Discontinuous Galerkin time-stepping and fast summation for fractional diffusion and wave equations

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Initial-boundary value problem

Fractional diffusion ($0 < \nu < 1$) or wave ($1 < \nu < 2$) equation

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathcal{Q}_\nu = f(x, t), \quad x \in \Omega \subseteq \mathbb{R}^d, \quad 0 < t < T.$$

Generalized flux

$$\mathcal{Q}_\nu(x, t) = -\partial_t^{1-\nu} K \nabla u, \quad K > 0.$$

Classical diffusion (heat) equation in the limit as $\nu \to 1$, since $Q_1 = -K\nabla u$.

Homogeneous Dirichlet or Neumann boundary condition, and initial condition

$$u(x, 0) = u_0(x) \quad \text{for } x \in \Omega.$$

Riemann–Liouville fractional derivative or integral

If $0 < \nu < 1$, then

$$\partial^{1-\nu} g(t) = \frac{\partial}{\partial t} \int_0^t \frac{(t-s)^{\nu-1}}{\Gamma(\nu)} g(s)\, ds.$$

If $1 < \nu < 2$, then

$$\partial^{1-\nu} g(t) = \int_0^t \frac{(t-s)^{\nu-2}}{\Gamma(\nu-1)} g(s)\, ds.$$

Kernel is weakly singular in both cases.

Weak formulation

Energy space $\dot{H}^1 = H_0^1(\Omega)$ or $H^1(\Omega)$.

First Green identity: if $v \in \dot{H}^1$ then

$$\int_\Omega [-\nabla \cdot (K\nabla u)] v \, dx = \int_\Omega K\nabla u \cdot \nabla v \, dx - \cancel{\int_{\partial\Omega} K \frac{\partial u}{\partial \mathbf{n}}} \, v.$$

Elliptic operator $Au = -\nabla \cdot (K\nabla u)$ and bilinear form

$$A(u, v) = \int_\Omega K\nabla u \cdot \nabla v \, dx = \langle Au, v \rangle.$$

Since $\langle \nabla \cdot \mathcal{Q}_\nu, v \rangle = A(\partial_t^{1-\nu} u, v)$, weak solution $u : (0, T) \to \dot{H}^1$ satisfies

$$\langle u'(t), v \rangle + A(\partial_t^{1-\nu} u, v) = \langle f(t), v \rangle \quad \text{for all } v \in \dot{H}^1.$$

Stability of the continuous problem

Putting $v = u(t)$ and integrating,

$$\int_0^T \langle u'(t), u(t)\rangle \, dt + \int_0^T A(\partial^{1-\nu} u(t), u(t))\, dt = \int_0^T \langle f(t), u(t)\rangle \, dt.$$

Can show via Laplace transforms that

$$\int_0^T A(\partial^{1-\nu} u(t), u(t))\, dt \geq 0,$$

and we easily deduce well-posedness:

$$\|u(t)\| \leq \|u_0\| + 2\int_0^t \|f(s)\|\, ds, \quad 0 \leq t \leq T.$$

Discontinuous piecewise polynomial approximation

Grid points

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

Subintervals

$$I_n = (t_{n-1}, t_n), \qquad k_n = t_n - t_{n-1}, \qquad 1 \le n \le N.$$

Basis for polynomials of degree at most $L - 1$,

$$\chi_1, \quad \chi_2, \quad \ldots, \quad \chi_L.$$

Basis function shifted to I_n,

$$\chi_{nl}(t) = \chi_l(\tau), \quad t = t_{n-1} + \tau k_n, \quad 0 < \tau < 1.$$

Seek approximate solution

$$u(x,t) \approx U(x,t) = \sum_{l=1}^{L} U^{nl}(x)\chi_{nl}(t), \quad t \in I_n.$$

Discontinuous Galerkin in time (DG)

One-sided limits and jump at t_n,

$$U^n_\pm = \lim_{t \to t_n^\pm} U(t), \qquad [U]^n = U^n_+ - U^n_-.$$

Require $U^0_- = u_0$ and, for $1 \le n \le N$,

$$\langle U^{n-1}_+, V^{n-1}_+ \rangle + \int_{I_n} \big[\langle U'(t), V(t) \rangle + A\big(\partial^{1-\nu} U(t), V(t)\big) \big]\, dt$$
$$= \langle U^{n-1}_-, V^{n-1}_+ \rangle + \int_{I_n} \langle f(t), V(t) \rangle \, dt$$

for every polynomial V of degree at most $L-1$ with coefficients in $\dot{H}^1$.

