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Convergence analysis of structure-preserving numerical methods for nonlinear Fokker–Planck equations with nonlocal interactions

Chenghua Duan[1,2] | Wenbin Chen[3] | Chun Liu[4] | Cheng Wang[5] | Shenggao Zhou[6]

[1]Department of Mathematics, Shanghai University, Shanghai, China

[2]Shanghai Center for Mathematical Sciences, Fudan University, Shanghai, China

[3]School of Mathematical Sciences and Shanghai Key Laboratory for Contemporary Applied Mathematics, Fudan University, Shanghai, China

[4]Department of Applied Mathematics, Illinois Institute of Technology, Chicago, Illinois, USA

[5]Department of Mathematics, The University of Massachusetts, North Dartmouth, Massachusetts, USA

[6]School of Mathematical Sciences and MOE-LSC, Shanghai Jiao Tong University, Shanghai, China

Correspondence
Cheng Wang, Department of Mathematics, The University of Massachusetts, North Dartmouth, MA 02747, USA.
Email: cwang1@umassd.edu

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A class of nonlinear Fokker–Planck equations with nonlocal interactions may include many important cases, such as porous medium equations with external potentials and aggregation–diffusion models. The trajectory equation of the Fokker–Plank equation can be derived based on an energetic variational approach. A structure-preserving numerical scheme that is mass conservative, energy stable, uniquely solvable, and positivity preserving at a theoretical level has also been designed in the previous work. Moreover, the numerical scheme is shown to satisfy the discrete energetic dissipation law and preserve steady states and has been observed to be second order accurate in space and first-order accurate time in various numerical experiments. In this work, we give the rigorous convergence analysis for the highly nonlinear numerical scheme. A careful higher order asymptotic expansion is needed to handle the highly nonlinear nature of the trajectory equation. In addition, two step error estimates (a rough estimate and a refined estimate) are necessary in the convergence proof. Different from a standard error estimate, the rough estimate is performed to control the nonlinear term. A few numerical results are also presented to verify the optimal convergence order and the preservation of equilibria.

KEYWORDS

convergence analysis, energy dissipation law, higher order asymptotic expansion, nonlocal Fokker–Planck equations, refined error estimate, rough error estimate, trajectory equation

MSC CLASSIFICATION

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1 | INTRODUCTION

The Fokker–Planck (FP) type of equations has been widely applied to describe phenomena arising from natural sciences and social sciences, including interacting gases, granular materials, cell migration and chemotaxis phenomena in biology, and collective motion of animals.[1–9] There are many important equations can be regarded as special cases of the FP equations, such as the porous medium equation and aggregation–diffusion equations. Interested readers are referred to the works[10–14] and references therein.

In this work, we consider the following initial-boundary value problem of the FP equations:

$$\begin{cases} \partial_t u = \partial_x \{ f(u) \partial_x [H'(u) + V(x) + W * u] \}, x \in \Omega \subset \mathbb{R}, t > 0, \\ u(x,0) = u_0(x), x \in \Omega, \\ f(u)\partial_x [H'(u) + V(x) + W * u] = 0, x \in \partial\Omega, t > 0, \end{cases} \tag{1.1}$$

where Ω is a bounded domain, $u(x,t) \geq 0$ represents the time-dependent probability density, $H(\cdot) : \mathbb{R}^+ \cup \{0\} \to \mathbb{R}$ describes the density of internal energy with $H''(\cdot) > 0$, $V(\cdot)$ is an external potential, $W(\cdot)$ is an even Lipschitz continuous function describing particle interactions, and $f : \mathbb{R}^+ \cup \{0\} \to \mathbb{R}^+ \cup \{0\}$ is a given increasing differentiable function with $f(0) = 0$ and $f'(0) \neq 0$.

There are three main properties for problem (1.1): non-negativity, mass conservation, and free-energy dissipation:

$$\frac{d}{dt} E^{total} = -\Delta \leq 0, \tag{1.2}$$

where

$$E^{total} := \int_\Omega H(u(x))dx + \int_\Omega u(x)V(x)dx + \frac{1}{2}\int_\Omega \int_\Omega W(x-y)u(x)u(y)dydx,$$

and

$$\Delta = \int_\Omega f(u) \left| \partial_x [H'(u) + V(x) + W * u] \right|^2 dx.$$

The free-energy dissipation (1.2) plays a critical role in analyzing the dynamics of the problem (1.1).[5,9,15,16] Hence, developing numerical methods, which can maintain a free-energy dissipation at a discrete level, non-negativity of the numerical density, and the mass conservation, is crucially desirable to address the problem, especially in the degenerate case.

