Discrete gradient structure of second-order integral averaged formula for integro-differential models

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Motivation

Linear and nonlinear integro-differential equations attract great interests in a wide range of disciplines in science and engineering. These models are formulated in integral form, including Riemann-Liouville fractional integral

$$(\mathcal{I}_t^{\beta} w)(t) := \int_0^t \omega_\beta(t-s) w(s) \, \mathrm{d}s \quad \text{with } \omega_\beta(t) := t^{\beta-1}/\Gamma(\beta)$$

and fractional Caputo derivative for $0 < \alpha < 1$

$$(\partial_t^{\alpha} w)(t) := (\mathcal{I}_t^{1-\alpha} w')(t) = \int_0^t \omega_{1-\alpha}(t-s) w'(s) \, \mathrm{d}s.$$

They exhibit multi-scaling time behavior, which makes them suitable for the description of different diffusive regimes and characteristic crossover dynamics in complex systems.

Time fractional phase field models

For example, the time-fractional phase field models

$$\partial_t^\alpha \Phi = M\frac{\delta E}{\delta \Phi}$$

where M is the mobility operator ($M := -I$ for L^2 gradient flow and $M := \Delta$ for H^{-1} gradient flow) and E is the free energy functional such as the Ginzburg-Landau energy functional

$$E[\Phi] := \int_\Omega \Big(\frac{\epsilon^2}{2}\left|\nabla\Phi\right|^2 + F(\Phi)\Big)\,\mathrm{d}\mathbf{x} \quad \text{with} \quad F(\Phi) := \frac{1}{4}(\Phi^2 - 1)^2.$$

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- Numerical properties: Tang-Yu-Zhou-SISC-2019, Ji-Liao-et al-2019, Ji-Liao-Zhang-2020, Quan-Tang-Yang-CSIAM-2020, Liao-Tang-Zhou-2020, Karaa-SINUM-2021, Liao-Tang-Zhou-2021, Quan-Wang-JCP-2022, ...

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$$\partial_t U = \int_0^t \kappa(t-s)\left[\Delta U + f(U)\right] \mathrm{d}s.$$

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- General kernels: McLean-Thomée-1993, Lubich-Sloan-Thomée-MC-1996, McLean-Thomée-JCAM-1996, Cuesta-Palencia-ANM-2003, ...
- Singular (fractional) kernels: Adolfsson-Enelund-Larsson-CMAME-2003, Cuesta-Lubich-Palencia-MC-2006, McLean-Mustapha-NM-2007, Mustapha-Mustapha-IMA-2010, Mustapha-Schötzau-IMA-2014, Golmankhaneh-Golmankhaneh-Baleanu-SignProc-2011, ...

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- In capturing the multi-scale behaviors in many of integro-differential equations, adaptive time-stepping strategies are practically useful. Especially in long-time simulations, a computationally efficient method should admit different time steps in different periods.

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General meshes Liao-McLean-Zhang-2019, Liao-Yan-Zhang-2019, Ji-Liao-et al-2019, Ji-Liao-Zhang-2020, Liao-Tang-Zhou-2020, Quan-Tang-Yang-CSIAM-2020, Liao-Tang-Zhou-2021, Quan-Wu-arXiv2205.06060-2022, Quan-Wu-arXiv2208.01384-2022,...

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Integral averaged formula

Consider $0 = t_0 < t_1 < \cdots < t_k < \cdots < t_N = T$ with $\tau_k := t_k - t_{k-1}$, $\tau := \max_{1\le k\le N} \tau_k$, $r_k := \tau_k/\tau_{k-1}$. Also, $w^{k-\frac{1}{2}} := (w^k + w^{k-1})/2$, $\nabla_\tau w^k := w^k - w^{k-1}$ and $\partial_\tau w^k := \nabla_\tau w^k/\tau_k$.

Let the piecewise constant approximation $(\Pi_0 w)(t) = w^{k-\frac{1}{2}}$ for $t_{k-1} < t \le t_k$. The integral averaged (Crank-Nicolson) formula of fractional Riemann-Liouville integral,

$$(\mathcal{I}_\tau^\beta w)^{n-\frac{1}{2}} := \frac{1}{\tau_n}\int_{t_{n-1}}^{t_n}\int_0^t \omega_\beta(t-s)(\Pi_0 w)\,\mathrm{d}s\,\mathrm{d}t \triangleq \sum_{k=1}^{n} a_{n-k}^{(\beta,n)}\tau_k w^{k-\frac{1}{2}},$$

where the associated discrete kernels $a_{n-k}^{(\beta,n)}$ are defined by

$$a_{n-k}^{(\beta,n)} := \frac{1}{\tau_n\tau_k}\int_{t_{n-1}}^{t_n}\int_{t_{k-1}}^{\min\{t,t_k\}} \omega_\beta(t-s)\,\mathrm{d}s\,\mathrm{d}t \quad \text{for } 1 \le k \le n.$$

L1$^+$ formula

Let the piecewise approximation $\Pi_1 w := \Pi_{1,k} w$ so that

$$(\Pi_1 w)'(t) = \partial_\tau w^k, \quad \text{for } t_{k-1} < t \le t_k \text{ and } k \ge 1.$$

The integral averaged formula (also called L1$^+$ formula) of fractional Caputo derivative is

$$(\partial_\tau^\alpha w)^{n-\frac{1}{2}} := \frac{1}{\tau_n}\int_{t_{n-1}}^{t_n}\int_0^t \omega_{1-\alpha}(t-s)(\Pi_1 w)'(s)\,\mathrm{d}s\,\mathrm{d}t \triangleq \sum_{k=1}^{n} a_{n-k}^{(1-\alpha,n)} \nabla_\tau w^k,$$

where the associated discrete kernels $a_{n-k}^{(1-\alpha,n)}$ are defined by

$$a_{n-k}^{(1-\alpha,n)} = \frac{1}{\tau_n \tau_k}\int_{t_{n-1}}^{t_n}\int_{t_{k-1}}^{\min\{t,t_k\}} \omega_{1-\alpha}(t-s)\,\mathrm{d}s\,\mathrm{d}t \quad \text{for } 1 \le k \le n.$$

