ANZIAM J. **62** (2020), 121–147
doi:10.1017/S1446181120000152

IMPLEMENTATION OF HIGH-ORDER, DISCONTINUOUS GALERKIN TIME STEPPING FOR FRACTIONAL DIFFUSION PROBLEMS

WILLIAM MCLEAN[1]

(Received 20 March, 2020; accepted 28 July, 2020; first published online 6 November, 2020)

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 specialized 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.

2020 *Mathematics subject classification*: primary 65M60; secondary 65D30.

Keywords and phrases: Gauss quadrature, finite-element method, Legendre polynomials, reconstruction, superconvergence.

1. Introduction

The discontinuous Galerkin (DG) method provides an effective numerical procedure for the time integration of diffusion problems. In the mid-1980s, Eriksson et al. [2] provided the first detailed error analysis, which has been subsequently extended and refined by numerous authors (see, for example, the articles [7, 16, 17] and the references therein). The DG method has also proved effective for time stepping of *fractional* diffusion problems [10, 13] of the form

$$\partial_t u + \partial_t^{1-\alpha} A u = f(t) \quad \text{for } 0 < t \le T \text{ with } u(0) = u_0. \tag{1.1}$$

Here, A is a linear, second-order, elliptic partial differential operator over a spatial domain Ω, 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

[1] School of Mathematics and Statistics, University of New South Wales, Sydney, NSW 2052 , Australia; e-mail: w.mclean@unsw.edu.au.

fractional time derivative is understood in the Riemann–Liouville sense [15]: for $t > 0$ and $\mu > 0$,

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

The partial integro-differential equation (1.1) arises in a variety of physical models [4, 12] 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 $1/t^{1+\alpha}$ as $t \to \infty$. The expected waiting time is therefore infinite, and the mean-square displacement turns out to be proportional to t^α. Standard Brownian motion is recovered in the limit as $\alpha \to 1$, when (1.1) reduces to the classical diffusion equation.

Our main concern in the present work is with the practical implementation of DG time stepping for (1.1) and, in particular, with the accurate evaluation of certain coefficients $H_{ij}^{n,n-\ell}$ used during the nth step. Section 2 introduces the DG method for the fractional ordinary differential equation (ODE) case of (1.1), 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

$$H_{11}^{n,0} = \int_{t_{n-1}}^{t_n} \frac{d}{dt}\biggl(\int_{t_{n-1}}^{t} \omega_\alpha(t-s)\,ds\biggr)\,dt$$

and

$$H_{11}^{n,n-\ell} = \int_{t_{n-1}}^{t_n} \frac{d}{dt}\biggl(\int_{t_{\ell-1}}^{t_\ell} \omega_\alpha(t-s)\,ds\biggr)\,dt \quad \text{for } 1 \le \ell \le n-1,$$

where $0 = t_0 < t_1 < t_2 < \cdots$ are the discrete time levels. Here, we can 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

$$H_{11}^{n,n-\ell} = \omega_{\alpha+1}(t_n - t_{\ell-1}) - \omega_{\alpha+1}(t_n - t_\ell) - \omega_{\alpha+1}(t_{n-1} - t_{\ell-1}) + \omega_{\alpha+1}(t_{n-1} - t_\ell), \tag{1.2}$$

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 prone to suffer from roundoff when evaluated in floating-point arithmetic if $n-\ell$ is large. Consider just the lowest-order case (1.2) with uniform time steps $t_n = nk$, so that

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

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 $\ell \le n-2$, 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,

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

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 discretization for the fractional partial differential equation (PDE) (1.1) and describes the structure of the linear system that must be solved at each time step. In Section 5, we specialize 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 $\widehat{U}$, called the "reconstruction" [7] of U. If U is a piecewise polynomial of degree at most $r-1$, then $\widehat{U}$ is a piecewise polynomial of degree at most r. For a classical diffusion problem, both U and $\widehat{U}$ are 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. Section 8 concludes the paper.

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

$$u' + \lambda \partial_t^{1-\alpha} u = f(t) \quad \text{for } 0 < t \leq T \text{ with } u(0) = u_0. \tag{2.1}$$

For the time discretization, we introduce a grid

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

and form the vector $\boldsymbol{t} = (t_0, t_1, \ldots, t_N)$. Let $k_n = t_n - t_{n-1}$ denote the length of the nth (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 $v : I \to \mathbb{R}$, write

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

provided the one-sided limits exist.

Given a vector $\boldsymbol{r} = (r_1, r_2, \ldots, r_N)$ of integers $r_n \geq 0$, the trial space $\mathcal{X} = \mathcal{X}(\boldsymbol{t}, \boldsymbol{r})$ consists of the functions $X : I \to \mathbb{R}$ 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 $U \in \mathcal{X}$ of (2.1) is then defined by [10, 13]

$$[\![U]\!]^{n-1} X_+^{n-1} + \int_{I_n} (U' + \lambda \partial_t^{1-\alpha} U) X \, dt = \int_{I_n} f X \, dt \tag{2.2}$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

for $X \in \mathbb{P}_{r_n-1}$ and $1 \le n \le N$, where, in the case $n = 1$, we set $U_-^0 = u_0$, so that $[\![U]\!]^0 = U_+^0 - U_-^0 = U_+^0 - u_0$. A general introduction to DG time stepping for classical diffusion problems may be found in the monograph of Thomée [18, Ch. 12].

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

$$U(t) = \sum_{j=1}^{r_n} U^{nj}\psi_{nj}(t) \quad \text{for } t \in I_n. \tag{2.3}$$

When $X = \psi_{ni}$,

$$U_+^{n-1}X_+^{n-1} + \int_{I_n} U'X\,dt = \sum_{j=1}^{r_n} G_{ij}^n U^{nj} \quad \text{and} \quad U_-^{n-1}X_+^{n-1} = \sum_{j=1}^{r_{n-1}} K_{ij}^{n,n-1}U^{n-1,j}$$

with coefficients given by

$$G_{ij}^n = \psi_{nj}(t_{n-1})\psi_{ni}(t_{n-1}) + \int_{I_n} \psi_{nj}'\psi_{ni}\,dt \tag{2.4}$$

and

$$K_{ij}^{n,n-1} = \psi_{n-1,j}(t_{n-1})\psi_{ni}(t_{n-1}). \tag{2.5}$$

Owing to the convolutional structure of the fractional derivative, it is convenient to introduce the notation $\bar{\ell} = n - \ell$ and define, if $t \in I_n$,

$$\rho_{j\alpha}^{n\bar{\ell}}(t) = \rho_{j\alpha}^{n,n-\ell}(t) = \int_{I_\ell} \omega_\alpha(t-s)\psi_{\ell j}(s)\,ds \quad \text{for } 1 \le \ell \le n-1$$

with

$$\rho_{j\alpha}^{n\bar{n}}(t) = \rho_{j\alpha}^{n0}(t) = \int_{t_{n-1}}^{t} \omega_\alpha(t-s)\psi_{nj}(s)\,ds.$$

We find that

$$\partial_t^{1-\alpha}U = \sum_{\ell=1}^{n}\sum_{j=1}^{r_\ell} U^{\ell j}(\rho_{j\alpha}^{n\bar{\ell}})'(t) \quad \text{for } t \in I_n$$

and thus

$$\int_{I_n} (\partial_t^{1-\alpha}U)X\,dt = \sum_{\ell=1}^{n}\sum_{j=1}^{r_\ell} H_{ij}^{n\bar{\ell}}U^{\ell j}, \quad \text{where} \quad H_{ij}^{n\bar{\ell}} = H_{ij}^{n,n-\ell} = \int_{I_n} (\rho_{j\alpha}^{n\bar{\ell}})'\psi_{ni}\,dt. \tag{2.6}$$

Hence, putting $F^{ni} = \int_{I_n} f\psi_{ni}\,dt$, the DG method (2.2) requires

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

$$\sum_{j=1}^{r_n}(G_{ij}^n + \lambda H_{ij}^{n0})U^{nj} = F^{ni} - \sum_{\ell=1}^{n-1}\sum_{j=1}^{r_\ell} \lambda H_{ij}^{n,n-\ell}U^{\ell j} + \begin{cases} \psi_{1i}(0)u_0, & n = 1, \\ \sum_{j=1}^{r_{n-1}} K_{ij}^{n,n-1}U^{n-1,j}, & 2 \le n \le N. \end{cases} \tag{2.7}$$

At the nth time step, this $r_n \times r_n$ linear system must be solved to determine U^{n1}, $U^{n2}, \dots, U^{nr_n}$ and hence $U(t)$ for $t \in I_n$.

REMARK 2.1. If we let $\alpha \to 1$, so that the fractional ODE in (2.1) reduces to the classical ODE $u' + \lambda u = f(t)$, then $H_{ij}^{n\bar\ell} = 0$ for $1 \le \bar\ell \le n-1$. Indeed, since $\omega_1(t) = 1$, we see that $\rho_{j\alpha}^{n\bar\ell}(t) = \int_{I_\ell} \psi_{\ell j}(s)\,ds$ is constant and so $(\rho_{j\alpha}^{n\bar\ell})'(t) = 0$ for $t \in I_n$. Moreover, $(\rho_{j\alpha}^{n0})'(t) = \psi_{nj}(t)$, so $H_{ij}^{n0} = \int_{I_n} \psi_{nj}\psi_{ni}\,dt$.