Many efforts have been devoted to the development of various numerical schemes for solving the FP equation (1.1), such as finite volume methods,[10,17–19] discontinuous Galerkin (DG) methods,[13,16,20,21] finite difference schemes,[14] particle methods,[22] evolving diffeomorphisms methods,[23] etc. One closely related theory is called the Poisson–Nernst–Planck (PNP) system, which can be regarded as a special case of the FP equations with the interaction kernel being the Green function of the Poisson's equation. There is a vast literature on the structure-preserving numerical methods for the PNP system. For instance, finite difference schemes based on the Slotboom transformation have been developed in the references.[24–27] Based on an H^{-1} gradient flow structure of the PNP system, a type of structure-preserving finite difference schemes have been proposed in Liu et al. and Qian et al.[28,29] There are structure-preserving finite element schemes are available as well.[30] The effort on the development of numerical schemes for the PNP system has also provided promising ideas for the development of structure-preserving numerical schemes for the nonlinear FP equations with nonlocal interactions.

In a more recent work,[12] the authors constructed a structure-preserving numerical scheme by an energetic variational approach, which is uniquely solvable, naturally respects mass conservation and positivity, and preserves steady states theoretically. Numerical simulations have revealed not only the preservation of physical structures, such as positivity, mass conservation, discrete energy dissipation, and steady states, but also the capability of solving *degenerate* cases effectively and robustly. Furthermore, the waiting time of free boundaries can be accurately and robustly computed, and blow-up singularity can be approximated up to a machine precision. Under certain smoothness assumptions, the numerical scheme has been demonstrated to be second-order accurate in space and first-order accurate in time, in various numerical experiments. In this paper, we will provide a rigorous proof of the optimal rate convergence analysis for the nonlinear numerical scheme. In particular, the highly nonlinear nature of the trajectory equation makes the convergence analysis very challenging. To overcome these difficulties, a higher order asymptotic expansion has to be applied to ensure a higher order consistency estimate, which is needed to obtain a discrete $W^{1,\infty}$ bound of the numerical solution. Similar ideas have been reported in earlier literature for incompressible fluid equations,[31–34] porous medium equation,[35,36] nonlocal gradient flow,[37] while the analysis presented in this work turns out to be more complicated, due to the lack of a linear diffusion term in the trajectory equation and an inclusion of a general nonlocal and external potential term. The two step estimates are needed to recover the nonlinear analysis:

- Step 1. A rough estimate for the discrete derivative of numerical solution, namely, $D_h x^{n+1}$ at time t^{n+1}, to control the nonlinear term;
- Step 2. A refined estimate for the numerical error function to obtain an optimal convergence order.

Different from a standard error estimate, the rough estimate controls the nonlinear term, which is an effective approach to handle the highly nonlinear term. A combination of rough error estimate and refined error estimate results in an optimal rate convergence estimate, which is the first such result for nonlinear FP equation. Extensive numerical results have verified the convergence order, even at steady state. Hence, we also confirm that the numerical scheme for the trajectory equation can preserve the equilibria.

This paper is organized as follows. The EnVarA and trajectory equation of the nonlinear FP equations are outlined in Section 2. The numerical scheme is described in Section 3. Subsequently, the proof of optimal rate convergence analysis is provided in Section 4. Section 5 presents a numerical example to verify the convergence order. Finally, some concluding remarks are made in Section 6.

2 | ENERGETIC VARIATIONAL APPROACH

In this section, we derive a trajectory equation for the nonlinear nonlocal FP equations by an energetic variational approach. We here recall some lemmas and key ingredients in our previous work[12] for the derivation of the trajectory equation.

