A unified design of energy stable schemes with variable steps for fractional gradient flows and nonlinear integro-differential equations

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Outline

1. Background

2. Discrete gradient structure

3. Application to time fractional Swift-Hohenberg model

4. Application to time fractional sine-Gordon model

5. Conclusion
Outline

1 Background

2 Discrete gradient structure

3 Application to time fractional Swift-Hohenberg model

4 Application to time fractional sine-Gordon model

5 Conclusion
Gradient flows

- Various physical and engineering problems are modeled by PDEs taking the form of gradient flows.
- Typical examples: interface dynamics $^1$, crystallization $^2$, pattern formation $^3$.

![Representative gradient flows](From PNAS, Vol. 119, No. 23, 2022)

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$$\frac{\partial u}{\partial t} = g\mu. \quad (1)$$
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- $\mu = \delta E/\delta u$: variational derivative of $E[u]$. 

Multiscale time behavior: fast-to-slow change during long-time simulation.
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- $\mathcal{G}$: nonpositive symmetric operators (e.g., $-I$, $\Delta$)
- Energy dissipation law

$$\frac{d}{dt} E[u] = \left\langle \frac{\delta E}{\delta u}, \frac{\partial u}{\partial t} \right\rangle = \left\langle \mu, \mathcal{G}\mu \right\rangle \leq 0.$$
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Numerical methods for gradient flows

Key concerns: energy stability, accuracy, efficiency.
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- Stabilization (C. Xu, T. Tang, SINUM, 2006)
- Invariant energy quadratization (X. Yang, JCP, 2016)
- Scalar auxiliary variable (J. Shen, J. Xu, J. Yang, JCP, 2018)
- Operator-splitting (Y. Cheng, JCP, 2015)
- Exponential time differencing (X. Li, L. Ju, X. Meng, CiCP, 2019)
- ...
Time fractional gradient flows

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\mathcal{D}_t^\alpha u = G\mu.
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\[
\mathcal{D}_t^\alpha u = \mathcal{G} \mu. \tag{2}
\]

- The Caputo fractional derivative of order \(0 < \alpha < 1\)

\[
\mathcal{D}_t^\alpha v(t) = \mathcal{I}^{1-\alpha} v'(t). \tag{3}
\]

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Time fractional gradient flows

- Time fractional models: describe diffusion with memory effect \(^4\).
- Time fractional gradient flows have been investigated recently \(^5\), \(^6\), \(^7\).
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D_t^\alpha u = G \mu. \tag{2}
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- The Caputo fractional derivative of order \(0 < \alpha < 1\)

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D_t^\alpha v(t) = I^{1-\alpha} v'(t). \tag{3}
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- The Riemann-Liouville fractional integral of order \(\beta > 0\)

\[
I^\beta v(t) = \int_0^t \omega_\beta(t-s)v(s)ds, \quad \text{with } \omega_\beta(t) = t^{\beta-1}/\Gamma(\beta). \tag{4}
\]

Numerical methods for time fractional gradient flows

  Energy boundedness

- L2-SAV and L2-IMEX schemes (C. Quan, B. Wang, JCP, 2022)
  Energy boundedness

- CQ scheme (S. Karaa, SINUM, 2021)
  Energy boundedness

- BDF-SAV scheme (H. Zhang, X. Jiang, Nonlinear Dyn, 2020)
  Modified energy dissipation law

- L1-stabilized and L1-SAV schemes (Z. Liu, X. Li, J. Huang, NMPDE, 2021)
  Modified energy dissipation law

- ...

Developed using the uniform time step sizes.
Adaptive time strategy

- Initial singularity of time fractional differential equations.
Adaptive time strategy

- **Initial singularity** of time fractional differential equations.
- **Multiscale time behavior** in long-time simulation.

![Graph showing energies with different fractional index](image)

**Figure 2**: Energies with different fractional index.
Adaptive time strategy

- **Initial singularity** of time fractional differential equations.
- **Multiscale time behavior in long-time simulation.**

![Graph showing energies with different fractional index](image)

**Figure 2**: Energies with different fractional index.

- **Practical way**: **Energy stable schemes with variable time steps**
Variable-step schemes for time fractional gradient flows

- **L1 type schemes**

- **L2-1\(\sigma\) type schemes**
  - L2-1\(\sigma\)-ExSAV scheme for TFMBE (D. Hou, C. Xu, JSC, 2022).

- **L1\(^+\) type schemes**
  - L1\(^+\) scheme for TFCH (J. Zhang, J. Zhao, J. Wang, CMA, 2020).

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One way: Positive-definiteness $\rightarrow$ Energy boundedness
Variable-step schemes for time fractional gradient flows

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**One way:** Positive-definiteness $\rightarrow$ Energy boundedness

**Further:** Asymptotic compatible discrete energy dissipation law?
Variable-step schemes for time fractional gradient flows

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One way: Positive-definiteness $\rightarrow$ Energy boundedness

Further: Asymptotic compatible discrete energy dissipation law?

Another way: Discrete gradient structure
Discrete gradient structure (DGS) view

For $\vec{x}^k = (x_1, x_2, \cdots, x_k)^T$ and a discrete temporal differential operator $D_\tau \vec{x}^k$, it seeks $c^* > 0$, two nonnegative quadratic functionals $P$ and $Q$, such that

$$x_k D_\tau \vec{x}^k = P[\vec{x}^k] - P[\vec{x}^{k-1}] + c^* x_k^2 + Q[\vec{x}^k].$$

(5)
Discrete gradient structure (DGS) view

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- Recent DGS results of nonuniform numerical schemes for time fractional gradient flows, e.g., L1 scheme, L1$_R$ scheme, L1$^+$ scheme, FBDF2 scheme.
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- ✓ Energy stability of variable-step schemes.
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- Recent DGS results of nonuniform numerical schemes for time fractional gradient flows, e.g., L1 scheme, L1$_R$ scheme, L1$^+$ scheme, FBDF2 scheme.

