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

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Outline

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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].

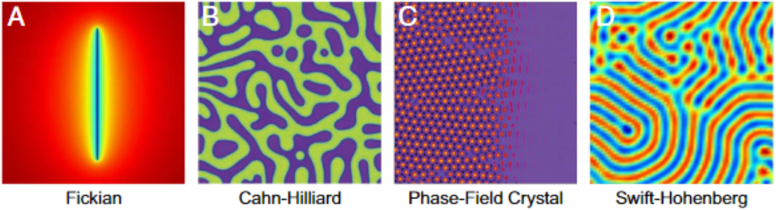

Figure 1: Representative gradient flows. (From *PNAS, Vol. 119, N0. 23, 2022*)

[1] G. Boussinot, E. Brener, Phys. Rev. E, 88 (2013), 022406.
[2] K. Elder, N. Provatas, J. Berry, P. Stefanovic, M. Grant, Phys. Rev. B, 75 (2007), 064107.
[3] L. Coelho, E. Vitral, J. Pontes, N. Mangiavacchi, Phys. D, (2021), 427.

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- Energy dissipation law

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- Multiscale time behavior: fast-to-slow change during long-time simulation.

Numerical methods for gradient flows

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- Convex-splitting (D. Eyre, MRS Proc, 1998)
- 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

- Time fractional models: describe diffusion with memory effect [4].

[4] T. Solomon, E. Weeks, H. Swinney, Phys. Rev. Lett, 71 (1993).
[5] Z. Li, H. Wang, D. Yang, J. Comput. Phys, 347 (2017), 20-38.
[6] M. Caputo, M. Fabrizio, J. Comput. Phys, 293 (2015), 400-408.
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- The Riemann-Liouville fractional integral of order $\beta > 0$

$$\mathcal{I}^\beta v(t) = \int_0^t \omega_\beta(t-s)v(s)\mathrm{d}s, \quad \text{with } \omega_\beta(t) = t^{\beta-1}/\Gamma(\beta). \tag{4}$$

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Numerical methods for time fractional gradient flows

- L1-stabilized scheme (T. Tang, H. Yu, T. Zhou, SISC, 2020)
  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)
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Developed using the uniform time step sizes.

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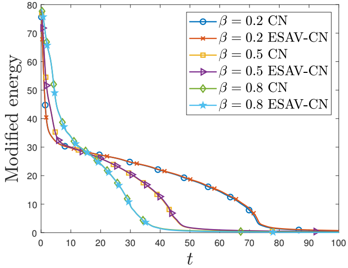

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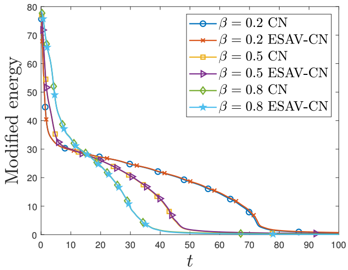

Figure 2: Energies with different fractional index.

- Practical way: Energy stable schemes with variable time steps

Variable-step schemes for time fractional gradient flows

- L1 type schemes
  - L1 scheme for TFAC (B. Ji, H.-L. Liao, L. Zhang, ACM, 2020).
  - L1-ExSAV scheme for TFAC (D. Hou, C. Xu, SISC, 2021).
  - L1-ESAV scheme for TFAC&TFCH (Y. Yu, J. Zhang, R. Qin, JSC, 2023).
- L2-1_σ type schemes
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  - L2-1_σ-ExSAV scheme for TFMBE (D. Hou, C. Xu, JSC, 2022).
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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

$$x_k D_\tau \vec{x}^k = P[\vec{x}^k] - P[\vec{x}^{k-1}] + c^* x_k^2 + Q[\vec{x}^k]. \tag{5}$$

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

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

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

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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 $1 \le n \le N$. 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

$$\mathcal{D}_\tau^\alpha v^n = \frac{1}{\tau_n}\int_{t_{n-1}}^{t_n}\int_0^t \omega_{1-\alpha}(t-s)(\Pi_1 v(s))'\mathrm{d}s\mathrm{d}t = \sum_{j=1}^{n} c_{n-j}^{(1-\alpha,n)}\delta_\tau v^j. \tag{7}$$

