Research Article

A Fast and Efficient Numerical Algorithm for the Nonlocal Conservative Swift–Hohenberg Equation

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In this paper, we consider a new Swift–Hohenberg equation, where the total mass of this model is conserved through a nonlocal Lagrange multiplier. Based on the operator splitting method and spectral method, a fast and efficient numerical algorithm is proposed. Three numerical examples in both two and three dimensions are provided to illustrate that the proposed algorithm is a practical, accurate, and efficient simulation tool for the nonlocal Swift–Hohenberg equation.

1. Introduction

The Swift–Hohenberg model [1] was first introduced by Swift and Hohenberg in studies of Rayleigh–Bénard convection and has become one of the paradigms of the nonlinear dynamical system leading to complex pattern formation. Recent applications of the Swift–Hohenberg equation have been extensively spanned in complex fluids and biological tissues [2, 3]. The Swift–Hohenberg model is derived by using the L^2 -gradient flow of the Lyapunov energy functional [4]

$$E(\phi) = \int_{\Omega} \left(\frac{\phi}{2} (\Delta + 1)^2 \phi + F(\phi) \right) dx, \quad (1)$$

where Ω is a bounded regular domain $[a, b]^n$ ($n = 1, 2, 3$) and ϕ is the density field. $F(u) = (1/4)\phi^4 - (\eta/3)\phi^3 - (\epsilon/2)\phi^2$ is the nonlinear smoothing potential, and $\eta \geq 0$ and $\epsilon > 0$ are constants with physical significance.

By taking the variational derivative of (1) in L^2 norm, the following Swift–Hohenberg equation is obtained:

$$\phi_t = -\frac{\delta E(\phi)}{\delta \phi} = -((\Delta + 1)^2 \phi + f(\phi)), \quad (\mathbf{x}, t) \in \Omega \times (0, T], \quad (2)$$

where $\delta E(\phi)/\delta \phi$ denotes the variational derivative and $f(u) = F'(u) = \phi^3 - \eta\phi^2 - \epsilon\phi$. Thus, the total energy $E(\phi)$ is not increasing with time

$$\frac{d}{dt} E(\phi) = \int_{\Omega} \frac{\delta E(\phi)}{\delta \phi} \frac{\partial \phi}{\partial t} dx = - \int_{\Omega} \left(\frac{\partial \phi}{\partial t} \right)^2 dx \leq 0. \quad (3)$$

The Swift–Hohenberg equation (2) is a fourth-order nonlinear partial differential equation, and we cannot generally obtain the analytic solution for the arbitrary initial conditions. Therefore, computer simulations play an essential role in understanding the dynamical behavior. Till now, a large number of works have been proposed to study the Swift–Hohenberg equation [5–12].

Since the Swift–Hohenberg model (2) is derived by using the L^2 -gradient flow, the total mass of the unknown variable is not conserved with time. However, in Elder's phase field crystal model, the phase field variable is interpreted as the density of atoms from the perspective of physical significance; thus, the total mass of the phase field variable is expected to be conserved, such as the Cahn–Hilliard equation [13, 14]. Zhang and Yang [15] very recently proposed a conservative Swift–Hohenberg equation with a nonlocal Lagrange multiplier to cancel out the variation in mass without influencing the original energy

law. The conservative Swift–Hohenberg equation is as follows:

$$\phi_t + (\Delta + 1)^2 \phi + f(\phi) - \frac{1}{|\Omega|} \int_{\Omega} (\phi + f(\phi)) d\mathbf{x} = 0, \quad (4)$$

$$(\mathbf{x}, t) \in \Omega \times (0, T],$$

subject to the initial condition

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \quad \mathbf{x} \in \overline{\Omega}, \quad (5)$$

The periodic boundary condition is adopted here since it is usually used to remove all boundary integrals (cf. [15]). Note that when $(1/|\Omega|) \int_{\Omega} (\phi + f(\phi)) d\mathbf{x} = 0$, equation (4) degenerates back to the standard Swift–Hohenberg model (2).