  ✓ Energy stability of variable-step schemes.

  ✓ Asymptotically compatible discrete energy dissipation law.
Fractional nonlinear integro-differential models

- Various physical processes in viscoelastic materials characterized by the nonlinear integro-differential equations \(^8,^9\).

\[ \frac{\partial u}{\partial t} + \mathcal{I}_{\alpha} \mu = 0, \]

with

\[ \mu = -\Delta u + f(u). \]

\[ (6) \]

Turn to a parabolic equation as \(\alpha \to 0\) plus

\[ \frac{\partial u}{\partial t} + \mu = 0, \]

with a dissipation law:

\[ \frac{d}{dt} E[u] \leq 0. \]

Turn to a hyperbolic equation as \(\alpha \to 1\) minus

\[ \frac{\partial^2 u}{\partial t^2} + \mu = 0, \]

with a conservation law:

\[ \frac{d}{dt} [E[u] + \frac{1}{2} \| u_t \|^2] = 0. \]

Many related numerical methods, see the monograph \[Brunner, Cambridge University Press, 2004\].


Fractional nonlinear integro-differential models

- Various physical processes in viscoelastic materials characterized by the nonlinear integro-differential equations \(^8,^9\).
- Consider the fractional integro-differential models with nonlinear memory

\[
\frac{\partial u}{\partial t} + \mathcal{I}^\alpha \mu = 0, \quad \text{with } \mu = -\Delta u + f(u). \tag{6}
\]

\(\alpha \rightarrow 0\) turn to a parabolic equation

\[
\frac{\partial u}{\partial t} + \mu = 0, \quad \text{with a dissipation law:} \quad \frac{d}{dt} E[u] \leq 0.
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\(\alpha \rightarrow 1\) turn to a hyperbolic equation

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\frac{\partial^2 u}{\partial t^2} + \mu = 0, \quad \text{with a conservation law:} \quad \frac{d}{dt} [E[u] + \frac{1}{2} \|u_t\|^2] = 0.
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- Turn to a parabolic equation as \(\alpha \to 0^+\)

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Fractional nonlinear integro-differential models

- Various physical processes in viscoelastic materials characterized by the nonlinear integro-differential equations \(^8,^9\).
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\frac{\partial u}{\partial t} + I^{\alpha} \mu = 0, \quad \text{with} \quad \mu = -\Delta u + f(u).
\]  

(6)

- Turn to a parabolic equation as \(\alpha \to 0^+\)

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\frac{\partial u}{\partial t} + \mu = 0, \quad \text{with a dissipation law:} \quad \frac{d}{dt} E[u] \leq 0.
\]

- Turn to a hyperbolic equation as \(\alpha \to 1^-\)

\[
\frac{\partial^2 u}{\partial t^2} + \mu = 0, \quad \text{with a conservation law:} \quad \frac{d}{dt} \left[ E[u] + \frac{1}{2} \| u_t \|^2 \right] = 0.
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Fractional nonlinear integro-differential models

- Various physical processes in viscoelastic materials characterized by the nonlinear integro-differential equations $^8,^9$.
- Consider the fractional integro-differential models with nonlinear memory

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- Turn to a parabolic equation as $\alpha \to 0^+$

\[ \frac{\partial u}{\partial t} + \mu = 0, \quad \text{with a dissipation law: } \frac{d}{dt}E[u] \leq 0. \]

- Turn to a hyperbolic equation as $\alpha \to 1^-$

\[ \frac{\partial^2 u}{\partial t^2} + \mu = 0, \quad \text{with a conservation law: } \frac{d}{dt} \left[ E[u] + \frac{1}{2} \|u_t\|^2 \right] = 0. \]

- Many related numerical methods, see the monograph [Brunner, Cambridge University Press, 2004].

Motivations

- A unified DGS for nonuniform integral averaged formulae of time fractional derivative and integral

\[ \mathcal{D}_t^\alpha u(t), \quad \mathcal{I}^\beta u(t). \]

- Variable-step energy stable schemes for time fractional gradient flow and nonlinear integro-differential equation

\[ \mathcal{D}_t^\alpha u = \mathcal{G} \mu, \quad \frac{\partial u}{\partial t} + \mathcal{I}^\alpha \mu = 0. \]

- Energy stability analysis of SAV-based variable-step numerical schemes.
Integral averaged formulae

- Consider $0 = t_1 < t_2 < \cdots < t_N = T$ with the step-sizes $\tau_n = t_n - t_{n-1}$ for $1 \leq n \leq N$. Denote by $r_n = \tau_n/\tau_{n-1}$ the adjacent step-size ratio.

- For any grid function $v^n = v(t_n)$, let $\delta_{\tau}v^n = v^n - v^{n-1}$, $\partial_{\tau}v^n = \delta_{\tau}v^n/\tau_n$ and $v^{n-\frac{1}{2}} = (v^n + v^{n-1})/2$.