Lemma 2.1. *If u(x, t) is the solution of (1.1), then u satisfies the corresponding energy dissipation law*

$$\frac{d}{dt}E^{total} = -\Delta, \tag{2.1}$$

where the total energy

$$E^{total} := \int_\Omega [H(u) + uV(x)]dx + \frac{1}{2}\int_\Omega\int_\Omega W(x-y)u(x)u(y)dydx,$$

and the entropy production

$$\Delta = \int_\Omega \frac{u^2}{f(u)}|\boldsymbol{v}|^2 dx,$$

with the velocity $\boldsymbol{v} = -\frac{f(u)}{u}\partial_x[H'(u) + V(x) + W * u]$. *If u satisfies the corresponding energy dissipation law (2.1) and a zero-flux boundary condition, then it can be shown by the Energetic Variational Approach that u(x, t) solves (1.1).*

The detailed proof has been provided in Duan et all.[12]; here, we only deduce the trajectory equation briefly.

(1) **Mass conservation**
The conservation equation of mass reads

$$u_t + \partial_x(u\mathbf{v}) = 0, \tag{2.2}$$

in the Eulerian coordinate, and can be expressed by

$$u(x(X,t),t) = \frac{u_0(X)}{\frac{\partial x(X,t)}{\partial X}}, \tag{2.3}$$

in the Lagrangian coordinate, where $u_0(X)$ is the initial condition and $\frac{\partial x(X,t)}{\partial X}$ is the *deformation gradient* in one dimension. In this work, we assume that the Jacobian of the flow map, $\frac{\partial x(X,t)}{\partial X}$, remains positive in the time evolution.

(2) **Least action principle**
The action functional is defined by

$$\begin{aligned}\mathcal{A}(x) := &- \int_0^{t^*}\int_\Omega H\left(\frac{u_0(X)}{\partial_X x}\right)\partial_X x\, dXdt - \int_0^{t^*}\int_\Omega u_0(X)V(x)dXdt \\ &- \frac{1}{2}\int_0^{t^*}\int_\Omega\int_\Omega u_0(X)u_0(Y)W(x-y)dXdYdt,\end{aligned}$$

where t^* denotes the time period under consideration. The conservative force in the Lagrangian coordinate can be obtained by taking the variational of $\mathcal{A}(x)$ with respect to x:

$$F_{con} := -\partial_X\left[\frac{u_0(X)}{\partial_X x}\cdot H' - H\right] - u_0(X)V'(x) - u_0(X)\int_\Omega W'(x(X,t)-y(Y,t))u_0(Y)dY.$$

(3) **Maximum dissipation law**
By the maximum dissipation law, i.e., the Onsager's Principle, we have the dissipation force by taking the variation of $\frac{1}{2}\Delta$ with respect to the velocity x_t in the Lagrangian coordinate, i.e.,

$$F_{dis} := \frac{\delta\left(\frac{1}{2}\Delta\right)}{\delta x_t} = \frac{u_0^2(X)}{\partial_X x}\cdot\frac{1}{f\left(\frac{u_0(X)}{\partial_X x}\right)}\cdot x_t.$$

(4) **Force balance**
According to the Newton's force balance law, we get the trajectory equation

$$\begin{aligned}\frac{u_0^2(X)}{\partial_X x}\cdot\frac{1}{f\left(\frac{u_0(X)}{\partial_X x}\right)}\cdot x_t = &- \partial_X\left[\frac{u_0(X)}{\partial_X x}H'\left(\frac{u_0(X)}{\partial_X x}\right) - H\left(\frac{u_0(X)}{\partial_X x}\right)\right] \\ &- u_0(X)V'(x) - u_0(X)\int_\Omega W'(x(X,t)-y(Y,t))u_0(Y)dY,\end{aligned} \tag{2.4}$$

which is supplemented with the initial condition

$$x(X,0) = X, X \in \Omega, \tag{2.5}$$

and the boundary condition

$$x|_{\partial\Omega} = X|_{\partial\Omega},\ t > 0. \tag{2.6}$$

Finally, the solution $u(x,t)$ to problem (1.1) can be obtained by (2.3).

3 | THE NUMERICAL SCHEME FOR THE TRAJECTORY EQUATION

A structure-preserving finite difference scheme has been proposed in Duan et al,[12] for the trajectory Equation (2.4) using the convex splitting method, which was first exploited by Eyre[38] to craft energy stable numerical schemes for the Allen–Cahn and Cahn–Hilliard equations. The basic idea is to treat the convex part implicitly and the concave part explicitly. This methodology has been widely used in the relevant algorithm by an Energetic Variational Approach.[12,39] In this section, we present the numerical scheme with a positive initial state directly.