Thus, approximate continuity at t_{n-1} enforced weakly.

Discontinuous Galerkin in time

- Eriksson, Johnson and Thomée, *Modél. Math. Anal. Numér.*, 19:611–643, 1985.
- McLean, Thomée and Walhbin, *J. Comput. Appl. Math.*, 69:49–69, 1996.
- Adolfsson , Enelund and Larsson, *Comput. Methods Appl. Mech. Engrg.*, 192:5285–5304, 2003.
- Mustapha and McLean, *Math. Comp.*, 78:1975–1995, 2009.
- Mustapha and McLean, *SIAM J. Numer. Anal.*, 51: 491–515, 2013.

Pros and cons of DG

Advantages:

- simple energy argument guarantees stability for arbitrary time steps;
- no need to enforce continuity across time levels;
- preserves smoothing property of fractional diffusion equation;
- superconvergence at the time levels if $L \geq 2$;
- *a posteriori* error estimation based on the dual problem.

Disadvantages:

- fully implicit method so need to solve $(LM) \times (LM)$ linear system at each time step;
- numerical solution is not continuous in time.

Simplest example: scalar problem, piecewise constants

Consider scalar-valued case $U : (0, T) \to \mathbb{R}$ (fractional ODE) with $L = 1$ (piecewise-constants). Then $U(t) = U_-^n = U_+^{n-1}$ and $U'(t) = 0$ for $t \in I_n$, so for all $V_-^n \in \mathbb{R}$,

$$\langle U_-^n, V_-^n \rangle + \int_{I_n} A\big(\partial^{1-\nu} U(t), V_-^n\big)\, dt = \langle U_-^{n-1}, V_-^n \rangle + \int_{I_n} \langle f(t), V_-^n \rangle\, dt.$$

This is just the implicit Euler method,

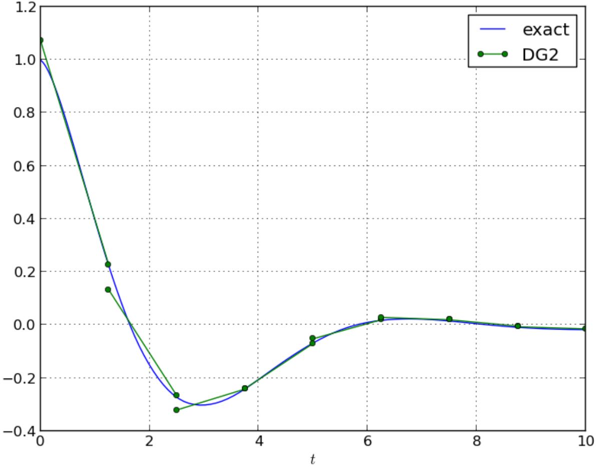
$$\frac{U_-^n - U_-^{n-1}}{k_n} + A \sum_{j=1}^{n} \beta_{nj} U_-^j = F^n,$$

with

$$F^n = \frac{1}{k_n} \int_{I_n} f(t)\, dt = \text{average value of } f \text{ on } I_n.$$

