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

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Outline

1. Intergal averaged formula and our results
   - Motivation
   - Integral averaged formula
   - The problem and our results

2. Derivation of discrete gradient structure
   - General kernels
   - Kernels of integral averaged formula

3. Application to time-fractional Allen-Cahn model

4. Application to time-fractional Klein-Gordon model

5. Further issues to be studied
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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**

\[
(I_t^\beta w)(t) := \int_0^t \omega_\beta(t-s)w(s)\,ds \quad \text{with} \quad \omega_\beta(t) := t^{\beta-1}/\Gamma(\beta)
\]

and **fractional Caputo derivative** for \(0 < \alpha < 1\)

\[
(\partial_t^\alpha w)(t) := (I_t^{1-\alpha} w')(t) = \int_0^t \omega_{1-\alpha}(t-s)w'(s)\,ds.
\]

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

\[ E[\Phi] := \int_{\Omega} \left( \frac{c^2}{2} |\nabla \Phi|^2 + F(\Phi) \right) \, dx \quad \text{with} \quad F(\Phi) := \frac{1}{4}(\Phi^2 - 1)^2. \]

- **Multiscale behaviors:** Chen-Zhao-et al-CPC-2018, Liu-Cheng-et al-CMA-2018, ...
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- **Multiscale behaviors:** Chen-Zhao-et al-CPC-2018, Liu-Cheng-et al-CMA-2018, ...
- **Theoretical analysis:** Du-Yang-Zhou-JSC-2020, Al-Maskari-Karaa-IMA-2021, Fritz-Rajendran-Wohlmuth-CMA-2022, ...
Fractional wave models

Another example, nonlinear fractional wave (integro-differential) equations

$$\partial_t U = \int_0^t \kappa(t-s) \left[ \Delta U + f(U) \right] \, ds.$$ 

There are many of related references, see

- **Monographs**: Brunner-Cambridge University Press-2004, Mainardi-Imperial College Press-2010, ...
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Adaptive time-stepping strategy

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

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- The theoretical verifications of energy dissipation law, stability and convergence on a general class of nonuniform time meshes are very desirable, see
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Integral averaged formula

Consider $0 = t_0 < t_1 < \cdots < t_k < \cdots < t_N = T$ with $\tau_k := t_k - t_{k-1}$, $\tau := \max_{1 \leq k \leq N} \tau_k$, $r_k := \tau_k / \tau_{k-1}$. 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 $t_{k-1} < t \leq t_k$. The integral averaged (Crank-Nicolson) formula of fractional Riemann-Liouville integral,

\[
(I^\beta_\tau w)^{n-\frac{1}{2}} := \frac{1}{\tau_n} \int_{t_{n-1}}^{t_n} \int_{0}^{t} \omega_\beta(t - s) (\Pi_0 w) \, ds \, dt \triangleq \sum_{k=1}^{n} a^{(\beta,n)}_{n-k} \tau_k w^{k-\frac{1}{2}},
\]

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

\[
a^{(\beta,n)}_{n-k} := \frac{1}{\tau_n \tau_k} \int_{t_{n-1}}^{t_n} \int_{t_{k-1}}^{\min\{t,t_k\}} \omega_\beta(t - s) \, ds \, dt \quad \text{for } 1 \leq k \leq n.
\]
Let the piecewise approximation $\Pi_1 w := \Pi_{1,k} w$ so that

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

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

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

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

$$a_{n-k}^{(1-\alpha,n)} = \frac{1}{\tau_n \tau_k} \int_{t_{n-1}}^{t_n} \int_{t_{k-1}}^{\min\{t,t_k\}} \omega_{1-\alpha}(t-s) \, ds \, dt \quad \text{for } 1 \leq k \leq n.$$
Positive-semidefinite-preserving approach