Firstly, we make certain assumptions: $\partial_X x > 0,\ H'' > 0$, and $H\left(\frac{u_0}{\partial_X x}\right)\partial_X x$ is convex. In addition, $V(x)$ and $W(x)$ can be split into a convex part and a concave part, i.e.,

$$V(x) := V_c(x) - V_e(x),$$

$$W(x) := W_c(x) - W_e(x),$$

where $V_c,\ W_c,\ V_e$, and W_e are convex functions.

We consider a uniform mesh $X_r = X(r) = X_0 + rh$, where r takes integer or half integer values, X_0 is the left endpoint of Ω, and $h = \frac{|\Omega|}{M}$ is the mesh spacing with $M \in \mathbb{N}^+$. Let $\mathcal{E}_M$ and $\mathcal{C}_M$ be the spaces of grid functions with domains being $\{X_i \,|\, i = 0, \ldots, M\}$ and $\{X_{i-\frac{1}{2}} \,|\, i = 1, \ldots, M\}$, respectively. At a component-wise level, these functions are identified via $l_i = l(X_i)$, $i = 0, \ldots, M$, for $l \in \mathcal{E}_M$, and $\phi_{i-\frac{1}{2}} = \phi\left(X_{i-\frac{1}{2}}\right)$, $i = 1, \ldots, M$, for $\phi \in \mathcal{C}_M$. Without causing any ambiguity, we denote $X = \{X_i \,|\, i = 0, \ldots, M\}$ for $X \in \mathcal{E}_M$.

We also recall the difference operators $D_h : \mathcal{E}_M \to \mathcal{C}_M$, $d_h : \mathcal{C}_M \to \mathcal{E}_M$, and $\tilde{D}_h : \mathcal{E}_M \to \mathcal{E}_M$, which are defined by

$$(D_h l)_{i-\frac{1}{2}} = (l_i - l_{i-1})/h,\ i = 1, \ldots, M, \tag{3.1}$$

$$(d_h \phi)_i = \left(\phi_{i+\frac{1}{2}} - \phi_{i-\frac{1}{2}}\right)/h,\ i = 1, \ldots, M-1, \tag{3.2}$$

$$(\tilde{D}_h l)_i = \begin{cases} (l_{i+1} - l_{i-1})/2h, & \text{i=1}, \ldots, M-1, \\ (l_{i+1} - l_i)/h, & i = 0, \\ (l_i - l_{i-1})/h, & i = M. \end{cases} \tag{3.3}$$

Let $l, g \in \mathcal{E}_M$ and $\phi, \varphi \in \mathcal{C}_M$. The discrete inner products are introduced on space $\mathcal{E}_M$ and $\mathcal{C}_M$:

$$\langle l, g \rangle_{\mathcal{E}} := h\left(\frac{1}{2} l_0 g_0 + \sum_{i=1}^{M-1} l_i g_i + \frac{1}{2} l_M g_M\right), \tag{3.4}$$

$$\langle \phi, \varphi \rangle_C := h \sum_{i=0}^{M-1} \phi_{i+\frac{1}{2}} \varphi_{i+\frac{1}{2}}. \tag{3.5}$$

It is straightforward to obtain the summation by parts formula

$$\langle l, d_h \phi \rangle_{\mathcal{E}} = -\langle D_h l, \phi \rangle_C, \text{with } l_0 = l_M = 0, \phi \in \mathcal{C}_M, l \in \mathcal{E}_M. \tag{3.6}$$

Meanwhile, the inverse inequality is valid:

$$\|l\|_\infty \le C_m \frac{\|l\|}{h^{1/2}},\ \|l\|_\infty := \max_{0 \le i \le M} \{|l_i|\},\ \forall l \in \mathcal{E}_M.$$

Let $Q := \{l \in \mathcal{E}_M \,|\, l_{i-1} < l_i, 1 \le i \le M;\ l_0 = X_0,\ l_M = X_M\}$ be an admissible set, in which particles are arranged in the order without twisting or exchanging. Its boundary set is defined by $\partial Q := \{l \in \mathcal{E}_M \,|\, l_{i-1} \le l_i, 1 \le i \le M$, and there exists $i_0 \in \{1, \ldots, M\}$ such that $l_{i_0} = l_{i_0 - 1};\ l_0 = X_0,\ l_M = X_M\}$. Clearly, $\bar{Q} := Q \cup \partial Q$ is a closed convex set.