The nonlocal term $(1/|\Omega|) \int_{\Omega} (\phi + f(\phi)) d\mathbf{x}$ can be understood as a nonlocal Lagrange multiplier for the mass constraint

$$\frac{d}{dt} M(\phi) = \frac{d}{dt} \int_{\Omega} \phi(\mathbf{x}, t) d\mathbf{x} = 0. \quad (6)$$

Furthermore, system (4) still satisfies energy dissipative law (3). Taking the L^2 inner product of (4) with ϕ_t , integrating by parts and using (6), we have

$$\begin{aligned} \frac{d}{dt} E(\phi) &= \int_{\Omega} (\phi(\Delta + 1)^2 + f(\phi)) \phi_t d\mathbf{x} \\ &= \int_{\Omega} \phi_t ((\Delta + 1)^2 \phi + f(\phi)) d\mathbf{x} - \frac{1}{|\Omega|} \int_{\Omega} (\phi \\ &\quad + f(\phi)) d\mathbf{x} \int_{\Omega} \phi_t d\mathbf{x} \\ &= - \int_{\Omega} (\phi_t)^2 d\mathbf{x} \leq 0, \end{aligned} \quad (7)$$

where $E(\phi)$ is defined by (1).

Compared to a large number of studies for the standard Swift–Hohenberg equation (2), there are few numerical results on the conservative Swift–Hohenberg equation (4) because the extra nonlocal term brings up substantial numerical challenges to developing fast and efficient algorithms. Zhang and Yang [15] proposed a second-order, unconditionally energy stable scheme by combining the invariant energy quadratization (IEQ) approach with the stabilization technique. The law of conservation of mass of the proposed scheme was not verified in this article [15].

In this work, we aim to develop a fast explicit algorithm based on the operator splitting method [14, 16, 17]. The main idea of the method is to solve problem (4) through three parts: the linear homogeneous heat equation was first solved via the Fourier spectral method and then the nonlinear part and the nonlocal equation were solved explicitly.

The rest of this paper is organized as follows. In Section 2, a fast explicit operator splitting method is proposed for solving (4). In Section 3, we test the accuracy and applicability of the obtained numerical method in three examples including a 3D example. Finally, we summarize the present work and discuss the future work in Section 4.

2. Time-Splitting Spectral Method

In this section, we present a time-splitting spectral method to simulate the asymptotic behavior of the solution of equation (4). The proposed method is based on the operator splitting method for the time and spectral method for the space. For simplicity, we only consider two-dimensional (2D) space. The 1D/3D case is defined analogously.

The operator splitting method for the conservative Swift–Hohenberg equation is constructed as follows. We rewrite equation (4) in the following abstract initial value problem:

$$u_t = \mathcal{A}u + \mathcal{B}u + \mathcal{C}u, \quad (8)$$

where the operators $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ are defined as

$$\begin{aligned} \mathcal{A}\phi &= -(\Delta + 1)^2 \phi, \\ \mathcal{B}u &= -f(\phi), \end{aligned} \quad (9)$$

$$\mathcal{C}u = \frac{1}{\Omega} \int_{\Omega} (\phi + f(\phi)) d\mathbf{x}.$$

Thus, we can evolve the solution from t to $t + \tau$ using the following first-order Lie–Trotter method [16]:

$$\phi(x, y, t + \tau) = \mathcal{S}_A^\tau \circ \mathcal{S}_B^\tau \circ \mathcal{S}_C^\tau \phi(x, y, t). \quad (10)$$

where $\mathcal{S}_A^\tau$, $\mathcal{S}_B^\tau$, and $\mathcal{S}_C^\tau$ are the exact solution operators associated with the nonlinear equation

$$\phi_t = -(\Delta + 1)^2 \phi, \quad (11)$$

the heat equation

$$\phi_t = -f(\phi), \quad (12)$$

and the Lagrange multiplier equation

$$\phi_t = \frac{1}{|\Omega|} \int_{\Omega} (\phi + f(\phi)) d\mathbf{x}, \quad (13)$$

respectively. Higher order splitting schemes can be found in [18, 19].

Before proceeding to present a fast explicit operator splitting method for (4), the exact solution operators $\mathcal{S}_A^\tau$, $\mathcal{S}_B^\tau$, and $\mathcal{S}_C^\tau$ are first replaced by their numerical approximations $\mathcal{S}_A^{\tau,h}$, $\mathcal{S}_B^{\tau,h}$, and $\mathcal{S}_C^{\tau,h}$, respectively.