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

\[
\sum_{j=1}^{n} \tau_j w^{j-\frac{1}{2}} \sum_{k=1}^{j} a_{j-k}^{(\beta,j)} \tau_k w^{k-\frac{1}{2}} = \sum_{j=1}^{n} \int_{t_{j-1}}^{t_j} w^{j-\frac{1}{2}} \int_{0}^{t} \omega_{\beta}(t - s)(\Pi_0 w) \, ds \, dt
\]

\[
= \int_{t_0}^{t_n} (\Pi_0 w) \, dt \int_{0}^{t} \omega_{\beta}(t - s)(\Pi_0 w) \, ds
\]

is a discrete analogue to the non-negative definiteness of kernel \( \omega_{\beta} \) (McLean-Thomée-1993, Lubich-Sloan-Thomée-MC-1996, McLean-Thomée-JCAM-1996)

\[
2I_1^1(wI_t^\beta w)(t) = 2 \int_{0}^{t} w(\mu) \, d\mu \int_{0}^{\mu} \omega_{\beta}(\mu - s)w(s) \, ds
\]

\[
= \int_{0}^{t} \int_{0}^{t} w(s)w(\mu)\omega_{\beta}(|\mu - s|) \, d\mu \, ds \geq 0
\]

for \( t > 0 \) and \( w \in C[0, T] \).
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But the regularity condition \( w \in C[0, T] \) is always inadequate since

\[ \Pi_0 w \not\in C[0, T]. \]

For the \( L^1^+ \) formula, the non-negative definiteness needs a severer condition

\[ (\Pi_1 w)' \in C[0, T]. \]
But the regularity condition \( w \in C[0, T] \) is always inadequate since
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For the \( L_{1^+} \) formula, the non-negative definiteness needs a severer condition
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(\Pi_1 w)' \in C[0, T].
\]

Tang, Yu and Zhou (SISC 2019) proved that the semipositive definiteness holds for
\[
w \in L^p(0, T) \quad \text{with} \quad p \geq \frac{2}{1 + \beta} \quad \text{for} \quad 0 < \beta < 1,
\]
which permits weakly singular functions like \( w = O(t^{\beta-1}) \) such that the \( L_{1^+} \) 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

\[
a_0^{(\beta,n)} := 2a_0^{(\beta,n)} \quad \text{and} \quad a_{n-j}^{(\beta,n)} := a_{n-j}^{(\beta,n)} \quad \text{for} \quad 1 \leq j \leq n - 1.
\]
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

\[
\sum_{j=k}^{n} p_{n-j}^{(\beta,n)} a_{j-k}^{(\beta,j)} \equiv 1 \quad \sum_{j=k}^{n} a_{n-j}^{(\beta,n)} r_{j-k}^{(\beta,j)} \equiv 1 \text{ for } 1 \leq k \leq n.
\]
Discrete gradient structure (DGS)

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\]

Step 3 Establish the discrete gradient structure in equality form

\[
2w_n \sum_{j=1}^{n} a_{n-j}^{(\beta,n)} w_j = \sum_{j=1}^{n} p_{n-j}^{(\beta,n)} v_j^2 - \sum_{j=1}^{n-1} p_{n-1-j}^{(\beta,n-1)} v_j^2 \\
+ \sum_{j=1}^{n-1} \left( \frac{1}{r_{p_{n-j}^{(\beta,n)}}} - \frac{1}{r_{p_{n-j-1}^{(\beta,n)}}} \right) \left( \sum_{k=1}^{j} r_{p_{n-k}^{(\beta,n)}} \nabla \tau v_k \right)^2
\]

where the sequence $v_j := \sum_{\ell=1}^{j} a_{j-\ell}^{(\beta,j)} w_{\ell}$.
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Continuous counterpart of DGS

Recall the Riemann-Liouville fractional derivative

\[ R^\beta_\partial t v := \partial_t I^{1-\beta}_t v \quad \text{for } 0 < \beta < 1. \]

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*

\[
2w(t)(I^\beta_t w)(t) = (R^\beta_\partial_t v^2)(t) \\
+ \frac{\beta \pi}{\sin \beta \pi} \int_0^t \omega_\beta(t - \xi) \left( \int_0^\xi \omega_{1-\beta}(t - s)v'(s) ds \right)^2 d\xi,
\]

*where \( v = I^\beta_t w \), such that*

\[
2 I_t (wI^\beta_t w)(t) \geq (I^{1-\beta}_t v^2)(t) > 0 \quad \text{for } v \neq 0.
\]
Proof of continuous DGS

Proof.