REMARK 2.2. Later we will show certain symmetry properties of H_{ij}^{n0} using the identity

$$\int_a^b \Big(\frac{\partial}{\partial t}\int_a^t \omega_\alpha(t-s)u(s)\,ds\Big)v(t)\,dt = -\int_a^b u(s)\Big(\frac{\partial}{\partial s}\int_s^b \omega_\alpha(t-s)v(t)\,dt\Big)\,ds. \tag{2.8}$$

In fact, a simple calculation using the substitution $x = t - s$ gives

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

and (2.8) follows after reversing the order of integration and then integrating by parts. Similarly,

$$\int_a^b \Big(\frac{\partial}{\partial t}\int_a^b \omega_\alpha(t-s)u(s)\,ds\Big)v(t)\,dt = -\int_a^b u(s)\Big(\frac{\partial}{\partial s}\int_a^b \omega_\alpha(t-s)v(t)\,dt\Big)\,ds.$$

Before discussing the general case in the next section, consider the power basis

$$\psi_{nj}(t) = \frac{1}{(j-1)!}\Big(\frac{t-t_{n-1}}{k_n}\Big)^{j-1} \quad \text{for } t \in I_n \text{ and } 1 \le j \le r_n,$$

which is arguably the simplest choice, as far as evaluation of G_{ij}^n, $H_{ij}^{n\ell}$ and $K_{ij}^{n,n-1}$ is concerned. We see from (2.4) that

$$G_{i1}^n = \delta_{i1} \quad \text{and} \quad G_{ij}^n = \frac{1}{(i-1)!\,(j-2)!\,(i+j-2)} \quad \text{for } j \ge 2$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

and from (2.5) that $K_{ij}^{n,n-1} = \delta_{i1}/(j-1)!$, so in this case both coefficients are independent of n. Turning to $H_{ij}^{n\bar{\ell}}$, observe that since $\psi_{\ell,1}(t) \equiv 1$,

$$\rho_{1\alpha}^{n\bar{\ell}}(t) = \begin{cases} \omega_{\alpha+1}(t-t_{\ell-1}) - \omega_{\alpha+1}(t-t_\ell) & \text{if } 1 \le \ell \le n-1, \\ \omega_{\alpha+1}(t-t_{n-1}) & \text{if } \ell = n. \end{cases}$$

For $j \ge 2$, we have $\psi_{\ell j}'(t) = k_\ell^{-1}\psi_{\ell,j-1}(t)$ and $\psi_{\ell,j}(t_{\ell-1}) = 0$, so, integrating by parts,

$$\rho_{j\alpha}^{n\bar{\ell}}(t) = \begin{cases} k_\ell^{-1}\rho_{j-1,\alpha+1}^{n\bar{\ell}}(t) - \psi_{\ell j}(t_\ell)\omega_{\alpha+1}(t-t_\ell) & \text{if } 1 \le \ell \le n-1, \\ k_n^{-1}\rho_{j-1,\alpha+1}^{n0}(t) & \text{if } \ell = n. \end{cases}$$

Repeating this process eventually yields

$$\begin{aligned} \rho_{j\alpha}^{n\bar{\ell}}(t) &= k_\ell^{-(j-1)}\rho_{1,\alpha+j-1}^{n\bar{\ell}}(t) - \sum_{p=0}^{j-2} k_\ell^{-p}\psi_{\ell,j-p}(t_\ell)\omega_{\alpha+p+1}(t-t_\ell) \\ &= k_\ell^{-(j-1)}[\omega_{\alpha+j}(t-t_{\ell-1}) - \omega_{\alpha+j}(t-t_\ell)] - \sum_{p=0}^{j-3} k_\ell^{-p}\psi_{\ell,j-p}(t_\ell)\omega_{\alpha+p+1}(t-t_\ell) \end{aligned} \tag{2.9}$$

for $1 \le \ell \le n-1$ with $\rho_{j\alpha}^{n0}(t) = k_n^{-(j-1)}\rho_{1,\alpha+j-1}^{n0}(t) = k_n^{-(j-1)}\omega_{\alpha+j}(t-t_{n-1})$. We define

$$\mathcal{D}_{i\mu}^{n\bar{\ell}} = \int_{I_n} \omega_\mu(t-t_\ell)\psi_{ni}(t)\,dt,$$

so that, recalling (2.6) and differentiating (2.9),

$$H_{ij}^{n\bar{\ell}} = k_\ell^{-(j-1)}[\mathcal{D}_{i,\alpha+j-1}^{n,\bar{\ell}+1} - \mathcal{D}_{i,\alpha+j-1}^{n,\bar{\ell}}] - \sum_{p=0}^{j-3} k_\ell^{-p}\psi_{\ell,j-p}(t_\ell)\mathcal{D}_{i,\alpha+p}^{n\bar{\ell}}$$

for $1 \le \ell \le n-1$, with $H_{ij}^{n0} = k_n^{-(j-1)}\mathcal{D}_{i,\alpha+j-1}^{n1}$, and repeated integration by parts gives

$$\mathcal{D}_{i\mu}^{n\bar{\ell}} = \sum_{q=0}^{i-1}(-1)^q k_n^{-q}[\omega_{\mu+q+1}(t-t_\ell)\psi_{n,i-q}(t)]_{t=t_{n-1}}^{t_n}.$$

In the case of a uniform step size $k_n = k = T/N$, we have $t_n - t_\ell = (n-\ell)k$ and find that

$$H_{ij}^{n\bar{\ell}} = k^\alpha H_{ij}^{\bar{\ell}} \quad \text{and} \quad \mathcal{D}_{i\mu}^{n\bar{\ell}} = k^\mu \mathcal{D}_{i\mu}^{\bar{\ell}},$$

where

$$H_{ij}^{\bar{\ell}} = \mathcal{D}_{i,\alpha+j-1}^{\bar{\ell}+1} - \mathcal{D}_{i,\alpha+j-1}^{\bar{\ell}} - \sum_{p=0}^{j-2} \frac{\mathcal{D}_{i,\alpha+p}^{\bar{\ell}}}{(j-p-1)!} \quad \text{for } 1 \le \ell \le n-1$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

with $H^0_{ij} = \mathcal{D}^1_{i,\alpha+j-1}$ and

$$\mathcal{D}^{\bar\ell}_{i\mu} = (-1)^{i-1}[\omega_{\mu+i}(\bar\ell) - \omega_{\mu+i}(\bar\ell - 1)] + \sum_{q=0}^{i-2} \frac{(-1)^q}{(i-q-1)!}\,\omega_{\mu+q+1}(\bar\ell).$$

However, as noted in the Introduction, if $\bar\ell = n - \ell$ is large then these formulae can suffer from cancellation of significant digits. In practice, the problem is most acute if we want to resolve the solution u accurately for t near zero, in which case a strong mesh grading is required so that the initial step sizes k_n are very small. For this reason, and also to allow a convenient treatment of other choices for the basis functions ψ_{nj}, in the following sections we consider efficient use of quadratures to evaluate the coefficients $H^{n\bar\ell}_{ij}$.

3. Evaluation of the coefficients

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

$$\mathsf{t}_n(\tau) = \tfrac{1}{2}[(1-\tau)t_{n-1} + (1+\tau)t_n]$$

and let $\Psi_{nj}(\tau) = \psi_{nj}(t)$ for $t = \mathsf{t}_n(\tau)$ and $-1 \le \tau \le 1$. In this way, (2.4) and (2.5) imply that

$$G^n_{ij} = \Psi_{nj}(-1)\Psi_{ni}(-1) + \int_{-1}^{1} \Psi'_{nj}(\tau)\Psi_{ni}(\tau)\,d\tau, \tag{3.1}$$

$$K^{n,n-1}_{ij} = \Psi_{n-1,j}(+1)\Psi_{ni}(-1). \tag{3.2}$$

Both of these coefficients are readily computed; the remainder of this section is devoted to $H^{n\bar\ell}_{ij}$. The formulae in the next lemma allow us to compute H^{n0}_{ij} to machine precision via Gauss–Legendre and Gauss–Jacobi quadrature [5].

LEMMA 3.1. *If we define the polynomial*

$$\Phi^n_{ij}(y) = \frac{1}{2}\int_{-1}^{1} \Psi_{nj}[(1-y)(1+z)/2 - 1]\Psi'_{ni}[1 - (1-y)(1-z)/2]\,dz,$$

then

$$H^{n0}_{ij} = \frac{(k_n/2)^\alpha}{\Gamma(\alpha)}\Big(\Psi_{ni}(1)\int_{-1}^{1}(1-\sigma)^\alpha\Psi_{nj}(\sigma)\,d\sigma - \int_{-1}^{1}(1+y)^{\alpha-1}(1-y)\Phi^n_{ij}(y)\,dy\Big).$$

PROOF. Since $\rho^{n0}_{j\alpha}(t_{n-1}) = 0$, integration by parts gives

$$\begin{aligned} H^{n0}_{ij} &= \int_{I_n} (\rho^{n0}_{j\alpha})'(t)\psi_{ni}(t)\,dt = \rho^{n0}_{j\alpha}(t_n)\psi_{ni}(t_n) - \int_{I_n}\rho^{n0}_{j\alpha}(t)\psi'_{ni}(t)\,dt \\ &= \rho^{n0}_{j\alpha}(t_n)\Psi_{ni}(1) - \int_{-1}^{1}\rho^{n0}_{j\alpha}(\mathsf{t}_n(\tau))\Psi'_{ni}(\tau)\,d\tau \end{aligned}$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

and, since $\mathrm{t}_n(\tau) - \mathrm{t}_n(\sigma) = (\tau - \sigma)k_n/2$, the substitution $s = \mathrm{t}_n(\sigma)$ yields

$$\begin{aligned}\rho_{j\alpha}^{n0}(\mathrm{t}_n(\tau)) &= \frac{k_n}{2}\int_{-1}^{\tau} \omega_\alpha(\mathrm{t}_n(\tau) - \mathrm{t}_n(\sigma))\Psi_{nj}(\sigma)\,d\sigma \\ &= \frac{(k_n/2)^\alpha}{\Gamma(\alpha)}\int_{-1}^{\tau}(\tau - \sigma)^{\alpha-1}\Psi_{nj}(\sigma)\,d\sigma. \qquad (3.3)\end{aligned}$$

Thus,

$$H_{ij}^{n0} = \frac{(k_n/2)^\alpha}{\Gamma(\alpha)}\Big(\Psi_{ni}(1)\int_{-1}^{1}(1-\sigma)^{\alpha-1}\Psi_{nj}(\sigma)\,d\sigma - B_{ij}^n\Big),$$