Positive-semidefinite-preserving approach

They come from the positive-semidefinite-preserving approach such that the corresponding real quadratic form

$$\sum_{j=1}^{n}\tau_j w^{j-\frac{1}{2}}\sum_{k=1}^{j}a_{j-k}^{(\beta,j)}\tau_k w^{k-\frac{1}{2}} = \sum_{j=1}^{n}\int_{t_{j-1}}^{t_j} w^{j-\frac{1}{2}}\int_0^t \omega_\beta(t-s)(\Pi_0 w)\,\mathrm{d}s\,\mathrm{d}t$$
$$= \int_{t_0}^{t_n}(\Pi_0 w)\,\mathrm{d}t\int_0^t \omega_\beta(t-s)(\Pi_0 w)\,\mathrm{d}s$$

is a discrete analogue to the non-negative definiteness of kernel ω_β (McLean-Thomée-1993, Lubich-Sloan-Thomée-MC-1996, McLean-Thomée-JCAM-1996)

$$2\,\mathcal{I}_t^1(w\,\mathcal{I}_t^\beta w)(t) = 2\int_0^t w(\mu)\,\mathrm{d}\mu\int_0^\mu \omega_\beta(\mu-s)w(s)\,\mathrm{d}s$$
$$= \int_0^t\int_0^t w(s)w(\mu)\omega_\beta(|\mu-s|)\,\mathrm{d}\mu\,\mathrm{d}s \ge 0$$

for $t>0$ and $w\in C[0,T]$.

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Positive-semidefinite-preserving approach

- But the regularity condition $w \in C[0, T]$ is always inadequate since

$$\Pi_0 w \notin C[0, T].$$

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- Tang, Yu and Zhou (SISC 2019) proved that the semipositive definiteness holds for

$$w \in L^p(0, T) \quad \text{with} \quad p \geq \frac{2}{1+\beta} \quad \text{for } 0 < \beta < 1,$$

which permits weakly singular functions like $w = O(t^{\beta-1})$ such that the L1$^+$ formula can naturally preserve the non-negative definiteness.

Discrete gradient structure (DGS)

In general, the non-negative definiteness of the real quadratic form

$$2\sum_{k=1}^{n} w_k \sum_{j=1}^{k} a_{k-j}^{(\beta,k)} w_j$$

is dependent on the discrete convolution kernels $a_{n-j}^{(\beta,n)}$, but should be independent of real sequences $\{w_k\}$. That is, *we want to determine the positive definiteness of these discrete convolution kernels without using the non-negative definiteness of continuous kernels.*

Step 1 Define the modified kernels

$$\mathsf{a}_0^{(\beta,n)} := 2a_0^{(\beta,n)} \quad \text{and} \quad \mathsf{a}_{n-j}^{(\beta,n)} := a_{n-j}^{(\beta,n)} \quad \text{for } 1 \le j \le n-1.$$

Step 2 For the modified kernels $a_{n-j}^{(\beta,n)}$, define the associated discrete (left-)complementary convolution (DCC) and right-complementary convolution (RCC) kernels

$$\sum_{j=k}^{n} p_{n-j}^{(\beta,n)} a_{j-k}^{(\beta,j)} \equiv 1 \quad \sum_{j=k}^{n} a_{n-j}^{(\beta,n)} {}^{r}p_{j-k}^{(\beta,j)} \equiv 1 \quad \text{for } 1 \leq k \leq n.$$

Step 2 For the modified kernels $a^{(\beta,n)}_{n-j}$, define the associated discrete (left-)complementary convolution (DCC) and right-complementary convolution (RCC) kernels

$$\sum_{j=k}^{n} p^{(\beta,n)}_{n-j} a^{(\beta,j)}_{j-k} \equiv 1 \quad \sum_{j=k}^{n} a^{(\beta,n)}_{n-j} {}^{r}p^{(\beta,j)}_{j-k} \equiv 1 \quad \text{for } 1 \le k \le n.$$

Step 3 Establish the discrete gradient structure in equality form

$$2w_n \sum_{j=1}^{n} a^{(\beta,n)}_{n-j} w_j = \sum_{j=1}^{n} p^{(\beta,n)}_{n-j} v_j^2 - \sum_{j=1}^{n-1} p^{(\beta,n-1)}_{n-1-j} v_j^2 + \sum_{j=1}^{n-1} \Big(\frac{1}{{}^{r}p^{(\beta,n)}_{n-j}} - \frac{1}{{}^{r}p^{(\beta,n)}_{n-j-1}} \Big) \Big(\sum_{k=1}^{j} {}^{r}p^{(\beta,n)}_{n-k} \nabla_\tau v_k \Big)^2$$

where the sequence $v_j := \sum_{\ell=1}^{j} a^{(\beta,j)}_{j-\ell} w_\ell$.

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Continuous counterpart of DGS

Recall the Riemann-Liouville fractional derivative ${}^R\partial_t^\beta := {}^{RL}_{0}\mathcal{D}_t^\beta$ defined by

$$ {}^R\partial_t^\beta v := \partial_t \mathcal{I}_t^{1-\beta} v \quad \text{for } 0 < \beta < 1. $$

We build up a continuous counterpart of DGS as follows,

Lemma 1

For $\beta \in (0,1)$ and an absolutely continuous function w, it holds that

$$ 2w(t)(\mathcal{I}_t^\beta w)(t) = \left({}^R\partial_t^\beta v^2\right)(t) + \frac{\beta\pi}{\sin\beta\pi}\int_0^t \omega_\beta(t-\xi)\Big(\int_0^\xi \omega_{1-\beta}(t-s)v'(s)\,\mathrm{d}s\Big)^2\,\mathrm{d}\xi, $$

where $v = \mathcal{I}_t^\beta w$, such that

$$ 2\,\mathcal{I}_t\big(w\mathcal{I}_t^\beta w\big)(t) \geq \big(\mathcal{I}_t^{1-\beta} v^2\big)(t) > 0 \quad \textit{for } v \neq 0. $$

Proof.