By the semigroup property, we have $w = R_{t}^{\beta} v = \partial_{t} I_{t}^{1-\beta} v$ and

$$w(t)(I_{t}^{\beta} w)(t) = v(t)(R_{t}^{\beta} v)(t).$$

Since $v(0) = 0$, $R_{t}^{\beta} v = \partial_{t}^{\beta} v$ and $R_{t}^{\beta} v^{2} = \partial_{t}^{\beta} v^{2}$. Then

$$J[v] := 2v(t)(R_{t}^{\beta} v)(t) - (R_{t}^{\beta} v^{2})(t)$$

$$= 2v(t) \frac{\partial}{\partial t} \int_{0}^{t} \omega_{1-\beta}(t-s)v(s) \, ds - \frac{\partial}{\partial t} \int_{0}^{t} \omega_{1-\beta}(t-s)v^{2}(s) \, ds$$

$$= 2 \int_{0}^{t} \omega_{1-\beta}(t-s)v'(s)[v(t) - v(s)] \, ds$$

$$= 2 \int_{0}^{t} \omega_{1-\beta}(t-s)v'(s) \int_{s}^{t} v'(<\xi>) \, d\xi \, ds$$

$$= 2 \int_{0}^{t} v'(\xi) \, d\xi \int_{0}^{\xi} \omega_{1-\beta}(t-s)v'(s) \, ds.$$
By taking
\[ u(\xi) := \int_0^\xi \omega_{1-\beta}(t-s)v'(s) \, ds \]
with \( u(0) = 0 \) and
\[ u'(\xi) = \omega_{1-\beta}(t-\xi)v'(\xi), \]
it is not difficult to derive that
\[ J[v] = \int_0^t \frac{u'(\xi)u(\xi)}{\omega_{1-\beta}(t-\xi)} \, d\xi = \int_0^t \Gamma(1-\beta)(t-\xi)^\beta \, du^2(\xi) \]
\[ = \Gamma(1-\beta)\Gamma(1+\beta) \int_0^t \omega_\beta(t-\xi)u^2(\xi) \, d\xi \]
\[ = \frac{\beta\pi}{\sin{\beta\pi}} \int_0^t \omega_\beta(t-\xi)u^2(\xi) \, d\xi. \]
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

\[
\theta_{0}^{(n)} := \frac{1}{a_{0}^{(n)}} \quad \text{and} \quad \theta_{n-k}^{(n)} := -\frac{1}{a_{0}^{(k)}} \sum_{j=k+1}^{n} \theta_{n-j}^{(n)} a_{j-k}^{(j)} \quad \text{for } 1 \leq k \leq n - 1.
\]

It is easy to check the following mutual orthogonality identities

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

where \( \delta_{nk} \) is the Kronecker delta symbol with \( \delta_{nk} = 0 \) if \( k \neq n \).
We define the discrete (left-)complementary convolution (DCC) kernels

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

and the right-complementary convolution (RCC) kernels

\[ r_{n-k}^{(n)} := \sum_{j=k}^{n} \theta_{n-j}^{(n)} \quad \text{for} \ 1 \leq k \leq n. \]

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

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

and \( a_{n-j}^{(n)} \) are complementary with respect to the RCC kernels \( r_{n-j}^{(n)} \),

\[ \sum_{j=k}^{n} a_{n-j}^{(n)} r_{j-k}^{(j)} \equiv 1 \quad \text{for} \ 1 \leq k \leq n. \]
DOC, DCC and RCC kernels

