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A Symmetric Discrete-Gradient Finite-Volume Method for Positive Drift–Diffusion Flows

Sergey Drominko[1,*] **Erina Kovachiskaya**[1]

[1] Faculty of Information Technology and Robotics, Vitebsk State Technological University, Belarus

Emails: Serdrominko1996@vsu.by; EriKovachi98rus@vsu.by

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ABSTRACT

Consider the periodic gradient flow

$$\partial_t u = \partial_x(m(u)\partial_x\mu), \qquad \mu = h'(u)+V, \qquad \mathscr{E}[u] = \int_0^1 \{h(u)+Vu\}\,\mathrm{d}x,$$

for strictly positive density u, convex entropy density h, and mobility $m>0$. We couple a centered finite-volume flux with a symmetric two-state approximation of the chemical potential. Its entropy component is the divided difference

$$\mathscr{D}_h(a,b) = \frac{h(a)-h(b)}{a-b}, \qquad \mathscr{D}_h(a,a) = h'(a),$$

which enforces the discrete chain rule exactly. With midpoint edge mobility and the logarithmic state $u_i^{n+1} = \exp z_i^{n+1}$, the nonlinear update is self-adjoint and, for every solved algebraic step, satisfies

$$\mathscr{E}_h^{n+1} - \mathscr{E}_h^n = -\Delta t \sum_i \mathscr{M}_{i+1/2}^{n+1/2} \frac{(\mu_{i+1}^{n+1/2} - \mu_i^{n+1/2})^2}{\Delta x} \le 0.$$

The flux telescopes to conserve mass, the logarithmic parametrization confines finite roots to the positive cone, and states satisfying $h'(u_i)+V_i = \text{const}$ are fixed points. A midpoint expansion gives second-order consistency in time; the centered flux gives the same order in space. For $h(u) = u(\log u - 1)$, a manufactured heat-flow calculation gives observed L^2 orders 1.998 and 1.999 under coupled refinement. In a confining Fokker–Planck test, the maximum mass defect is 3.20×10^{-14} and the energy identity is satisfied within 1.42×10^{-14}. Replacing $\mathscr{D}_h$ by the midpoint chemical potential in the same one-step problem produces an energy-balance defect 1.60×10^{-2}, isolating the role of the temporal discrete gradient.

Keywords: Discrete gradient ▪ Finite volume method ▪ Drift–diffusion equation ▪ Gradient flow ▪ Free-energy dissipation ▪ Positivity ▪ Time symmetry

1. INTRODUCTION

Nonlinear drift–diffusion equations often carry more mathematical structure than their parabolic form alone suggests. For a density $u>0$ on the one-dimensional torus $\mathbb{T} = \mathbb{R}/\mathbb{Z}$, the equation

$$\partial_t u = \partial_x \big(m(u)\partial_x[h'(u)+V]\big) \tag{1}$$

combines a conservation law, a positivity constraint, an equilibrium relation, and a Lyapunov functional. If

$$\mathscr{E}[u] = \int_{\mathbb{T}} \big(h(u)+Vu\big)\,\mathrm{d}x, \qquad \mu = \frac{\delta\mathscr{E}}{\delta u} = h'(u)+V, \tag{2}$$

then smooth solutions satisfy

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}[u(t)] = -\int_{\mathbb{T}} m(u)|\partial_x\mu|^2\,\mathrm{d}x \le 0, \\ &\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{T}} u\,\mathrm{d}x = 0. \end{aligned} \tag{3}$$

The question addressed here is whether a second-order, centered finite-volume update can reproduce the algebraic identity in (3) *exactly at the fully discrete level*, while keeping every computed state in $(0,\infty)$ and retaining a symmetric time map.

The difficulty lies in the temporal chain rule. A midpoint approximation $h'((a+b)/2)(a-b)$ is second-order accurate but is not equal to $h(a)-h(b)$ unless h is quadratic. The mismatch is cubic:

$$h(a)-h(b)-h'\left(\frac{a+b}{2}\right)(a-b) = \frac{h'''(\xi)}{24}(a-b)^3, \tag{4}$$

for an intermediate ξ when $h \in C^3$. Thus a spatial discretization may be perfectly conservative and yet the fully discrete entropy calculation inherits a nonzero remainder. The device used below is the two-point discrete gradient

$$\mathscr{D}_h(a,b) = \begin{cases} \dfrac{h(a)-h(b)}{a-b}, & a \ne b, \\ h'(a), & a = b, \end{cases} \tag{5}$$

which is symmetric in (a,b) and satisfies

$$\mathscr{D}_h(a,b)(a-b) = h(a)-h(b) \tag{6}$$

without approximation.