We recall the fully nonlinear discrete scheme as follows: Given $x^n \in \mathcal{Q}$, find $x^{n+1} = (x_0^{n+1}, \dots, x_N^{n+1}) \in \mathcal{Q}$ such that

$$
\begin{aligned}
\frac{u_{0_i}^2}{\tilde{D}_h x_i^n} \cdot \frac{1}{f\left(\frac{u_{0_i}}{\tilde{D}_h x_i^n}\right)} \cdot \frac{x_i^{n+1} - x_i^n}{\tau} = &- d_h\left[\frac{u_0}{D_h x^{n+1}} \cdot H'\left(\frac{u_0}{D_h x^{n+1}}\right) - H\left(\frac{u_0}{D_h x^{n+1}}\right)\right]_i \\
&- u_{0_i} V_c'(x_i^{n+1}) + u_{0_i} V_e'(x_i^n) \\
&- u_{0_i}\left\langle W_c'(x_i^{n+1} - y^{n+1}), u_0(Y)\right\rangle_{\mathcal{E}} \\
&+ u_{0_i}\left\langle W_e'(x_i^n - y^n), u_0(Y)\right\rangle_{\mathcal{E}}, \; 1 \le i \le M-1,
\end{aligned}
\tag{3.7}
$$

where $x_i^n := x(X_i, t^n)$, $n = 1, \dots, N$. In fact $y^n = y(Y, t^n)$, $n = 1, \dots, N$. To make the algorithm clearer, we write x^n in the following descriptions.

The corresponding boundary conditions are

$$
x_0^n = X_0, x_M^n = X_M. \tag{3.8}
$$

Also, we recall the Newton's iteration method that has been developed in[12] to solve the nonlinear difference Equations 3.7 and (3.8).

Newton's iteration. Set $x^{n+1,0} = x^n$. For $k = 0, 1, 2, \dots$, update $x^{n+1,k+1} = x^{n+1,k} + \delta_x$, where δ_x solves equations

$$
\begin{aligned}
&\frac{u_{0_i}^2}{\tilde{D}_h x_i^n} \cdot \frac{1}{f\left(\frac{u_{0_i}}{\tilde{D}_h x_i^n}\right)} \cdot \frac{x_i^{n+1,k} + \delta_{x_i} - x_i^n}{\tau} \\
&= - d_h\left[\frac{u_0}{D_h x^{n+1,k}} \cdot H'\left(\frac{u_0}{D_h x^{n+1,k}}\right) - H\left(\frac{u_0}{D_h x^{n+1,k}}\right)\right]_i + d_h\left[\left(\frac{u_0^2}{(D_h x^{n+1,k})^3} H''\right) D_h \delta_x\right]_i \\
&- u_{0_i} V_c'(x_i^{n+1,k}) - u_{0_i} V_c''(x_i^{n+1,k})\delta_{x_i} + u_{0_i} V_e'(x_i^n) - u_{0_i}\left\langle W_c'(x_i^{n+1,k} - x^{n+1,k}), u_0(X)\right\rangle_{\mathcal{E}} \\
&- u_{0_i}\left\langle W_c''(x_i^{n+1} - x^{n+1}), u_0(X)\right\rangle_{\mathcal{E}} \delta_{x_i} + u_{0_i}\left\langle W_c''(x_i^{n+1} - x^{n+1})\delta_x, u_0(X)\right\rangle_{\mathcal{E}} \\
&+ u_{0_i}\left\langle W_e'(x_i^n - x^n), u_0(X)\right\rangle_{\mathcal{E}}, \; 1 \le i \le M-1,
\end{aligned}
\tag{3.9}
$$

with boundary conditions $\delta_{x_0} = \delta_{x_M} = 0$.