**DOC kernels**

$$\theta_{n-k}^{(n)}$$

**DCC kernels**

$$p_{n-k}^{(n)} = \sum_{i=k}^{n} \theta_{i-k}^{(i)}$$

**Definition:**

$$\sum_{i=k}^{n} \theta_{n-i}^{(n)} a_{i-k}^{(i)} \equiv \delta_{nk}$$

**Orthogonal:**

$$\sum_{i=k}^{n} a_{n-i}^{(n)} \theta_{i-k}^{(i)} \equiv \delta_{nk}$$

**Right-complementary identity:**

$$\sum_{i=k}^{n} a_{n-i}^{(n)} r_{p_{i-k}}^{(i)} \equiv 1$$

**Left-complementary identity:**

$$\sum_{i=k}^{n} p_{n-i}^{(n)} a_{i-k}^{(i)} \equiv 1$$

**RCC kernels**

$$r_p_{n-k}^{(n)} = \sum_{i=k}^{n} \theta_{n-i}^{(n)}$$

**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 $1 \leq j \leq n - 1$, then the DCC kernels $p_{n-k}^{(n)} \geq 0$. 
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 $1 \leq j \leq n - 1$, then the DCC kernels $p_{n-k}^{(n)} \geq 0$.

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 $1 \leq j \leq n - 1$, and satisfy a class of logarithmic convexity, $a_{j-1}^{(n-1)} a_j^{(n)} \geq a_j^{(n-1)} a_{j+1}^{(n)}$ for $1 \leq j \leq n - 2$, 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 $\sigma_{\text{min}} \in [0, 2)$,

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

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

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

(\text{Row decrease}) \quad a_{j-1}^{(n)} \geq a_j^{(n)} > 0 \quad \text{for} \quad 1 \leq j \leq n - 1;
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\]

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

- **(Row decrease)** \( a_{j-1}^{(n)} \geq a_j^{(n)} > 0 \) for \( 1 \leq j \leq n - 1 \);
- **(Column decrease)** \( a_{j-1}^{(n-1)} > a_j^{(n)} \) for \( 1 \leq j \leq n - 1 \);
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 $\sigma_{\text{min}} \in [0, 2)$,

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

(Row decrease) $a_{j-1}^{(n)} \geq a_{j}^{(n)} > 0 \quad \text{for } 1 \leq j \leq n - 1$;

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

(Logarithmic convexity) $a_{j-1}^{(n-1)} a_{j+1}^{(n)} \geq a_{j}^{(n-1)} a_{j}^{(n)} \quad \text{for } 1 \leq j \leq n - 2$. 
Theorem 5 (continue)

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

$$2 w_n \sum_{j=1}^{n} \chi_{n-j}^{(n)} w_j = \sum_{k=1}^{n} p_{n-k}^{(n)} v_k^2 - \sum_{k=1}^{n-1} p_{n-k-1}^{(n-1)} v_k^2 + \sigma_{\min} \chi_{0}^{(n)} w_n^2$$

$$+ \sum_{j=1}^{n-1} \left( \frac{1}{r p_{n-j}^{(n)}} - \frac{1}{r p_{n-j-1}^{(n)}} \right) \left[ \sum_{k=1}^{j} r p_{n-k}^{(n)} (v_k - v_{k-1}) \right]^2,$$

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

$$2 \sum_{k=1}^{n} w_k \sum_{j=1}^{k} \chi_{k-j}^{(k)} w_j \geq \sum_{j=1}^{n} p_{n-j}^{(n)} v_j^2 + \sigma_{\min} \sum_{k=1}^{n} \chi_{0}^{(k)} w_k^2.$$
Skeleton proof of DGS

Proof.

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

\[
wn = \sum_{k=1}^{n} \theta_{n-k} v_k = r_{p_0}^{(n)} v_n + \sum_{k=1}^{n-1} (r_{p_{n-k}}^{(n)} - r_{p_{n-k-1}}^{(n)}) v_k = \sum_{k=1}^{n} r_{p_{n-k}}^{(n)} \nabla_\tau v_k.
\]