By the semigroup property, we have $w = {}^R\partial_t^\beta v = \partial_t \mathcal{I}_t^{1-\beta} v$ and

$$w(t)(\mathcal{I}_t^\beta w)(t) = v(t)({}^R\partial_t^\beta v)(t).$$

Since $v(0) = 0$, ${}^R\partial_t^\beta v = \partial_t^\beta v$ and ${}^R\partial_t^\beta v^2 = \partial_t^\beta v^2$. Then

$$\begin{aligned}
J[v] :=& 2v(t)({}^R\partial_t^\beta v)(t) - \big({}^R\partial_t^\beta v^2\big)(t) \\
=& 2v(t)\frac{\partial}{\partial t}\int_0^t \omega_{1-\beta}(t-s)v(s)\,\mathrm{d}s - \frac{\partial}{\partial t}\int_0^t \omega_{1-\beta}(t-s)v^2(s)\,\mathrm{d}s \\
=& 2\int_0^t \omega_{1-\beta}(t-s)v'(s)\big[v(t)-v(s)\big]\,\mathrm{d}s \\
=& 2\int_0^t \omega_{1-\beta}(t-s)v'(s)\int_s^t v'(\xi)\,\mathrm{d}\xi\,\mathrm{d}s \\
=& 2\int_0^t v'(\xi)\,\mathrm{d}\xi\int_0^\xi \omega_{1-\beta}(t-s)v'(s)\,\mathrm{d}s.
\end{aligned}$$

Proof of continuous DGS

Continue.

By taking

$$u(\xi) := \int_0^{\xi} \omega_{1-\beta}(t-s)v'(s)\,\mathrm{d}s$$

with $u(0) = 0$ and

$$u'(\xi) = \omega_{1-\beta}(t-\xi)v'(\xi),$$

it is not difficult to derive that

$$\begin{aligned} J[v] &= 2\int_0^t \frac{u'(\xi)u(\xi)}{\omega_{1-\beta}(t-\xi)}\,\mathrm{d}\xi = \int_0^t \Gamma(1-\beta)(t-\xi)^{\beta}\,\mathrm{d}u^2(\xi) \\ &= \Gamma(1-\beta)\Gamma(1+\beta)\int_0^t \omega_{\beta}(t-\xi)u^2(\xi)\,\mathrm{d}\xi \\ &= \frac{\beta\pi}{\sin\beta\pi}\int_0^t \omega_{\beta}(t-\xi)u^2(\xi)\,\mathrm{d}\xi. \end{aligned}$$

It leads to the claimed equality. □

To seek the discrete counterpart of Lemma 1, we introduce some discrete tools for any kernels $\{a_{n-j}^{(n)}\}_{j=1}^{n}$. The associated discrete orthogonality convolution (DOC) kernels $\theta_{n-k}^{(n)}$ are defined by

$$\theta_0^{(n)} := \frac{1}{a_0^{(n)}} \quad \text{and} \quad \theta_{n-k}^{(n)} := -\frac{1}{a_0^{(k)}} \sum_{j=k+1}^{n} \theta_{n-j}^{(n)} a_{j-k}^{(j)} \quad \text{for } 1 \le k \le n-1.$$

It is easy to check the following mutual orthogonality identities

$$\sum_{j=k}^{n} \theta_{n-j}^{(n)} a_{j-k}^{(j)} \equiv \delta_{nk} \quad \text{and} \quad \sum_{j=k}^{n} a_{n-j}^{(n)} \theta_{j-k}^{(j)} \equiv \delta_{nk} \quad \text{for } 1 \le k \le n,$$

where δ_{nk} is the Kronecker delta symbol with $\delta_{nk} = 0$ if $k \ne n$.

We define the discrete (left-)complementary convolution (DCC) kernels

$$p_{n-k}^{(n)} := \sum_{j=k}^{n} \theta_{j-k}^{(j)} \quad \text{for } 1 \le k \le n,$$

and the right-complementary convolution (RCC) kernels

$$^{r}p_{n-k}^{(n)} := \sum_{j=k}^{n} \theta_{n-j}^{(n)} \quad \text{for } 1 \le k \le n.$$

The DCC kernels $p_{n-j}^{(n)}$ are complementary with respect to $a_{n-j}^{(n)}$,

$$\sum_{j=k}^{n} p_{n-j}^{(n)} a_{j-k}^{(j)} \equiv 1 \quad \text{for } 1 \le k \le n;$$

and $a_{n-j}^{(n)}$ are complementary with respect to the RCC kernels $^{r}p_{n-j}^{(n)}$,

$$\sum_{j=k}^{n} a_{n-j}^{(n)}\, {}^{r}p_{j-k}^{(j)} \equiv 1 \quad \text{for } 1 \le k \le n.$$

DOC, DCC and RCC kernels

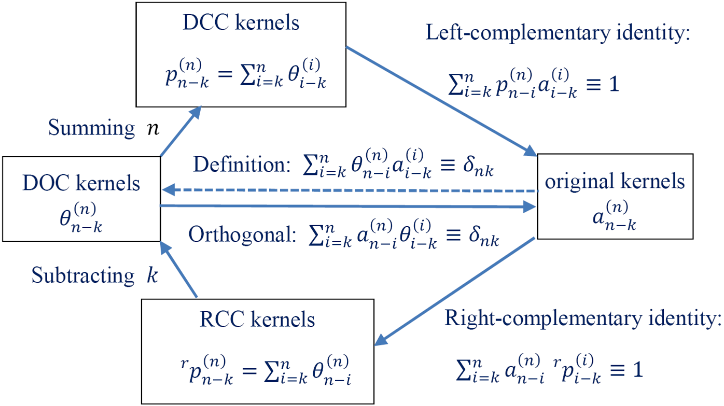

Figure: The relationship diagram of DOC, DCC and RCC kernels.