Then one obtains the numerical density $\{u_i^n\}_{i=0}^M := \{u(x_i, t^n)\}_{i=0}^M$, $n = 1, \dots, N$ from (2.3) by

$$
u_i^n = \frac{u_0(X_i)}{(x_{i+1}^{n+1} - x_{i-1}^{n+1})/(2h)}, \; 1 \le i \le M-1, \text{ and} \tag{3.10}
$$

$$
u_0^n = \frac{u_0(X_0)}{(x_1^{n+1} - x_0^{n+1})/h}, \; u_M^n = \frac{u_0(X_M)}{(x_M^{n+1} - x_{N-1}^{n+1})/h}. \tag{3.11}
$$

The mass conservation of $\{u_i^n\}_{i=0}^M$, obtained from (3.10)-(3.11), has been proven in Duan et al.[12]

4 | THE OPTIMAL RATE CONVERGENCE ANALYSIS

In this section, the second-order spatial convergence and the first-order temporal convergence will be theoretically justified for the proposed numerical scheme (3.7). We first introduce a higher order approximate expansion of the exact solution, since a consistency estimate (second-order in space and first order in time) is not able to control the discrete $W^{1,\infty}$ norm of the numerical solution. Also see the related works in the earlier literature,[28,31–34,40–46] etc.

Lemma 4.1. *Denote x_e as the exact solution to (2.4). Assume that $\partial_X x_e \geq C_0 > 0$. Consider a higher order approximate solution in the form of*

$$z := x_e + \tau w_\tau^{(1)} + \tau^2 w_\tau^{(2)} + h^2 w_h, \tag{4.1}$$

where $w_\tau^{(1)}, w_\tau^{(2)}, w_h \in C^\infty(\Omega; 0, T)$. Then, there exists a small $\tau_0 > 0$, such that $\forall \tau, h \leq \tau_0$, $D_h z > 0$, where τ and h are the time step and the spatial mesh sizes, respectively.

The detail of the proof can be found in Duan et al.[36]

Theorem 4.2. *The initial condition $u_0(X)$, external potential $V(x)$, interaction kernel $W(x)$, the density of internal energy $H(u)$, and mobility $f(u)$ are assumed to satisfy the following conditions:*

1. $0 < b_{u_0} \leq u_0(X) \leq B_{u_0}$, *where* $b_{u_0}, B_{u_0} > 0$ *are constants;*
2. $V_c(\cdot)$, $V_e(\cdot)$, $W_c(\cdot)$, $W_e(\cdot) \in W^{3,\infty}(\Omega)$ *with upper bounds;*
3. $H(\cdot) \in W^{3,\infty}([0,\infty))$ *with* $H'(\cdot) > 0$ *and* $H''(\cdot) > 0$;
4. $f(\cdot) \in W^{2,\infty}([0,\infty))$.

Denote by $x_e := x_e(X_e, t) \in \Omega$ the exact solution to the trajectory Equation (2.4) with sufficient regularity and $x := x(X,t) \in Q$ the numerical solution to the numerical scheme (3.7). The numerical error function is defined by

$$e_i^n = x_{e_i}^n - x_i^n, \; 0 \leq i \leq M, \; n = 0, \dots, N. \tag{4.2}$$

Under the linear refinement requirement $C_1 h \leq \tau \leq C_2 h$, we have the following estimates:

- $e^n = (e_0^n, \dots, e_M^n)$ *satisfies*

$$\|e^n\| := \langle e^n, e^n \rangle_{\mathcal{E}} \leq C(\tau + h^2).$$

- $\tilde{D}_h e^n = (\tilde{D}_h e_0^n, \dots, \tilde{D}_h e_M^n)$ *satisfies*

$$\|\tilde{D}_h e^n\| \leq C(\tau + h^2).$$

Moreover, the numerical error between the numerical solution u^n and exact solution u_e^n to the problem (1.1) is estimated by

$$\|u^n - u_e^n\| \leq C(\tau + h^2), \; n = 0, \dots, N,$$

where C is a positive constant, h is the grid spacing, and τ is the time step size.