Recent structure-preserving discretizations have established strong results for finite-volume cross-diffusion systems, aggregation–diffusion equations, Poisson–Nernst–Planck models, and nonlinear Fokker–Planck equations [1, 2, 3, 4, 5, 6]. Positivity through exponential variables has also proved effective in entropy-based Galerkin constructions [7]. Maximum-bound and variational formulations broaden this viewpoint beyond a single diffusion model [8, 9, 10, 11]. The distinction developed here is temporal: rather than deriving an energy inequality from a one-sided time discretization, the chemical potential itself is replaced by an exact two-state discrete derivative of the entropy. This is the step that permits simultaneous time symmetry and an equality-form free-energy law.

The resulting scheme couples a general convex entropy with a positive symmetric mobility mean while preserving the finite-volume conservation mechanism. A summation-by-parts calculation gives an equality-form discrete energy law rather than an inequality with a temporal remainder. Positivity is built into the unknown through a logarithmic parametrization, and the update is self-adjoint under $(u^n,u^{n+1},\Delta t) \mapsto (u^{n+1},u^n,-\Delta t)$. The analysis also identifies the discrete Onsager operator, its nullspace and spectral bounds, the fixed-mass equilibrium, a local positive solution branch, and the second-order truncation structure. Numerical calculations are used only to test these statements: an exact heat solution measures convergence, a confining potential tests mass and free-energy identities, and a matched midpoint calculation isolates the chain-rule defect.

Section 2 places the construction in the recent structure-preserving literature. Sections 3–5 develop the model, discretization, and analysis. Sections 6 and 7 report the numerical tests and discuss their implications; the final section states the conclusions.

2. RELATED WORK

A common objective in numerical diffusion is to retain at least part of the continuous entropy structure after discretization. Entropy-diminishing finite volumes for cross-diffusion have been accompanied by convergence analysis and discrete functional inequalities [1, 2, 12]. Fully discrete aggregation–diffusion methods can preserve nonnegativity and dissipate a discrete free energy, while subsequent analysis establishes convergence under suitable hypotheses [3, 4]. Related finite-difference constructions for Poisson–Nernst–Planck and Maxwell–Stefan systems exploit positivity, variational structure, or constrained optimization [5, 10].

The same structural program appears in several discretization families. Structure-preserving schemes for nonlinear or anisotropic Fokker–Planck equations have been developed through energetic variational formulations and fitted fluxes [9, 13]. Multispecies nonlocal gradient flows admit conservative finite-volume schemes with positive states and energy control [11]. Entropy-preserving space–time Galerkin methods provide another route for cross-diffusion systems [14]; Lagrange-multiplier approaches impose positivity, bounds, and conservation constraints while retaining second-order accuracy [15, 16]. On the analytical side, discrete gradient-flow structures themselves can converge to Fokker–Planck gradient flows under evolutionary Γ-convergence [17].

More recent developments sharpen bounds, entropy mechanisms, and higher-order time discretization. The discrete boundedness-by-entropy framework supplies a vector-valued chain rule for finite-volume cross-diffusion [18], while saturation models combine finite-volume bounds with free-energy dissipation [19]. Maximum-bound-preserving integrating-factor Runge–Kutta methods provide high-order time integration for semilinear parabolic equations [20]. Stabilized variants preserve the maximum bound unconditionally through third order [21], and cut-off postprocessing yields arbitrarily high-order maximum-bound-preserving, energy-stable schemes for Allen–Cahn problems [22].

The method below differs in three coupled choices: a cell-centered finite-volume flux, a symmetric two-state entropy derivative, and an exponential state variable. None of these ingredients alone is new. Their combination, however, produces an especially transparent identity: the fully discrete free-energy decrement is exactly the negative edge dissipation, not an inequality containing a temporal remainder. The construction is therefore useful as a small mathematical model for isolating what is gained by an exact temporal chain rule.

3. MATHEMATICAL MODEL

Let $h \in C^4((0,\infty))$ be strictly convex,

$$h''(s) > 0, \qquad s > 0, \tag{7}$$

and let $m : (0,\infty) \to (0,\infty)$ be continuous. The potential $V \in C^3(\mathbb{T})$ is time independent. Equation (1) can be written

$$\partial_t u + \partial_x J = 0, \qquad J = -m(u)\partial_x \mu, \qquad \mu = h'(u) + V. \tag{8}$$

Under periodic boundary conditions, integration by parts yields (3).

