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The original energy dissipation law of the R-SAV approach for gradient flows[☆]Jie Shen^{ID*}, Chengchao Zhao^{ID}

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ABSTRACT

The scalar auxiliary variable (SAV) approach is widely utilized to construct energy-stable numerical schemes for gradient flows. Its relaxed version (R-SAV) further enhances numerical accuracy by directly linking the updated auxiliary variable to the original energy. Although numerical experiments have suggested that the original energy in the R-SAV scheme exhibits a dissipative property under sufficiently small time steps, a rigorous theoretical proof has been lacking. This work fills this gap by providing a complete proof of the original energy dissipation law for a first-order R-SAV scheme applied to general gradient flows. The proof centers on establishing a key inequality that circumvents the need for an L^∞ -norm bound on the numerical solution. By leveraging the inherent relaxation step of the R-SAV approach, the dissipative property is rigorously proved through mathematical induction. Numerical experiments validate the theoretical results.

1. Introduction

Many scientific and engineering problems can be described by gradient flow equations. These equations are generally derived from the thermodynamic variation of a system's free energy and are governed by a dissipative dynamical path. A typical form of the gradient flow energy functional is given by

$$E(\phi) = \int_{\Omega} \left(\frac{1}{2} \mathcal{L}\phi \cdot \phi + F(\phi) \right) dx. \quad (1)$$

where \mathcal{L} is a self-adjoint linear symmetric nonnegative operator in $L^2(\Omega)$ and $F(\phi)$ is a nonlinear potential, Ω is a bounded domain in \mathbb{R}^d , (\cdot, \cdot) is the inner product in $L^2(\Omega)$, and $\|\cdot\|$ is the associated norm in $L^2(\Omega)$. The gradient flow associated with the above free energy can be written as

$$\phi_t = -\mathcal{G}\mu, \quad \mu = \frac{\delta E}{\delta \phi} = \mathcal{L}\phi + F'(\phi), \quad (2)$$

where \mathcal{G} is a symmetric positive operator in $L^2(\Omega)$. The equation is supplemented with the boundary condition: periodic, or $\phi|_{\partial\Omega} = 0$, or $\frac{\partial\phi}{\partial n} = 0$ if $\mathcal{G} = I$; periodic, or $\frac{\partial\phi}{\partial n} = \frac{\partial\mu}{\partial n} = 0$ if $\mathcal{G} = -\Delta$. With these boundary conditions, the above gradient flow system satisfies the following energy dissipation law:

$$\frac{d}{dt} E(\phi) = \left(\frac{\delta E}{\delta \phi}, \phi_t \right) = -(\mathcal{G}\mu, \mu). \quad (3)$$

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A highly desirable property of numerical algorithms for the dissipative systems (2) is to be able to satisfy the energy dissipation law, which is crucial to eliminating numerical results that are not physical. In the last few decades, a large body of research has been devoted to developing efficient energy-stable numerical schemes [1–6]. In particular, the SAV approach has attracted significant attention due to its simplicity, efficiency, accuracy, and broad applicability. Building upon this method, the relaxed SAV (R-SAV) approach introduced in [7,8] incorporates a relaxation step that directly links the updated SAV to the original energy, thereby further enhancing the computational accuracy.

Ample numerical evidence from [7,8] indicates that the original energy of the R-SAV scheme is also dissipative when the time step is sufficiently small. However, only the dissipation law for the modified energy has been rigorously established. It is therefore desirable to derive the original energy dissipation law for the R-SAV approach.

This paper presents a rigorous proof of the original energy dissipation law for a first-order R-SAV scheme applied to (2) under sufficiently small time steps. The success of the proof hinges on two key elements: firstly, we derive a pivotal inequality (Lemma 1) that circumvents the need for L^∞ -norm estimates of the numerical solution; secondly, in contrast to original SAV methods, the relaxation step in the R-SAV approach directly links the auxiliary variable to the original energy at the current time step, enabling effective control of the SAV by the numerical solutions ϕ^n and ϕ^{n-1} when the time step is sufficiently small. By integrating these two key aspects with mathematical induction, we successfully prove the dissipation of the original energy. It is important to note that the proof presented herein cannot be directly extended to the original SAV scheme, due to the absence of a direct linkage between the auxiliary variable and the original energy. Extensions of the results presented in this paper to the original SAV schemes and higher-order R-SAV schemes will be the subject of a future study.