Piecewise linears for fractional ODE

Take $\nu = 3/2,\ T = 10,\ A = 1,\ u_0 = 1,\ f \equiv 0,\ L = 2,\ N = 8.$



U^n_- converges faster than U^n_+

Compare

$$E^N_- = \max_{1 \le n \le N} |U^n_- - u(t_n)| = O(k^{\rho_-})$$

and

$$E^N_+ = \max_{0 \le n \le N-1} |U^n_+ - u(t_n)| = O(k^{\rho_+})$$

N	E^N_-	ρ_-	E^N_+	ρ_+
20	0.83E-05		0.47E-02	
40	0.12E-05	2.820	0.17E-02	1.482
80	0.16E-06	2.864	0.59E-03	1.493
160	0.22E-07	2.897	0.21E-03	1.498
320	0.29E-08	2.924	0.74E-04	1.499
640	0.37E-09	2.943	0.26E-04	1.500

Non-uniform time steps

Put

$$t_n = (n/N)^q T, \qquad q \geq 1.$$

With $q = 1.5$ we observe $\rho_- = 3$ (superconvergence) and $\rho_+ = 2$ (optimal).

N	E_-^N	ρ_-	E_+^N	ρ_+
20	0.11E-04		0.16E-02	
40	0.15E-05	2.877	0.40E-03	1.976
80	0.20E-06	2.921	0.10E-03	1.989
160	0.26E-07	2.947	0.25E-04	1.995
320	0.33E-08	2.963	0.63E-05	1.998
640	0.42E-09	2.973	0.16E-05	1.999

Spatial discretization

Conforming finite element space $S_h \subseteq \dot{H}^1$.

Spatially discrete solution $u_h : (0, T) \to S_h$ satisfies

$$\langle u_h'(t), v\rangle + A(\partial_t^{1-\nu} u_h, v) = \langle f(t), v\rangle \quad \text{for all } v \in S_h,$$

with $u_h(0) = u_{0h} \approx u_h$ and $u_{0h} \in S_h$.

Basis $\vartheta_1, \vartheta_2, \ldots, \vartheta_M$ for S_h, so that

$$u(x,t) \approx u_h(x,t) = \sum_{m=1}^{M} U_m(t)\vartheta_m(x).$$

E.g., for a nodal basis,

$$\vartheta_m(x_p) = \delta_{mp} \quad \text{and} \quad U_m(t) = u_h(x_m, t).$$

Method of lines

Mass matrix $\mathbf{M} = [M_{pm}]$ and stiffness matrix $\mathbf{S} = [S_{pm}]$ with entries

$$M_{pm} = \langle \vartheta_m, \vartheta_p \rangle \quad \text{and} \quad S_{pm} = A(\vartheta_m, \vartheta_p)$$

for $1 \leq p \leq M$ and $1 \leq m \leq M$.

Stiff system of (ordinary) integrodifferential equations

$$\sum_{m=1}^{M} \Big(M_{pm} U_m'(t) + S_{pm} \partial_t^{1-\nu} U_m(t) \Big) = \langle f(t), \vartheta_p \rangle, \quad 1 \leq p \leq M,$$

or equivalently,

$$\mathbf{M}\mathbf{U}'(t) + \mathbf{S}\partial_t^{1-\nu}\mathbf{U}(t) = \mathbf{F}(t),$$

with $\mathbf{U}(0) = \mathbf{U}_{0h}$.

Fully discrete solution

Seek $U_h : [0, T] \to S_h$ satisfying $U^0_{h-} = u_{0h}$ and, for $1 \le n \le N$,

$$\langle U^{n-1}_+, V^{n-1}_+ \rangle + \int_{I_n} \big[\langle U'(t), V(t) \rangle + A\big(\partial^{1-\nu} U(t), V(t)\big) \big] \, dt$$
$$= \langle U^{n-1}_-, V^{n-1}_+ \rangle + \int_{I_n} \langle f(t), V(t) \rangle \, dt$$

for every polynomial V of degree at most $L-1$ with coefficients in S_h. Writing

$$U_h(x,t) = \sum_{m=1}^{M} \sum_{l=1}^{L} U^{nl}_m \chi_{nl}(t) \vartheta_m(x) \quad x \in \Omega, \; t \in I_n,$$

we obtain for $2 \le n \le N$ a linear system of the form

$$(\mathbf{M} \otimes \boldsymbol{\alpha} + \mathbf{S} \otimes \boldsymbol{\beta}_{nn}) \mathbf{U}^n = \mathbf{F}^n + (\mathbf{M} \otimes \gamma) \mathbf{U}^{n-1} - \sum_{j=1}^{n-1} (\mathbf{S} \otimes \boldsymbol{\beta}_{nj}) \mathbf{U}^j.$$