Step 1 ($\mathcal{S}_A^\tau \longrightarrow \mathcal{S}_A^{\tau,h}$). We first consider the fully discrete scheme for (11). The following spatial grid is introduced:

$$\Omega_h^{\text{per}} = \{(x_i, y_j) = (a + ih, a + jh), \quad 0 \leq i, j \leq N - 1\}, \quad (14)$$

for the periodic condition, where $h = (b - a)/N$. Let $u_{j,k}^k = u(x_i, y_j, k\tau)$, where $\tau = T/K$ is the time step and M is the total number of time steps.

Based on the theory of spectral method [20], the solution to equation (11) derived with periodic boundary conditions can be represented by the following band-limited Fourier series:

$$\begin{aligned}\mathcal{F}_N^{-1}[\tilde{\phi}(t)](x, y) &:= (P_N \phi)(x, y, t) \\ &= \sum_{p=-N/2}^{N/2} \sum_{q=-N/2}^{N/2} \tilde{\phi}_{p,q}(t) \varphi_{p,q}(x, y),\end{aligned}\quad (15)$$

where

$$\varphi_{p,q} = \exp\left(i \frac{2p\pi(x-a)}{b-a} + i \frac{2q\pi(y-a)}{b-a}\right), \quad (16)$$

and by using the following Fourier expansion, the fast Fourier transform (FFT) may be used to calculate the Fourier coefficients $\{\tilde{\phi}_{p,q}(t)\}$ from the discrete function values $\{\phi_{i,j}(t)\}$:

$$\begin{aligned}\mathcal{F}_N[\phi(t)](p, q) &:= \tilde{\phi}_{p,q}(t) = \frac{h^2}{C_p^{\text{per}} C_q^{\text{per}} (b-a)^2} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \phi_{i,j} \\ &\cdot (t) \varphi_{p,q}(x_i, y_j),\end{aligned}\quad (17)$$

and C_p^{per} and C_q^{per} are, respectively, defined as

$$C_r^{\text{per}} = \begin{cases} 2, & |r| = \frac{N}{2}, \\ 1, & |r| < \frac{N}{2}. \end{cases} \quad (18)$$

Substituting (15) into (11), we obtain the following system of ordinary differential equations for the discrete (pq) -th Fourier coefficients:

$$\frac{d\tilde{\phi}_{p,q}(t)}{dt} = -(\lambda_{p,q} + 1)^2 \tilde{\phi}_{p,q}(t), \quad (19)$$

where

$$\lambda_{p,q} = -\left(\left(\frac{2p\pi}{b-a}\right)^2 + \left(\frac{2q\pi}{b-a}\right)^2\right), \quad p, q = 0, \pm 1, \pm 2, \dots, \pm \frac{N}{2}. \quad (20)$$

The above equation is solved analytically by the variable separation method with an initial condition $\tilde{\phi}_{p,q}^k$, and then the solution $\tilde{\phi}_{p,q}^{k+1}$ is obtained as follows:

$$\tilde{\phi}_{p,q}^{k+1} = \exp\left(-\tau(\lambda_{p,q} + 1)^2\right) \tilde{\phi}_{p,q}^k. \quad (21)$$

Hence, we have

$$\phi^{k+1} = \mathcal{F}_N^{-1}\left\{\exp\left(-\tau(\lambda_{p,q} + 1)^2\right) \mathcal{F}_N[\phi^k](p, q)\right\}. \quad (22)$$

The errors between $P_N \phi$ and ϕ can be measured in Sobolev spaces. For this purpose, we denote by $H_p^s(\Omega)$ the subspace of $H^s(\Omega)$, which consists of functions with derivatives of order up to $s-1$ being periodic on Ω . The main approximation result is stated below.

Theorem 1 (see [20]). For any $\phi \in H_p^s(\Omega)$ and $s \geq 0$, it holds that

$$\|P_N \phi - \phi\| \leq CN^{-s} |\phi|_s, \quad (23)$$

This theorem indicates that the projection $P_N \phi$ is the best approximation of ϕ in all Sobolev spaces $H_p^s(\Omega)$. For further references about the spectral method, we refer to [20].