Lemma 2 (DCC)

If the positive kernels $a_j^{(n)}$ *are monotonically decreasing with respect to the subscript index* j, *that is,* $a_{j-1}^{(n)} > a_j^{(n)}$ *for* $1 \le j \le n-1$, *then the DCC kernels* $p_{n-k}^{(n)} \ge 0$.

Discrete convolution tools-DCC&RCC

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Lemma 3 (RCC)

If the positive kernels $a_j^{(n)}$ *are monotonically decreasing with respect to the superscript index* n*,* $a_{j-1}^{(n-1)} > a_j^{(n)}$ *for* $1 \le j \le n-1$*, and satisfy a class of logarithmic convexity,* $a_{j-1}^{(n-1)} a_{j+1}^{(n)} \ge a_j^{(n-1)} a_j^{(n)}$ *for* $1 \le j \le n-2$*, then the RCC kernels* ${}^r p_j^{(n)}$ *are positive and monotonically decreasing with respect to* j*.*

Theorem 4

For any fixed index $n \geq 2$ and any discrete convolution kernels $\{\chi_{n-j}^{(n)}\}_{j=1}^{n}$, consider the following auxiliary kernels for a constant $\sigma_{\min} \in [0, 2)$,

$$a_0^{(n)} := (2 - \sigma_{\min})\chi_0^{(n)} \quad \text{and} \quad a_{n-j}^{(n)} := \chi_{n-j}^{(n)} \quad \text{for } 1 \leq j \leq n-1.$$

Assume that the auxiliary kernels $a_{n-j}^{(n)}$ satisfy the following assumptions:

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(Column decrease) $\quad a_{j-1}^{(n-1)} > a_j^{(n)} \quad \text{for } 1 \leq j \leq n-1;$

(Logarithmic convexity) $\quad a_{j-1}^{(n-1)} a_{j+1}^{(n)} \geq a_j^{(n-1)} a_j^{(n)} \quad \text{for } 1 \leq j \leq n-2.$

DGS

Theorem 5 (continue)

Let $p^{(n)}_{n-j}$ and ${}^{r}p^{(n)}_{n-j}$ be the associated DCC and RCC kernels, respectively, with respect to $a^{(n)}_{n-j}$. Then the following DGS holds,

$$2w_n\sum_{j=1}^{n}\chi^{(n)}_{n-j}w_j=\sum_{k=1}^{n}p^{(n)}_{n-k}v_k^2-\sum_{k=1}^{n-1}p^{(n-1)}_{n-k-1}v_k^2+\sigma_{\min}\chi^{(n)}_0w_n^2+\sum_{j=1}^{n-1}\Big(\frac{1}{{}^{r}p^{(n)}_{n-j}}-\frac{1}{{}^{r}p^{(n)}_{n-j-1}}\Big)\Big[\sum_{k=1}^{j}{}^{r}p^{(n)}_{n-k}(v_k-v_{k-1})\Big]^2,$$

where $v_k:=\sum_{\ell=1}^{k}a^{(k)}_{k-\ell}w_\ell$ so that $\chi^{(n)}_{n-k}$ are positive definite,

$$2\sum_{k=1}^{n}w_k\sum_{j=1}^{k}\chi^{(k)}_{k-j}w_j\geq\sum_{j=1}^{n}p^{(n)}_{n-j}v_j^2+\sigma_{\min}\sum_{k=1}^{n}\chi^{(k)}_0w_k^2.$$

Skeleton proof of DGS

Proof.

For any real sequence $\{w_k\}_{k=1}^n$, let $v_0 := 0$ and $v_j := \sum_{k=1}^j a_{j-k}^{(j)} w_k$ for $1 \le j \le n$. With the help of orthogonality identity, $w_k = \sum_{j=1}^k \theta_{k-j}^{(k)} v_j$. Then one applies the definition of RCC kernels to find

$$w_n = \sum_{k=1}^n \theta_{n-k}^{(n)} v_k = {}^r p_0^{(n)} v_n + \sum_{k=1}^{n-1} ({}^r p_{n-k}^{(n)} - {}^r p_{n-k-1}^{(n)}) v_k = \sum_{k=1}^n {}^r p_{n-k}^{(n)} \nabla_\tau v_k.$$

By following the proof of (Liao-McLean-Zhang-2019, Lemma A.1),

$$\begin{aligned} 2v_n \sum_{k=1}^n {}^r p_{n-k}^{(n)} \nabla_\tau v_k &= \sum_{k=1}^n {}^r p_{n-k}^{(n)} \nabla_\tau v_k^2 + \frac{1}{{}^r p_0^{(n)}} \Big(\sum_{k=1}^n {}^r p_{n-k}^{(n)} \nabla_\tau v_k \Big)^2 \\ &+ \sum_{j=1}^{n-1} \Big(\frac{1}{{}^r p_{n-j}^{(n)}} - \frac{1}{{}^r p_{n-j-1}^{(n)}} \Big) \Big(\sum_{k=1}^j {}^r p_{n-k}^{(n)} \nabla_\tau v_k \Big)^2. \end{aligned}$$

Outline

Integral averaged kernels

The discrete kernels of integral averaged formula,

$$a_{n-k}^{(\beta,n)} := \frac{1}{\tau_n\tau_k}\int_{t_{n-1}}^{t_n}\int_{t_{k-1}}^{\min\{t,t_k\}} \omega_\beta(t-s)\,\mathrm{d}s\,\mathrm{d}t \quad \text{for } 1 \le k \le n.$$