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:

$$\begin{aligned}B_{ij}^n &= \int_{-1}^{1}\int_{-1}^{\tau}(1+y)^{\alpha-1}\Psi_{nj}(\tau - y - 1)\,dy\,\Psi_{ni}'(\tau)\,d\tau \\ &= \int_{-1}^{1}(1+y)^{\alpha-1}\int_{y}^{1}\Psi_{nj}(\tau - y - 1)\Psi_{ni}'(\tau)\,d\tau\,dy.\end{aligned}$$

The substitution $\tau = [(1-z)y + (1+z)]/2$ then yields

$$\int_{y}^{1}\Psi_{nj}(\tau - y - 1)\Psi_{ni}'(\tau)\,d\tau = (1-y)\Phi_{ij}^n(y),$$

implying the desired formula for H_{ij}^{n0}. □

To evaluate $H_{ij}^{n,n-\ell}$ for $\ell \le n-1$, we introduce the notation

$$t_{n-1/2} = \mathrm{t}_n(0) = (t_{n-1} + t_n)/2 \quad \text{and} \quad D_{n\bar\ell} = D_{n,n-\ell} = t_{n-1/2} - t_{\ell-1/2},$$

with $\Delta_{n\bar\ell}(\tau,\sigma) = \Delta_{n,n-\ell}(\tau,\sigma) = (\tau k_n - \sigma k_\ell)/(2D_{n\bar\ell})$, so that

$$\mathrm{t}_n(\tau) - \mathrm{t}_\ell(\sigma) = D_{n\bar\ell}(1 + \Delta_{n\bar\ell}(\tau,\sigma)).$$

LEMMA 3.2. *If* $1 \le \ell \le n-1$, *then*

$$H_{ij}^{n\bar\ell} = \frac{D_{n\bar\ell}^{\alpha-1}}{\Gamma(\alpha)}\frac{k_\ell}{2}[\Psi_{ni}(1)\mathcal{A}_j^{n\bar\ell}(1) - \Psi_{ni}(-1)\mathcal{A}_j^{n\bar\ell}(-1) - C_{ij}^{n\bar\ell}],$$

where

$$\mathcal{A}_j^{n\bar\ell}(\tau) = \int_{-1}^{1}[1 + \Delta_{n\bar\ell}(\tau,\sigma)]^{\alpha-1}\Psi_{\ell j}(\sigma)\,d\sigma \quad \text{and} \quad C_{ij}^{n\bar\ell} = \int_{-1}^{1}\Psi_{ni}'(\tau)\mathcal{A}_j^{n\bar\ell}(\tau)\,d\tau.$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

PROOF. Integrating by parts,

$$H_{ij}^{n\bar{\ell}} = \rho_{j\alpha}^{n\bar{\ell}}(t_n)\psi_{ni}(t_n) - \rho_{j\alpha}^{n\bar{\ell}}(t_{n-1})\psi_{ni}(t_{n-1}) - \int_{I_n} \rho_{j\alpha}^{n\bar{\ell}}(t)\psi'_{ni}(t)\,dt$$
$$= \rho_{j\alpha}^{n\bar{\ell}}(\mathrm{t}_n(1))\Psi_{ni}(1) - \rho_{j\alpha}^{n\bar{\ell}}(\mathrm{t}_n(-1))\Psi_{ni}(-1) - \int_{-1}^{1} \rho_{j\alpha}^{n\bar{\ell}}(\mathrm{t}_n(\tau))\Psi'_{ni}(\tau)\,d\tau$$

and the substitution $s = \mathrm{t}_\ell(\sigma)$ gives

$$\rho_{j\alpha}^{n\bar{\ell}}(\mathrm{t}_n(\tau)) = \frac{D_{n\bar{\ell}}^{\alpha-1}}{\Gamma(\alpha)} \frac{k_\ell}{2} \int_{-1}^{1} (1 + \Delta_{n\bar{\ell}}(\tau,\sigma))^{\alpha-1}\Psi_{\ell j}(\sigma)\,d\sigma,$$

so the formula for $H_{ij}^{n\bar{\ell}}$ follows at once. □

Notice that

$$1 + \Delta_{n\bar{\ell}}(1,\sigma) = \frac{2(t_n - t_\ell) + (1-\sigma)k_\ell}{k_n + 2(t_{n-1} - t_\ell) + k_\ell} > 0 \quad \text{for } 1 \le \ell \le n-1,$$

so the integrand of $\mathcal{A}_{ij}^{n\bar{\ell}}(1)$ is always a smooth function of σ. However,

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

so the integrands of $\mathcal{A}_j^{n\bar{\ell}}(-1)$ and $C_j^{n\bar{\ell}}$ are weakly singular if $\bar{\ell} = 1$ (that is, if $\ell = n-1$). The next lemma provides alternative expressions that are amenable to Gauss–Jacobi and Gauss–Legendre quadrature.

LEMMA 3.3. *Let $\varrho_n = k_n/k_{n-1}$. Then*

$$\mathcal{A}_j^{n1}(1) = (1+\varrho_n)^{1-\alpha} \int_{-1}^{1} (2\varrho_n + 1 - \sigma)^{\alpha-1}\Psi_{n-1,j}(\sigma)\,d\sigma,$$
$$\mathcal{A}_j^{n1}(-1) = (1+\varrho_n)^{1-\alpha} \int_{-1}^{1} (1-\sigma)^{\alpha-1}\Psi_{n-1,j}(\sigma)\,d\sigma,$$
$$C_{ij}^{n1} = (1+\varrho_n)^{1-\alpha}\bigg[\int_{-1}^{1} (1+\tau)^{\alpha}\Psi'_{ni}(\tau) \int_0^1 (\varrho_n + z)^{\alpha-1}\Psi_{n-1,j}(1 - z(1+\tau))\,dz\,d\tau$$
$$+ \int_{-1}^{1} (1-\sigma)^{\alpha}\Psi_{n-1,j}(\sigma) \int_0^1 (\varrho_n z + 1)^{\alpha-1}\Psi'_{ni}(z(1-\sigma) - 1)\,dz\,d\sigma\bigg].$$

PROOF. The formulae for $\mathcal{A}_j^{n\bar{\ell}}(\pm 1)$ follow from

$$1 + \Delta_{n1}(1,\sigma) = \frac{2k_n + (1-\sigma)k_{n-1}}{k_n + k_{n-1}} \quad \text{and} \quad 1 + \Delta_{n1}(-1,\sigma) = \frac{(1-\sigma)k_{n-1}}{k_n + k_{n-1}}.$$

To deal with $C_{ij}^{n,1}$, we begin by mapping $[-1,1]^2$ onto $[0,2]^2$ with the substitution $(\tau,\sigma) = (x-1, 1-y)$. In this way, the singularity at $(\tau,\sigma) = (-1,1)$ moves

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

to $(x, y) = (0, 0)$, and

$$C_{ij}^{n1} = \int_0^2 \int_0^2 [1 + \Delta_{n1}(x-1, 1-y)]^{\alpha-1} \Psi_{n-1,j}(1-y)\Psi'_{ni}(x-1)\, dx\, dy$$

with $1 + \Delta_{n1}(x-1, 1-y) = (xk_n + yk_{n-1})/(k_n + k_{n-1})$. By splitting the integration domain $[0, 2]^2$ into the triangular halves where $x > y$ and $x < y$,

$$\begin{aligned} C_{ij}^{n1} &= \int_0^2 \Psi'_{ni}(x-1) \int_0^x \left(\frac{xk_n + yk_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi_{n-1,j}(1-y)\, dy\, dx \\ &\quad + \int_0^2 \Psi_{n-1,j}(1-y) \int_0^y \left(\frac{xk_n + yk_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi'_{ni}(x-1)\, dx\, dy. \end{aligned} \tag{3.4}$$

The substitution $y = zx$ transforms the inner integral in the first term of (3.4) 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

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

Thus,

$$\begin{aligned} C_{ij}^{n1} &= \int_0^2 x^\alpha \Psi'_{ni}(x-1) \int_0^1 \left(\frac{k_n + zk_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi_{n-1,j}(1-zx)\, dz\, dx \\ &\quad + \int_0^2 y^\alpha \Psi_{n-1,j}(1-y) \int_0^1 \left(\frac{zk_n + k_{n-1}}{k_n + k_{n-1}}\right)^{\alpha-1} \Psi'_{ni}(zy-1)\, dz\, dy \end{aligned}$$

and the substitutions $x = 1 + \tau$ and $y = 1 - \sigma$ now yield the desired formula for C_{ij}^{n1}. □

We also have the following alternative representation.

LEMMA 3.4. *If* $1 \le \ell \le n-2$, *then*

$$H_{ij}^{n\bar{\ell}} = -\frac{1-\alpha}{\Gamma(\alpha)} \frac{k_n k_\ell}{4} D_{n\bar{\ell}}^{\alpha-2} \int_{-1}^1 \Psi_{ni}(\tau) \int_{-1}^1 [1 + \Delta_{n\bar{\ell}}(\tau, \sigma)]^{\alpha-2} \Psi_{\ell j}(\sigma)\, d\sigma\, d\tau.$$

PROOF. If $1 \le \ell \le n-2$, then $(\rho_{j\alpha}^{n\bar{\ell}})'(t) = \int_{I_\ell} \omega_{\alpha-1}(t-s)\psi_{\ell j}(s)\, ds$ for $t > t_\ell$ and so

$$H_{ij}^{n\bar{\ell}} = \int_{I_n} \psi_{ni}(t) \int_{I_\ell} \omega_{\alpha-1}(t-s)\psi_{\ell j}(s)\, ds. \tag{3.5}$$

The result now follows via the substitutions $t = \mathrm{t}_n(\tau)$ and $s = \mathrm{t}_\ell(\sigma)$, noting that $\Gamma(\alpha) = (\alpha-1)\Gamma(\alpha-1)$. □

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

REMARK 3.5. If the time levels are uniformly spaced, and if the reference basis functions are the same for each subinterval, say

$$k_\ell = k, \quad r_\ell = r \quad \text{and} \quad \Psi_{\ell j} = \Psi_j \quad \text{for } 1 \le \ell \le n \quad \text{and} \quad 1 \le j \le r,$$

then $D_{n\bar\ell} = \bar\ell k$ and $\Delta_{n\bar\ell}(\tau,\sigma) = (\tau-\sigma)/(2\bar\ell)$, so the formulae of Lemma 3.2 show that $H_{ij}^{n\bar\ell}$ depends on n and ℓ only through the difference $\bar\ell = n-\ell$ (for further details, see Example 5.5 in Section 5).