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

$$c_{n-j}^{(\alpha,n)} = \frac{1}{\tau_n\tau_j}\int_{t_{n-1}}^{t_n}\int_{t_{j-1}}^{\min\{t,t_j\}} \omega_\alpha(t-s)\mathrm{d}s\mathrm{d}t, \quad \text{for } 1 \le j \le n. \tag{8}$$

Integral averaged formulae

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

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

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

Outline

Modified convolution kernels of nonuniform integral averaged formulae

- 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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- Denote

$$\hat{c}_0^{(\alpha,n)} = 2c_0^{(\alpha,n)} \quad \text{and} \quad \hat{c}_{n-j}^{(\alpha,n)} = c_{n-j}^{(\alpha,n)} \quad \text{for } 1 \le j \le n-1. \tag{10}$$

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- Such that

$$\hat{c}_0^{(\alpha,n)} > \hat{c}_1^{(\alpha,n)} > \hat{c}_2^{(\alpha,n)} > \cdots > \hat{c}_{n-1}^{(\alpha,n)}.$$

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) $\hat{c}_{n-j-1}^{(\alpha,n)} \geq \hat{c}_{n-j}^{(\alpha,n)} > 0$ for $1 \leq j \leq n-1$;

If the adjacent step-size ratios r_{n+1} and r_n for $n \geq 2$ fulfill the following relation

$$r_{n+1} \geq r_\alpha(r_n) = \left[\frac{2h(r_n)-h(2r_n)}{r_n^\alpha(4-2^{1+\alpha})}\right]^{\frac{1}{\alpha}}, \quad (11)$$

then the auxiliary kernels $\hat{c}_{n-j}^{(\alpha,n)}$ satisfy

(2) $\hat{c}_{n-1-j}^{(\alpha,n-1)} > \hat{c}_{n-j}^{(\alpha,n)}$ for $1 \leq j \leq n-1$;

(3) $\hat{c}_{n-2-j}^{(\alpha,n-1)} - \hat{c}_{n-1-j}^{(\alpha,n-1)} > \hat{c}_{n-j-1}^{(\alpha,n)} - \hat{c}_{n-j}^{(\alpha,n)}$ 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

$$2q_n \sum_{j=1}^{n} \omega_{n-j}^{(n)} q_j = G[\vec{q}_n] - G[\vec{q}_{n-1}] + \theta\omega_0^{(n)} q_n^2 + Y[\vec{q}_n], \quad \text{for } n \geq 1. \tag{12}$$

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)

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

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

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

- DGS $\to$ 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

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

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- Geometric convexity in [H.-L. Liao, N. Liu, P. Lyu, SINUM, 2023]

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

- A different DGS under another step-size ratio restriction

$$r_{n+1} \geq \hat{r}_\alpha(r_n) = \left[\frac{(2^\alpha - 1)h(r_n)}{h(2r_n) - 2h(r_n)}\right]^{\frac{1}{1-\alpha}}. \tag{14}$$

Comparison

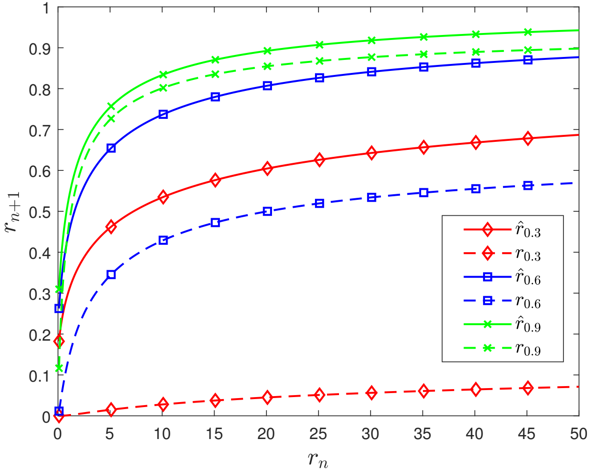

Figure 3: Comparisons of the step-size ratio constraints (11) with (14).