- $\Pi_1 v$: piecewise-linear interpolation on each subinterval $[t_{n-1}, t_n]$, the integral averaged formula for the Caputo derivative

$$D^\alpha_{\tau}v^n = \frac{1}{\tau_n} \int_{t_{n-1}}^{t_n} \int_0^t \omega_{1-\alpha}(t-s)(\Pi_1 v(s))' ds dt = \sum_{j=1}^{n} c^{(1-\alpha,n)}_{n-j} \delta_{\tau} v^j. \quad (7)$$

- The discrete convolution kernels $c^{(\alpha,n)}_{n-j}$ are given by

$$c^{(\alpha,n)}_{n-j} = \frac{1}{\tau_n \tau_j} \int_{t_{n-1}}^{t_n} \int_{t_{j-1}}^{\min\{t,t_j\}} \omega_{\alpha}(t-s) ds dt, \quad \text{for } 1 \leq j \leq n. \quad (8)$$
Integral averaged formulae

- $\Pi_0 v$: piecewise-constant interpolation on each subinterval $[t_{n-1}, t_n]$, the integral averaged formula for the Riemann-Liouville fractional integral

$$\mathcal{I}_\tau^\beta \bar{v}^n = \frac{1}{\tau_n} \int_{t_{n-1}}^{t_n} \int_0^t \omega_\beta(t - s) \Pi_0 v(s) ds dt = \sum_{j=1}^n c_{n-j}^{(\beta,n)} \tau_j \bar{v}^j,$$  \hspace{1cm} (9)

where the piecewise-constants $\bar{v}^n$ are flexible according to the problem.
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It is observed that

\[ c_0^{(\alpha,n)} - c_1^{(\alpha,n)} = \frac{r_n}{\Gamma(2 + \alpha) \tau_n^{1-\alpha}} \left[ 1 + 1/r_n + 1/r_n^{1+\alpha} - (1 + 1/r_n)^{1+\alpha} \right]. \]

Thus \( c_0^{(\alpha,n)} > c_1^{(\alpha,n)} \) when \( \alpha \to 0 \) but \( c_0^{(\alpha,n)} < c_1^{(\alpha,n)} \) when \( \alpha \to 1 \).
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Denote

\[ \hat{c}_0^{(\alpha,n)} = 2c_0^{(\alpha,n)} \quad \text{and} \quad \hat{c}_{n-j}^{(\alpha,n)} = c_{n-j}^{(\alpha,n)} \quad \text{for} \ 1 \leq j \leq n - 1. \quad (10) \]
It is observed that
\[
c_0^{(\alpha,n)} - c_1^{(\alpha,n)} = \frac{r_n}{\Gamma(2 + \alpha)\tau_n^{1-\alpha}} \left[ 1 + 1/r_n + 1/r_n^{1+\alpha} - (1 + 1/r_n)^{1+\alpha} \right].
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Thus \(c_0^{(\alpha,n)} > c_1^{(\alpha,n)}\) when \(\alpha \to 0\) but \(c_0^{(\alpha,n)} < c_1^{(\alpha,n)}\) when \(\alpha \to 1\).

Denote
\[
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\]
\begin{equation}
\hat{c}_0^{(\alpha,n)} > \hat{c}_1^{(\alpha,n)} > \hat{c}_2^{(\alpha,n)} > \cdots > \hat{c}_{n-1}^{(\alpha,n)}.
\end{equation}
Properties of modified kernels $\hat{c}_{n-j}^{(\alpha,n)}$

The three algebraic properties of the modified kernels $\hat{c}_{n-j}^{(\alpha,n)}$ are listed below.

**Theorem 1**

For $0 < \alpha < 1$, the auxiliary kernels $\hat{c}_{n-j}^{(\alpha,n)}$ defined in (10) satisfy

1. $\hat{c}_{n-j}^{(\alpha,n)} \geq \hat{c}_{n-j}^{(\alpha,n)} > 0$ for $1 \leq j \leq n - 1$;
2. If the adjacent step-size ratios $r_{n+1}$ and $r_n$ for $n \geq 2$ fulfill the following relation
   
   $$r_{n+1} \geq r_{\alpha}(r_n) = \left[ \frac{2h(r_n) - h(2r_n)}{r_n^{\alpha}(4 - 2^{1+\alpha})} \right]^{\frac{1}{\alpha}},$$
   
   then the auxiliary kernels $\hat{c}_{n-j}^{(\alpha,n)}$ satisfy
3. $\hat{c}_{n-1-j}^{(\alpha,n-1)} > \hat{c}_{n-j}^{(\alpha,n)}$ for $1 \leq j \leq n - 1$;
4. $\hat{c}_{n-2-j}^{(\alpha,n-1)} - \hat{c}_{n-1-j}^{(\alpha,n-1)} > \hat{c}_{n-j-1}^{(\alpha,n)} - \hat{c}_{n-j}^{(\alpha,n)}$ for $1 \leq j \leq n - 2$. 
Technical lemma

For given $n \geq 2$ and a positive sequence $\omega_{n-j}^{(n)} (1 \leq j \leq n)$, introduce

$$\hat{\omega}_0^{(n)} = (2 - \theta)\omega_0^{(n)}, \quad \theta \in [0, 2),$$

$$\hat{\omega}_{n-j}^{(n)} = \omega_{n-j}^{(n)}, \quad 1 \leq j \leq n - 1.$$

Lemma 1 [H.-L. Liao, N. Liu, X. Zhao, arXiv, 2022]

If the modified kernels $\hat{\omega}_{n-j}^{(n)}$ satisfy:

1. $\hat{\omega}_{n-j-1}^{(n)} \geq \hat{\omega}_{n-j}^{(n)}$,
2. $\hat{\omega}_{n-1-j}^{(n-1)} \geq \hat{\omega}_{n-j}^{(n)}$,
3. $\hat{\omega}_{n-2-j}^{(n-1)} - \hat{\omega}_{n-1-j}^{(n-1)} \geq \hat{\omega}_{n-1-j}^{(n)} - \hat{\omega}_{n-j}^{(n)}$,

then

$$2q_n \sum_{j=1}^{n} \omega_{n-j}^{(n)} q_j = G[\vec{q}_n] - G[\vec{q}_{n-1}] + \theta \omega_0^{(n)} q_n^2 + Y[\vec{q}_n], \quad \text{for} \ n \geq 1.$$ (12)
**Theorem 2 (DGS of nonuniform integral averaged formulae)**