4. Spatial discretization

The initial-boundary value problem (1.1) is known to be well posed [6, 8, 11]. 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 $u : (0,T] \to H_0^1(\Omega)$ satisfies

$$\langle \partial_t u, v\rangle + a(\partial_t^{1-\alpha} u, v) = \langle f(t), v\rangle \quad \text{for } v \in H_0^1(\Omega) \text{ and } 0 < t \le T.$$

We choose a finite-dimensional subspace $V_n \subseteq H_0^1(\Omega)$ for $0 \le n \le N$ and form the vector $\boldsymbol{V} = (V_1,\ldots,V_N)$. For example, V_n might be a (conforming) finite-element space constructed using a triangulation of Ω. Our trial space $\mathcal{X} = \mathcal{X}(\boldsymbol{t},\boldsymbol{r},\boldsymbol{V})$ then consists of the functions $X : I \to H_0^1(\Omega)$ 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. Generalizing (2.2), the DG solution $U \in \mathcal{X}$ of (1.1) satisfies

$$\langle [\![U]\!]^{n-1}, X_+^{n-1}\rangle + \int_{I_n} \langle \partial_t U, X\rangle\,dt + \int_{I_n} a(\partial_t^{1-\alpha} U, X)\,dt = \int_{I_n} \langle f(t), X\rangle\,dt \tag{4.1}$$

for $X \in \mathbb{P}_{r_n-1}(I_n; V_n)$ and $1 \le n \le N$, with $U_-^0 = U_0$ 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 (2.3), the coefficient U^{nj} is now a function in V_n, so there exist real numbers U_q^{nj} such that

$$U^{nj}(x) = \sum_{q=1}^{P_n} U_q^{nj} \phi_{nq}(x) \quad \text{for } x \in \Omega;$$

for example, $U_q^{nj} = U^{nj}(x_{nq})$ if x_{nq} is the qth free node of a finite-element mesh and if ϕ_{nq} is the corresponding nodal basis function. Similarly, for the discrete initial data, there are real numbers U_{0q} such that

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

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

Choosing $X(x,t) = \psi_{ni}(t)\phi_{nq}(x)$ in (4.1), we find that the equations (2.7) for time stepping the scalar problem generalize to

$$\sum_{j=1}^{r_n}\sum_{q=1}^{P_n}(G_{ij}^n M_{pq}^{nn} + H_{ij}^{n0}A_{pq}^{nn})U_q^{nj} = F_p^{ni} - \sum_{\ell=1}^{n-1}\sum_{j=1}^{r_\ell}\sum_{q=1}^{P_\ell} H_{ij}^{n,n-\ell}A_{pq}^{n\ell}U_q^{\ell j}$$
$$+\begin{cases}\psi_{1i}(0)\displaystyle\sum_{q=1}^{P_0}M_{pq}^{10}U_{0q}, & n=1,\\ \displaystyle\sum_{j=1}^{r_{n-1}}\sum_{q=1}^{P_{n-1}}K_{ij}^{n,n-1}M_{pq}^{n,n-1}U_q^{n-1,j}, & 2\le n\le N,\end{cases} \tag{4.2}$$

where

$$M_{pq}^{n\ell} = \langle\phi_{\ell q},\phi_{np}\rangle,\quad A_{pq}^{n\ell} = a(\phi_{\ell q},\phi_{np}),\quad F_p^{ni} = \int_{I_n}\langle f(t),\phi_{np}\rangle\psi_{ni}(t)\,dt.$$

By introducing the $P_n \times P_\ell$ mass matrix $\boldsymbol{M}^{n\ell} = [M_{pq}^{n\ell}]$ and stiffness matrix $\boldsymbol{A}^{n\ell} = [A_{pq}^{n\ell}]$, and forming the column vectors $\boldsymbol{U}^{nj} = [U_1^{nj}, U_2^{nj}, \dots, U_{P_n}^{nj}]^\top$, $\boldsymbol{F}^{nj} = [F_1^{nj}, F_2^{nj}, \dots, F_{P_n}^{nj}]^\top$ and $\boldsymbol{U}_0 = [U_{01}, U_{02}, \dots, U_{0P_0}]^\top$, we can rewrite the equations (4.2) as

$$\sum_{j=1}^{r_n}(G_{ij}^n\boldsymbol{M}^{nn} + H_{ij}^{n0}\boldsymbol{A}^{nn})\boldsymbol{U}^{nj} = \boldsymbol{F}^{ni} - \sum_{\ell=1}^{n-1}\sum_{j=1}^{r_\ell}H_{ij}^{n,n-\ell}\boldsymbol{A}^{n\ell}\boldsymbol{U}^{\ell j}$$
$$+\begin{cases}\psi_{1i}(0)\boldsymbol{M}^{10}\boldsymbol{U}_0, & n=1,\\ \displaystyle\sum_{j=1}^{r_{n-1}}K_{ij}^{n,n-1}\boldsymbol{M}^{n,n-1}\boldsymbol{U}^{n-1,j}, & 2\le n\le N.\end{cases} \tag{4.3}$$

To write (4.3) even more compactly, define the $r_n \times r_n$ matrix $\boldsymbol{G}^n = [G_{ij}^n]$ and the $r_n \times r_\ell$ matrix $\boldsymbol{H}^{n\bar{\ell}} = [H_{ij}^{n\bar{\ell}}]$, together with the (block) column vectors $\boldsymbol{U}^n = [\boldsymbol{U}^{n1}, \boldsymbol{U}^{n2}, \dots, \boldsymbol{U}^{nr_n}]^\top$ and $\boldsymbol{F}^n = [\boldsymbol{F}^{n1}, \boldsymbol{F}^{n2}, \dots, \boldsymbol{F}^{nr_n}]^\top$. We also form the $r_n \times r_{n-1}$ matrix $\boldsymbol{K}^{n,n-1} = [K_{ij}^{n,n-1}]$ and the column vector $\boldsymbol{\psi}_+^{\boldsymbol{0}} = [\psi_{11}(0), \psi_{12}(0), \dots, \psi_{1r_n}(0)]^\top$. By utilizing the Kronecker product, the linear system (4.3) then takes the form

$$(\boldsymbol{G}^n\otimes\boldsymbol{M}^{nn} + \boldsymbol{H}^{n0}\otimes\boldsymbol{A}^{nn})\boldsymbol{U}^n = \boldsymbol{F}^n - \sum_{\ell=1}^{n-1}(\boldsymbol{H}^{n,n-\ell}\otimes\boldsymbol{A}^{n\ell})\boldsymbol{U}^\ell$$
$$+\begin{cases}(\boldsymbol{\psi}_+^0\otimes\boldsymbol{M}^{10})\boldsymbol{U}_0, & n=1,\\ (\boldsymbol{K}^{n,n-1}\otimes\boldsymbol{M}^{n,n-1})\boldsymbol{U}^{n-1,j}, & 2\le n\le N.\end{cases} \tag{4.4}$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

5. Legendre polynomials

Let $P_0, P_1, P_2, \ldots$ denote the Legendre polynomials with the standard normalization $P_j(1) = 1$ for all $j \geq 0$. By choosing

$$\Psi_{nj}(\tau) = P_{j-1}(\tau), \tag{5.1}$$

we obtain a convenient and well-conditioned basis for $\mathbb{P}_{r_n-1}$ with the properties

$$\int_{-1}^{1} \Psi_{nj}(\tau)\Psi_{ni}(\tau)\, d\tau = \frac{2\delta_{ij}}{2j-1} \quad \text{and} \quad \Psi_{nj}(-\tau) = (-1)^{j-1}\Psi_{nj}(\tau).$$

LEMMA 5.1. *With the choice of basis functions in* (5.1),

$$\Psi_{nj}(1) = 1 \quad \textit{and} \quad \Psi_{nj}(-1) = (-1)^{j-1}, \tag{5.2}$$

and the coefficients (3.1) *and* (3.2) *are given by*

$$K_{ij}^{n,n-1} = (-1)^{i-1} \quad \textit{and} \quad G_{ij}^{n} = \begin{cases} (-1)^{i+j} & \textit{if } i \geq j, \\ 1 & \textit{if } i < j. \end{cases}$$

PROOF. The properties (5.2) follow from $P_j(1) = 1$ and $P_j(-1) = (-1)^j$. Hence, the formula for $K_{ij}^{n,n-1}$ follows from (3.2) and, by (3.1),

$$G_{ij}^{n} = (-1)^{i+j} + E_{ij} \quad \text{where } E_{ij} = \int_{-1}^{1} P'_{j-1}(\tau)P_{i-1}(\tau)\, d\tau.$$

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

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

and hence $G_{ij}^{n} = 1$. □

EXAMPLE 5.2. If $r_n = 4$ and $r_{n-1} = 3$, then

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

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

LEMMA 5.3. *With the choice of basis functions in* (5.1),

$$H_{ji}^{n0} = (-1)^{i+j} H_{ij}^{n0} \quad \textit{for } i, j \in \{1, 2, \ldots, r_n\}.$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