Step 2 ($\mathcal{S}_B^\tau \longrightarrow \mathcal{S}_B^{\tau,h}$). Now we propose a first-order difference scheme for solving equation (12) in $[t_k, t_{k+1}]$. Note that if $|\phi| \neq 0$, equation (12) can be rewritten as

$$\frac{\phi_t}{\phi} = -(\phi^2 - \eta\phi - \epsilon). \quad (24)$$

Taking the integral from t_k to t_{k+1} on both sides of the above equation with respect to t , we have

$$\ln \phi^{k+1} - \ln \phi^k = - \int_{t_k}^{t_{k+1}} (\phi^2 - \eta\phi - \epsilon) dt. \quad (25)$$

Note that $\int_{t_k}^{t_{k+1}} (\phi^2 - \eta\phi - \epsilon) dt = \tau((\phi^k)^2 - \eta\phi^k - \epsilon) + O(\tau^2)$, and then we obtain a first-order explicit finite difference scheme for (12)

$$\phi^{k+1} = \phi^k \exp\left(-\tau((\phi^k)^2 - \eta\phi^k - \epsilon)\right). \quad (26)$$

It is clear that if $|\phi| = 0$, the above formula is also derived.

Step 3 ($\mathcal{S}_C^\tau \longrightarrow \mathcal{S}_C^{\tau,h}$). Equation (12) involves solving a nonlocal Lagrange multiplier equation. For convenience, we denote $\beta(\phi) = \int_{\Omega} (\phi + f(\phi)) dx$. Then, we employ the backward difference method for equation (13) in $[t_k, t_{k+1}]$ with an initial condition ϕ^k ; this gives

$$\frac{\phi^{k+1} - \phi^k}{\tau} = \frac{1}{|\Omega|} \beta(\phi^{k+1}). \quad (27)$$

Summing both sides of equation (27) over i and j , and by the property of mass conservation $h^2 \sum_{i,j=0}^{N-1} \phi_{ij}^0 = h^2 \sum_{i,j=0}^{N-1} \phi_{ij}^{k+1}$, we obtain

$$\beta(\phi^{k+1}) = \frac{h^2}{\tau} \left(\sum_{i,j=0}^{N-1} \phi_{ij}^0 - \sum_{i,j=0}^{N-1} \phi_{ij}^k \right). \quad (28)$$

A similar idea has also been mentioned in [21].

Combining (27) and (28), a first-order explicit finite difference scheme for (13) is obtained:

$$\phi^{k+1} = \phi^k + \frac{h^2}{|\Omega|} \left(\sum_{i,j=0}^{N-1} \phi_{ij}^0 - \sum_{i,j=0}^{N-1} \phi_{ij}^k \right). \quad (29)$$

Then, based on equations (10), (22), (26), and (29), we obtain the following fast explicit operator splitting schemes:

TABLE 1: Convergence rate with $h = 1/2$ and different M for Problem 1 at $T = 1$.

$M =$		10	20	40	80	160
$\epsilon = 0.05$	Err_{L^∞}	$8.14e-5$	$1.78e-5$	$4.18e-6$	$1.01e-6$	$2.49e-7$
	Rate_{L^∞}	—	2.19	2.09	2.05	2.02
$\eta = 0.05$	Err_{L^2}	$1.30e-3$	$2.95e-4$	$7.04e-5$	$1.72e-5$	$4.25e-6$
	Rate_{L^2}	—	2.14	2.07	2.03	2.02
$\epsilon = 0.25$	Err_{L^∞}	$4.61e-3$	$1.10e-3$	$2.66e-4$	$6.52e-5$	$1.62e-5$
	Rate_{L^∞}	—	2.07	2.05	2.03	2.01
$\eta = 2$	Err_{L^2}	$3.69e-2$	$9.16e-3$	$2.27e-3$	$5.63e-4$	$1.40e-4$
	Rate_{L^2}	—	2.01	2.01	2.01	2.01
$\epsilon = 0.5$	Err_{L^∞}	$1.25e-4$	$3.30e-5$	$8.43e-6$	$2.13e-6$	$5.34e-7$
	Rate_{L^∞}	—	1.92	1.97	1.99	1.99
$\eta = 0.5$	Err_{L^2}	$1.78e-3$	$4.23e-4$	$1.03e-4$	$2.54e-5$	$6.32e-6$
	Rate_{L^2}	—	2.08	2.04	2.02	2.01