Under the step-size ratio constraint (11), we have the following discrete gradient structure of the integral averaged formulae (7) and (9)

\[
\langle v_n, \sum_{j=1}^{n} c_{n-j}^{(\alpha,n)} v_j \rangle = \mathcal{F}_\alpha[\bar{v}_n] - \mathcal{F}_\alpha[\bar{v}_{n-1}] + \mathcal{R}_\alpha[\bar{v}_n], \quad \text{for } n \geq 2. \tag{13}
\]

\[
\mathcal{F}_\alpha[\bar{v}_n] = \frac{1}{2} \sum_{j=1}^{n-1} \left( \hat{c}_{n-j-1}^{(\alpha,n)} - \hat{c}_{n-j}^{(\alpha,n)} \right) \left\| \sum_{k=j+1}^{n} v_k \right\|^2 + \frac{1}{2} \hat{c}_{n-1}^{(\alpha,n)} \left\| \sum_{k=1}^{n} v_k \right\|^2,
\]

\[
\mathcal{R}_\alpha[\bar{v}_n] = \frac{1}{2} \sum_{j=1}^{n-2} \left( \hat{c}_{n-j-2}^{(\alpha,n-1)} - \hat{c}_{n-j-1}^{(\alpha,n-1)} - \hat{c}_{n-j-1}^{(\alpha,n)} + \hat{c}_{n-j}^{(\alpha,n)} \right) \left\| \sum_{k=j+1}^{n-1} v_k \right\|^2 + \frac{1}{2} \left( \hat{c}_{n-2}^{(\alpha,n-1)} - \hat{c}_{n-1}^{(\alpha,n)} \right) \left\| \sum_{k=1}^{n-1} v_k \right\|^2.
\]

- **DGS** → the positive-definiteness of the nonuniform integral averaged formulae
- The lower bound of \( r_n \) is less than 1; no requirement for the upper bound
Comparison

- **Algebraic convexity** in Theorem 1

\[
\hat{c}_{n-2-j}^{(\alpha,n-1)} - \hat{c}_{n-1-j}^{(\alpha,n-1)} > \hat{c}_{n-j-1}^{(\alpha,n)} - \hat{c}_{n-j}^{(\alpha,n)}
\]
Comparison

- **Algebraic convexity** in Theorem 1
  \[
  \hat{c}_{n-2-j} - \hat{c}_{n-1-j} > \hat{c}_{n-j-1} - \hat{c}_{n-j}
  \]

- **Geometric convexity** in [H.-L. Liao, N. Liu, P. Lyu, SINUM, 2023]
  \[
  \hat{c}_{n-2-j} \hat{c}_{n-j} \geq \hat{c}_{n-1-j} \hat{c}_{n-j-1}.
  \]
Comparison

- **Algebraic convexity** in Theorem 1

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\[
\hat{c}_{n-2-j} \hat{c}_{n-j} \geq \hat{c}_{n-1-j} \hat{c}_{n-j-1}.
\]

- A different DGS under another step-size ratio restriction

\[
r_{n+1} \geq \hat{r}_\alpha(r_n) = \left[ \frac{(2^\alpha - 1)h(r_n)}{h(2r_n) - 2h(r_n)} \right]^{\frac{1}{1-\alpha}}.
\]

(14)
Figure 3: Comparisons of the step-size ratio constraints (11) with (14).
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Consider the TFSH model of order $\alpha \in (0, 1)$

$$\mathcal{D}_t^\alpha u = -\mu, \quad (x, t) \in \Omega \times (0, T]$$

subjected to the periodic boundary conditions.

- $u(x, t)$: the density field of atoms in a binary mixture on the domain $\Omega$.
- Free energy $E[u]$

$$E[u] = \int_\Omega \frac{1}{2} u(1 + \Delta)^2 u + F(u) \, dx, \text{ with } F(u) = \frac{1}{4} u^4 - \frac{g}{3} u^3 + \frac{\epsilon}{2} u^2. \quad (16)$$

- $g, \epsilon$: two nonnegative physical parameters.
Variable-step CN scheme for TFSH model

- Using the integral averaged formula for Caputo derivative, the variable-step Crank-Nicolson (CN) scheme

\[ D_\tau^\alpha u^n = -\mu^{n-\frac{1}{2}}, \quad \text{with} \quad \mu^{n-\frac{1}{2}} = (1 + \Delta)^2 u^{n-\frac{1}{2}} + \Psi(u^n, u^{n-1}). \]  

(17)

- The nonlinear term \( f(u) = F'(u) \) is implicitly treated

\[ \Psi(u^n, u^{n-1}) = \frac{F(u^n) - F(u^{n-1})}{u^n - u^{n-1}} \]

\[ = \frac{1}{2} u^{n-\frac{1}{2}} [(u^n)^2 + (u^{n-1})^2] - g \frac{(u^n)^2 + u^n u^{n-1} + (u^{n-1})^2}{3} - \epsilon u^{n-\frac{1}{2}}. \]

- The CN scheme (17) is uniquely solvable when \( \tau_n \leq \frac{\alpha}{\sqrt{\Gamma(3-\alpha)(g^2 + 3\epsilon)}}. \)
Energy dissipation law of variable-step CN scheme

Taking the inner product of variable-step CN scheme (17) with $\delta \tau u^n$.

$$\langle D_\tau^{\alpha} u^n, \delta \tau u^n \rangle = \left\langle \sum_{j=1}^{n} c_{n-j}^{(\alpha,n)} \delta \tau u^n, \delta \tau u^n \right\rangle$$

$$= \mathcal{F}_{1-\alpha} [\delta \tau u^n] - \mathcal{F}_{1-\alpha} [\delta \tau u^{n-1}] + \mathcal{R}_{1-\alpha} [\delta \tau u^n],$$

$$\langle \mu^{n-\frac{1}{2}}, \delta \tau u^n \rangle = E[u^n] - E[u^{n-1}].$$

**Theorem 3**

Under the step-size ratio restriction (11), the variable-step CN scheme (17) preserves the following discrete energy dissipation law

$$\partial_\tau E_\alpha[u^n] = -\frac{1}{\tau_n} \mathcal{R}_{1-\alpha} [\delta \tau u^n], \quad \text{for } 1 \leq n \leq N,$$