PROOF. We see from (3.3) that $(\rho^{n\bar{\ell}}_{i\alpha})(\mathrm{t}_n(\tau)) = (k_n/2)^\alpha (BP_{i-1})(\tau)$, where $(Bv)(\tau) = \int_{-1}^{\tau} \omega_\alpha(\tau-\sigma)v(\sigma)\,d\sigma$, so, by (2.8),

$$H^{n0}_{ji} = \Big(\frac{k_n}{2}\Big)^\alpha \int_{-1}^{1} (BP_{i-1})'(\tau)P_{j-1}(\tau)\,d\tau = -\Big(\frac{k_n}{2}\Big)^\alpha \int_{-1}^{1} P_{i-1}(\sigma)(B^*P_{j-1})'(\sigma)\,d\sigma$$

with $(B^*v)(\sigma) = \int_\sigma^1 \omega_\alpha(\tau-\sigma)v(\tau)\,d\tau$. Let $(RV)(\tau) = V(-\tau)$. A short calculation shows that $RB^* = BR$, so

$$\begin{aligned}(B^*P_{j-1})'(-\sigma) &= -\frac{d}{d\sigma}[(B^*P_{j-1})(-\sigma)] = -\frac{d}{d\sigma}(RB^*P_{j-1})(\sigma)\\ &= -(BRP_{j-1})'(\sigma) = (-1)^j(BP_{j-1})'(\sigma)\end{aligned}$$

and, therefore, using the substitution $\sigma = -x$,

$$\begin{aligned}H^{n0}_{ji} &= (-1)^{j+1}\Big(\frac{k_n}{2}\Big)^\alpha \int_{-1}^{1} P_{i-1}(-x)(BP_{j-1})'(x)\,dx\\ &= (-1)^{i+j}\Big(\frac{k_n}{2}\Big)^\alpha \int_{-1}^{1} (BP_{j-1})'(x)P_{i-1}(x)\,dx = (-1)^{i+j}H^{n0}_{ij},\end{aligned}$$

as claimed. □

REMARK 5.4. In the limit as $\alpha \to 1$, we see from Remark 2.1 that

$$H^{n0}_{ij} \to \int_{I_n} \psi_{nj}(t)\psi_{ni}(t)\,dt = \frac{k_n}{2}\int_{-1}^{1} \Psi_j(\tau)\Psi_i(\tau)\,d\tau = \frac{k_n\delta_{ij}}{2j-1}.$$

EXAMPLE 5.5. Consider the uniform case $k_n = k$, $r_n = r$ and $\Psi_{nj} = \Psi_j$ for $1 \le n \le N$ (as in Remark 3.5) with $\Psi_j(\tau) = P_{j-1}(\tau)$ as above. We then have

$$H^{n\bar{\ell}}_{ij} = k^\alpha H^{\bar{\ell}}_{ij} \quad \text{for } 1 \le \ell \le n \le N \text{ and } i,j \in \{1,2,\ldots,r\},$$

where, by Lemma 3.1,

$$H^0_{ij} = \frac{1}{2^\alpha\Gamma(\alpha)}\Big(\int_{-1}^{1}(1-\sigma)^\alpha P_{j-1}(\sigma)\,d\sigma - \int_{-1}^{1}(1+y)^{\alpha-1}(1-y)\Phi_{ij}(y)\,dy\Big) \tag{5.3}$$

with

$$\Phi_{ij}(y) = \frac{1}{2}\int_{-1}^{1} P_{j-1}\Big(\frac{1}{2}(1-y)(1+z)-1\Big)P'_{i-1}\Big(1-\frac{1}{2}(1-y)(1-z)\Big)\,dz \tag{5.4}$$

and, by Lemma 3.2,

$$H^{\bar{\ell}}_{ij} = \frac{\bar{\ell}^{\alpha-1}}{2\Gamma(\alpha)}\big(\mathcal{A}^{\bar{\ell}}_j(1) + (-1)^i\mathcal{A}^{\bar{\ell}}_j(-1) - C^{\bar{\ell}}_{ij}\big) \quad \text{for } \ell \ge 1$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

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

$$\mathcal{A}_j^{\bar\ell}(\tau) = \int_{-1}^{1} (1 + \Delta_{\bar\ell}(\tau - \sigma))^{\alpha-1} P_{j-1}(\sigma)\, d\sigma \quad \text{and} \quad C_{ij}^{\bar\ell} = \int_{-1}^{1} P'_{i-1}(\tau)\mathcal{A}_j^{n\bar\ell}(\tau)\, d\tau.$$

Moreover, Lemma 3.3 provides alternative expressions when $\bar\ell = 1$:

$$\begin{aligned} \mathcal{A}_j^{1}(1) &= 2^{1-\alpha} \int_{-1}^{1} (3 - \sigma)^{\alpha-1} P_{j-1}(\sigma)\, d\sigma, \\ \mathcal{A}_j^{1}(-1) &= 2^{1-\alpha} \int_{-1}^{1} (1 - \sigma)^{\alpha-1} P_{j-1}(\sigma)\, d\sigma \end{aligned} \tag{5.5}$$

and

$$\begin{aligned} C_{ij}^{1} = 2^{1-\alpha}\Big(&\int_{-1}^{1} (1+\tau)^{\alpha} P'_{i-1}(\tau) \int_{0}^{1} (1+z)^{\alpha-1} P_{j-1}(1 - z(1+\tau))\, dz\, d\tau \\ &+ \int_{-1}^{1} (1-\sigma)^{\alpha} P_{j-1}(\sigma) \int_{0}^{1} (z+1)^{\alpha-1} P'_{i-1}(z(1-\sigma) - 1)\, dz\, d\sigma \Big). \end{aligned} \tag{5.6}$$

Likewise, Lemma 3.4 provides an alternative expression for $\bar\ell \geq 2$:

$$H_{ij}^{\bar\ell} = -\frac{1-\alpha}{4\Gamma(\alpha)}\, \bar\ell^{\alpha-2} \int_{-1}^{1} P_{i-1}(\tau) \int_{-1}^{1} (1 + \Delta_{\bar\ell}(\tau - \sigma))^{\alpha-2} P_{j-1}(\sigma)\, d\sigma\, d\tau. \tag{5.7}$$

Finally, by arguing as in the proof of Lemma 5.3, we can show that

$$H_{ji}^{\bar\ell} = (-1)^{i+j} H_{ij}^{\bar\ell} \quad \text{for all } \bar\ell \geq 0. \tag{5.8}$$

6. Reconstruction

Throughout this section, we continue to use the Legendre basis (5.1). We may have some insight into the DG method by considering the trivial case of (1.1) when $A = 0$, that is, $\partial_t u = f(t)$ for $0 < t \leq T$ with $u(0) = u_0$. The DG scheme (4.1) then reduces to

$$\langle [\![U]\!]^{n-1}, X_+^{n}\rangle + \int_{I_n} \langle \partial_t U, X\rangle\, dt = \int_{I_n} \langle \partial_t u, X\rangle\, dt \tag{6.1}$$

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

$$\mathcal{Q}_{n\ell} = \mathcal{P}_n \mathcal{P}_{n-1} \cdots \mathcal{P}_{\ell+1} \quad \text{for } 0 \leq \ell \leq n-1.$$

LEMMA 6.1. *If $A = 0$, then for $1 \leq n \leq N$ the* DG *solution $U \in \mathcal{X}$ satisfies*

$$U_-^n - \mathcal{P}_n u(t_n) = \mathcal{Q}_{n0}(U_0 - \mathcal{P}_0 u_0) + \sum_{\ell=0}^{n-1} \mathcal{Q}_{n\ell}(\mathcal{P}_\ell - I)u(t_\ell). \tag{6.2}$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

PROOF. Integrating by parts in (6.1),

$$\langle U_-^n - u(t_n), X_-^n\rangle = \langle U_-^{n-1} - u(t_{n-1}), X_+^{n-1}\rangle + \int_{I_n} \langle U - u, \partial_t X\rangle\, dt. \tag{6.3}$$

Given $v \in V_n$, by choosing the constant function $X(t) = v$ for $t \in I_n$ we deduce that $\langle U_-^n - u(t_n), v\rangle = \langle U_-^{n-1} - u(t_{n-1}), v\rangle$ and so

$$\mathcal{P}_n(U_-^n - u(t_n)) = \mathcal{P}_n(U_-^{n-1} - u(t_{n-1})).$$

Since $\mathcal{P}_n U_-^n = U_-^n$,

$$\begin{aligned} U_-^n - \mathcal{P}_n u(t_n) &= \mathcal{P}_n(\mathcal{P}_{n-1} + I - \mathcal{P}_{n-1})\{U_-^{n-1} - u(t_{n-1})\} \\ &= \mathcal{P}_n\{U_-^{n-1} - \mathcal{P}_{n-1}u(t_{n-1})\} + \mathcal{P}_n(\mathcal{P}_{n-1} - I)u(t_{n-1}) \end{aligned}$$

and, in particular, (6.2) holds for $n = 1$:

$$U_-^1 - \mathcal{P}_1 u(t_1) = \mathcal{P}_1(U_0 - \mathcal{P}_0 u_0) + \mathcal{P}_1(\mathcal{P}_0 - I)u_0 = \mathcal{Q}_{10}(U_0 - \mathcal{P}_0 u_0) + \mathcal{Q}_{10}(\mathcal{P}_0 - I)u_0.$$

The general case follows by finite induction on n. □

For the remainder of this section, we will assume that

$$U_0 = \mathcal{P}_0 u_0 \quad \text{and} \quad V_0 \supseteq V_1 \supseteq V_2 \supseteq \cdots \supseteq V_N. \tag{6.4}$$

Hence, $\mathcal{P}_{\ell+1}(\mathcal{P}_\ell - I) = 0$ for $0 \le \ell \le N-1$, so $\mathcal{Q}_{n\ell} = \mathcal{P}_n$ and, by Lemma 6.1,

$$U_-^n = \mathcal{P}_n u(t_n) \quad \text{for } 0 \le n \le N. \tag{6.5}$$

Therefore, by (6.3),

$$\int_{I_n} \langle U - u, \partial_t X\rangle\, dt = 0 \quad \text{for all } X \in \mathbb{P}_n(I_n; V_n), \tag{6.6}$$

leading to the following explicit representation for U.