A principal example is the linear-mobility entropy pair

$$h(u) = u(\log u - 1), \qquad m(u) = u, \tag{9}$$

for which $\mu = \log u + V$ and

$$\partial_t u = \partial_{xx} u + \partial_x(uV_x). \tag{10}$$

For prescribed mass $M_0 > 0$, the equilibrium is

$$u_\infty(x) = \frac{M_0 e^{-V(x)}}{\int_{\mathbb{T}} e^{-V(y)}\,\mathrm{d}y}. \tag{11}$$

The discrete analysis uses a symmetric mobility mean. Let $\mathsf{A} : (0,\infty)^2 \to (0,\infty)$ satisfy

$$\mathsf{A}(a,b) = \mathsf{A}(b,a), \qquad \mathsf{A}(a,a) = a. \tag{12}$$

The arithmetic mean is used in the computations. Other positive symmetric means leave the energy proof unchanged.

Lemma 1 (Two-state entropy derivative)**.** *For $h \in C^3((0,\infty))$, the map (5) obeys*

$$\mathscr{D}_h(a,b) = \mathscr{D}_h(b,a), \tag{13}$$

$$\mathscr{D}_h(a,b)(a-b) = h(a) - h(b), \tag{14}$$

$$\mathscr{D}_h(a,b) = h'\left(\frac{a+b}{2}\right) + O((a-b)^2). \tag{15}$$

For (9),

$$\mathscr{D}_h(a,b) = \int_0^1 \log\big((1-\theta)b + \theta a\big)\,\mathrm{d}\theta. \tag{16}$$

Proof. Symmetry and (14) are immediate. Put $m = (a+b)/2$ and $d = a-b$. The fundamental theorem of calculus gives

$$\mathscr{D}_h(a,b) = \frac{1}{d}\int_{-d/2}^{d/2} h'(m+s)\,\mathrm{d}s.$$

Because $h \in C^3$, Taylor expansion of h' about m gives $h'(m+s) = h'(m) + h''(m)s + O(s^2)$. The odd term integrates to zero on the symmetric interval, so $\mathscr{D}_h(a,b) = h'(m) + O(d^2)$, proving (15). Equation (16) follows by applying the same integral identity to $h'(u) = \log u$. □

4. NUMERICAL METHOD

Partition $\mathbb{T}$ into N cells of width $\Delta x = 1/N$. Cell values at t_n are denoted u_i^n, with periodic indexing. Introduce

$$\bar{u}_i^{n+1/2} = \frac{u_i^{n+1} + u_i^n}{2}, \qquad \mu_i^{n+1/2} = \mathscr{D}_h(u_i^{n+1}, u_i^n) + V_i. \tag{17}$$

The positive edge mobility is

$$\mathscr{M}_{i+1/2}^{n+1/2} = \mathsf{A}\Big(m(\bar{u}_i^{n+1/2}), m(\bar{u}_{i+1}^{n+1/2})\Big). \tag{18}$$

Define the edge flux

$$J_{i+1/2}^{n+1/2} = -\mathscr{M}_{i+1/2}^{n+1/2}\frac{\mu_{i+1}^{n+1/2} - \mu_i^{n+1/2}}{\Delta x}. \tag{19}$$

The update is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{J_{i+1/2}^{n+1/2} - J_{i-1/2}^{n+1/2}}{\Delta x} = 0. \tag{20}$$

Positivity is imposed at the algebraic level by solving for

$$u_i^{n+1} = e^{z_i^{n+1}}, \qquad z_i^{n+1} \in \mathbb{R}. \tag{21}$$

Thus no evaluation of h or h' occurs outside their positive domain. This transformation does not by itself prove global existence of a nonlinear root. It states a precise admissibility result: every finite root of the transformed system corresponds to a strictly positive density.

The discrete energy and mass are

$$\mathscr{E}_h^n = \Delta x \sum_{i=0}^{N-1}\big(h(u_i^n) + V_i u_i^n\big), \qquad M_h^n = \Delta x \sum_{i=0}^{N-1} u_i^n. \tag{22}$$

For (9), the nonlinear residual in z is smooth for finite z, and the implementation uses the arithmetic edge mean

$$\mathscr{M}_{i+1/2}^{n+1/2} = \tfrac{1}{2}(\bar{u}_i^{n+1/2} + \bar{u}_{i+1}^{n+1/2}).$$