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

\[
2v_n \sum_{k=1}^{n} r_{p_{n-k}}^{(n)} \nabla_\tau v_k = \sum_{k=1}^{n} r_{p_{n-k}}^{(n)} \nabla_\tau v_k^2 + \frac{1}{r_{p_0}^{(n)}} \left( \sum_{k=1}^{n} r_{p_{n-k}}^{(n)} \nabla_\tau v_k \right)^2
\]

\[
+ \sum_{j=1}^{n-1} \left( \frac{1}{r_{p_{n-j}}^{(n)}} - \frac{1}{r_{p_{n-j-1}}^{(n)}} \right) \left( \sum_{k=1}^{j} r_{p_{n-k}}^{(n)} \nabla_\tau v_k \right)^2.
\]
Outline

1. Intergal averaged formula and our results
   - Motivation
   - Integral averaged formula
   - The problem and our results

2. Derivation of discrete gradient structure
   - General kernels
   - Kernels of integral averaged formula

3. Application to time-fractional Allen-Cahn model

4. Application to time-fractional Klein-Gordon model

5. Further issues to be studied
Integral averaged kernels

The discrete kernels of integral averaged formula,

\[ a_{n-k}^{(\beta,n)} := \frac{1}{\tau_n \tau_k} \int_{t_{n-1}}^{t_n} \int_{t_{k-1}}^{\min\{t,t_k\}} \omega_\beta(t-s) \, ds \, dt \quad \text{for } 1 \leq k \leq n. \]

The integral mean-value theorem yields

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

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

$$r_{k+1} \geq r_\ast(r_k) := \sqrt{\frac{(2^\beta - 1)\rho(r_k)}{\rho(2r_k) - \rho(r_k)}}$$

for $k \geq 2$,

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

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

for $n \geq 2$. 
Corollary 8

Let the adjacent step-ratios satisfy the following condition

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

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

\[
2w_n \sum_{j=1}^{n} a_{n-j}^{(\beta,n)} w_j = \sum_{j=1}^{n} p_{n-j}^{(\beta,n)} v_j^2 - \sum_{j=1}^{n-1} p_{n-1-j}^{(\beta,n-1)} v_j^2 \\
+ \sum_{j=1}^{n-1} \left( \frac{1}{rp_{n-j}^{(\beta,n)}} - \frac{1}{rp_{n-j-1}^{(\beta,n)}} \right) \left( \sum_{k=1}^{j} r p_{n-k}^{(\beta,n)} \nabla \tau v_k \right)^2
\]

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

1. Intergal averaged formula and our results
   - Motivation
   - Integral averaged formula
   - The problem and our results

2. Derivation of discrete gradient structure
   - General kernels
   - Kernels of integral averaged formula

3. Application to time-fractional Allen-Cahn model

4. Application to time-fractional Klein-Gordon model

5. Further issues to be studied
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 \( \kappa \) is the mobility coefficient and \( E \) is the Ginzburg-Landau functional

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

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

\[ E(t) \leq E(0). \]

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

\[(\partial_t^\alpha E)(t) \leq 0 \quad \text{for } t > 0,\]

and a weighted energy dissipation law,

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

where \(E(\theta t) = E[\Phi(\cdot, \theta t)]\) 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

\[\frac{d}{dt} \mathcal{E}_{\text{nonlocal}}(t) \leq 0.\]
Recently, we obtain a local energy law (Liao-Tang-Zhou-2021, Liao-Zhu-Wang-2022)

\[
\frac{d}{dt} \left( E[\Phi] + \frac{\kappa}{2} I^\alpha_t \|\mu\|^2 \right) + \frac{\kappa}{2} \omega_\alpha(t) \|\mu\|^2 \leq 0.
\]

\[\mathcal{E}_\alpha[\Phi] : \text{a global energy may not be physical}\]

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

\[
\frac{d}{dt} E[\Phi] + \kappa \|\mu\|^2 \leq 0,
\]

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

\[
\mathcal{E}_\alpha[\Phi] \to E[\Phi] + \frac{1}{2} \int_0^t \|\mu\|^2 \, ds, \quad \text{as } \alpha \to 1.
\]
Continuous energy dissipation law

Applying Lemma 1, one gets an improved energy dissipation law

\[
\frac{dE_\alpha}{dt} + \frac{(1 - \alpha)\pi}{2\kappa \sin(1 - \alpha)\pi} \int_0^t \omega_{1-\alpha}(t - \xi) \left\| \int_0^\xi \omega_\alpha(t - s) v'(s) \, ds \right\|^2 \, d\xi = 0,
\]