LEMMA 6.2. *If $A = 0$ and (6.4) holds, then*

$$U(t) = \sum_{j=1}^{r_n-1} a_{nj}\psi_{nj}(t) + \tilde{a}_n \psi_{nr_n}(t) \quad \textit{for } t \in I_n, \tag{6.7}$$

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

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

orthogonality property of the ψ_{nj} (see Remark 5.4). The formula for $\tilde{a}_n$ follows from (6.5), because $\psi_{nj}(t_n) = P_{j-1}(1) = 1$ for all j. □

We have a Peano kernel G_r [3, Ch. 5, Section 2.4] for the Fourier–Legendre expansion of degree r,

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

assuming that $f : [-1,1] \to \mathbb{R}$ is C^{r+1}, and also a Peano kernel $\mathsf{M}_j(\tau)$ for the jth coefficient:

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

Thus, if $t = \mathsf{t}_n(\tau)$ and $s = \mathsf{t}_n(\sigma)$, and if we define the local Peano kernels

$$\mathsf{g}_{nr}(t,s) = (k_n/2)^r \mathsf{G}_r(\tau,\sigma) \quad \text{and} \quad \mathsf{m}_{nj}(t) = (k_n/2)^{j-2}\mathsf{M}_j(\tau),$$

then

$$\mathcal{P}_n u(t) = \sum_{j=1}^{r_n+1} a_{nj}\psi_{nj}(t) + \int_{I_n} \mathsf{g}_{nr_n}(t,s)\mathcal{P}_n u^{(r_n+1)}(s)\, ds \quad \text{for } t \in I_n \tag{6.8}$$

and

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

It follows that $a_{nj} = O(k_n^{j-1})$, provided u is C^{j-1} on $\bar{I}_n$.

THEOREM 6.3. *Assume that $A = 0$ and the conditions in (6.4). If $u : \bar{I}_n \to L^2(\Omega)$ is C^{r_n+1}, then $a_{n,r_n+1} = O(k_n^{r_n})$ and*

$$\mathcal{P}_n u(t) - U(t) = a_{n,r_n+1}[\psi_{n,r_n+1}(t) - \psi_{n,r_n}(t)] + O(k_n^{r_n+1}) \quad \textit{for } t \in I_n. \tag{6.9}$$

PROOF. Subtracting (6.7) from (6.8),

$$\mathcal{P}_n u(t) - U(t) = (a_{n,r_n} - \tilde{a}_n)\psi_{nr_n}(t) + a_{n,r_n+1}\psi_{n,r_n+1}(t) + O(k_n^{r_n+1})$$

for $t \in I_n$. Since $U_-^n = \mathcal{P}_n u(t_n)$ and $\psi_{n,r_n}(t_n) = \psi_{n,r_n+1}(t_n) = 1$, taking the limit as $t \to t_n$ yields $a_{n,r_n} - \tilde{a}_n = -a_{n,r_n+1} + O(k_n^{r_n+1})$. □

COROLLARY 6.4. $\mathcal{P}_n [\![U]\!]^{n-1} = 2(-1)^{r_n+1} a_{n,r_n+1} + O(k_n^{r_n+1})$.

PROOF. As $t \to t_{n-1}^+$, the left-hand side of (6.9) tends to

$$\begin{aligned}\mathcal{P}_n u(t_{n-1}) - U_+^{n-1} &= \mathcal{P}_n(I - \mathcal{P}_{n-1} + \mathcal{P}_{n-1})u(t_{n-1}) - U_+^{n-1} = \mathcal{P}_n U_-^{n-1} - U_+^{n-1} \\ &= -\mathcal{P}_n(U_+^{n-1} - U_-^{n-1}) = -\mathcal{P}_n [\![U]\!]^{n-1}\end{aligned}$$

and, on the right-hand side, $\psi_{n,r_n+1}(t) - \psi_{n,r_n}(t)$ tends to

$$P_{r_n}(-1) - P_{r_n-1}(-1) = (-1)^{r_n} - (-1)^{r_n-1} = 2(-1)^{r_n}. \qquad \square$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

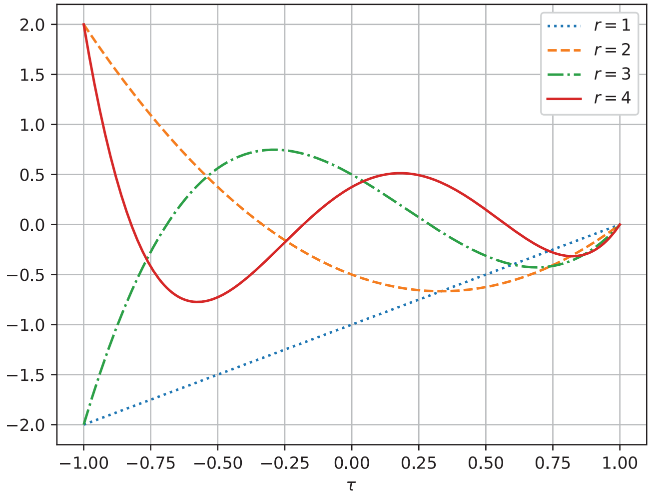

FIGURE 1. The polynomials $P_r(\tau) - P_{r-1}(\tau)$.

In light of Theorem 6.3, we consider the polynomials

$$\psi_{n,r_n+1}(t) - \psi_{n,r_n}(t) = \Psi_{r_n+1}(\tau) - \Psi_{r_n}(\tau) = P_{r_n}(\tau) - P_{r_n-1}(\tau).$$

As illustrated in Figure 1, there are $r+1$ points

$$-1 = \tau_{r0} < \tau_{r1} < \cdots < \tau_{rr} = 1$$

such that $(P_r - P_{r-1})(\tau_{rj}) = 0$ for $1 \le j \le r$. In fact, the r zeros $\tau_{r1}, \tau_{r2}, \ldots, \tau_{rr}$ are the points of a right-Radau quadrature rule [5, Ch. 9] on the interval $[-1, 1]$. We put

$$t^*_{nj} = \mathrm{t}_n(\tau_{r_nj}) \quad \text{for } 0 \le j \le r_n, \tag{6.10}$$

so that $t_{n-1} = t^*_{n0} < t^*_{n1} < \cdots < t^*_{nr_n} = t_n$ and $\psi_{n,r_n+1}(t^*_{nj}) - \psi_{n,r_n}(t^*_{nj}) = 0$ for $1 \le j \le r_n$.

From Theorem 6.3, $\mathcal{P}_n u(t) - U(t) = O(k_n^{r_n})$ for general $t \in I_n$, but $\mathcal{P}_n u(t^*_{nj}) - U(t^*_{nj}) = O(k_n^{r_n+1})$ for $1 \le j \le r_n$. Let $\widehat{\mathcal{X}}$ 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 $1 \le n \le N$. The "reconstruction" $\widehat{U} \in \widehat{\mathcal{X}}$ of $U \in \mathcal{X}$ is then defined by requiring that

$$\widehat{U}(t^*_{nj}) = U(t^*_{nj}) \quad \text{for } 1 \le j \le r_n - 1$$

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

$$\widehat{U}^{n-1}_+ = \mathcal{P}_n U^{n-1}_- \quad \text{and} \quad \widehat{U}^n_- = U^n_-.$$

Since $\widehat{U}|_{I_n}$ 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 $\widehat{U}$ is continuous at t_{n-1} if $V_{n-1} = V_n$, because $\mathcal{P}_n U^{n-1}_- = U^{n-1}_-$.

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

Makridakis and Nochetto [7] introduced the reconstruction in their analysis of a posteriori error bounds for parabolic PDEs. Since the polynomial $(U - \widehat{U})|_{I_n}$ has degree at most r_n and vanishes at t^*_{nj} for $1 \le n \le r_n$, it must be a multiple of $\psi_{n,r_n+1} - \psi_{nr_n}$. In fact, by taking limits as $t \to t^+_{n-1}$,

$$U(t) - \widehat{U}(t) = \tfrac{1}{2}(-1)^{r_n}\mathcal{P}_n[\![U]\!]^{n-1}[\psi_{n,r_n+1}(t) - \psi_{n,r_n}(t)] \quad \text{for } t \in I_n. \tag{6.11}$$

At the same time, by Theorem 6.3 and Corollary 6.4,

$$U(t) - \mathcal{P}_n u(t) = \tfrac{1}{2}(-1)^{r_n}\mathcal{P}_n[\![U]\!]^{n-1}[\psi_{n,r_n+1}(t) - \psi_{n,r_n}(t)] + O(k_n^{r_n+1}) \quad \text{for } t \in I_n, \tag{6.12}$$

implying that $\widehat{U} - \mathcal{P}_n u$ 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 $\widehat{U}$ in nontrivial cases of the fractional diffusion problem (1.1), that is, with $A \ne 0$. We hope that something similar to (6.12) 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 (2.3) and (6.11) imply that

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

where

$$\widehat{U}^{nj} = \begin{cases} U^{nj}, & 1 \le j \le r_n - 1, \\ U^{nr_n} + \tfrac{1}{2}(-1)^{r_n}\mathcal{P}_n[\![U]\!]^{n-1}, & j = r_n, \\ \tfrac{1}{2}(-1)^{r_n+1}\mathcal{P}_n[\![U]\!]^{n-1}, & j = r_n + 1 = \hat{r}_n. \end{cases}$$

7. Numerical experiments

A Julia package [9] provides functions to evaluate the coefficients G^n_{ij}, $K^{n,n-1}_{ij}$ and $H^{n\bar{\ell}}_{ij}$ 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 $\boldsymbol{H}^{\bar{\ell}}$ 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 5.5 apply. To get a sense of how the matrix entries $H^{\bar{\ell}}_{ij}$ behave, we computed