4.1 Discrete Onsager operator

The flux form can be written without indices. Let $G \in \mathbb{R}^{N\times N}$ be the periodic difference operator

$$(Gq)_{i+1/2} = \frac{q_{i+1} - q_i}{\Delta x}, \qquad G\mathbf{1} = 0, \tag{23}$$

and define the diagonal edge matrix

$$W^{n+1/2} = \operatorname{diag}\big(\mathscr{M}_{1/2}^{n+1/2}, \ldots, \mathscr{M}_{N-1/2}^{n+1/2}\big). \tag{24}$$

Then the discrete Onsager operator

$$K^{n+1/2} = G^\top W^{n+1/2} G \tag{25}$$

is symmetric and positive semidefinite, and (20) becomes

$$\frac{u^{n+1} - u^n}{\Delta t} = -K^{n+1/2}\mu^{n+1/2}. \tag{26}$$

This representation separates thermodynamics from transport: the discrete gradient supplies the exact temporal chain rule, whereas K supplies a symmetric nonnegative dissipation metric.

Proposition 2 (Spectrum of the discrete transport operator)**.** *Suppose* $0 < m_0 \le \mathscr{M}_{i+1/2} \le m_1$. *Then*

$$K = K^\mathsf{T} \succeq 0, \qquad \ker K = \operatorname{span}\{\mathbf{1}\}, \tag{27}$$

and, on the zero-mean subspace,

$$m_0 \lambda_{1,h} \|q\|_2^2 \le q^\mathsf{T} K q \le \frac{4m_1}{\Delta x^2} \|q\|_2^2, \tag{28}$$

where $\lambda_{1,h} = 4\Delta x^{-2} \sin^2(\pi/N)$. *Consequently,*

$$\kappa_+(K) \le \frac{m_1}{m_0 \sin^2(\pi/N)} \tag{29}$$

for the spectral condition number restricted to constants' orthogonal complement.

Proof. From (25), $q^\mathsf{T} K q = \|W^{1/2} G q\|_2^2 \ge 0$. Positive edge weights imply $Gq = 0$ exactly when q is constant. The lower estimate follows from the first nonzero eigenvalue of the periodic difference Laplacian $G^\mathsf{T} G$; the upper estimate follows from $\lambda_{\max}(G^\mathsf{T} G) = 4/\Delta x^2$. Dividing the two bounds gives (29). □

5. THEORETICAL ANALYSIS

5.1 Conservation and exact dissipation

Theorem 3 (Mass and free energy)**.** *Assume that a positive solution of* (20) *exists and that* (18) *is positive. Then*

$$M_h^{n+1} = M_h^n, \tag{30}$$

and

$$\mathscr{E}_h^{n+1} - \mathscr{E}_h^n = -\Delta t\, \mathscr{D}_h^{n+1/2}, \tag{31}$$

where

$$\mathscr{D}_h^{n+1/2} = \sum_i \mathscr{M}_{i+1/2}^{n+1/2} \frac{(\mu_{i+1}^{n+1/2} - \mu_i^{n+1/2})^2}{\Delta x} \ge 0. \tag{32}$$

Proof. Summing (20) over i and using periodicity cancels all fluxes, proving (30). Multiply (20) by $\Delta x\, \mu_i^{n+1/2}$ and sum. By (14),

$$\begin{aligned}\Delta x \sum_i \mu_i^{n+1/2}(u_i^{n+1} - u_i^n) &= \Delta x \sum_i \{h(u_i^{n+1}) - h(u_i^n) \\ &\qquad + V_i(u_i^{n+1} - u_i^n)\} \\ &= \mathscr{E}_h^{n+1} - \mathscr{E}_h^n.\end{aligned}$$

Periodic summation by parts gives

$$\sum_i \mu_i (J_{i+1/2} - J_{i-1/2}) = -\sum_i (\mu_{i+1} - \mu_i) J_{i+1/2}.$$

Substitution of (19) yields (31). □

Corollary 4. *For* $\Delta t > 0$, $\mathscr{E}_h^{n+1} \le \mathscr{E}_h^n$ *with no time-step restriction in the algebraic energy estimate.*

The qualification "in the algebraic energy estimate" is important: existence and convergence of the nonlinear solver are separate questions. The theorem does not convert a failed nonlinear solve into a valid time step.