The rest of this paper is organized as follows. Section 2 provides a brief review of the R-SAV approach. In Section 3, we first establish a key inequality and then present and prove our main result, namely the original energy dissipation theorem. Finally, Section 4 presents numerical experiments to validate the theoretical results.

2. A brief review of the R-SAV approach

Assuming $E_1(\phi) := \int_\Omega F(\phi) dx \geq 1 - C_0, \forall \phi$ for some $C_0 > 0$. By introducing a SAV $r(t) = \sqrt{E_1(\phi) + C_0}$, (2) can be reformulated as

$$\begin{cases} \phi_t = -\mathcal{G}\mu, \\ \mu = \mathcal{L}\phi + \frac{r(t)}{\sqrt{E_1(\phi) + C_0}} F'(\phi) \\ r_t = \frac{1}{2\sqrt{E_1(\phi) + C_0}} (F'(\phi), \phi_t). \end{cases} \quad (4)$$

Taking the inner products of the first two equations in (4) with μ and $-\phi_t$, respectively, and making use of the third equation, we derive the following modified energy dissipation law:

$$\frac{d}{dt} \tilde{E}(\phi) = -(\mathcal{G}\mu, \mu), \quad (5)$$

where $\tilde{E}(\phi) = \int_\Omega \frac{1}{2} \mathcal{L}\phi \cdot \phi dx + r^2$ is the modified energy. Let $\phi^n := \phi^n(x)$ denote the numerical approximation of $\phi(t, x)$ at $t = t_n$. Then, a first-order SAV scheme for the modified system is given by

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\tau} = -\mathcal{G}\mu^{n+1}, \\ \mu^{n+1} = \mathcal{L}\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1(\phi^n) + C_0}} F'(\phi^n) \\ r^{n+1} - r^n = \frac{1}{2\sqrt{E_1(\phi^n) + C_0}} (F'(\phi^n), \phi^{n+1} - \phi^n). \end{cases} \quad (6)$$

Taking the inner products of the first two equations in (6) with $\tau\mu^{n+1}$ and $-(\phi^{n+1} - \phi^n)$, and using the third equation, we have the following energy dissipation law:

$$\tilde{E}^{n+1} - \tilde{E}^n \leq -\tau(\mathcal{G}\mu^{n+1}, \mu^{n+1}), \quad \forall n \geq 0, \quad (7)$$

where the modified energy at time level n is defined as

$$\tilde{E}^n := \int_\Omega \frac{1}{2} \mathcal{L}\phi^n \cdot \phi^n dx + (r^n)^2. \quad (8)$$

Based on the SAV scheme (6), the R-SAV scheme is constructed as follows:

Step 1: Compute the solution $(\phi^{n+1}, \tilde{r}^{n+1})$ using the original SAV method:

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\tau} = -\mathcal{G}\mu^{n+1}, \\ \mu^{n+1} = \mathcal{L}\phi^{n+1} + \frac{\tilde{r}^{n+1}}{\sqrt{E_1(\phi^n) + C_0}} F'(\phi^n) \\ \tilde{r}^{n+1} - r^n = \frac{1}{2\sqrt{E_1(\phi^n) + C_0}} (F'(\phi^n), \phi^{n+1} - \phi^n). \end{cases} \tag{9}$$

Step 2: Update the SAV r^{n+1} by a relaxation:

$$r^{n+1} = \theta^{n+1}\tilde{r}^{n+1} + (1 - \theta^{n+1})\sqrt{E_1(\phi^{n+1}) + C_0}, \quad \theta^{n+1} \in \mathcal{V}^{n+1}. \tag{10}$$

Here \mathcal{V}^{n+1} is the admissible set defined by

$$\mathcal{V}^{n+1} := \{ \theta \in [0, 1] \mid \tilde{E}^{n+1} - \tilde{E}^n \leq -(1 - \gamma)\tau(\mathcal{G}\mu^{n+1}, \mu^{n+1}) \}, \tag{11}$$

where $\gamma \in [0, 1]$ is a tunable parameter. Note that (7) implies $1 \in \mathcal{V}^{n+1}$ for all $n \geq 0$, guaranteeing that \mathcal{V}^{n+1} is always nonempty. Therefore, the R-SAV scheme (9)–(10) is unconditionally energy stable.