(18)

where the modified energy $E_\alpha[\cdot] = E[u^n] + \mathcal{F}_{1-\alpha} [\delta \tau u^n]$. 
Asymptotic compatibility of variable-step CN scheme

- As $\alpha \to 1^-$, $c_0^{(1-\alpha,n)} \to 1/\tau_n$ and $c_j^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n - 1$. 
Asymptotic compatibility of variable-step CN scheme

- As $\alpha \to 1^-$, $c_{0}^{(1-\alpha,n)} \to 1/\tau_n$ and $c_{j}^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n - 1$.
- The CN scheme (17) reduces to the CN scheme for classical SH model

$$\partial_\tau u^n = -\mu^{n-\frac{1}{2}}, \quad \text{for } n \geq 1,$$  \hspace{1cm} (19)

which holds that

$$\partial_\tau E[u^n] = -\|\mu^{n-\frac{1}{2}}\|^2, \quad \text{for } n \geq 1.$$  \hspace{1cm} (20)
Asymptotic compatibility of variable-step CN scheme

- As $\alpha \to 1^-$, $c_0^{(1-\alpha,n)} \to 1/\tau_n$ and $c_j^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n - 1$.
- The CN scheme (17) reduces to the CN scheme for classical SH model

$$\partial_\tau u^n = -\mu^{n-\frac{1}{2}}, \quad \text{for } n \geq 1,$$

which holds that

$$\partial_\tau E[u^n] = -\|\mu^{n-\frac{1}{2}}\|^2, \quad \text{for } n \geq 1. \quad (20)$$

- Moreover, $\hat{c}_0^{(1-\alpha,n)} \to 2/\tau_n$ and $\hat{c}_j^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n - 1$. 


Asymptotic compatibility of variable-step CN scheme

- As $\alpha \to 1^-$, $c_0^{(1-\alpha,n)} \to 1/\tau_n$ and $c_j^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n - 1$.
- The CN scheme (17) reduces to the CN scheme for classical SH model

$$\partial_\tau u^n = -\mu^{n-\frac{1}{2}}, \quad \text{for } n \geq 1,$$

which holds that

$$\partial_\tau E[u^n] = -\|\mu^{n-\frac{1}{2}}\|^2, \quad \text{for } n \geq 1.$$

Moreover, $\hat{c}_0^{(1-\alpha,n)} \to 2/\tau_n$ and $\hat{c}_j^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n - 1$.
- The energy dissipation law (18) reduces to

$$\partial_\tau E[u^n] = -\|\partial_\tau u^n\|^2, \quad \text{for } n \geq 1,$$

which is the same as (20).
Asymptotic compatibility of variable-step CN scheme

As $\alpha \to 1^-$, $c_0^{(1-\alpha,n)} \to 1/\tau_n$ and $c_j^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n-1$.

The CN scheme (17) reduces to the CN scheme for classical SH model

$$\partial_\tau u^n = -\mu^{n-\frac{1}{2}}, \text{ for } n \geq 1,$$

which holds that

$$\partial_\tau E[u^n] = -||\mu^{n-\frac{1}{2}}||^2, \text{ for } n \geq 1. \quad (20)$$

Moreover, $\hat{c}_0^{(1-\alpha,n)} \to 2/\tau_n$ and $\hat{c}_j^{(1-\alpha,n)} \to 0$ for $1 \leq j \leq n-1$.

The energy dissipation law (18) reduces to

$$\partial_\tau E[u^n] = -||\partial_\tau u^n||^2, \text{ for } n \geq 1,$$

which is the same as (20).

The discrete energy dissipation law of variable-step CN scheme is asymptotically compatible.
The proposed DGS is also useful to develop SAV-based variable-step energy stable linear schemes.

Introduce an exponential SAV (ESAV, see, Z. Liu, X. Li, SISC, 2020)

\[ s(t) = \exp(E_1[u]) = \exp \left( \int_{\Omega} \frac{1}{4} u^4 - \frac{g}{3} u^3 + \frac{\epsilon}{2} u^2 \, dx \right), \]

and denote \( \sigma(u, s) = \frac{s(t)}{\exp(E_1[u])} f(u) \).

The TFSH model (15) is transformed into the expanded system

\[ \mathcal{D}_t^\alpha u = -\mu, \quad (21a) \]
\[ \mu = (1 + \Delta)^2 u + \sigma(u, s), \quad (21b) \]
\[ (\ln s)_t = \langle \sigma(u, s), u_t \rangle. \quad (21c) \]
Variable-step ESAV-CN scheme for TFSH model

- Using the integral averaged formula for (21a) and the standard Crank-Nicolson discretization for (21c).
- Variable-step ESAV Crank-Nicolson (ESAV-CN) scheme

\[ D_\tau^\alpha u^n = -\mu^{n-\frac{1}{2}}, \]  
\[ \mu^{n-\frac{1}{2}} = (1 + \Delta)^2 u^{n-\frac{1}{2}} + \sigma(\bar{u}^{n-\frac{1}{2}}, \bar{s}^{n-\frac{1}{2}}), \]  
\[ \ln s^n - \ln s^{n-1} = \left\langle \sigma(\bar{u}^{n-\frac{1}{2}}, \bar{s}^{n-\frac{1}{2}}), u^n - u^{n-1} \right\rangle. \]