5.2 Positive states and equilibria

Proposition 5 (Positive-state parametrization)**.** *If* $z^{n+1} \in \mathbb{R}^N$ *is a finite solution of the transformed system obtained from* (20) *and* (21), *then* $u_i^{n+1} > 0$ *for every cell i. For the logarithmic entropy* (9), *all terms in* (5) *are consequently well defined.*

Proof. The exponential map has range $(0,\infty)$. The second statement follows from (16). □

Proposition 6 (Equilibrium consistency)**.** *Let* $u_i^* > 0$ *satisfy*

$$h'(u_i^*) + V_i = C \tag{33}$$

for some constant C. Then $u^n = u^*$ *implies* $u^{n+1} = u^*$ *is a solution of* (20) *for every* Δt.

Proof. At $u^{n+1} = u^n = u^*$, (5) reduces to $h'(u_i^*)$. Hence $\mu_i = C$, every edge flux vanishes, and (20) is satisfied. □

Proposition 7 (Unique fixed-mass equilibrium)**.** *Assume* $h'' > 0$ *and fix a discrete mass* $M_0 > 0$. *If the range of* h' *contains every value* $C - V_i$ *needed below, there is at most one positive vector* u^* *satisfying*

$$h'(u_i^*) + V_i = C, \qquad \Delta x \sum_i u_i^* = M_0. \tag{34}$$

For the entropy (9), *this equilibrium exists explicitly:*

$$u_i^* = \frac{M_0 e^{-V_i}}{\Delta x \sum_j e^{-V_j}}. \tag{35}$$

Proof. Strict convexity makes h' strictly increasing, hence $(h')^{-1}$ is strictly increasing on its range. Thus

$$F(C) = \Delta x \sum_i (h')^{-1}(C - V_i)$$

is strictly increasing wherever defined. The mass equation $F(C) = M_0$ therefore has at most one solution. For $h'(u) = \log u$, substitution gives (35). □

Theorem 8 (Local solvability of the positive branch)**.** *Let* $u^n \in (0,\infty)^N$ *and suppose* h, m, *and the mobility mean are continuously differentiable on a neighborhood of* u^n. *Then there exists* $\tau_0 > 0$ *such that, for* $|\Delta t| < \tau_0$, *the transformed nonlinear system has a locally unique finite solution* z^{n+1} *near* $\log u^n$. *Hence the corresponding branch satisfies* $u^{n+1} > 0$.

Proof. Multiply (20) by Δt and define

$$\mathscr{F}(z,\tau) = e^z - u^n + \tau \mathscr{L}(e^z, u^n),$$

where $\mathscr{L}$ denotes the periodic finite-volume flux divergence constructed from (17)–(19). At $\tau = 0$, $\mathscr{F}(\log u^n, 0) = 0$, while

$$D_z \mathscr{F}(\log u^n, 0) = \operatorname{diag}(u_0^n, \ldots, u_{N-1}^n)$$

is nonsingular. The finite-dimensional implicit-function theorem supplies a unique smooth local branch $z(\tau)$ for sufficiently small $|\tau|$. Exponentiation gives positivity. □

Proposition 9 (Coercive dissipation and strict decay)**.** *Assume $\mathscr{M}_{i+1/2}^{n+1/2} \geq m_0 > 0$. Let*

$$\bar{\mu} = \frac{1}{N}\sum_i \mu_i^{n+1/2}, \qquad \lambda_{1,h} = \frac{4}{\Delta x^2}\sin^2\left(\frac{\pi}{N}\right).$$

Then

$$\mathscr{D}_h^{n+1/2} \geq m_0 \lambda_{1,h} \Delta x \sum_i (\mu_i^{n+1/2} - \bar{\mu})^2. \tag{36}$$

Consequently, the energy decrement in (31) vanishes if and only if the discrete chemical potential is constant.

Proof. The periodic discrete Poincaré inequality for the centered graph Laplacian gives

$$\sum_i \frac{(\mu_{i+1}-\mu_i)^2}{\Delta x} \geq \lambda_{1,h}\Delta x \sum_i (\mu_i - \bar{\mu})^2.$$

Multiplication by the mobility lower bound proves (36). Since every edge weight is positive on the connected periodic grid, $\mathscr{D}_h = 0$ is equivalent to $\mu_{i+1} = \mu_i$ for all i. □

Proposition 10 (Relative-energy identity for the logarithmic entropy)**.** *Let (9) hold, and let u and u^* have the same discrete mass, with u^* given by (35). Then*

$$\mathscr{E}_h(u) - \mathscr{E}_h(u^*) = \Delta x \sum_i \left[u_i \log\frac{u_i}{u_i^*} - u_i + u_i^*\right] \geq 0. \tag{37}$$

Proof. The equilibrium relation is $\log u_i^* + V_i = C$. Subtract the two discrete energies and write

$$\begin{aligned}\mathscr{E}_h(u) - \mathscr{E}_h(u^*) = \Delta x \sum_i \left[u_i \log\frac{u_i}{u_i^*} - u_i + u_i^*\right] \\ + C\Delta x \sum_i (u_i - u_i^*).\end{aligned}$$

The last term vanishes by equal mass. Nonnegativity follows from $r\log r - r + 1 \geq 0$. □

5.3 Time symmetry

Let $\mathscr{R}(u^+, u^-; \tau)$ denote the vector residual in (20) with $u^{n+1} = u^+$, $u^n = u^-$, and $\Delta t = \tau$.