Remark 1 (Optimal Choice for θ^n). The relaxation parameter θ^{n+1} can be selected as the solution to the following constrained minimization problem:

$$\theta^{n+1} = \min_{\theta \in [0, 1]} \theta, \quad \text{s.t., } (r^{n+1}(\theta))^2 \leq \tilde{E}^n - \frac{1}{2} \|\mathcal{L}^{1/2}\phi^{n+1}\|^2 - (1 - \gamma)\tau(\mathcal{G}\mu^{n+1}, \mu^{n+1}),$$

where

$$r^{n+1}(\theta) := \theta\tilde{r}^{n+1} + (1 - \theta)Q(\phi^{n+1}) \quad \text{and} \quad Q(\phi) := \sqrt{E_1(\phi) + C_0}.$$

This problem can be rewritten in the simplified form:

$$\theta^{n+1} = \min_{\theta \in [0, 1]} \theta, \quad \text{s.t., } f(\theta) = a\theta^2 + b\theta + c \leq 0, \tag{12}$$

with coefficients given by

$$\begin{aligned} a &= (\tilde{r}^{n+1} - Q(\phi^{n+1}))^2, & b &= 2Q(\phi^{n+1})(\tilde{r}^{n+1} - Q(\phi^{n+1})), \\ c &= Q(\phi^{n+1})^2 - \tilde{E}^n + \frac{1}{2} \|\mathcal{L}^{1/2}\phi^{n+1}\|^2 + (1 - \gamma)\tau(\mathcal{G}\mu^{n+1}, \mu^{n+1}). \end{aligned}$$

If $a = 0$, we set $\theta^{n+1} = 0$. If $a > 0$, we observe that $f(1) \leq -\gamma\tau(\mathcal{G}\mu^{n+1}, \mu^{n+1}) \leq 0$. It follows that $f(\theta)$ has at least one real root, and $f(\theta) \leq 0$ for any $\theta \in ((-b - \sqrt{b^2 - 4ac})/(2a), 1)$. In this case, we choose

$$\theta^{n+1} = \max \left\{ 0, \frac{-b - \sqrt{b^2 - 4ac}}{2a} \right\}. \tag{13}$$

3. The original energy dissipation law of the R-SAV scheme

In this section, we establish the original energy dissipation law for the R-SAV scheme (9)–(10). We first present a key auxiliary result. In the remainder of this paper, we denote the space $H^1(\Omega)$ by H^1 for brevity.

Lemma 1. Let $v, w \in H^1$. Then for any $\epsilon > 0$, the following inequality holds:

$$\int_{\Omega} v^2 |w|^p \, dx \leq \epsilon \|v\|_{H^1}^2 + \frac{C_1}{\epsilon} \|v\|^2 \|w\|_{H^1}^{2p}, \tag{14}$$

where $C_1 := (2 + |\Omega|)C_{\Omega}^{2p+2}/4$ and $p > 0$ arbitrary if $d = 1, 2$; $0 < p \leq 2$ if $d = 3$.

Proof. By Hölder’s inequality, we obtain

$$\int_{\Omega} v^2 |w|^p \, dx \leq \left(\int_{\Omega} v^6 \, dx \right)^{1/6} \left(\int_{\Omega} (v|w|^p)^{6/5} \, dx \right)^{5/6}.$$

From the Sobolev embedding theorem, for any $q \geq 1$ if $d = 1, 2$, and $1 \leq q \leq 6$ if $d = 3$, we have

$$\left(\int_{\Omega} |w|^q \, dx \right)^{1/q} \leq C_{\Omega} \|w\|_{H^1}. \tag{15}$$

Applying Young’s inequality yields

$$\int_{\Omega} v^2 |w|^p \, dx \leq \epsilon \|v\|_{H^1}^2 + \frac{C_{\Omega}^2}{4\epsilon} \left(\int_{\Omega} (v|w|^p)^{6/5} \, dx \right)^{5/3}. \tag{16}$$

Now, applying Hölder’s inequality again to the last term in (16), we get

$$\left(\int_{\Omega} (v|w|^p)^{6/5} dx\right)^{5/3} \leq \|v\|^2 \left(\int_{\Omega} |w|^{3p} dx\right)^{2/3}. \tag{17}$$

Furthermore, for $0 < q < 1$, Hölder’s inequality implies

$$\int_{\Omega} |w|^q dx \leq |\Omega|^{1-q} \left(\int_{\Omega} |w| dx\right)^q \leq (|\Omega| + 1) \left(\int_{\Omega} |w| dx\right)^q. \tag{18}$$

Combining (15) and (18), we deduce

$$\left(\int_{\Omega} |w|^{3p} dx\right)^{2/3} \leq (2 + |\Omega|) C_{\Omega}^{2p} \|w\|_{H^1}^{2p}, \tag{19}$$

which together with (16) and (17) complete the proof. \square

We now state the original energy dissipation law for the R-SAV scheme (9)–(10) in the following theorem.