Computational cost

At the nth time step, we must use $O(nLM)$ operations to compute the RHS, and (at least) $O(LM)$ operations to solve the $(LM) \times (LM)$ linear system.

For N times steps, the cost is thus $O(N^2 LM)$ operations.

Also use $O(NLM)$ active memory locations.

For a classical diffusion equation, total cost is only $O(NLM)$ operations and $O(LM)$ active memory locations.

Conclusion: solving a fractional diffusion equation costs N times as much as solving a classical diffusion equation.

Fast time stepping algorithms for fractional DEs

- Ford and Simpson, *Numer. Algorithms* 26:333–346, 2001.
- Diethelm and Freed, *Comput. Math. Appl.* 51: 51–72, 2006.
- Schädle, López-Fernández and Lubich, *SIAM J. Sci. Comput.* 28:421–438, 2006
- Deng, *J. Comput. Appl. Math.* 206: 174–188, 2007.
- Li, *SIAM J. Sci. Comput.* 31: 4696–4714, 2010.

Degenerate kernel

For simplicity, restrict to fractional ODE ($M = 1$) and use piecewise-constants ($L = 1$) in time.

Need a fast way to evaluate

$$\int_{I_n} \int_0^{t_{n-1}} \beta(t, s) U(s)\, ds\, dt = \sum_{j=1}^{n-1} \beta_{nj} U_-^j.$$

Easy for β of the form

$$\beta(t, s) = \sum_{r=1}^{R} \phi_r(t) \psi_r(s)$$

because

$$\beta_{nj} = \int_{I_n} \int_{I_j} \beta(t, s)\, ds\, dt = \sum_{r=1}^{R} \phi_{rn} \psi_{rj},$$

where

$$\phi_{rn} = \int_{I_n} \phi_r(t)\, dt, \quad \psi_{rj} = \int_{I_j} \psi_r(s)\, ds.$$

Degenerate kernel

Compute the sum as

$$\sum_{j=1}^{n-1} \beta_{nj} U_-^j = \sum_{j=1}^{n-1} \sum_{r=1}^{R} \phi_{rn} \psi_{rj} U_-^j = \sum_{r=1}^{R} \phi_{rn} \Psi_r^{n-1}(U)$$

where

$$\Psi_r^{n-1}(U) = \sum_{j=1}^{n-1} \psi_{rj} U_-^j = \psi_{r,n-1} U_-^{n-1} + \Psi_r^{n-2}(U).$$

At nth time step, overwrite $\Psi_r^{n-2}(U)$ with $\Psi_r^{n-1}(U)$, and compute sum using $O(R)$ operations.

Reduces total cost from $O(N^2)$ operations and $O(N)$ storage to $O(RN)$ operations and $O(R)$ storage.

Weakly singular kernel

But fractional wave equation has the kernel

$$\beta(t, s) = \frac{(t - s)^{\nu - 2}}{\Gamma(\nu - 1)}, \quad 1 < \nu < 2.$$

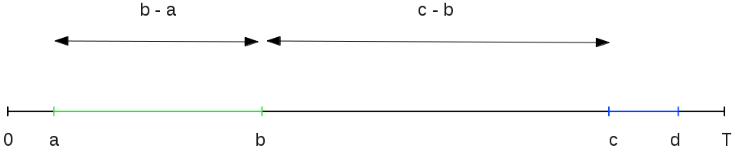
Key idea: if $t \in I_n$ and $s \in I_j$ are well-separated, then we can approximate $\beta(t, s)$ by a degenerate kernel.