- \( \bar{u}^{n-\frac{1}{2}} = (1 + \frac{r_n}{2})u^{n-1} - \frac{r_n}{2}u^{n-2} \) and \( \bar{s}^{n-\frac{1}{2}} = (1 + \frac{r_n}{2})s^{n-1} - \frac{r_n}{2}s^{n-2} \) are explicit second order approximations for \( u(t_{n-1/2}) \) and \( s(t_{n-1/2}) \).
Energy dissipation law of variable-step ESAV-CN scheme

Taking the inner product of (22a) and (22b) with $\delta \tau u^n$.

$$\langle D_\tau^\alpha u^n, \delta \tau u^n \rangle = \mathcal{F}_{1-\alpha}[\delta \tau u^n] - \mathcal{F}_{1-\alpha}[\delta \tau u^{n-1}] + \mathcal{R}_{1-\alpha}[\delta \tau u^n].$$

$$\langle \mu^{n-\frac{1}{2}}, \delta \tau u^n \rangle = \frac{1}{2} \left( \| (1 + \Delta)u^n \|^2 - \| (1 + \Delta)u^{n-1} \|^2 \right) + \ln s^n - \ln s^{n-1}.$$

**Theorem 4**

If the step-size ratio constraint (11) is satisfied, the variable-step ESAV-CN scheme (22) preserves the energy dissipation law

$$\partial_\tau \tilde{E}_\alpha[u^n] = -\frac{1}{\tau_n} \mathcal{R}_{1-\alpha}[\delta \tau u^n], \text{ for } 1 \leq n \leq N,$$

(23)

where the modified energy $\tilde{E}_\alpha[\cdot]$ is defined as

$$\tilde{E}_\alpha[u^n] = \frac{1}{2} \| (1 + \Delta)u^n \|^2 + \ln s^n + \mathcal{F}_{1-\alpha}[\delta \tau u^n].$$

(24)
As \( \alpha \to 1^- \), the ESAV-CN scheme (22) reduces to the ESAV-based Crank-Nicolson scheme for the classical SH model.

The discrete energy dissipation law is asymptotically compatible with the classical counterpart

\[
\partial_\tau \hat{E} = -\|\partial_\tau u^n\|^2,
\]

where \( \hat{E}[u^n] = \frac{1}{2}\|(1 + \Delta)u^n\|^2 + \ln s^n \).
Numerical experiments

**Example 1**

*(Convergence test).* Consider a forced TFSH model: \( D_t^\alpha u = -\mu + f(x, t) \) until \( T = 1 \) in the domain \( \Omega = (0, 2\pi)^2 \) with parameters \( g = 1 \) and \( \epsilon = 0.2 \). The exact solution \( u = t^\sigma \sin x \sin y / \Gamma(1 + \sigma) \).

- **Space:** Fourier pseudo-spectral method.
- **Time:** graded mesh \( t_n = T(n/N)^\gamma \). Optimal second-order when \( \gamma \geq \frac{2}{\sigma} \).
Numerical experiments

Table 1: Convergence rates of CN scheme and ESAV-CN scheme with $(\alpha, \sigma) = (0.4, 0.6)$. 

<table>
<thead>
<tr>
<th></th>
<th>$N$</th>
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<th></th>
<th>$\gamma = 2/\sigma$</th>
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<td>Rate</td>
<td>$e(N)$</td>
<td>Rate</td>
<td>$e(N)$</td>
<td>Rate</td>
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<td>3.90e-3</td>
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<td>1.53e-2</td>
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<td>1.98</td>
<td>2.63e-4</td>
<td>1.98</td>
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### Numerical experiments

Table 2: Convergence rates of CN scheme and ESAV-CN scheme with \((\alpha, \sigma) = (0.8, 0.4)\).

<table>
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<tr>
<th></th>
<th>(N)</th>
<th>(\gamma = 3)</th>
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<th>(\gamma = 2/\sigma)</th>
<th>Rate</th>
<th>(\gamma = 6)</th>
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<td></td>
<td>(e(N))</td>
<td></td>
<td>(e(N))</td>
<td></td>
</tr>
<tr>
<td>CN</td>
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<td>3.65e-3</td>
<td>-</td>
<td>6.36e-4</td>
<td>-</td>
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<td>1.95</td>
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<td>1.21</td>
<td>5.16e-4</td>
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<td>7.27e-3</td>
<td>1.97</td>
</tr>
<tr>
<td></td>
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<td>3.01e-4</td>
<td>1.20</td>
<td>1.31e-4</td>
<td>1.98</td>
<td>1.86e-4</td>
<td>1.98</td>
</tr>
</tbody>
</table>
Numerical experiments

Example 2

*(Energy stability).* Consider the TFSH model with \( g = 1 \), \( \epsilon = 0.25 \) and the initial value

\[
\begin{align*}
  u_0(x) &= 0.07 - 0.02 \cos \left( \frac{\pi(x - 12)}{16} \right) \sin \left( \frac{\pi(y - 1)}{16} \right) \\
  &\quad + 0.02 \cos^2 \left( \frac{\pi(x + 10)}{32} \right) \sin^2 \left( \frac{\pi(y + 3)}{32} \right) - 0.01 \sin^2 \left( \frac{\pi x}{8} \right) \sin^2 \left( \frac{\pi(y - 6)}{8} \right).
\end{align*}
\]

in \( \Omega = (0, 32)^2 \) until \( T = 500 \).

- Adaptive time strategy

\[
\tau_{n+1} = \max\{\tau_*, r_\alpha(r_n)\tau_n\}, \quad \tau_* = \max\left\{ \tau_{\min}, \frac{\tau_{\max}}{\sqrt{1 + \lambda\|\partial_t u^n\|^2}} \right\}
\]

- \( \tau_{\min} = 10^{-3}, \tau_{\max} = 10^{-1}, \lambda = 10^2 \).
Figure 4: Energies of CN scheme and ESAV-CN scheme with different $\alpha$. 