Theorem 2. Assume that there exists a constant C such that $\|\phi\|_{H^1}^2 \leq C\|\mathcal{L}^{1/2}\phi\|^2$; $|F'(\phi)| \leq \mathcal{R}(1 + |\phi|^{p+1})$ and $|F''(\phi)| \leq \mathcal{R}(1 + |\phi|^p)$ with $0 < p \leq 2$ if $d = 3$ and $p > 0$ if $d = 1, 2$. Then there exists a uniform constant $\tau^* > 0$, independent of n and the final time T , such that for any $\tau \leq \tau^*$, the R-SAV scheme (9)–(10) admits the following original energy dissipation law

$$E(\phi^{n+1}) - E(\phi^n) \leq -(1 - \gamma)\tau(G\mu^{n+1}, \mu^{n+1}), \quad \forall n \geq 0, \tag{20}$$

where $\gamma \in [0, 1]$ is the parameter in (11).

Proof. We now prove the theorem by mathematical induction. Assume that $0 \in \mathcal{V}^k$ ($1 \leq k \leq n$), that is, $r^k = \sqrt{E_1(\phi^k) + C_0}$. We now consider the case of $k = n + 1$. Taking the inner products of the first two equations in (9) with $\tau\mu^{n+1}$ and $-(\phi^{n+1} - \phi^n)$ respectively, we obtain

$$\begin{aligned} E(\phi^{n+1}) - E(\phi^n) + \frac{1}{2}\|\mathcal{L}^{1/2}(\phi^{n+1} - \phi^n)\|^2 - (F(\phi^{n+1}) - F(\phi^n), 1) \\ + \frac{\bar{r}^{n+1}}{\sqrt{E_1(\phi^n) + C_0}} (F'(\phi^n), \phi^{n+1} - \phi^n) = -\tau(G\mu^{n+1}, \mu^{n+1}). \end{aligned} \tag{21}$$

By Taylor expansion, we have

$$(F(\phi^{n+1}) - F(\phi^n), 1) = (F'(\phi^n), \phi^{n+1} - \phi^n) + \frac{1}{2}(F''(\xi^n), (\phi^{n+1} - \phi^n)^2),$$

where $\xi^n = \theta\phi^{n+1} + (1 - \theta)\phi^n$ and $\theta := \theta(x) \in [0, 1], \forall x \in \Omega$. Substituting into (21) yields

$$E(\phi^{n+1}) - E(\phi^n) + \frac{1}{2}\|\mathcal{L}^{1/2}(\phi^{n+1} - \phi^n)\|^2 + I_1 + I_2 = -\tau(G\mu^{n+1}, \mu^{n+1}). \tag{22}$$

where

$$I_1 := -\frac{1}{2}(F''(\xi^n), (\phi^{n+1} - \phi^n)^2), \quad I_2 := \left(\frac{\bar{r}^{n+1}}{\sqrt{E_1(\phi^n) + C_0}} - 1\right)(F'(\phi^n), \phi^{n+1} - \phi^n). \tag{23}$$

From (11) we have the uniform bound

$$\|\phi^n\|_{H^1}^2 \leq C\|\mathcal{L}^{1/2}\phi^n\|^2 \leq 2C\bar{E}^n \leq 2CE^0, \quad \forall n \geq 0. \tag{24}$$

Since $|F''(\xi^n)| \leq \mathcal{R}(1 + |\xi^n|^p)$ and $\|\xi^n\|_{H^1} \leq \|\theta\phi^{n+1}\|_{H^1} + \|(1 - \theta)\phi^n\|_{H^1}$, from (24) and Lemma 1, we have

$$|I_1| \leq \frac{\epsilon\mathcal{R}}{2}\|\phi^{n+1} - \phi^n\|_{H^1}^2 + \frac{\mathcal{R}}{2}\left(1 + \frac{(4CE^0)^p C_1}{\epsilon}\right)\|\phi^{n+1} - \phi^n\|^2. \tag{25}$$