Theorem 11 (Self-adjoint update)**.** *If the mobility mean satisfies (12), then*

$$\mathscr{R}(u^-, u^+; -\tau) = \mathscr{R}(u^+, u^-; \tau). \tag{38}$$

Consequently, an exactly solved forward step followed by an exactly solved step of size $-\tau$ returns the initial state whenever the relevant algebraic branch is unique.

Proof. The quotient $(u^+ - u^-)/\tau$ is invariant under simultaneous interchange of the two states and sign reversal of τ. The arithmetic state $\bar{u}$, the divided difference $\mathscr{D}_h$, and the symmetric edge mobility are unchanged by interchange of u^+ and u^-. Hence the flux is unchanged and (38) follows. □

5.4 Second-order consistency

Theorem 12 (Local consistency)**.** *Assume u is a strictly positive C^4 solution of (1), $h \in C^4$, $m \in C^3$, $V \in C^3$, and the symmetric mean A is C^2 in a neighborhood of the relevant diagonal states. Inserting exact cell-center values at t_n and t_{n+1} into (20) gives a residual*

$$\mathscr{T}_i^{n+1/2} = O(\Delta t^2 + \Delta x^2) \tag{39}$$

uniformly on compact time intervals on which u stays bounded away from zero.

Proof. At $t_{n+1/2} = t_n + \Delta t/2$,

$$\begin{aligned}\frac{u(t_{n+1}) - u(t_n)}{\Delta t} &= u_t(t_{n+1/2}) + O(\Delta t^2),\\ \bar{u}^{n+1/2} &= u(t_{n+1/2}) + O(\Delta t^2).\end{aligned}$$

Lemma 1 and $u(t_{n+1}) - u(t_n) = O(\Delta t)$ yield

$$\mathscr{D}_h(u(t_{n+1}), u(t_n)) = h'(u(t_{n+1/2})) + O(\Delta t^2).$$

Smoothness of m and A, together with symmetry and $\mathsf{A}(a,a) = a$, gives the same temporal order and a second-order edge approximation of the mobility. Centered differences of the midpoint chemical potential and the conservative flux divergence are second-order in space. Substitution into (1) proves (39). □

The distinction between (5) and a midpoint chemical potential is now explicit. Both are second-order consistent, but only (5) enforces (14). For nonquadratic h, equation (4) predicts a nonzero one-step energy defect even when the nonlinear residual is driven to machine accuracy.

Table 1. Coupled space–time refinement for (40).

N	Δt	L^2 err.	Order	L^∞ err.
20	1.00×10^{-2}	1.8932×10^{-4}	–	2.6887×10^{-4}
40	5.00×10^{-3}	4.7401×10^{-5}	1.998	6.8030×10^{-5}
80	2.50×10^{-3}	1.1855×10^{-5}	1.999	1.7059×10^{-5}

6. NUMERICAL EXPERIMENTS

The tests use the manufactured and confining PDE benchmarks specified below. The nonlinear system is solved in the logarithmic variable z by a trust-region least-squares iteration. The accompanying code records the input grids, step histories, solver residuals, and tabulated outputs.

6.1 Manufactured heat-flow test

Set $V = 0$ and use (9). Then (10) reduces to $u_t = u_{xx}$. On $\mathbb{T}$ choose

$$\begin{aligned}u(x,0) &= 1 + 0.2\cos(2\pi x),\\ u(x,t) &= 1 + 0.2e^{-4\pi^2 t}\cos(2\pi x).\end{aligned} \tag{40}$$

The final time is $T = 0.05$ and $\Delta t = 0.2\Delta x$. Errors are computed at cell centers.

6.2 Confining Fokker–Planck test

For a genuinely nonconstant chemical potential, set

$$\begin{aligned}V(x) &= 1.5\cos(2\pi x),\\ u(x,0) &= 1 + 0.45\cos(4\pi x - 0.3).\end{aligned} \tag{41}$$

Table 2. Structural audit for the confining problem (41).

