_{nj}^*$ for $1 \leq j \leq 3$) than at the left endpoint ($t_{n0}^* = t_{n-1}$).

In Table 2, we show how the quantities

$$E_{\text{max}}^j = \max_{1 \leq n \leq N} (t_{nj}^*)^{r-\alpha} E_j^n$$

(36)
Figure 4: Absolute errors in the reconstruction $\hat{U}(t)$ for $0 \leq t \leq T = 2$, and in the dG solution $U(t)$ for $t = t^*_n$, using piecewise quadratics ($r = 3$) and $N = 5$ uniform subintervals; see (31).

behave as $N$ grows. These results, together with similar computations using other choices of $\alpha$ and $r \geq 2$, lead us to conjecture that, in general, using a constant time step $k$,

$$E^n_0 \leq C(t^*_n)^{\alpha-r}k^r \quad \text{for} \quad 2 \leq n \leq N,$$

whereas

$$E^n_j \leq C(t^*_n)^{\alpha-r}k^{r+\alpha} \quad \text{for} \quad 1 \leq n \leq N \quad \text{and} \quad 1 \leq j \leq r,$$

and that, consequently,

$$|\hat{U}(t) - u(t)| \leq Ct^{\alpha-r}k^{r+\alpha} \quad \text{for} \quad t_1 \leq t \leq T.$$

However, using piecewise-constants ($r = 1$) we do not observe any super-convergence, with both $E^n_{0\text{max}}$ and $E^n_{1\text{max}}$ behaving like $C t^{1-\alpha}k$, albeit with a noticeably smaller constant in the case of $E^n_{1\text{max}}$.

To suppress the growth in the error as $t$ approaches 0, we can use a graded mesh of the form

$$t_n = (n/N)^qT \quad \text{for} \quad 0 \leq n \leq N,$$

(37)
Table 3: Maximum error in the reconstruction \( \hat{U}(t) \) for \( 0 \leq t \leq T = 1 \), using piecewise quadratics \((r = 3)\) for four choices of the mesh grading exponent \( q \); see (37).

| \( N \) | \( q = 1 \) | \( q = 3 \) | \( q = 5 \) | \( q = 6 \) |
|---|---|---|---|---|
| 8 | 1.1e-02 | 1.4e-03 | 4.1e-04 | 7.1e-04 |
| 16 | 6.0e-03 | 0.84 | 3.8e-04 | 1.89 | 5.2e-05 | 2.95 | 9.1e-05 | 2.97 |
| 32 | 4.3e-03 | 0.50 | 1.3e-04 | 1.50 | 7.9e-06 | 2.72 | 1.0e-05 | 3.19 |
| 64 | 3.0e-03 | 0.50 | 4.7e-05 | 1.50 | 1.4e-06 | 2.51 | 9.8e-07 | 3.35 |
| 128 | 2.1e-03 | 0.50 | 1.7e-05 | 1.50 | 2.5e-07 | 2.50 | 9.2e-08 | 3.41 |
| 256 | 1.5e-03 | 0.50 | 5.9e-06 | 1.50 | 4.3e-08 | 2.50 | 8.4e-09 | 3.45 |

with a suitable grading exponent \( q \geq 1 \). Table 3 shows the maximum error in the reconstruction, i.e., \( \max_{0 \leq t \leq T} |\hat{U}(t) - u(t)| \), together with the associated convergence rates, for four choices of \( q \) and using \( T = 1 \) as the final time. These errors appear to be of order \( k \min(3, q_0) \) where \( k = \max_{1 \leq n \leq N} k_n \leq CN^{-1} \). We conjecture that, in general,

\[
|\hat{U}(t) - u(t)| \leq C k \min(r + \alpha, q_0) \quad \text{for} \ 0 \leq t \leq T, \ \text{provided} \ r \geq 2. \quad (38)
\]