We now estimate $|I_2|$. From the third equation in (6) and the induction hypothesis $r^n = \sqrt{E_1(\phi^n) + C_0}$, we have

$$\frac{\bar{r}^{n+1}}{\sqrt{E_1(\phi^n) + C_0}} - 1 = \frac{(F'(\phi^n), \phi^{n+1} - \phi^n)}{2(E_1(\phi^n) + C_0)}. \tag{26}$$

By the Sobolev embedding theorem and (24), we obtain

$$\|F'(\phi^n)\|^2 \leq 2\mathcal{R}^2(|\Omega| + \int_{\Omega} |\phi^n|^{2p+2} dx) \leq 2\mathcal{R}^2(|\Omega| + C_{\Omega}^{2p+2}\|\phi^n\|_{H^1}^{2p+2}) \leq \mathcal{R}^2 C_2, \tag{27}$$

where $C_2 := 2(|\Omega| + (2CC_{\Omega}E^0)^{2p+2})$. Substituting (26) and (27) into (23) gives

$$|I_2| \leq \frac{\mathcal{R}^2 C_2}{2}\|\phi^{n+1} - \phi^n\|^2, \tag{28}$$

where we have used the assumption $E_1(\phi^n) + C_0 \geq 1$. Now, inserting (25) and (28) into (22), and choosing $\epsilon = \frac{1}{2C\mathcal{R}}$, we derive

$$E(\phi^{n+1}) - E(\phi^n) + \tau(G\mu^{n+1}, \mu^{n+1}) + \frac{1}{4C}\|\nabla(\phi^{n+1} - \phi^n)\|^2 \leq C_3\|\phi^{n+1} - \phi^n\|^2, \tag{29}$$

where $C_3 = \mathcal{R}/2 + C\mathcal{R}^2(4CE^0)^p C_1 + R^2 C_2/2$, and we have used the inequality $\|\phi\|_{H^1}^2 \leq C\|\mathcal{L}^{1/2}\phi\|^2$. Define $C^* := CC_3^2 + C_3$ and $\tau^* := \gamma/C^*$. We now analyze the L^2 and H^{-1} gradient flow cases separately.

For L^2 gradient flow (i.e., $\mathcal{G} = I$), it follows from the first equation in (9) that

$$\|\phi^{n+1} - \phi^n\|^2 = \tau^2(G\mu^{n+1}, \mu^{n+1}). \tag{30}$$

Taking $\tau \leq \tau^* \leq \gamma/C_3$, inequality (29) implies that $0 \in \mathcal{V}^{n+1}$.

For the H^{-1} gradient flow, it follows from the first equation in (9) that

$$\|\phi^{n+1} - \phi^n\|^2 = \tau^2\|\Delta\mu^{n+1}\|^2, \quad \text{and} \quad \|\nabla(\phi^{n+1} - \phi^n)\|^2 = \tau^2\|\nabla\Delta\mu^{n+1}\|^2. \tag{31}$$

Substituting (31) into (29) yields

$$E(\phi^{n+1}) - E(\phi^n) + \tau\|\nabla\mu^{n+1}\|^2 + \frac{\tau^2}{4C}\|\nabla\Delta\mu^{n+1}\|^2 \leq C_3\tau^2\|\Delta\mu^{n+1}\|^2.$$

Note that

$$\|\Delta\mu^{n+1}\|^2 = -\int_{\Omega} \nabla\Delta\mu^{n+1} \cdot \nabla\mu^{n+1} \, dx \leq \frac{1}{4CC_3}\|\nabla\Delta\mu^{n+1}\|^2 + CC_3\|\nabla\mu^{n+1}\|^2.$$

Combining the above inequalities, we obtain

$$E(\phi^{n+1}) - E(\phi^n) \leq -(1 - CC_3^2\tau)\tau\|\nabla\mu^{n+1}\|^2. \tag{32}$$

Taking $\tau \leq \tau^* \leq \gamma/(CC_3^2)$, we conclude that $0 \in \mathcal{V}^{n+1}$.