(a) Original energy

(b) Modified energy

(c) Adaptive step-sizes
Numerical experiments

Table 3: Comparisons of CN scheme and ESAV-CN scheme using adaptive strategy.

<table>
<thead>
<tr>
<th></th>
<th>$\alpha = 0.5$</th>
<th></th>
<th>$\alpha = 0.7$</th>
<th></th>
<th>$\alpha = 0.9$</th>
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<tr>
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<td>Time step</td>
<td>CPU(s)</td>
<td>Time step</td>
<td>CPU(s)</td>
<td>Time step</td>
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<td>CN</td>
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<td>ESAV-CN</td>
<td>6477</td>
<td>92.6</td>
<td>7567</td>
<td>107.5</td>
<td>8959</td>
</tr>
</tbody>
</table>
1. Background

2. Discrete gradient structure

3. Application to time fractional Swift-Hohenberg model

4. Application to time fractional sine-Gordon model

5. Conclusion
Consider the time fractional sine-Gordon (TFSG) model
\[ \phi_t + \mathcal{I}^\beta \varsigma = 0, \quad (x, t) \in \Omega \times (0, T] \]  
subjected to the periodic boundary conditions.

\( \varsigma = \delta \mathcal{E} / \delta \phi \) with \( \mathcal{E}[\phi] \) defined by
\[ \mathcal{E}[\phi] = \int_\Omega \frac{\epsilon}{2} |\nabla \phi|^2 + F(\phi) dx, \quad \text{with } F(\phi) = 1 - \cos \phi. \]  

When \( \beta \to 1^- \), the TFSG model recovers the classical sine-Gordon wave equation: \( \phi_{tt} = \epsilon \Delta \phi - \sin u \), which satisfies
\[ \frac{d}{dt} \left[ \mathcal{E}[\phi] + \frac{1}{2} \| \phi_t \|^2 \right] = 0. \]
Using the integral averaged formula for Riemann-Liouville fractional integral, the variable-step CN scheme for TFSG model

\[ \partial_{\tau} \phi^n + \mathcal{I}_{\tau}^{\beta} \zeta^n = 0, \quad \text{with} \quad \zeta^n = -\epsilon \Delta \phi^{n-\frac{1}{2}} - \Psi(\phi^n, \phi^{n-1}), \quad (28) \]

where \( \Psi(\phi^n, \phi^{n-1}) = \frac{\cos \phi^n - \cos \phi^{n-1}}{\phi^n - \phi^{n-1}}. \)

The variable-step CN scheme (28) is uniquely solvable when \( \tau_n \leq 1 + \beta \sqrt{\Gamma(2 + \beta)}. \)
Energy dissipation law of variable-step CN scheme

Taking the inner product of variable-step CN scheme (28) with $\tau_n \tilde{s}^n$.

$$
\langle I^\beta \tilde{s}^n, \tau_n \tilde{s}^n \rangle = \left\langle \sum_{j=1}^{n} c_{n-j}^{(\beta,n)} \tau_j \tilde{s}^j, \tau_n \tilde{s}^n \right\rangle
$$

$$
= \mathcal{F}_\beta[\tau_n \tilde{s}^n] - \mathcal{F}_\beta[\tau_n \tilde{s}^{n-1}] + \mathcal{R}_\beta[\tau_n \tilde{s}^n],
$$

$$
\langle \partial_\tau \phi^n, \tau_n \tilde{s}^n \rangle = \mathcal{E}[\phi^n] - \mathcal{E}[\phi^{n-1}].
$$

Theorem 5

If the step-size ratio restriction (11) is satisfied, the variable-step CN scheme (28) preserves the following energy dissipation law

$$
\partial_\tau \mathcal{E}_\beta[\phi^n] = -\frac{1}{\tau_n} \mathcal{R}_\beta[\tau_n \tilde{s}^n], \quad \text{for } 1 \leq n \leq N,
$$

(29)

where the modified energy $\mathcal{E}_\beta[\cdot]$ is defined as

$$
\mathcal{E}_\beta[\phi^n] = \mathcal{E}[\phi^n] + \mathcal{F}_\beta[\tau_n \tilde{s}^n].
$$

(30)
Asymptotic compatibility of variable-step CN scheme

- As $\beta \to 1^-$, the CN scheme (28) degrades into the CN scheme for the classical SG model

$$\partial_\tau \phi^n + \frac{\tau_n}{2} \bar{\varsigma}^n + \sum_{j=1}^{n-1} \tau_j \bar{\varsigma}^j = 0, \quad \text{for } n \geq 1,$$

which holds that

$$\hat{\mathcal{E}}[\phi^n] = \hat{\mathcal{E}}[\phi^{n-1}], \quad \text{for } n \geq 1, \quad (31)$$

where $\hat{\mathcal{E}}[\phi^n] = \mathcal{E}[\phi^n] + \frac{1}{2} \| \sum_{j=1}^{n} \tau_j \bar{\varsigma}^j \|^2$. 

Moreover, $\mathcal{E}_\beta[\phi^n] \to \hat{\mathcal{E}}[\phi^n]$, and the energy dissipation law degrades into conservation law (31).

Both discrete energy and energy dissipation law are asymptotically compatible.
Asymptotic compatibility of variable-step CN scheme

- As $\beta \to 1^-$, the CN scheme (28) degrades into the CN scheme for the classical SG model

$$\partial_t \phi^n + \frac{\tau_n}{2} \zeta^n + \sum_{j=1}^{n-1} \tau_j \zeta^j = 0, \text{ for } n \geq 1,$$

which holds that

$$\hat{E}[^n \phi] = \hat{E}[\phi^{n-1}], \text{ for } n \geq 1,$$

(31)

where $\hat{E}[^n \phi] = E[^n \phi] + \frac{1}{2} \| \sum_{j=1}^{n} \tau_j \zeta^j \|^2$.