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

and

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

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

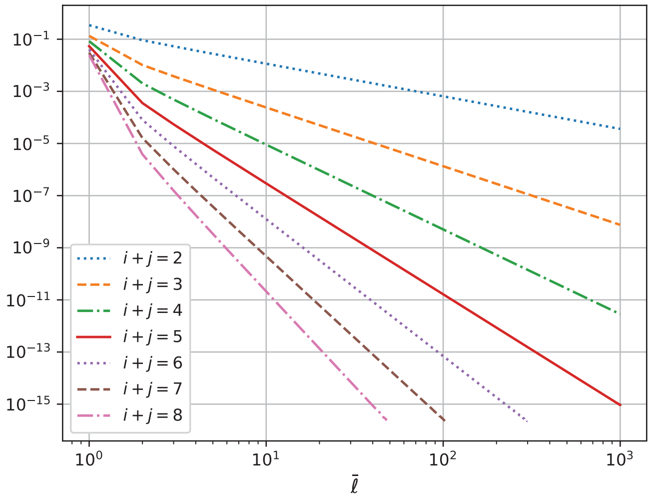

FIGURE 2. Decay of $\max_{i+j=m} |H^{\bar{\ell}}_{ij}|$ for increasing m and $\bar{\ell}$, when $\alpha = 3/4$.

which illustrate the property (5.8). The factor $(1 + \Delta_{\bar{\ell}}(\tau - \sigma))^{\alpha-2}$ in (5.7) becomes very smooth as $\bar{\ell}$ increases, with the result that $H^{\bar{\ell}}_{ij}$ decays rapidly to zero as $i + j$ increases. Even for $\bar{\ell} = 2$,

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

and Figure 2 illustrates 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 $M_\sigma = \lceil j/2 \rceil$ and $M_y = \lceil (i + j)/2 \rceil - 1$ points for the integrals with respect to σ and y in (5.3), and using $M_z = \lceil (i + j)/2 \rceil - 1$ points for the integral with respect to z in (5.4). Similarly, to compute $\mathcal{A}^1_j(-1)$ in (5.5), it suffices to use $M_\sigma = \lceil j/2 \rceil$ points, although the other terms in H^1_{ij} may require more points. Let $H^1_{ij}(M)$ denote the value of H^1_{ij} computed by applying M-point Gauss rules to compute $\mathcal{A}^1_j(1)$ in (5.5) and C^1_{ij} in (5.6) (that is, M^2 Gauss points for the double integral). Likewise, for $\ell \geq 2$, let $H^{\bar{\ell}}_{ij}(M)$ denote the value of $H^{\bar{\ell}}_{ij}$ computed by applying M-point Gauss rules to (5.7). For a given absolute tolerance `atol`, let $M^{\bar{\ell}}_r(\texttt{atol})$ denote the smallest M for which

$$|H^{\bar{\ell}}_{ij}(M) - H^{\bar{\ell}}_{ij}(12)| < \texttt{atol} \quad \text{for all } i, j \in \{1, 2, \ldots, r\}.$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

TABLE 1. Numbers of Gauss points $M_r^{\bar\ell}(\texttt{atol})$ in each variable required for $\texttt{atol} = 10^{-14}$, when $\alpha = 3/4$.

r	$\bar\ell = 1$	$\bar\ell = 2$	$\bar\ell = 10$	$\bar\ell = 100$	$\bar\ell = 1000$
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

Table 1 lists some values of $M_r^{\bar\ell}(\texttt{atol})$ for $\texttt{atol} = 10^{-14}$. Unsurprisingly, fewer quadrature points are needed as $\bar\ell$ increases. In any case, the computational cost of computing the coefficients is negligible in comparison with the overall cost of assembling and solving the linear system (4.4) for any realistic spatial discretization.

7.2. A fractional ODE We consider the initial-value problem (2.1) in the case

$$\alpha = 1/2, \quad \lambda = 1/2, \quad f(t) = \cos \pi t, \quad u_0 = 1, \quad T = 2, \tag{7.1}$$

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 $E_\alpha(z) = \sum_{n=0}^\infty z^n/\Gamma(1+n\alpha)$ denotes the Mittag-Leffler function [15]. 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 $E_{1/2}(-x) = \operatorname{erfcx}(x) = e^{x^2}\operatorname{erfc}(x)$ 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,

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

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 $m \ge 1$, the mth 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 $1 \le j \le 3$) than at the left end point ($t_{n0}^* = t_{n-1}$).

In Table 2, we show how the quantities

$$E_j^{\max} = \max_{1\le n\le N} (t_{nj}^*)^{r-\alpha} E_j^n \tag{7.2}$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

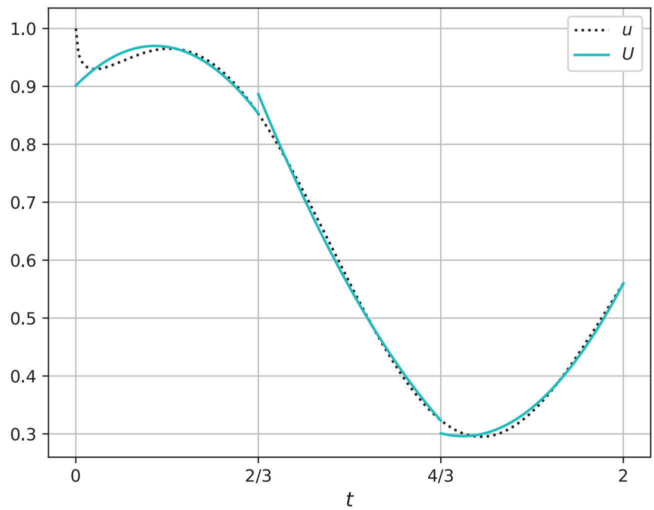

FIGURE 3. The exact solution u of (2.1) in the case (7.1), together with the piecewise-quadratic ($r = 3$) DG solution with $N = 3$ subintervals.

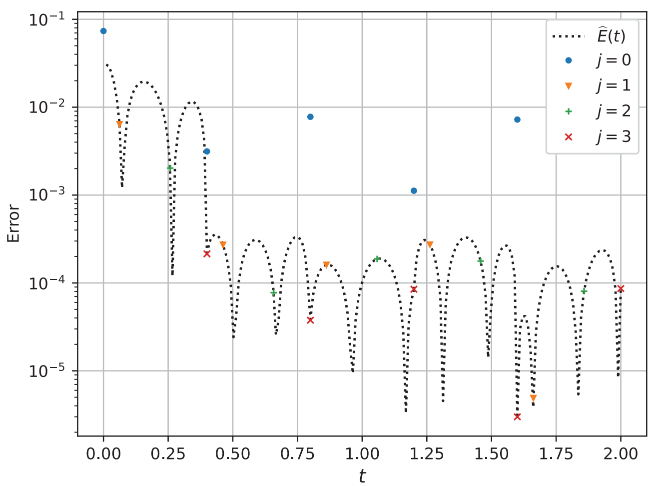

FIGURE 4. Absolute errors in the reconstruction $\widehat{U}(t)$ for $0 \le t \le T = 2$, and in the DG solution $U(t)$ for $t = t^*_{nj}$, using piecewise quadratics ($r = 3$) and $N = 5$ uniform subintervals (see (6.10)).

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

$$E_0^n \le C(t^*_{n0})^{\alpha-r}k^r \quad \text{for } 2 \le n \le N,$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

TABLE 2. Maximum weighted errors (7.2) at the points t_{nj}^* using piecewise quadratics ($r = 3$) on a uniform grid.

N	$E_0^{\max}$		$E_1^{\max}$		$E_2^{\max}$		$E_3^{\max}$	
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

TABLE 3. Maximum error in the reconstruction $\widehat{U}(t)$ for $0 \le t \le T = 1$, using piecewise quadratics ($r = 3$) for four choices of the mesh grading exponent q (see (7.3)).

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

whereas

$$E_j^n \le C(t_{nj}^*)^{\alpha-r}k^{r+\alpha} \quad \text{for } 1 \le n \le N \text{ and } 1 \le j \le r$$

and that, consequently,

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

However, using piecewise constants ($r = 1$) we do not observe any superconvergence, with both $E_0^{\max}$ and $E_1^{\max}$ behaving like $Ct_n^{1-\alpha}k$, albeit with a noticeably smaller constant in the case of $E_1^{\max}$.

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

$$t_n = (n/N)^q T \quad \text{for } 0 \le n \le N \tag{7.3}$$

with a suitable grading exponent $q \ge 1$. Table 3 shows the maximum error in the reconstruction, that is, $\max_{0\le t\le T} |\widehat{U}(t) - u(t)|$, 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 $k^{\min(3.5,q\alpha)}$, where $k = \max_{1\le n\le N} k_n \le CN^{-1}$. We conjecture that, in general,

$$|\widehat{U}(t) - u(t)| \le Ck^{\min(r+\alpha,q\alpha)} \quad \text{for } 0 \le t \le T \text{ provided } r \ge 2. \tag{7.4}$$

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

7.3. A fractional PDE Consider the elliptic operator $A = -\partial^2/\partial x^2$ for the one-dimensional spatial domain $\Omega = (0, L)$. To construct a reference solution, we exploit the 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

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

where $\omega = z^{\alpha/2}$ and $g(x,z) = z^{\alpha-1}[u_0(x) + \tilde{f}(x,z)]$. The variation-of-parameters formula leads to the integral representation

$$\begin{aligned}\tilde{u}(x,z) &= \frac{\sinh \omega(L-x)}{\omega \sinh \omega L} \int_0^x g(\xi,z) \sinh \omega\xi\,d\xi \\ &\quad + \frac{\sinh \omega x}{\omega \sinh \omega L} \int_x^L g(\xi,z) \sinh \omega(L-\xi)\,d\xi\end{aligned}$$

and the Laplace inversion formula then gives

$$u(x,t) = \frac{1}{2\pi i} \int_\Gamma e^{zt} \tilde{u}(x,z)\,dz \tag{7.5}$$

for a contour Γ homotopic to the imaginary axis and passing to the right of all singularities of the integrand.