$$\left\{ \begin{array}{l} \phi^{k+1,(1)} = \mathcal{F}_N \left\{ \exp \left(-\tau (\lambda_{p,q} + 1)^2 \right) \mathcal{F}_N^{-1} [\phi^k] (p, q) \right\}, \\ \phi^{k+1,(2)} = \phi^{k+1,(1)} \exp \left(-\tau \left((\phi^k)^2 - \eta \phi^k - \epsilon \right) \right), \\ \phi^{k+1} = \phi^{k+1,(2)} + \frac{h^2}{|\Omega|} \left(\sum_{i,j=0}^{N-1} \phi_{ij}^0 - \sum_{i,j=0}^{N-1} \phi_{ij}^{k,(2)} \right). \end{array} \right. \quad (30)$$

The derivation of algorithm (30) shows that the temporal truncation error has the form $(C_1 \tau + C_2 \tau^2)$. Based on this observation, we can use the following Richardson's extrapolation technique:

$$\phi_w^K = 2\phi^{2K} - \phi^K, \quad (31)$$

to eliminate the leading term $O(\tau)$, where ϕ^K and ϕ^{2K} are the numerical solutions at the final time level calculated using time step sizes $\tau = T/K$ and $\tau = T/2K$, respectively. Thus, we obtain a high-order numerical solution ϕ_w^K with second-order temporal accuracy.

In addition, we define the discrete inner product

$$(f, g) := h^2 \sum_{i,j=0}^{N-1} f_{i,j} g_{i,j} \quad (32)$$

and discrete $\|\cdot\|_\infty$ norm and $\|\cdot\|_2$ norm

$$\begin{aligned} \|f\|_\infty &= \max_{0 \leq i,j \leq N-1} |f_{i,j}|, \\ \|f\|_2 &= \sqrt{(f, f)}. \end{aligned} \quad (33)$$

Theorem 2. Scheme (30) satisfies the discrete mass conservation law

$$M^k = M^0, \quad k = 1, 2, \dots, K, \quad (34)$$

where $M^k = h^2 \phi_{i,j}^k$.

Proof. Taking discrete inner product of the third equation of (30) with 1, summing over i and j , we have

$$\begin{aligned} (\phi^{k+1}, 1) &= (\phi^{k+1,(2)}, 1) + \left(\frac{h^2}{|\Omega|} \left(\sum_{i,j=0}^{N-1} \phi_{ij}^0 - \sum_{i,j=0}^{N-1} \phi_{ij}^{k,(2)} \right), 1 \right) \\ &= (\phi^0, 1). \end{aligned} \quad (35)$$

This completes the proof. $\square$

3. Numerical Experiments

In this section, three numerical experiments are carried out to study the accuracy and efficiency of the proposed method. The L^∞ -norm error (denoted as Err_{L^∞}) and the L^2 -norm error (denoted as Err_{L^2}) of the numerical solutions are computed, respectively, by the following formulas:

$$\begin{aligned} \text{Err}_{L^\infty} &= \|\phi^{M+1} - \phi(x, y, T)\|_\infty, \\ \text{Err}_{L^2} &= \|\phi^{M+1} - \phi(x, y, T)\|_2. \end{aligned} \quad (36)$$

Problem 1 (convergence test). In order to verify the temporal numerical accuracy, we consider an example on $[0, 64]^2 \times (0, 1]$ with various ϵ and η , and the initial condition is as follows:

$$\phi_0(x, y) = \sin\left(\frac{8\pi}{128}x\right) \cos\left(\frac{8\pi}{128}y\right). \quad (37)$$

We use $h = 1/2$, so the spatial discretization errors are negligible compared with the time discretization error. The computational results at $T = 1$ for various ϵ and η are presented in Table 1. One may see that the convergence rate is close to 2 for all cases, which coincides with what we expected.

Problem 2 (effects of ϵ and η on energy stability and pattern formation). Various related works have been proposed for the Swift-Hohenberg equation, and most of them considered the case of $\eta = 0$ except [9, 10]. In order to show the effects of ϵ and η on pattern formation, we use a benchmark simulation for the conservative Swift-Hohenberg equation,

FIGURE 1: $\phi(x, y, 2000)$ and the curves of mass M and energy E with different time steps τ for Problem 2: (a) $\tau = 10$, (b) $\tau = 5$, (c) $\tau = 1$, (d) $\tau = 0.5$, and (e) $\tau = 0.1$.