- Moreover, $E_\beta[^n \phi] \to \hat{E}[\phi^n]$, and the energy dissipation law degrades into conservation law (31).
Asymptotic compatibility of variable-step CN scheme

- As $\beta \to 1^-$, the CN scheme (28) degrades into the CN scheme for the classical SG model

$$
\partial_{\tau} \phi^n + \frac{\tau_n}{2} \bar{\varsigma}^n + \sum_{j=1}^{n-1} \tau_j \bar{\varsigma}^j = 0, \quad \text{for } n \geq 1,
$$

which holds that

$$
\hat{E}[\phi^n] = \hat{E}[\phi^{n-1}], \quad \text{for } n \geq 1, \quad (31)
$$

where $\hat{E}[\phi^n] = E[\phi^n] + \frac{1}{2} \| \sum_{j=1}^{n} \tau_j \bar{\varsigma}^j \|^2$.

- Moreover, $E_\beta[\phi^n] \to \hat{E}[\phi^n]$, and the energy dissipation law degrades into conservation law (31).

- Both discrete energy and energy dissipation law are asymptotically compatible
The variable-step ESAV-CN scheme based on the integral averaged formula

\[ \partial_\tau \phi^n + I_\tau^\beta \bar{\varsigma}^n = 0, \]

\[ \bar{\varsigma}^n = -\epsilon \Delta \phi^{n-\frac{1}{2}} + \eta(\bar{\phi}^{n-\frac{1}{2}}, \bar{r}^{n-\frac{1}{2}}), \]

\[ \ln r^n - \ln r^{n-1} = \langle \eta(\bar{\phi}^{n-\frac{1}{2}}, \bar{r}^{n-\frac{1}{2}}), \phi^n - \phi^{n-1} \rangle. \]

where

\[ r(t) = \exp(E_2(t)) = \exp\left(\int_{\Omega} 1 - \cos \phi \, dx\right), \]

\[ \eta(\phi, r) = \frac{r(t)}{\exp(E_2(t))} f(\phi). \]
Energy dissipation law of variable-step ESAV-CN scheme

Taking the inner product of variable-step CN scheme (32a)–(32b) with $\tau_n \bar{\varsigma}^n$.

$$
\langle \partial_\tau \phi^n, \tau_n \bar{\varsigma}^n \rangle = \frac{\epsilon}{2} \| \nabla \phi^n \|^2 - \frac{\epsilon}{2} \| \nabla \phi^{n-1} \|^2 + \ln r^n - \ln r^{n-1}.
$$

$$
\langle I_\tau ^{\beta} \bar{\varsigma}^n, \tau_n \bar{\varsigma}^n \rangle = \mathcal{F}_\beta [\tau_n \bar{\varsigma}^n] - \mathcal{F}_\beta [\tau_n \bar{\varsigma}^{n-1}] + \mathcal{R}_\beta [\tau_n \bar{\varsigma}^n].
$$

Theorem 6

Under the step-size ratio constraint (11), the variable-step ESAV-CN scheme (32) possesses the following energy dissipation law

$$
\partial_\tau \tilde{\mathcal{E}}_\beta [\phi^n] = -\frac{1}{\tau_n} \mathcal{R}_\beta [\tau_n \bar{\varsigma}^n], \quad \text{for} \ 1 \leq n \leq N,
$$

(33)

where the modified energy $\tilde{\mathcal{E}}_\beta [\cdot]$ is defined as

$$
\tilde{\mathcal{E}}_\beta [\phi^n] = \frac{\epsilon}{2} \| \nabla \phi^n \|^2 + \ln r^n + \mathcal{F}_\beta [\tau_n \bar{\varsigma}^n].
$$

(34)

Both discrete energy and energy dissipation law are asymptotically compatible.
Numerical experiments

Example 3

(Convergence test). Consider the TFSG model with the initial value $u_0(x) = \pi \sin(2x) \sin(2y)$ in $\Omega = (-3, 3)^2$ until $T = 1, \epsilon = 0.1$.

Table 4: Errors and convergence rates of CN scheme and ESAV-CN scheme with $\beta = 0.3$.

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<tr>
<th>$N$</th>
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<th>$\gamma = 3$</th>
<th>$\gamma = 4$</th>
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<td>1.50e-4</td>
</tr>
<tr>
<td>ESAV-CN</td>
<td></td>
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<tr>
<td>20</td>
<td>1.01e-2</td>
<td>-</td>
<td>1.99e-2</td>
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<tr>
<td>40</td>
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<td>1.99</td>
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<td>6.64e-4</td>
<td>1.99</td>
<td>1.40e-3</td>
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<tr>
<td>160</td>
<td>1.70e-4</td>
<td>1.98</td>
<td>3.51e-4</td>
</tr>
</tbody>
</table>
Numerical experiments

Example 4

(Energy stability). Take $\Omega = (-10, 10)^2$ and $\epsilon = 0.04$. The initial value $u_0(x) = 4 \tanh \left[ \exp \left( 3 - \sqrt{x^2 + y^2} \right) \right]$. 

![Figure 5: Energies of CN scheme and ESAV-CN scheme with different $\beta$.](image)
Comparison

**Figure 6:** Modified energies of the proposed schemes for TFSG model and the original conservative energy of sine-Gordon model.
Outline

1. Background

2. Discrete gradient structure

3. Application to time fractional Swift-Hohenberg model

4. Application to time fractional sine-Gordon model

5. Conclusion
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- A unified DGS for the nonuniform integral averaged formulae of time fractional derivative and integral.
- Theoretical framework of variable-step energy stable numerical schemes for fractional gradient flows and nonlinear integro-differential equations.
- SAV-type variable-step scheme and energy stability analysis.

Future work: extended to other gradient flows, such as TFCH, TFMBE model.


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Thanks for your attention!

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