The integral mean-value theorem yields

$$a_0^{(\beta,n)} = \frac{\tau_n^{\beta-1}}{\Gamma(2+\beta)} \quad \text{and} \quad a_1^{(\beta,n)} > a_2^{(\beta,n)} > \cdots > a_{n-1}^{(\beta,n)} \quad \text{for } n \ge 2.$$

A direct calculation gives

$$a_0^{(\beta,n)} - a_1^{(\beta,n)} = \frac{r_n}{\Gamma(2+\beta)\tau_n^{1-\beta}}\left[1 + 1/r_n + 1/r_n^{1+\beta} - (1+1/r_n)^{1+\beta}\right].$$

It is seen that $a_0^{(\beta,n)} > a_1^{(\beta,n)}$ as $\beta \to 0$, while $a_0^{(\beta,n)} < a_1^{(\beta,n)}$ as $\beta \to 1$.

Lemma 6

The kernels $a_{n-k}^{(\beta,n)}$ *fulfill* $2a_0^{(\beta,n)} > a_1^{(\beta,n)} > a_2^{(\beta,n)} > \cdots > a_{n-1}^{(\beta,n)} > 0.$

Integral averaged kernels

Lemma 6

The kernels $a_{n-k}^{(\beta,n)}$ *fulfill* $2a_0^{(\beta,n)} > a_1^{(\beta,n)} > a_2^{(\beta,n)} > \cdots > a_{n-1}^{(\beta,n)} > 0.$

Lemma 7

Let the adjacent step-ratios satisfy the following condition

$$r_{k+1} \geq r_*(r_k) := \sqrt[1-\beta]{\frac{(2^\beta - 1)\rho(r_k)}{\rho(2r_k) - \rho(r_k)}} \quad \text{for } k \geq 2,$$

where the function $\rho(z) := (z+1)^{1+\beta} - z^{1+\beta} - 1$ *and* $r_*(z) < 1$ *for any* $z > 0$. *Then the discrete convolution kernels* $a_{n-k}^{(\beta,n)}$ *fulfill*

$$\frac{a_1^{(\beta,n)}}{2a_0^{(\beta,n-1)}} < \frac{a_2^{(\beta,n)}}{a_1^{(\beta,n-1)}} < \cdots < \frac{a_{n-1}^{(\beta,n)}}{a_{n-2}^{(\beta,n-1)}} < 1 \quad \text{for } n \geq 2.$$

DGS for integral averaged kernels

Corollary 8

Let the adjacent step-ratios satisfy the following condition

$$r_{k+1} \geq r_*(r_k) := \sqrt[1-\beta]{\frac{(2^\beta - 1)\rho(r_k)}{\rho(2r_k) - \rho(r_k)}} \quad \text{for } k \geq 2,$$

where $r_*(z) < 1$ *for any* $z > 0$. *It holds that*

$$2w_n \sum_{j=1}^{n} a_{n-j}^{(\beta,n)} w_j = \sum_{j=1}^{n} \mathsf{p}_{n-j}^{(\beta,n)} v_j^2 - \sum_{j=1}^{n-1} \mathsf{p}_{n-1-j}^{(\beta,n-1)} v_j^2 + \sum_{j=1}^{n-1} \Big(\frac{1}{{}^r\mathsf{p}_{n-j}^{(\beta,n)}} - \frac{1}{{}^r\mathsf{p}_{n-j-1}^{(\beta,n)}} \Big) \Big(\sum_{k=1}^{j} {}^r\mathsf{p}_{n-k}^{(\beta,n)} \nabla_\tau v_k \Big)^2$$

where the sequence $v_j := \sum_{\ell=1}^{j} a_{j-\ell}^{(\beta,j)} w_\ell$. *Thus the discrete kernels* $a_{n-k}^{(\beta,n)}$ *are positive definite.*

Outline

Continuous energy dissipation law

Consider the time-fractional Allen-Cahn model

$$\partial_t^\alpha \Phi = -\kappa\mu \quad \text{with} \quad \mu := \frac{\delta E}{\delta \Phi} = f(\Phi) - \epsilon^2 \Delta\Phi,$$

where κ is the mobility coefficient and E is the Ginzburg-Landau functional

$$E[\Phi] := \int_\Omega \Big(\frac{\epsilon^2}{2}\left|\nabla\Phi\right|^2 + F(\Phi)\Big)\,\mathrm{d}\mathbf{x} \quad \text{with} \quad F(\Phi) := \frac{1}{4}\Big(\Phi^2 - 1\Big)^2.$$

Tang, Yu and Zhou (Tang-Yu-Zhou-SISC-2019) derived an energy law

$$E(t) \le E(0).$$

This energy dissipation law is globally in time and not asymptotically compatible in the $\alpha \to 1$ limit.

Continuous energy dissipation law

Quan et al (Quan-Tang-Yang-CSIAM-2020, Quan-Tang-Yang-2020) derived a time-fractional energy dissipation law

$$\left(\partial_t^\alpha E\right)(t) \leq 0 \quad \text{for } t > 0,$$

and a weighted energy dissipation law,

$$\frac{\mathrm{d}E_\varpi}{\mathrm{d}t} \leq 0 \quad \text{for } t > 0 \quad \text{where} \quad E_\varpi(t) := \int_0^1 \varpi(\theta)E(\theta t)\,\mathrm{d}\theta,$$

where $E(\theta t) = E\left[\Phi\left(\cdot, \theta t\right)\right]$ is a weighted Ginzburg–Landau energy.