Outline

Time fractional Swift-Hohenberg (TFSH) model

- Consider the TFSH model of order $\alpha \in (0,1)$

$$\mathcal{D}_t^\alpha u = -\mu, \quad (\mathbf{x}, t) \in \Omega \times (0, T] \tag{15}$$

subjected to the periodic boundary conditions.

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

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

- g, ϵ: two nonnegative physical parameters.

Variable-step CN scheme for TFSH model

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

$$\mathcal{D}_\tau^\alpha u^n = -\mu^{n-\frac{1}{2}}, \quad \text{with } \mu^{n-\frac{1}{2}} = (1+\Delta)^2 u^{n-\frac{1}{2}} + \Psi(u^n, u^{n-1}). \tag{17}$$

- 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 $\tau_n \le \sqrt[\alpha]{\frac{6}{\Gamma(3-\alpha)(g^2+3\epsilon)}}$.

Energy dissipation law of variable-step CN scheme

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

$$\begin{aligned}\langle \mathcal{D}_\tau^\alpha u^n, \delta_\tau u^n\rangle &= \left\langle \sum_{j=1}^{n} c_{n-j}^{(\alpha,n)} \delta_\tau u^n, \delta_\tau u^n \right\rangle \\ &= \mathcal{F}_{1-\alpha}[\delta_\tau u^n] - \mathcal{F}_{1-\alpha}[\delta_\tau u^{n-1}] + \mathcal{R}_{1-\alpha}[\delta_\tau u^n], \\ \langle \mu^{n-\frac{1}{2}}, \delta_\tau u^n\rangle &= E[u^n] - E[u^{n-1}].\end{aligned}$$

Theorem 3

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

$$\partial_\tau E_\alpha[u^n] = -\frac{1}{\tau_n}\mathcal{R}_{1-\alpha}[\delta_\tau u^n], \quad \text{for } 1 \le n \le N, \tag{18}$$

where the modified energy $E_\alpha[\cdot] = E[u^n] + \mathcal{F}_{1-\alpha}[\delta_\tau u^n]$.

Asymptotic compatiblity of varibale-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 $1 \le j \le n-1$.

Asymptotic compatiblity of varibale-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 $1 \le j \le n-1$.
- The CN scheme (17) reduces to the CN scheme for classical SH model

$$\partial_\tau u^n = -\mu^{n-\frac{1}{2}}, \quad \text{for } n \ge 1, \tag{19}$$

which holds that

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

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

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

which is the same as (20).

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- The energy dissipation law (18) reduces to

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

which is the same as (20).

- The discrete energy dissipation law of variable-step CN scheme is asymptotically compatible.

Variable-step ESAV-CN scheme for TFSH model

- 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)

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

  and denote $\sigma(u,s) = \frac{s(t)}{\exp(E_1[u])} f(u)$.
- The TFSH model (15) is transformed into the expanded system

$$\mathcal{D}_t^\alpha u = -\mu, \tag{21a}$$

$$\mu = (1+\Delta)^2 u + \sigma(u,s), \tag{21b}$$

$$(\ln s)_t = \langle \sigma(u,s), u_t \rangle. \tag{21c}$$

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

$$\mathcal{D}_\tau^\alpha u^n = -\mu^{n-\frac{1}{2}}, \tag{22a}$$

$$\mu^{n-\frac{1}{2}} = (1+\Delta)^2 u^{n-\frac{1}{2}} + \sigma(\bar{u}^{n-\frac{1}{2}}, \bar{s}^{n-\frac{1}{2}}), \tag{22b}$$

$$\ln s^n - \ln s^{n-1} = \left\langle \sigma(\bar{u}^{n-\frac{1}{2}}, \bar{s}^{n-\frac{1}{2}}), u^n - u^{n-1} \right\rangle. \tag{22c}$$

- $\bar{u}^{n-\frac{1}{2}} = (1+\frac{r_n}{2})u^{n-1} - \frac{r_n}{2}u^{n-2}$ 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 $\delta_\tau u^n$.