Leads to a variant of the panel clustering algorithm for boundary element methods (Hackbusch and Nowak, *Numer. Math.* 54: 463–491, 1989).

Well-separated intervals

Suppose

$$0 \le a < s \le b < c \le t \le d \le T \quad \text{and} \quad \frac{b-a}{c-b} \le \eta \le 1.$$



Change of variable

$$s = \tfrac{1}{2}\big[(1-\sigma)a + (1+\sigma)b\big]$$

takes $\sigma \in [-1, 1]$ to $s \in [a, b]$.

Tchebyshev interpolation

Denote the Tchebyshev points for $[a, b]$ by

$$s_r^{a,b} = \tfrac{1}{2}\big[(1-\sigma_r)a + (1+\sigma_r)b\big], \qquad \sigma_r = \cos\frac{(r+\frac{1}{2})\pi}{R+1},$$

for $0 \le r \le R$. For $s \in [a, b]$ and $t \in [c, d]$,

$$\beta(t, s) \approx \beta^{a,b}(t, s) = {\sum_{r=0}^{R}}' \phi_r^{a,b}(t)\psi_r^{a,b}(s)$$

where

$$\phi_r^{a,b}(t) = \frac{2}{R+1}\sum_{q=0}^{R} \beta(t, s_q^{a,b})\, T_r(\sigma_q), \qquad \psi_r^{a,b}(s) = T_r(\sigma).$$

Can use fast cosine transform to evaluate $\phi_r^{a,b}(t)$ for $0 \le r \le R$ because

$$T_r(\sigma_q) = \cos\frac{q(r+\frac{1}{2})\pi}{R+1}.$$

Tchebyshev interpolation

Local degenerate kernel satisfies

$$\beta(t, s_r^{a,b}) = \beta^{a,b}(t, s_r^{a,b}), \qquad 0 \le r \le R,$$

and standard error estimate for Tchebyshev interpolation of analytic functions gives

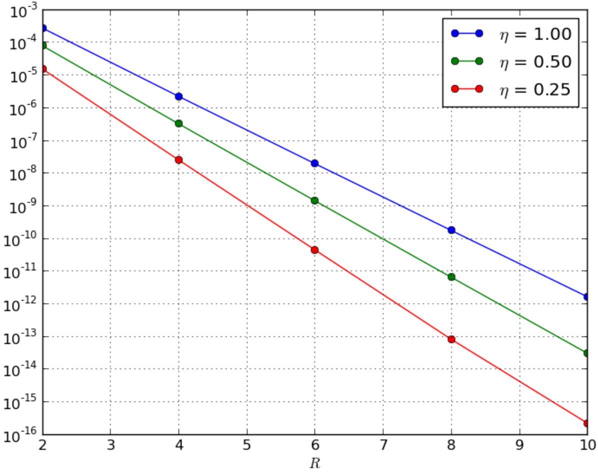
$$\left|\beta^{a,b}(t,s) - \beta(t,s)\right| = O(\rho^{-R})$$

for

$$s \in I_j \subseteq [a,b], \qquad t \in I_n \subseteq [c,d], \qquad \frac{b-a}{c-b} \le \eta^{-1},$$

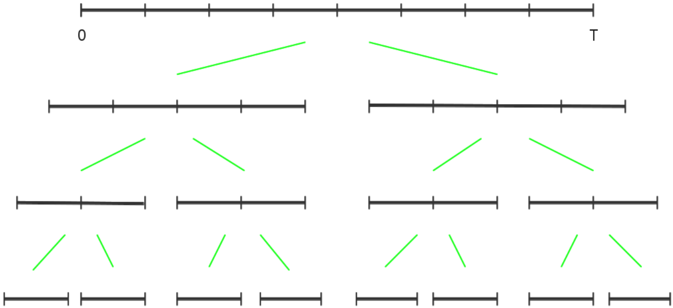
with $\rho > 1$ satisfying $\rho + \rho^{-1} < 4\eta^{-1} - 2$.

