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

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

Bilinear form

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

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

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

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,

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

Require

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

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

Weakly enforce continuity at t_{n-1}.

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.
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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 $X_-^n \in \mathbb{R}$,

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

This is just the implicit Euler method,

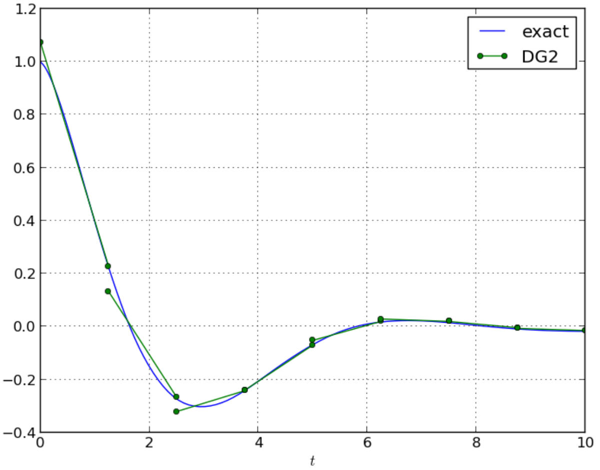
$$\frac{U_-^n - U_-^{n-1}}{k_n} + A \sum_{j=1}^{n} \beta_{nj} U_-^j = F^n,$$

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 wave equation

Take $\nu = 3/2$, $T = 6$, $A = 1$, $u_0 = 1$, $f \equiv 0$. $L = 1$, $N = 8$.



U_-^n converges faster than U_+^n

Compare

$$E_+^N = \max_{0 \le n \le N-1} |U_+^n - u(t_n)| = O(k^{\rho_+})$$

and

$$E_-^N = \max_{1 \le n \le N} |U_-^n - u(t_n)| = O(k^{\rho_-})$$

N	E_-	ρ_-	E_+	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_-	ρ_-	E_+	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 $1 \leq m \leq M$.

System of (ordinary) integrodifferential equations

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

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

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

for every polynomial X of degree at most L with coefficients in S_h, with $U_{h-}^0 = u_{0h}$. Writing

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

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

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

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 $O(N^2LM)$ 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

- Hackbusch and Nowak, *Numer. Math.* 54: 463–491, 1989.
- 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
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Degenerate kernel

For simplicity, restrict to scalar ($M = 1$) problem with 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 if 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.

Reduce 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

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

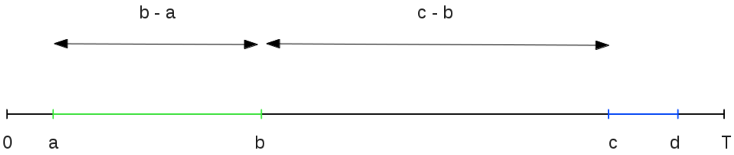
Key idea: if $t \in I_n$ and $s \in I_j$ are well-separated, then we can approximate $\beta(t,s)$ by a degenerate kernel.

Leads to a variant of the panel clustering algorithm for boundary element methods (Hackbusch and Nowak, 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 $t \in [c, d]$,

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

where

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

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

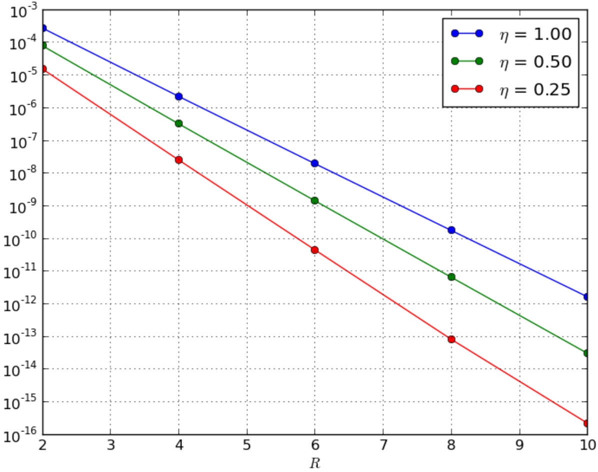
$$\left|\beta^{a,b}(t,s) - \beta(t,s)\right| = O(\rho^{-R})$$

for

$$s \in I_j \subseteq [a,b] \quad \text{and} \quad t \in I_n \subseteq [c,d],$$

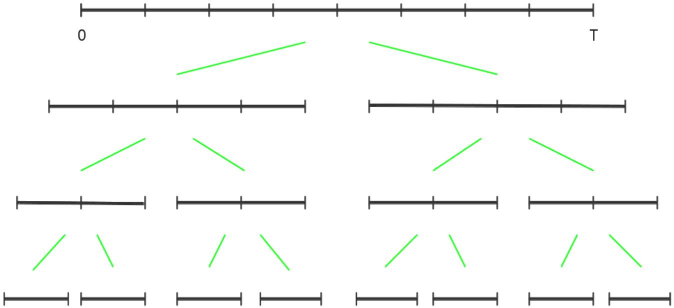
with $\rho > 1$ satisfying $\rho + \rho^{-1} < 4\eta^{-1} - 2$.

Accuracy in practice



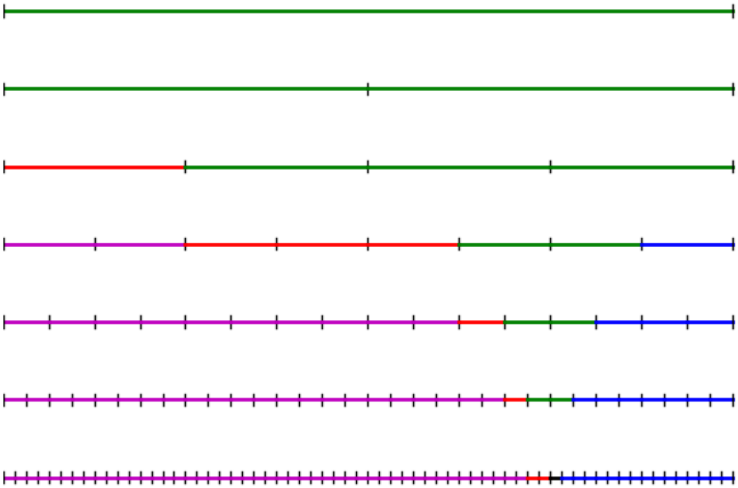
Cluster tree

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 $[t_0, t_{n-1}]$.



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