### 7.3 A fractional PDE

Consider the elliptic operator \( A = -\partial^2 / \partial x^2 \) for the 1D spatial domain \( \Omega = (0, L) \). To construct a reference solution, we exploit fact that the Laplace transform of \( u \),

\[
\tilde{u}(x, z) = \int_0^\infty e^{-zt} u(x,t) \, dt,
\]

satisfies the two-point boundary-value problem

\[
\omega^2 \tilde{u} - \tilde{u}_{xx} = g(x, z) \quad \text{for} \ 0 < x < L, \ \text{with} \ \tilde{u}(0, z) = 0 = \tilde{u}(L, z),
\]

where

\[
\omega = z^{\alpha/2} \quad \text{and} \quad g(x, z) = z^{\alpha-1} [u_0(x) + \tilde{f}(x, z)].
\]

The variation-of-parameters formula leads to the integral representation

\[
\tilde{u}(x, z) = \frac{\sinh \omega (L - x)}{\omega \sinh \omega L} \int_0^x g(x, z) \sinh \omega \xi \, d\xi
\]
Figure 5: The reference solution for the 1D problem with data given by (40) and (41).

\[
\tilde{u}(x,z) = C_0 \frac{\rho_1(x) \sinh \omega(L - x) + \rho_1(L - x) \sinh \omega x}{z} + \frac{C_f}{z(z+1)^2} \frac{\rho_2(x) \sinh \omega(L - x) + \rho_2(L - x) \sinh \omega x}{\sinh \omega L},
\]

and the Laplace inversion formula then gives

\[
u(x,t) = \frac{1}{2\pi i} \int_\Gamma e^{zt} \tilde{u}(x,z) \, dz,
\]

for a contour \( \Gamma \) homotopic to the imaginary axis and passing to the right of all singularities of the integrand.

We choose as data the functions

\[
u_0(x) = C_0 x(L - x) \quad \text{and} \quad f(x,t) = C_f te^{-t},
\]

for constants \( C_0 \) and \( C_f \), and find that

\[
u(x,t) = 1 \frac{\sinh \omega x}{\omega \sinh \omega L} \int_x^L g(x,z) \sinh \omega \xi \, d\xi,
\]
Figure 6: Comparison of the jumps $\|\|U\|_{n-1}\|$ with the dG error $\|U(t) - u(t)\|$ and the reconstruction error $\|\widehat{U}(t) - u(t)\|$. Top: a uniform mesh with $N = 12$ time steps. Bottom: a graded mesh with $N = 40$ time steps.
where
\[ \rho_1(x) = (\omega x (L - x) - 2\omega^{-1}) \cosh \omega x + (2x - L) \sinh \omega x + 2\omega^{-1} \]
and
\[ \rho_2(x) = \cosh \omega x - 1. \]

To evaluate the contour integral \[39\] we apply an optimised equal-weight quadrature rule that arises after deforming \( \Gamma \) into the left branch of a hyperbola \[16\]. Figure 5 shows the reference solution over the time interval \([0, 2]\) in the case
\[ \alpha = 0.6, \quad L = 2, \quad C_0 = 1, \quad C_f = 2. \quad (41) \]

In Figure 6, we plot the \( L_2 \)-norms of the jumps, \( \|U\|^{n-1} \), together with the errors in \( U(t) \) and its reconstruction \( \hat{U}(t) \). The dG method used piecewise-quadratics \( (r = 3) \), first with a uniform mesh of \( N = 12 \) subintervals (top), and then with a non-uniform mesh of \( N = 40 \) subintervals (bottom). In both cases, the spatial discretisation used (continuous) piecewise cubics on a uniform grid with 20 subintervals. Since \( u_0 \) is a quadratic polynomial in this instance, we simply put \( U_0 = u_0 \). Consistent with our conjecture \[33\], we observe that
\[ \sup_{t_{n-1} < t < t_n} \|U(t) - u(t)\| \approx \|U\|^{n-1}. \]

Motivated by our conjecture \[38\], the second mesh was graded for \( 0 \leq t_n \leq 1 \) by taking \( q = (r + \alpha)/\alpha \), \( N = 34 \) and \( T = 1 \) in the formula \[37\], followed by a uniform mesh on the other half \([1, 2]\) of the time interval. We see that the mesh grading is effective at resolving the solution for \( t \) near zero, albeit with a substantial increase in the overall computational cost.

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