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

\[
E_\alpha[\Phi] := E[\Phi] + \frac{\kappa}{2} I_t^\alpha \|\mu\|^2 = E[\Phi] + \frac{\kappa}{2} I_t^\alpha \|\frac{\delta E}{\delta \Phi}\|^2.
\]

As \( \alpha \to 1 \), \( \int_0^\xi \omega_\alpha(t - s) v'(s) \, ds \to v(\xi) \), and the above law degrades into

\[
\frac{d}{dt} \left( E[\Phi] + \frac{\kappa}{2} I_t^1 \|\mu\|^2 \right) + \frac{\kappa}{2} \|\mu\|^2 = \frac{dE}{dt} + \kappa \|\mu\|^2 = 0,
\]

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

\[
(\partial^\alpha_T \phi)^{n-\frac{1}{2}} = -\kappa \mu^{n-\frac{1}{2}} \quad \text{with} \quad \mu^{n-\frac{1}{2}} = f(\phi)^{n-\frac{1}{2}} - \epsilon^2 \Delta \phi^{n-\frac{1}{2}} \quad \text{for } n \geq 1.
\]

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

\[
\langle f(\phi)^{n-\frac{1}{2}}, \nabla_T \phi^n \rangle = \langle F(\phi^n), 1 \rangle - \langle F(\phi^{n-1}), 1 \rangle.
\]

**Theorem 9**

If \(\tau_n \leq \alpha \sqrt{\frac{2}{\kappa \Gamma(3-\alpha)}}\), the Crank-Nicolson scheme is uniquely solvable.
Discrete energy dissipation law

We define the following discrete variational energy

\[
E_\alpha[\phi^n] := E[\phi^n] + \frac{1}{2\kappa} \sum_{j=1}^{n} p_{n-j}^{(1-\alpha,n)} \|v^j\|^2 \quad \text{with} \quad v^j := \sum_{\ell=1}^{j} a_{j-\ell}^{(1-\alpha,j)} \nabla_\tau \phi^\ell,
\]

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*

\[
\partial_\tau E_\alpha[\phi^n] + \frac{1}{2\kappa \tau} \sum_{j=1}^{n-1} \left( \frac{1}{r^{(1-\alpha,n)}_{p_{n-j}}} - \frac{1}{r^{(1-\alpha,n)}_{p_{n-j-1}}} \right) \| \sum_{k=1}^{j} r^{(1-\alpha,n)}_{p_{n-k}} \nabla_\tau v^k \|^2 = 0.
\]
Asymptotical compatibility

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

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

The DCC and RCC kernels $p_{n-k}^{(0,n)} = \tau_k/2$ and $r_{p_{n-k}}^{(0,n)} = \tau_n/2$ for $1 \leq k \leq n$. The discrete variational energy degrades into

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

and the discrete energy dissipation law in Theorem 10 degrades into

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

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

Liao Hong-lin (NUAA)  
CSRC  
Aug 11-13, 2022  
39 / 51
Example: TFAC

An adaptive step criterion based on the solution variation

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

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 $u_{0} = \text{rand}(x)$. 
Example: TFAC

An adaptive step criterion based on the solution variation

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

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

Figure: Numerical results for different fractional orders $\alpha$. 

(a) energy $E[\phi^n]$

(b) energy $E_\alpha[\phi^n]$

(c) steps $\tau_n$
Outline

1. Intergal averaged formula and our results
   - Motivation
   - Integral averaged formula
   - The problem and our results

2. Derivation of discrete gradient structure
   - General kernels
   - Kernels of integral averaged formula

3. Application to time-fractional Allen-Cahn model

4. Application to time-fractional Klein-Gordon model

5. Further issues to be studied
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 $\beta \in (0, 1)$,

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

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

$$E[U] := \int_\Omega \left( \frac{\epsilon^2}{2} |\nabla U|^2 + F(U) \right) \, dx \quad \text{with} \quad F(U) := \frac{1}{4} \left( U^2 - 1 \right)^2.$$

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 $\alpha = 1 + \beta \in (1, 2)$. 