Δt	$\min u$	Mass defect	$\max \Delta\mathscr{E}_h^+$	Identity defect
10^{-2}	0.13946	4.44×10^{-16}	0	3.82×10^{-16}
5×10^{-3}	0.13976	1.11×10^{-15}	0	7.63×10^{-16}
2.5×10^{-3}	0.13984	3.20×10^{-14}	0	1.42×10^{-14}

Table 3. Approach to the discrete equilibrium at $T = 0.1$.

Δt	$\mathscr{E}_h(T)$	$\mathscr{H}_h(T)$	$\|u-u_\infty\|_{1,h}$
10^{-2}	-1.4987718	1.5561×10^{-5}	3.6635×10^{-3}
5×10^{-3}	-1.4987686	1.8725×10^{-5}	4.0160×10^{-3}
2.5×10^{-3}	-1.4987678	1.9580×10^{-5}	4.1070×10^{-3}

Table 4. One-step energy accounting at $\Delta t = 0.02$. The balance defect is $(\mathscr{E}_h^{n+1} - \mathscr{E}_h^n) + \Delta t\, \mathscr{D}_h$.

Potential	$\Delta\mathscr{E}_h$	$\mathscr{D}_h$	Balance defect
Discrete gradient	-0.4577775	22.88887	-5.55×10^{-17}
Midpoint	-0.4600863	23.80570	1.6028×10^{-2}

Table 5. Forward–backward reversal error on $N = 80$.

Δt	L^2 reversal	L^∞ reversal
10^{-2}	8.81×10^{-15}	4.88×10^{-14}
5×10^{-3}	5.63×10^{-14}	2.16×10^{-13}
2.5×10^{-3}	2.62×10^{-14}	1.11×10^{-13}

normalized to unit discrete mass. With (9), the equilibrium is proportional to e^{-V}. Computations use $N = 40$, $T = 0.1$, and three time steps. The relative entropy reported below is

$$\mathscr{H}_h(u \mid u_\infty) = \Delta x \sum_i \left[u_i \log \frac{u_i}{u_{\infty,i}} - u_i + u_{\infty,i} \right]. \tag{42}$$

The initial free energy is -0.9479978. The final values are -1.4987718, -1.4987686, and -1.4987678 for decreasing Δt. The relative entropy falls from 0.5507896 to 1.56×10^{-5}, 1.87×10^{-5}, and 1.96×10^{-5}, respectively. The small non-monotonic variation across time steps reflects a fixed spatial grid and comparison at finite T; it is not used as an order estimate.

Equation (37) shows that $\mathscr{H}_h$ is not an auxiliary diagnostic: on the fixed-mass manifold it is exactly the discrete free-energy gap to equilibrium.

6.3 Isolating the temporal chain rule

To distinguish exact energy accounting from generic dissipation, one step of size $\Delta t = 0.02$ is taken on $N = 80$ for (41). The proposed $\mathscr{D}_h$ is compared with

$$\mu_i^{n+1/2} = \log\left(\frac{u_i^{n+1} + u_i^n}{2}\right) + V_i, \tag{43}$$

while every other component of the solver is unchanged.

Both steps decrease the energy in this example; Table 4 is therefore not a claim that midpoint evaluation is unstable. Its purpose is narrower. The divided difference turns the free-energy calculation into an identity, whereas the midpoint approximation retains the cubic chain-rule remainder in (4).

6.4 Time-symmetry check

Theorem 11 is tested with $V(x) = 0.7\cos(2\pi x)$ and $u(x,0) = 1 + 0.25\sin(2\pi x) + 0.1\cos(4\pi x)$, again normalized to unit mass. A forward step is followed by a step of the negative time increment.

7. RESULTS AND DISCUSSION

The numerical evidence separates consistency, structural stability, and nonlinear solvability. First, Table 1 supports the formal estimate (39): halving both mesh width and time step reduces the L^2 error by factors 3.994 and 3.999. The corresponding L^∞ orders are 1.983 and 1.996. Across these runs the maximum mass defect is 2.95×10^{-14}, the density remains positive, and no positive energy increment is observed.

Second, the nonlinear potential test confirms the algebraic statements of Theorem 3. At the smallest step, the largest mass discrepancy is 3.20×10^{-14} and the largest absolute defect in (31) is 1.42×10^{-14}. These scales are several orders below the physical energy change. Positivity is not marginal: the smallest value over the reported trajectories remains approximately 0.14. The decrease of (42) by more than four orders of magnitude is consistent with approach toward the discrete analogue of (11).