Some other nonlocal energy forms were also proposed in (Li-Salgado-arXiv:2101.00541v1, Fritz-Khristenko-Wohlmuth-arXiv 2106.10985, Li-Quan-Xu-arXiv 2106.11163) for the desired local energy law like

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\mathrm{nonlocal}}(t) \leq 0.$$

Continuous energy dissipation law

Recently, we obtain a local energy law (Liao-Tang-Zhou-2021,Liao-Zhu-Wang-2022)

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\underbrace{E[\Phi]+\frac{\kappa}{2}\mathcal{I}_t^{\alpha}\|\mu\|^2}_{\mathcal{E}_\alpha[\Phi]\,:\ \text{a global energy may not be physical}}\Big)+\frac{\kappa}{2}\omega_\alpha(t)\|\mu\|^2\le 0.$$

It is asymptotically compatible (but not exactly) with the classical energy dissipation law (equality). As the fractional order $\alpha \to 1$,

$$\frac{\mathrm{d}}{\mathrm{d}t}E[\Phi]+\kappa\|\mu\|^2\le 0,$$

but $\mathcal{E}_\alpha[\Phi]$ is not asymptotically compatible with the free energy

$$\mathcal{E}_\alpha[\Phi] \ \rightarrow\ E[\Phi]+\frac{1}{2}\int_0^t \|\mu\|^2\,\mathrm{d}s, \quad \text{as } \alpha\to 1.$$

Applying Lemma 1, one gets an improved energy dissipation law

$$\frac{\mathrm{d}E_\alpha}{\mathrm{d}t} + \frac{(1-\alpha)\pi}{2\kappa\sin(1-\alpha)\pi}\int_0^t \omega_{1-\alpha}(t-\xi)\Big\|\int_0^\xi \omega_\alpha(t-s)v'(s)\,\mathrm{d}s\Big\|^2\,\mathrm{d}\xi = 0,$$

where $v = \partial_t^\alpha \Phi = -\kappa\mu$ and the nonlocal (variational) energy

$$E_\alpha[\Phi] := E[\Phi] + \frac{\kappa}{2}\mathcal{I}_t^\alpha\|\mu\|^2 = E[\Phi] + \frac{\kappa}{2}\mathcal{I}_t^\alpha\Big\|\frac{\delta E}{\delta\Phi}\Big\|^2.$$

As $\alpha \to 1$, $\int_0^\xi \omega_\alpha(t-s)v'(s)\,\mathrm{d}s \to v(\xi)$, and the above law degrades into

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(E[\Phi] + \frac{\kappa}{2}\mathcal{I}_t^1\|\mu\|^2\Big) + \frac{\kappa}{2}\|\mu\|^2 = \frac{\mathrm{d}E}{\mathrm{d}t} + \kappa\|\mu\|^2 = 0,$$

which is just the energy dissipation law of Allen-Cahn model. The new energy law is asymptotically compatible (exactly) as $\alpha \to 1$.

Crank-Nicolson ($L1^+$) scheme

By applying the $L1^+$ formula, we have the Crank-Nicolson scheme

$$(\partial_\tau^\alpha \phi)^{n-\frac{1}{2}} = -\kappa\mu^{n-\frac{1}{2}} \quad \text{with} \quad \mu^{n-\frac{1}{2}} = f(\phi)^{n-\frac{1}{2}} - \epsilon^2\Delta\phi^{n-\frac{1}{2}} \quad \text{for } n \geq 1.$$

Here, $f(\phi)^{n-\frac{1}{2}}$ is the standard second-order approximation defined by

$$f(\phi)^{n-\frac{1}{2}} := \frac{1}{2}\left[(\phi^n)^2 + (\phi^{n-1})^2\right]\phi^{n-\frac{1}{2}} - \phi^{n-\frac{1}{2}}$$

such that

$$\langle f(\phi)^{n-\frac{1}{2}}, \nabla_\tau \phi^n\rangle = \langle F(\phi^n), 1\rangle - \langle F(\phi^{n-1}), 1\rangle.$$

Theorem 9

If $\tau_n \leq \sqrt[\alpha]{\frac{2}{\kappa\Gamma(3-\alpha)}}$, the Crank-Nicolson scheme is uniquely solvable.

We define the following discrete variational energy

$$E_\alpha[\phi^n] := E[\phi^n] + \frac{1}{2\kappa}\sum_{j=1}^{n} \mathsf{p}_{n-j}^{(1-\alpha,n)}\left\|v^j\right\|^2 \quad \text{with } v^j := \sum_{\ell=1}^{j} \mathsf{a}_{j-\ell}^{(1-\alpha,j)}\nabla_\tau\phi^\ell,$$

where $E[\phi^n]$ is the original Ginzburg-Landau energy.

Theorem 10

Under the step-ratio constraint $r_{k+1} \geq r_*(r_k)$, the variable-step Crank-Nicolson scheme is energy stable in the sense that

$$\partial_\tau E_\alpha[\phi^n] + \frac{1}{2\kappa\tau_n}\sum_{j=1}^{n-1}\Big(\frac{1}{{}^r\mathsf{p}_{n-j}^{(1-\alpha,n)}} - \frac{1}{{}^r\mathsf{p}_{n-j-1}^{(1-\alpha,n)}}\Big)\Big\|\sum_{k=1}^{j} {}^r\mathsf{p}_{n-k}^{(1-\alpha,n)}\nabla_\tau v^k\Big\|^2 = 0.$$

Asymptotical compatiblity

As $\alpha \to 1$, $a_0^{(0,n)} = 1/\tau_n$ and $a_{n-k}^{(0,n)} = 0$ for $1 \le k \le n-1$. The L1$^+$ scheme degrades into the Crank-Nicolson scheme

$$\partial_\tau \phi^n = -\kappa\mu^{n-\frac{1}{2}} \quad \text{with} \quad \mu^{n-\frac{1}{2}} = f(\phi)^{n-\frac{1}{2}} - \epsilon^2\Delta\phi^{n-\frac{1}{2}} \quad \text{for } n \ge 1.$$

The DCC and RCC kernels $\mathrm{p}_{n-k}^{(0,n)} = \tau_k/2$ and ${}^r\mathrm{p}_{n-k}^{(0,n)} = \tau_n/2$ for $1 \le k \le n$. The discrete variational energy degrades into

$$E_\alpha[\phi^n] \quad \longrightarrow \quad E[\phi^n] + \frac{1}{\kappa}\sum_{j=1}^{n} \tau_j \left\|\partial_\tau \phi^j\right\|^2 \quad \text{as } \alpha \to 1;$$

and the discrete energy dissipation law in Theorem 10 degrades into

$$\partial_\tau E\left[\phi^n\right] + \frac{1}{\kappa}\left\|\partial_\tau \phi^n\right\|^2 = 0 \quad \text{for } n \ge 1.$$

Our energy law is asymptotically compatible (exactly) as $\alpha \to 1$.