$$\langle \mathcal{D}_\tau^\alpha u^n, \delta_\tau u^n \rangle = \mathcal{F}_{1-\alpha}[\delta_\tau u^n] - \mathcal{F}_{1-\alpha}[\delta_\tau u^{n-1}] + \mathcal{R}_{1-\alpha}[\delta_\tau u^n].$$
$$\langle \mu^{n-\frac{1}{2}}, \delta_\tau u^n \rangle = \frac{1}{2}\left(\|(1+\Delta)u^n\|^2 - \|(1+\Delta)u^{n-1}\|^2\right) + \ln s^n - \ln s^{n-1}.$$

Theorem 4

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

$$\partial_\tau \tilde{E}_\alpha[u^n] = -\frac{1}{\tau_n}\mathcal{R}_{1-\alpha}[\delta_\tau u^n], \quad \text{for } 1 \le n \le N, \tag{23}$$

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

$$\tilde{E}_\alpha[u^n] = \frac{1}{2}\|(1+\Delta)u^n\|^2 + \ln s^n + \mathcal{F}_{1-\alpha}[\delta_\tau u^n]. \tag{24}$$

Asymptotic compatiblity of variable-step ESAV-CN scheme

- 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: $\mathcal{D}_t^\alpha u = -\mu + f(\mathbf{x}, t)$ 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 $(\alpha, \sigma) = (0.4, 0.6)$.

	N	$\gamma = 2$		$\gamma = 2/\sigma$		$\gamma = 4$	
		$e(N)$	Rate	$e(N)$	Rate	$e(N)$	Rate
CN	80	3.90e-3	-	1.77e-4	-	2.00e-4	-
	160	1.69e-3	1.21	4.46e-5	2.01	5.01e-5	2.02
	320	7.34e-4	1.21	1.12e-5	2.00	1.26e-5	2.01
	640	3.19e-4	1.20	2.81e-6	2.00	3.15e-6	2.00
ESAV-CN	80	4.38e-3	-	1.09e-2	-	1.53e-2	-
	160	1.70e-3	1.37	2.84e-3	1.97	4.00e-3	1.97
	320	7.36e-4	1.21	7.30e-4	1.97	1.03e-3	1.97
	640	3.20e-4	1.20	1.86e-4	1.98	2.63e-4	1.98

Numerical experiments

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

	N	$\gamma = 3$		$\gamma = 2/\sigma$		$\gamma = 6$	
		$e(N)$	Rate	$e(N)$	Rate	$e(N)$	Rate
CN	80	3.65e-3	-	6.36e-4	-	5.07e-4	-
	160	1.59e-4	1.21	1.64e-4	1.99	1.25e-4	2.06
	320	6.90e-4	1.21	4.17e-5	2.00	3.07e-5	2.05
	640	3.01e-4	1.20	1.05e-5	2.00	7.50e-6	2.04
ESAV-CN	80	3.77e-3	-	7.56e-3	-	1.05e-2	-
	160	1.59e-4	1.26	2.00e-3	1.96	2.80e-3	1.95
	320	6.91e-4	1.21	5.16e-4	1.97	7.27e-3	1.97
	640	3.01e-4	1.20	1.31e-4	1.98	1.86e-4	1.98

Numerical experiments

Example 2

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

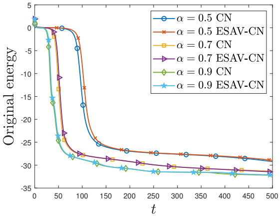
$$u_0(\mathbf{x}) = 0.07 - 0.02\cos\left(\frac{\pi(x-12)}{16}\right)\sin\left(\frac{\pi(y-1)}{16}\right) + 0.02\cos^2\left(\frac{\pi(x+10)}{32}\right)\sin^2\left(\frac{\pi(y+3)}{32}\right) - 0.01\sin^2\left(\frac{\pi x}{8}\right)\sin^2\left(\frac{\pi(y-6)}{8}\right).$$