Third, Table 4 explains why the discrete gradient is more than a stylistic replacement of a midpoint. With the same grid, time step, potential, mobility, and nonlinear solve, the midpoint chemical potential leaves a balance error of 1.60×10^{-2}, while (5) reduces the same quantity to roundoff. Equation (4) predicts precisely this qualitative distinction. Exact dissipation is therefore obtained from a local chain-rule design rather than from tuning a global stabilization parameter.

Proposition 9 sharpens the interpretation of the confining test. As long as the numerical trajectory remains in a compact positive interval, the arithmetic mobility has a positive lower bound. The exact decrement therefore controls the discrete variance of the chemical potential through (36). Together with Proposition 7, this excludes a non-equilibrium stationary state on the connected periodic mesh. For the logarithmic model the same gap is measured exactly by (37), which is why the last column of Table 3 can be read as an equilibrium diagnostic rather than merely a statistical distance.

The matrix form (26) adds an operator-level interpretation. Proposition 2 shows that the discrete transport operator has exactly the constant mode in its nullspace and is coercive on the fixed-mass subspace. The bound (29) also quantifies the expected mesh dependence of unpreconditioned algebraic solves: for fixed mobility contrast, the nonzero spectral condition number grows like $O(N^2)$. This estimate is independent of the particular entropy and therefore isolates a spatial linear-algebra issue from the nonlinear thermodynamic map.

The local existence result in Theorem 8 also clarifies the role of the nonlinear solve. The logarithmic transformation guarantees that the local branch issuing from a positive state remains inside the positive cone for sufficiently small time increments. It does not assert that arbitrary large steps possess a unique solution. This separation between structural algebra and nonlinear global solvability is useful in practice: failure of a nonlinear iteration should be handled by step control, not by modifying the density after the solve.

The forward–backward experiment is likewise structural rather than physical. Diffusion should not normally be integrated backward as an evolution problem. Here the negative step is used only to test the algebraic adjoint relation (38). Reversal errors between 10^{-14} and 10^{-13} are consistent with the theorem and nonlinear-solver tolerance. This symmetry is also the reason a second-order temporal expansion arises naturally despite the exact energy decay for positive time steps.

There are limitations. The analysis is one-dimensional and periodic; boundary terms must be redesigned for no-flux, Robin, or reservoir conditions. The positivity statement is conditional on a finite root of the logarithmic nonlinear system and does not constitute a global existence theorem for arbitrary Δt. Degenerate mobilities that vanish at $u = 0$ require additional care because the logarithmic parametrization never represents the boundary of the positive cone. Multicomponent systems introduce noncommuting mobility matrices and generally require a vector discrete chain rule, a setting in which entropy-based finite-volume analysis is substantially more delicate [18]. Finally, the scheme is fully implicit. Its structural simplicity comes at the cost of a nonlinear solve at every step, so preconditioning and scalable multidimensional solvers are natural subjects for further work.

These restrictions do not affect the underlying design principle. If a dissipative PDE contains a separable entropy contribution, replacing the time-centered variational derivative by its exact two-state discrete gradient can remove the temporal chain-rule remainder without sacrificing centered accuracy. The spatial method then needs only a compatible discrete integration-by-parts identity and positive mobility. This division of labor is useful when constructing schemes in which the origin of each preserved property should remain visible.

8. CONCLUSION

A symmetric finite-volume discretization has been developed for positive drift–diffusion gradient flows. The method uses the divided difference of the entropy in time, a centered positive mobility in space, and a logarithmic state variable. The resulting update conserves total mass and satisfies the exact equality

$$\mathscr{E}_h^{n+1} - \mathscr{E}_h^n = -\Delta t\, \mathscr{D}_h^{n+1/2},$$

with $\mathscr{D}_h^{n+1/2} \geq 0$. It is equilibrium consistent, self-adjoint under time reversal, and second-order consistent in time and space for smooth positive solutions.

The numerical tests were designed to verify these statements separately rather than to maximize benchmark performance. Coupled refinement produced second-order errors for an exact heat solution. A nonlinear Fokker–Planck test retained positive states, conserved mass to near machine precision, and reproduced the discrete energy law to roundoff. The midpoint comparison showed that second-order centering alone does not provide the exact energy identity: the discrete gradient is the component that closes the chain rule. These results motivate extensions to multidimensional meshes, nonperiodic boundaries, and matrix-valued mobilities, where the same algebraic principle can be combined with more elaborate spatial discretizations.

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