We choose as data the functions

$$u_0(x) = C_0 x(L-x) \quad \text{and} \quad f(x,t) = C_f t e^{-t} \tag{7.6}$$

for constants C_0 and C_f, and find that

$$\begin{aligned}\tilde{u}(x,z) &= \frac{C_0}{z} \frac{\rho_1(x) \sinh \omega(L-x) + \rho_1(L-x) \sinh \omega x}{\sinh \omega L} \\ &\quad + \frac{C_f}{z(z+1)^2} \frac{\rho_2(x) \sinh \omega(L-x) + \rho_2(L-x) \sinh \omega x}{\sinh \omega L},\end{aligned}$$

where we have $\rho_1(x) = (\omega x(L-x) - 2\omega^{-1}) \cosh \omega x + (2x - L) \sinh \omega x + 2\omega^{-1}$ and $\rho_2(x) = \cosh \omega x - 1$. To evaluate the contour integral (7.5), we apply an optimized equal-weight quadrature rule that arises after deforming Γ into the left branch of an hyperbola [19]. Figure 5 shows the reference solution over the time interval $[0, 2]$ in the case

$$\alpha = 0.6, \quad L = 2, \quad C_0 = 1, \quad C_f = 2. \tag{7.7}$$

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 $\widehat{U}(t)$. The DG method used piecewise quadratics ($r = 3$), first with a uniform mesh of $N = 12$ subintervals (top) and then with a nonuniform mesh of $N = 40$ subintervals (bottom). In both cases, the spatial discretization used

https://doi.org/10.1017/S1446181120000152 Published online by Cambridge University Press

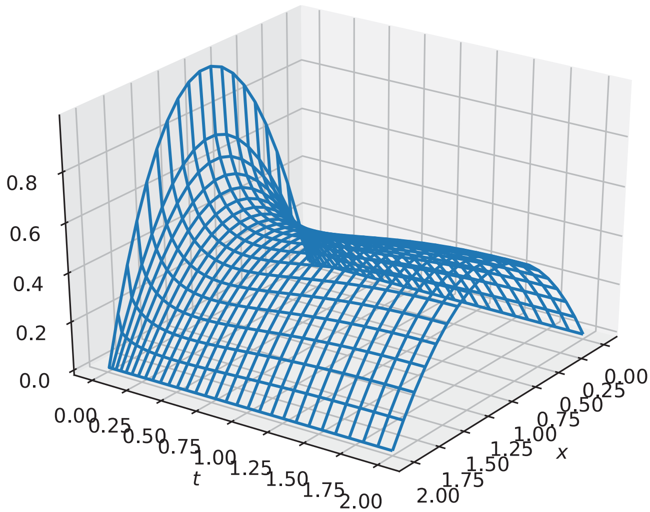

FIGURE 5. The reference solution for the one-dimensional problem with data given by (7.6) and (7.7).

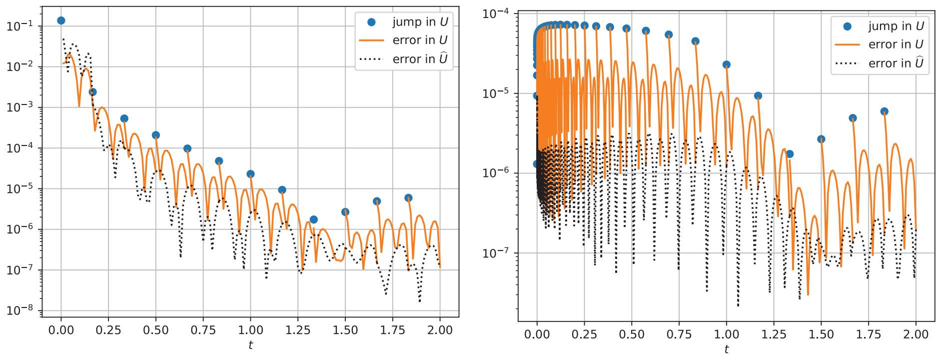

FIGURE 6. Comparison of the jumps $\|[\![U]\!]^{n-1}\|$ with the DG error $\|U(t) - u(t)\|$ and the reconstruction error $\|\widehat{U}(t) - u(t)\|$. Left: a uniform mesh with $N = 12$ time steps. Right: a graded mesh with $N = 40$ time steps.

(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 (6.12), we observe that

$$\sup_{t_{n-1}<t<t_n} \|U(t) - u(t)\| \approx \|[\![U]\!]^{n-1}\|.$$

Motivated by our conjecture (7.4), the second mesh was graded for $0 \le t_n \le 1$ by taking $q = (r + \alpha)/\alpha$, $N = 34$ and $T = 1$ in the formula (7.3), 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.

We conclude by noting that the conjectures above are stronger than what has been proved in the literature. Mustapha [13, Theorem 5] was able to show an error bound in $L_\infty(L_2)$ of at best $O(k^{r-\mu})$ with $\mu = 1 - \alpha/2$ for $r \geq 3$, and $\mu = (1-\alpha)/2$ for $r = 2$, using a sufficiently strong mesh grading, but pointed out that in practice the rate is observed to be optimal (that is, $\mu = 0$). For the piecewise-linear case $r = 2$, convergence of at best $O(k^{1+2\alpha}\log k^{-1})$ has been proved [14, Theorem 4.3] for the nodal value U^n_-. The rate is better than the optimal $O(k^2)$, when $1/2 < \alpha < 1$, but in practice one observes $O(k^{r+\alpha})$ superconvergence for the full range $0 < \alpha < 1$. There appear to be no a priori superconvergence results for the error at the interior Radau points t^*_{nj} $(1 \leq j \leq r_n - 1)$. For the classical diffusion equation ($\alpha = 1$), U^n_- is known to be superconvergent of order at best k^{2r-1} (assuming that $r_n = r$ is fixed) but with a constant factor that may blow up as $t \to 0$, depending on the regularity of the data [2, Theorem 3].

8. Conclusion

We have described in detail a practical implementation of DG time stepping for fractional diffusion problems, and demonstrated that the high accuracy of the DG solution U can be further improved by post processing to form the reconstruction $\widehat{U}$. Moreover, the jumps $[\![U]\!]^{n-1}$ provide an easily computed error estimator for $U|_{I_n}$ that could form the basis for automatic step-size control. A complete theoretical justification for the observed convergence behaviour is, however, not yet available.

Acknowledgement

This project was supported by a University of New South Wales Faculty Research Grant (PS47152/IR001/MATH).

References

[1] M. G. Duffy, "Quadrature over a pyramid or cube of integrands with a singularity at a vertex", *SIAM J. Numer. Anal.* **19** (1962) 1260–1262; doi:10.1137/0719090.

[2] K. Eriksson, C. Johnson and V. Thomée, "Time discretization of parabolic problems by the discontinuous Galerkin method", *ESAIM: M2AN* **19** (1985) 611–643; doi:10.1051/m2an/1985190406111.

[3] G. Hämmerlin and K.-H. Hoffmann, *Numerical mathematics* (Springer, New York, 1962); ISBN: 978-1-4612-4442-4.

[4] J. Klafter and I. M. Sokolov, *First steps in random walks* (Oxford University Press, Oxford, 2011); ISBN 9780199234868.

[5] V. I. Krylov, *Approximate calculation of integrals*, *ACM Monogr.* (Macmillan, New York, 1962); ISBN: 978-0-4861-5467-1.

[6] K-N. Le, W. McLean and M. Stynes, "Existence, uniqueness and regularity of the solution of the time-fractional Fokker–Planck equation with general forcing", *Commun. Pure Appl. Anal.* **18** (2019) 2765–2787; doi:10.3934/cpaa.2019124.

[7] C. Makridakis and R. H. Nochetto, "A posteriori error analysis for higher order dissipative methods for evolution problems", *Numer. Math.* **1004** (2006) 489–514; doi:10.1007/s00211-006-0013-6.

[8] W. McLean, "Regularity of solutions to a time-fractional diffusion equation", *ANZIAM J.* **52** (2010) 123–138; doi:10.1017/S1446181111000617.

[9] W. McLean, *FractionalTimeDG: Generate coefficient arrays needed for discontinuous Galerkin time-stepping of fractional diffusion problems (Github,* 2020*)*; https://github.com/billmclean/FractionalTimeDG.jl

[10] W. McLean and K. Mustapha, "Convergence analysis of a discontinuous Galerkin method for a sub-diffusion equation", *Numer. Algorithms* **52** (2009) 69–88; doi:10.1007/s11075-008-9258-8.

[11] W. McLean, K. Mustapha, R. Ali and O. Knio, "Well-posedness of time-fractional advection–diffusion–reaction equations", *Fract. Calc. Appl. Anal.* **22** (2019) 918–944; doi:10.1515/fca-2019-0050.

[12] R. Metzler and J. Klafter, "The random walk's guide to anomalous diffusion: a fractional dynamics approach", *Phys. Rep.* **339** (2000) 1–77; doi:10.1016/S0370-1573(00)00070-3.

[13] K. Mustapha, "Time-stepping discontinuous Galerkin methods for fractional diffusion problems", *Numer. Math.* **130** (2015) 497–516; doi:10.1007/s00211-014-0669-2.

[14] K. Mustapha and W. McLean, "Superconvergence of a discontinuous Galerkin method for fractional diffusion and wave equations", *SIAM J. Numer. Anal.* **51** (2013) 491–515; doi:10.1137/120880719.

[15] K. B. Oldham and J. Spanier, *The fractional calculus* (Academic Press, New York, 1974); ISBN: 978-0-0809-5620-6.

[16] L. Schmutz and T. P. Wihler, "The variable-order discontinuous Galerkin time stepping scheme for parabolic evolution problems is uniformly L^∞-stable", *SIAM J. Numer. Anal.* **57** (2019) 293–319; doi:10.1137/17M1158835.

[17] D. Schötzau and C. Schwab, "Time discretization of parabolic problems by the hp-version of the discontinuous Galerkin finite element method", *SIAM J. Numer. Anal.* **38** (2001) 837–875; doi:10.1137/S0036142999352394:.

[18] V. Thomée, *Galerkin finite element methods for parabolic problems* (Springer, Berlin–Heidelberg, 2006); ISBN: 978-3-540-33121-6.

[19] J. A. C. Weideman and L. N. Trefethen, "Parabolic and hyperbolic contours for computing the Bromwich integral", *Math. Comp.* **76** (2007) 1341–1356; doi:10.1090/S0025-5718-07-01945-X.