Example: TFAC

An adaptive step criterion based on the solution variation

$$\tau_{ada} = \max\left\{\tau_{\min}, \frac{\tau_{\max}}{\sqrt{1+\eta\left\|\partial_\tau \phi^n\right\|^2}}\right\},$$

where the uniform size $\tau = 0.005$, $\tau_{\max} = 10^{-1}$ and $\tau_{\min} = 10^{-3}$.

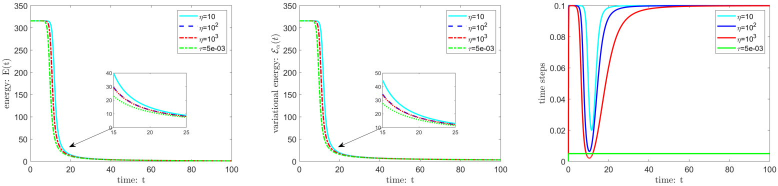
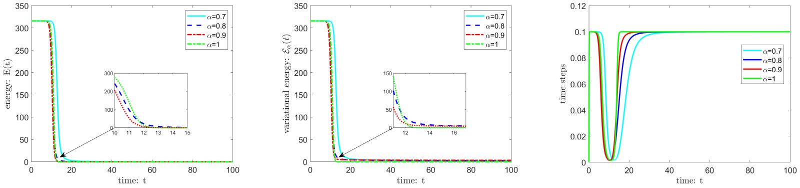


Figure: The energies $E(t)$, $E_\alpha(t)$ and adaptive steps for $u_0 = \mathrm{rand}(\mathbf{x})$.

An adaptive step criterion based on the solution variation

$$\tau_{ada} = \max\left\{\tau_{\min}, \frac{\tau_{\max}}{\sqrt{1+\eta\left\|\partial_\tau \phi^n\right\|^2}}\right\},$$

where we set $\tau_{\max} = 10^{-1}$, $\tau_{\min} = 10^{-3}$ and $\eta = 10^3$.



(a) energy $E[\phi^n]$ (b) energy $E_\alpha[\phi^n]$ (c) steps τ_n

Figure: Numerical results for different fractional orders α.

Outline

Continuous energy dissipation law

We consider the following Klein-Gordon-type fractional wave equation (Adolfsson-Enelund-Larsson-2003,Golmankhaneh-Golmankhaneh-Baleanu-2011) with the fractional order $\beta \in (0, 1)$,

$$\partial_t U + \mathcal{I}_t^{\beta} \zeta = 0 \quad \text{with } \zeta := \frac{\delta E}{\delta U} = f(U) - \epsilon^2 \Delta U,$$

where $f(U) = F'(U)$ and the associated energy $E[U]$ is defined by

$$E[U] := \int_{\Omega} \Big(\frac{\epsilon^2}{2} |\nabla U|^2 + F(U) \Big) \, \mathrm{d}\mathbf{x} \quad \text{with} \;\; F(U) := \frac{1}{4} \Big(U^2 - 1 \Big)^2.$$

This model is intermediate between the Allen-Cahn-type diffusion equation $(\beta = 0)$ and the Klein-Gordon-type wave equation $(\beta = 1)$, and it can be termed as a nonlinear fractional PDE with the Caputo time derivative of order $\alpha = 1 + \beta \in (1, 2)$.

Continuous energy dissipation law

Typically, in the limit $\beta \to 1$, the above model recovers the classical Klein-Gordon equation $\partial_t^2 U = \epsilon^2 \Delta U - f(U)$. As well-known, it admits the energy conservation law (Li-Vu Quoc-SINUM-1995)

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} = 0,$$

where the Hamiltonian energy $\mathcal{E}$ is defined by

$$\mathcal{E}[U] := E[U] + \frac{1}{2}\|\partial_t U\|^2.$$

Therefore, it is natural to ask whether the time-fractional Klein-Gordon equation also maintains a similar energy law, and whether the second-order time-stepping scheme based on integral averaged formula can also maintain the corresponding energy law at the discrete time levels.

Continuous energy dissipation law

Applying Lemma 1, we get an energy dissipation law

$$\frac{\mathrm{d}\mathcal{E}_\beta}{\mathrm{d}t} + \frac{\beta\pi}{2\sin\beta\pi}\int_0^t \omega_\beta(t-\xi)\Big\|\int_0^\xi \omega_{1-\beta}(t-s)v'(s)\,\mathrm{d}s\Big\|^2\,\mathrm{d}\xi = 0,$$

where the nonlocal energy

$$\mathcal{E}_\beta[U] := E[U] + \frac{1}{2}\mathcal{I}_t^{1-\beta}\big\|\partial_t U\big\|^2 \quad \text{for } t > 0.$$

As the fractional order $\beta \to 1$, one has

$$\mathcal{E}_\beta[U] \to \mathcal{E}[U] = E[U] + \frac{1}{2}\|\partial_t U\|^2.$$

The energy dissipation law degrades into the energy conservation law of the classical Klein-Gordon model

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} = 0.$$

Both the nonlocal energy $\mathcal{E}_\beta[U]$ and the energy dissipation law are asymptotically compatible in the limit $\beta \to 1$.