Accuracy in practice



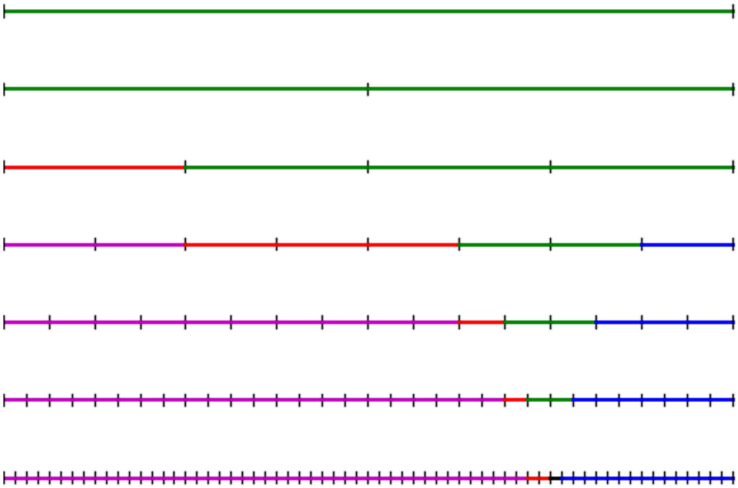
Cluster tree

A cluster is a set $\mathcal{C} = \{I_j, I_{j+1}, \dots, I_n\}$ $(1 \leq j \leq n \leq N)$ of consecutive subintervals.



Admissible cover

Given I_n and $\eta \in (0, 1]$, a simple recursive procedure constructs a unique minimal admissible cover for $[t_0, t_{n-1}]$.



A regularity property of the cluster tree

Definition

The generation of a cluster is defined recursively by

$$\mathrm{Gen}(\mathcal{C}) = 1 + \mathrm{Gen}\big(\mathrm{Parent}(\mathcal{C})\big),$$

with $\mathrm{Gen}(\mathcal{C}) = 0$ if $\mathcal{C} = \{I_1, I_2, \ldots, I_N\}$ is the root cluster.

Definition

For integers $G \geq 1$ and $Q \geq 2$, the cluster tree is (G, Q)-uniform if there exist constants $0 < \lambda < \Lambda$ such that for every cluster $\mathcal{C}$,

1. $0 \leq \mathrm{Gen}(\mathcal{C}) \leq G$;
2. either $\mathcal{C}$ has Q children or else $\mathcal{C}$ is a leaf;
3. $\lambda T Q^{-\ell} \leq \mathrm{Len}(\mathcal{C}) \leq \Lambda T Q^{-\ell}$ if $\ell = \mathrm{Gen}(\mathcal{C})$.
4. $\bigcup\{\mathcal{C} : \mathrm{Gen}(\mathcal{C}) = \ell\} = \{I_1, I_2, \ldots, I_N\}$ for $0 \leq \ell \leq G$.

Computational cost

Theorem

If the cluster tree is (G, Q)-uniform, then the fast summation algorithm

- *evaluates the RHS for $1 \leq n \leq N$ using order $R\eta^{-1}NQ(G + NQ^{-G})LM$ operations,*
- *requires no more than order $R\eta^{-1}QGLM$ active memory locations during any one time step.*

Corollary

If $N = Q^G$ then the cost is order $LMN \log N$ operations and order $LM \log N$ active memory.

CPU times for piecewise constants, 2D problem

Fractional diffusion equation ($\nu = 1/2$), $N = 16000$ times steps, $\Omega = (0,1) \times (0,1)$, bilinear finite elements with $M = 6241$ degrees of freedom, Taylor expansions of kernel.

.

	Slow	Fast		
r	—	4	5	6
Error	0.129E-03	0.789E-03	0.129E-03	0.129E-03
Setup	49.0 s	0.64 s	0.66 s	0.70 s
RHS	916.2 s	16.76 s	20.48 s	23.09 s
Solver	7.7 s	7.17 s	6.87 s	7.13 s
Total	972.9 s	24.57 s	28.02 s	30.91 s