FIGURE 2: Continued.

FIGURE 2: Snapshots of ϕ at different time steps for Problem 2: (a) $\phi(x, y, 0)$, (b) $\phi(x, y, 100)$, (c) $\phi(x, y, 200)$, (d) $\phi(x, y, 600)$, (e) $\phi(x, y, 1000)$, and (f) $\phi(x, y, 2000)$.

FIGURE 3: The curves of energy E with different ϵ , η , and time steps τ for Problem 2: (a) $\epsilon = 0.025, \eta = 0.1$, (b) $\epsilon = 0.025, \eta = 0.5$, (c) $\epsilon = 0.025, \eta = 0.99$, (d) $\epsilon = 0.25, \eta = 0.1$, (e) $\epsilon = 0.25, \eta = 0.5$, (f) $\epsilon = 0.25, \eta = 0.99$, (g) $\epsilon = 0.5, \eta = 0.1$, (h) $\epsilon = 0.5, \eta = 0.5$, and (i) $\epsilon = 0.5, \eta = 0.99$.

FIGURE 4: Snapshots of ϕ at different time periods for Problem 3: (a) $\phi(x, y, 10)$, (b) $\phi(x, y, 100)$, (c) $\phi(x, y, 300)$, (d) $\phi(x, y, 400)$, and (e) $\phi(x, y, 1000)$.

FIGURE 5: The curves of (a) mass M and (b) energy E for Problem 3.

i.e., the phase transition behaviors. We set the 2D computational domain as $[0, 128]^2$ and discretize it by using $h = 1$. The initial condition reads as

$$\phi_0(x, y) = 0.07(1 + \text{rand}(x, y)), \quad (38)$$

where $\text{rand}(x, y)$ is a random number in the range of $[-1, 1]$.

We first perform a numerical experiment with $\epsilon = 0.025$ and $\eta = 0.1$ for the stability study of the proposed method. Figure 1 shows the $x - y - \phi$ plots at $T = 2000$ with different time steps, and the corresponding curves of mass M and energy E are also presented. These results suggest that the

proposed method satisfies mass conservation and is unconditionally stable. The only drawback is that the method is conditionally energy stable.

Secondly, with the same parameters and $\tau = 0.1$, we present the snapshots of phase transition behaviors of the density field $\phi(x, y, t)$ at different computational time steps in Figure 2.

Finally, the relationship between energy stability and the parameters ϵ and η is examined. Figure 3 shows the evolution of the energies using different ϵ , η , and time steps. The results in Figure 3 suggest that the proposed method is conditionally energy stable. We can see from this figure that

the energy $E(\phi)$ is mainly affected by the value of ϵ rather than η , and small time step τ is needed to keep the energy law (7) for large ϵ .

Problem 3 (the conservative Swift–Hohenberg equation in 3D). We consider the evolution of ϕ in 3D space using the proposed method. The initial condition on $[0, 40]^3$ is

$$\phi_0(x, y, z) = \sin\left(\frac{8\pi x}{128}\right)\cos\left(\frac{8\pi y}{128}\right)\cos\left(\frac{8\pi z}{128}\right). \quad (39)$$

We take the simulation parameters

$$\begin{aligned} T &= 1000, \\ \epsilon &= 0.25, \\ \eta &= 0.05, \\ h &= 1, \\ \tau &= \frac{1}{3}. \end{aligned} \quad (40)$$

In Figure 4, we display the evolution of the phase field at different time periods. From the results, it can be seen that our method is applicable to 3D conservative Swift–Hohenberg equation. Moreover, the curves of mass M and energy E are also presented in Figure 5.

4. Conclusions

In this paper, we developed a second-order, linear, and mass conservation algorithm for solving the nonlocal Swift–Hohenberg equation by combining the operator splitting technique with the Fourier spectral method. A variety of numerical experiments were presented to demonstrate the stability and the accuracy of the developed method. In particular, it is applicable to various problems with a mass conservation constraint.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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