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

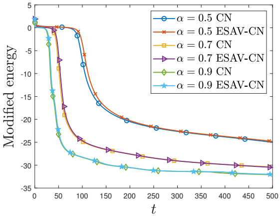
- Adaptive time strategy

$$\tau_{n+1} = \max\{\tau_*, r_\alpha(r_n)\tau_n\}, \quad \tau_* = \max\left\{\tau_{\text{min}}, \frac{\tau_{\text{max}}}{\sqrt{1+\lambda\|\partial_\tau u^n\|^2}}\right\} \tag{25}$$

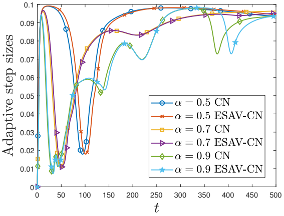
- $\tau_{\text{min}} = 10^{-3}$, $\tau_{\text{max}} = 10^{-1}$, $\lambda = 10^2$.



(a) Original energy



(b) Modified energy



(c) Adaptive step-sizes

Figure 4: Energies of CN scheme and ESAV-CN scheme with different α.

Numerical experiments

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

	$\alpha = 0.5$		$\alpha = 0.7$		$\alpha = 0.9$	
	Time step	CPU(s)	Time step	CPU(s)	Time step	CPU(s)
CN	6496	220.4	7574	215.6	8980	224.8
ESAV-CN	6477	92.6	7567	107.5	8959	126.2

Outline

Time fractional sine-Gordon model

- Consider the time fractional sine-Gordon (TFSG) model

$$\phi_t + \mathcal{I}^{\beta}\varsigma = 0, \quad (\mathbf{x}, t) \in \Omega \times (0, T] \tag{26}$$

  subjected to the periodic boundary conditions.
- $\varsigma = \delta\mathcal{E}/\delta\phi$ with $\mathcal{E}[\phi]$ defined by

$$\mathcal{E}[\phi] = \int_{\Omega} \frac{\epsilon}{2}|\nabla\phi|^2 + F(\phi)\mathrm{d}\mathbf{x}, \quad \text{with } F(\phi) = 1 - \cos\phi. \tag{27}$$

- When $\beta \to 1^{-}$, the TFSG model recovers the classical sine-Gordon wave equation: $\phi_{tt} = \epsilon\Delta\phi - \sin u$, which satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathcal{E}[\phi] + \frac{1}{2}\|\phi_t\|^2\right] = 0.$$

Variable-step CN scheme for TFSG model

- Using the integral averaged formula for Riemann-Liouvile fractional integral, the variable-step CN scheme for TFSG model

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

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 $\tau_n \leq \sqrt[1+\beta]{\Gamma(2+\beta)}$.

Energy dissipation law of variable-step CN scheme

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

$$\langle \mathcal{I}_\tau^\beta \bar{\varsigma}^n, \tau_n\bar{\varsigma}^n\rangle = \left\langle \sum_{j=1}^{n} c_{n-j}^{(\beta,n)} \tau_j \bar{\varsigma}^j, \tau_n\bar{\varsigma}^n \right\rangle$$
$$= \mathcal{F}_\beta[\tau_n\bar{\varsigma}^n] - \mathcal{F}_\beta[\tau_n\bar{\varsigma}^{n-1}] + \mathcal{R}_\beta[\tau_n\bar{\varsigma}^n],$$
$$\langle \partial_\tau \phi^n, \tau_n\bar{\varsigma}^n\rangle = \mathcal{E}[\phi^n] - \mathcal{E}[\phi^{n-1}].$$

Theorem 5

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

$$\partial_\tau \mathcal{E}_\beta[\phi^n] = -\frac{1}{\tau_n}\mathcal{R}_\beta[\tau_n\bar{\varsigma}^n], \quad \text{for } 1 \le n \le N, \tag{29}$$

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

$$\mathcal{E}_\beta[\phi^n] = \mathcal{E}[\phi^n] + \mathcal{F}_\beta[\tau_n\bar{\varsigma}^n]. \tag{30}$$

Asymptotic compatiblity 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

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

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

Asymptotic compatiblity of variable-step CN scheme

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  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).