Liao Hong-lin (NUAA)
CSRC
Aug 11-13, 2022 43 / 51
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)

$$\frac{dE}{dt} = 0,$$

where the Hamiltonian energy $E$ is defined by

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

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.
Applying Lemma 1, we get an energy dissipation law
\[
\frac{d\mathcal{E}_\beta}{dt} + \frac{\beta \pi}{2 \sin \beta \pi} \int_0^t \omega_\beta(t - \xi) \left\| \int_0^\xi \omega_1(t - s)v'(s) \, ds \right\|^2 \, d\xi = 0,
\]
where the nonlocal energy
\[
\mathcal{E}_\beta[U] := E[U] + \frac{1}{2} \mathcal{I}_t^{1-\beta} \left\| \partial_t U \right\|^2 \quad \text{for } t > 0.
\]
As the fractional order \( \beta \to 1 \), one has
\[
\mathcal{E}_\beta[U] \to \mathcal{E}[U] = E[U] + \frac{1}{2} \left\| \partial_t U \right\|^2.
\]
The energy dissipation law degrades into the energy conservation law of the classical Klein-Gordon model
\[
\frac{d\mathcal{E}}{dt} = 0.
\]
Both the nonlocal energy \( \mathcal{E}_\beta[U] \) and the energy dissipation law are asymptotically compatible in the limit \( \beta \to 1 \).
By applying the integral averaged formula $I^\beta_\tau$, we have a Crank-Nicolson scheme for the Klein-Gordon-type fractional wave equation

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

**Theorem 11**

*If $\tau_n \leq \frac{1+\sqrt{2\Gamma(2+\beta)}}{1}$, the Crank-Nicolson scheme is uniquely solvable.*
Discrete energy dissipation law

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

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

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

**Theorem 12**

*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*

$$\partial_\tau \mathcal{E}_\beta[u^n] + \frac{1}{2 \tau_n} \sum_{j=1}^{n-1} \left( \frac{1}{r p_{n-j}^{(\beta,n)}} - \frac{1}{r p_{n-j-1}^{(\beta,n)}} \right) \left\| \sum_{k=1}^{j} r p_{n-k}^{(\beta,n)} \nabla \tau v^k \right\|^2 = 0.$$
Asymptotical compatibility

As $\beta \to 1$, $a_0^{(1,n)} = 1/2$ and $a_{n-k}^{(1,n)} = 1$ for $1 \leq k \leq n - 1$. 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 $\tau_n \leq 2$. 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

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

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

\[
p_0^{(1,n)} = 1 \quad \text{and} \quad p_{n-k}^{(1,n)} = 0 \quad \text{for} \quad 1 \leq k \leq n - 1,
\]

\[
r_0^{(1,n)} = 1 \quad \text{and} \quad r_{n-k}^{(1,n)} = 0 \quad \text{for} \quad 1 \leq k \leq n - 1.
\]

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

\[
E_{\beta}[u^n] \rightarrow E[u^n] + \frac{1}{2} \|v^n\|^2 \quad \text{as} \quad \beta \rightarrow 1;
\]

and the discrete energy dissipation law in Theorem 12 degrades into

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

Both the discrete energy and energy dissipation law are asymptotically compatible in the limit $\beta \rightarrow 1$. 
For the DGS decomposition, we impose a sufficient step-ratio condition

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

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

\[ r_{k+1} \geq r_g(r_k) := (1 + 5r_k^{-\beta})^{-1}. \]

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

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

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

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

\[ r_{k+1} \geq r_g(r_k) := (1 + 5r_k^{-\beta})^{-1}. \]

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

- We build the discrete gradient structure of \( L_1^+ \) formula. How about other discrete Cauplo formulas, such as variable-step \( L_2-1_\sigma \) (Alikhanov-JCP-2015, Liao-McLean-Zhang-2021) and variable-step \( L_1-2 \) (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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