Since $r^0 = \sqrt{E_1(\phi^0) + C_0}$, the same argument shows that $0 \in \mathcal{V}^1$ (details omitted). The proof is thus completed by mathematical induction. \square

Remark 2. The genetic constant \mathcal{R} can be very large for realistic physical models. For example, for the Allen-Cahn equation where $F(\phi) = \frac{1}{2\epsilon}(1 - \phi^2)^2$, $\mathcal{R} = \mathcal{O}(\epsilon^{-2})$. From the above analysis, it follows that the admissible time-step threshold satisfies $\tau^* = \mathcal{O}(\mathcal{R}^{-2}) = \mathcal{O}(\epsilon^4)$. Therefore, the present analytical technique still exhibits a strong dependence on ϵ . This strong dependence mainly arises from the theoretical analysis itself, in particular from the use of Young’s inequality in the proof. Improving the ϵ -scaling of the stability threshold will be considered in future work.

Remark 3. The growth assumptions imposed on F in Theorem 2 are satisfied by a broad class of polynomial-type potentials, including the widely used Ginzburg–Landau potentials. It is worth noting that certain singular potentials, such as the Flory–Huggins potential, do not satisfy these polynomial growth conditions due to the singular behavior of their derivatives near the pure phases. Extending the present analysis to such singular potentials would require additional techniques and constitutes an interesting direction for future research.

4. Numerical experiments

We now provide a numerical example to demonstrate the original energy dissipation law of the R-SAV approach. We consider the Cahn–Hilliard equation

$$\phi_t = \Delta\mu, \quad \mu = \frac{\delta E}{\delta\phi} = -\Delta\phi + \frac{1}{\epsilon^2}(\phi^3 - \phi), \tag{33}$$

with periodic boundary condition and the initial condition

$$\phi(0, x) = 0.3 + 0.01 \text{rand}(x), \quad \text{rand}(x) : \text{uniform random distribution in } [-1, 1].$$

The algorithm is performed in the bounded domain $\Omega = (0, 2\pi)^2$ using the spatial Fourier-pseudospectral discretization with N_f Fourier modes for each direction. We define an indicator function as follows:

$$\chi := \begin{cases} 1, & \text{if } \max_{0 \leq n \leq T/\tau} (E^{n+1} - E^n) > \epsilon, \\ 0, & \text{otherwise,} \end{cases}$$

where E^n denotes the original energy and the tolerance is set to $\epsilon = 1 \times 10^{-13}$. Clearly, the original energy dissipation law is deemed satisfied when $\chi = 0$.

Fig. 1 illustrates the variation of the indicator χ with the time step size τ . In the simulations, the interface width parameter is chosen as $\epsilon^2 = 0.03, 0.06$, the relaxation parameters as $\gamma = 0.1, 0.5, 1$, the Fourier modes as $N_f = 32, 128$ and the final time as $T = 10$. The results show that for sufficiently small time steps, the R-SAV schemes with different values of γ all satisfy the original energy dissipation law, in agreement with the theoretical results in Theorem 2. Furthermore, we observe that the maximum time step size τ^* preserving the original energy dissipation is independent of the number of Fourier modes N_f , but depends on interface width parameter ϵ .

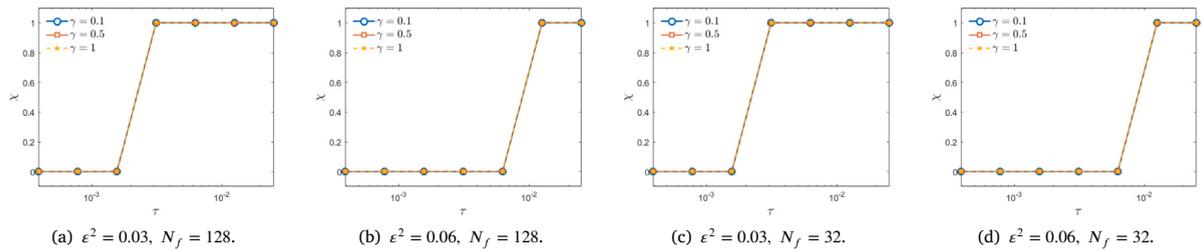


Fig. 1. Behavior of the indicator function χ with respect to the time step size τ : $\chi = 0$ indicates that the original energy dissipation law is satisfied; otherwise, $\chi = 1$.

Data availability

No data was used for the research described in the article.

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