Crank-Nicolson scheme

By applying the integral averaged formula $\mathcal{I}_\tau^\beta$, we have a Crank-Nicolson scheme for the Klein-Gordon-type fractional wave equation

$$\partial_\tau u^n + (\mathcal{I}_\tau^\beta \zeta)^{n-\frac{1}{2}} = 0 \quad \text{with} \quad \zeta^{n-\frac{1}{2}} = f(u)^{n-\frac{1}{2}} - \epsilon^2 \Delta u^{n-\frac{1}{2}}.$$

Theorem 11

If $\tau_n \le \sqrt[1+\beta]{2\Gamma(2+\beta)}$, the Crank-Nicolson scheme is uniquely solvable.

With the original energy $E\left[u^n\right]=\frac{\epsilon^2}{2}\left\|\nabla u^n\right\|^2+\frac{1}{4}\left\|(u^n)^2-1\right\|^2$, we define the following discrete analogue of $\mathcal{E}_\beta[u]$,

$$\mathcal{E}_\beta[u^n]:=E[u^n]+\frac{1}{2}\sum_{j=1}^{n}\mathsf{p}_{n-j}^{(\beta,n)}\left\|v^j\right\|^2,$$

where $v^j:=\sum_{\ell=1}^{j}\mathsf{a}_{j-\ell}^{(\beta,j)}\tau_\ell\zeta^{\ell-\frac{1}{2}}$.

Theorem 12

Under the step-ratio constraint $r_{k+1}\ge r_*(r_k)$, the variable-step Crank-Nicolson scheme is energy stable in the sense that

$$\partial_\tau\mathcal{E}_\beta[u^n]+\frac{1}{2\tau_n}\sum_{j=1}^{n-1}\Big(\frac{1}{{}^r\mathsf{p}_{n-j}^{(\beta,n)}}-\frac{1}{{}^r\mathsf{p}_{n-j-1}^{(\beta,n)}}\Big)\Big\|\sum_{k=1}^{j}{}^r\mathsf{p}_{n-k}^{(\beta,n)}\nabla_\tau v^k\Big\|^2=0.$$

Asymptotical compatiblity

As $\beta \to 1$, $a_0^{(1,n)} = 1/2$ and $a_{n-k}^{(1,n)} = 1$ for $1 \le k \le n-1$. The above numerical scheme degrades into the Crank-Nicolson scheme

$$\partial_\tau u^n + \frac{\tau_n}{2}\zeta^{n-\frac{1}{2}} + \sum_{j=1}^{n-1} \tau_j \zeta^{j-\frac{1}{2}} = 0 \quad \text{with} \quad \zeta^{n-\frac{1}{2}} = f(u)^{n-\frac{1}{2}} - \epsilon^2 \Delta u^{n-\frac{1}{2}}$$

This numerical scheme is uniquely solvable if $\tau_n \le 2$. This numerical scheme can be formulated into

$$\partial_\tau u^n + w^{n-\frac{1}{2}} = 0$$

by introducing $w^n := \sum_{k=1}^n \tau_k \zeta^{k-\frac{1}{2}}$. With the fact $w^n - w^{n-1} = \tau_n \zeta^{n-\frac{1}{2}}$, it is easy to establish a discrete energy conservation law

$$E[u^n] + \frac{1}{2}\|w^n\|^2 = E[u^{n-1}] + \frac{1}{2}\|w^{n-1}\|^2 \quad \text{for } n \ge 1.$$

Asymptotical compatiblity

The modified kernels $a_{n-k}^{(1,n)} = 1$ for $1 \le k \le n$. The associated DOC kernels $\theta_0^{(1,n)} = 1$, $\theta_1^{(1,n)} = -1$ and $\theta_{n-k}^{(1,n)} = 0$ for $1 \le k \le n-2$. Then the corresponding DCC and RCC kernels read

$$\mathrm{p}_0^{(1,n)} = 1 \quad \text{and} \quad \mathrm{p}_{n-k}^{(1,n)} = 0 \quad \text{for } 1 \le k \le n-1,$$
$$^r\mathrm{p}_0^{(1,n)} = 1 \quad \text{and} \quad ^r\mathrm{p}_{n-k}^{(1,n)} = 0 \quad \text{for } 1 \le k \le n-1.$$

With $v^n := \sum_{k=1}^n \tau_k \zeta^{k-\frac{1}{2}}$, the discrete energy degrades into

$$\mathcal{E}_\beta[u^n] \quad \longrightarrow \quad E[u^n] + \frac{1}{2}\|v^n\|^2 \quad \text{as } \beta \to 1;$$

and the discrete energy dissipation law in Theorem 12 degrades into

$$\partial_\tau \left(E\left[u^n\right] + \frac{1}{2}\|v^n\|^2 \right) = 0 \quad \text{for } n \ge 1.$$

Both the discrete energy and energy dissipation law are asymptotically compatible in the limit $\beta \to 1$.

Some further issues

- For the DGS decomposition, we impose a sufficient step-ratio condition

$$r_{k+1} \geq \sqrt[1-\beta]{\frac{(2^\beta - 1)\rho(r_k)}{\rho(2r_k) - \rho(r_k)}}.$$

Numerical tests support that the following weak condition is also sufficient,

$$r_{k+1} \geq r_g(r_k) := \left(1 + 5r_k^{-\beta}\right)^{-1}.$$

Nonetheless, we are not able to present a rigorous proof.

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Nonetheless, we are not able to present a rigorous proof.

- We build the discrete gradient structure of $L1^+$ formula. How about other discrete Caupto formulas, such as variable-step L2-1_{σ} (Alikhanov-JCP-2015, Liao-McLean-Zhang-2021) and variable-step L1-2 (fractional BDF2-like) formulas (Gao-Sun-Zhang-JCP-2014, Lv-Xu-SISC-2016, Liao-McLean-Zhang-2019) ?

Thank you for your attention !

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