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

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  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

Variable-step ESAV-CN scheme for TFSG model

- The variable-step ESAV-CN scheme based on the integral averaged formula

$$\partial_\tau \phi^n + \mathcal{I}_\tau^\beta \bar{\varsigma}^n = 0, \tag{32a}$$

$$\bar{\varsigma}^n = -\epsilon \Delta \phi^{n-\frac{1}{2}} + \eta(\bar{\phi}^{n-\frac{1}{2}}, \bar{r}^{n-\frac{1}{2}}), \tag{32b}$$

$$\ln r^n - \ln r^{n-1} = \left\langle \eta(\bar{\phi}^{n-\frac{1}{2}}, \bar{r}^{n-\frac{1}{2}}), \phi^n - \phi^{n-1} \right\rangle . \tag{32c}$$

where

$$r(t) = \exp(E_2(t)) = \exp(\int_\Omega 1 - \cos\phi \mathrm{d}\mathbf{x}),$$

$$\eta(\phi, r) = \frac{r(t)}{\exp(E_2(t))} f(\phi).$$

Energy dissipation law of variable-step ESAV-CN scheme

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

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

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

Theorem 6

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

$$\partial_\tau \tilde{\mathcal{E}}_\beta[\phi^n] = -\frac{1}{\tau_n}\mathcal{R}_\beta[\tau_n \bar{\varsigma}^n], \quad \text{for } 1 \le n \le N, \tag{33}$$

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

$$\tilde{\mathcal{E}}_\beta[\phi^n] = \frac{\epsilon}{2}\|\nabla \phi^n\|^2 + \ln r^n + \mathcal{F}_\beta[\tau_n \bar{\varsigma}^n]. \tag{34}$$

Both discrete energy and energy dissipation law are asymptotically compatible

Numerical experiments

Example 3

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

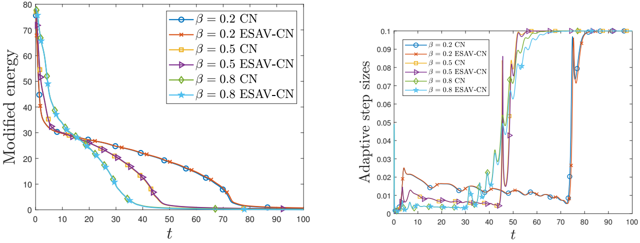
Table 4: Errors and convergence rates of CN scheme and ESAV-CN scheme with $\beta = 0.3$.

	N	$\gamma = 2$		$\gamma = 3$		$\gamma = 4$	
		$e(N)$	Rate	$e(N)$	Rate	$e(N)$	Rate
CN	20	4.07e-3	-	7.87e-3	-	1.28e-2	-
	40	1.09e-3	1.94	2.14e-3	1.95	3.56e-3	1.95
	80	2.87e-4	1.94	5.72e-4	1.94	9.63e-4	1.94
	160	7.52e-5	1.94	1.50e-4	1.95	2.56e-4	1.94
ESAV-CN	20	1.01e-2	-	1.99e-2	-	3.26e-2	-
	40	2.60e-3	1.99	5.28e-3	1.99	8.85e-3	1.99
	80	6.64e-4	1.99	1.40e-3	1.98	2.32e-3	1.99
	160	1.70e-4	1.98	3.51e-4	1.98	5.99e-4	1.98

Numerical experiments

Example 4

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



(a) Modified energy (b) Adaptive step-sizes

Figure 5: Energies of CN scheme and ESAV-CN scheme with different β.

Comparison

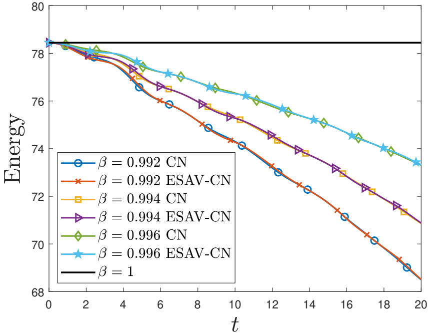


Figure 6: Modified energies of the proposed schemes for TFSG model and the original conservative energy of sine-Gordon model.

Outline

Conclusion

- 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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