Proof of Theorem 4.2. A higher order Taylor expansion of the fully discrete scheme in both time and space reveals that

$$\begin{aligned}
&\frac{u_0^2(X_{e_i})}{\tilde{D}_h x_{e_i}^n} \cdot \frac{1}{f\left(\frac{u_0(X_{e_i})}{\tilde{D}_h x_{e_i}^n}\right)} \cdot \frac{x_{e_i}^{n+1} - x_{e_i}^n}{\tau} \\
&= - d_h \left[\frac{u_0(X_e)}{D_h x_e^{n+1}} H'\left(\frac{u_0(X_e)}{D_h x_e^{n+1}}\right) - H\left(\frac{u_0(X_e)}{D_h x_e^{n+1}}\right) \right]_i \\
&\quad - u_0(X_{e_i}) V_c'(x_{e_i}^{n+1}) + u_0(X_{e_i}) V_e'(x_{e_i}^n) \\
&\quad - u_0(X_{e_i}) \left\langle W_c'(x_{e_i}^{n+1} - x_e^{n+1}), u_0(X_e) \right\rangle_{\mathcal{E}} + u_0(X_{e_i}) \left\langle W_e'(x_{e_i}^n - x_e^n), u_0(X_e) \right\rangle_{\mathcal{E}} \\
&\quad + \tau l_i^{(1)} + \tau^2 l_i^{(2)} + \tau^3 l_i^{(3)} + h^2 g_i^{(1)} + h^4 g_i^{(2)}, \; 1 \leq i \leq M-1,
\end{aligned}$$

with the boundary points $x_{e_0}^{n+1} = X_{e_0}$ and $x_{e_M}^{n+1} = X_{e_M}$. These high order derivative terms satisfying $\|l^{(1)}\|$, $\|l^{(2)}\|$, $\|l^{(3)}\|$, $\|g^{(1)}\|$, $\|g^{(2)}\| \leq C_e$, with C_e being dependent on the exact solution.

The constructed approximate solution $z:=z(Z,t)$ satisfies the following numerical scheme with a higher order truncation error:

$$
\begin{aligned}
\frac{u_0^2(Z_i)}{\tilde{D}_h z_i^n}\cdot\frac{1}{f\left(\frac{u_0(Z_i)}{\tilde{D}_h z_i^n}\right)}\cdot\frac{z_i^{n+1}-z_i^n}{\tau} = & -d_h\left[\frac{u_0(Z)}{D_h z^{n+1}}H'\left(\frac{u_0(Z)}{D_h z^{n+1}}\right)-H\left(\frac{u_0(Z)}{D_h z^{n+1}}\right)\right]_i \\
& - u_0(Z_i)V_c'(z_i^{n+1}) + u_0(Z_i)V_e'(z_i^n) \\
& - u_0(Z_i)\left\langle W_c'(z_i^{n+1}-z^{n+1}), u_0(Z)\right\rangle_{\mathcal{E}} \\
& + u_0(Z_i)\left\langle W_e'(z_i^{n}-z^{n}), u_0(Z)\right\rangle_{\mathcal{E}} \\
& + \tau^3 l_i^* + h^4 g_i^*,\ 1\le i\le M-1,
\end{aligned}
\tag{4.3}
$$

with boundary conditions $z_0^{n+1}=Z_0$ and $z_M^{n+1}=Z_M$ for $n=0,1,\dots,N-1$. Here, l^* and g^* depend on $l^{(1)},\ l^{(2)},\ l^{(3)}$, $g^{(1)},\ g^{(2)}$, and derivatives of $w_\tau^{(1)}$, $w_\tau^{(2)}$, and w_h.

The correction term $w_\tau^{(1)}\in C^\infty(\Omega;0,T)$ is given by the following linear equation

$$
\begin{aligned}
&\frac{u_0^2(X_e)}{\partial_X x_e}\cdot\frac{1}{f\left(\frac{u_0(X_e)}{\partial_X x_e}\right)}\cdot\partial_t w_\tau^{(1)} + G_1(x_e)\cdot\partial_X w_\tau^{(1)}\cdot\partial_t x_e \\
&= \partial_X\left[\frac{u_0^2(X_e)}{(\partial_X x_e)^3}\cdot H''\cdot\partial_X w_\tau^{(1)}\right] - u_0(X_e)\left(V_c''(x_e)+\int_\Omega W_c''(x_e-y_e)u_0(Y)dY\right)\cdot w_\tau^{(1)} \\
&+ u_0(X_e)\left(V_e''(x_e)+\int_\Omega W_e''(x_e-y_e)u_0(Y)dY\right)\cdot w_\tau^{(1)} - l^{(1)}, \\
&\quad \text{with } w_\tau^{(1)}|_{\partial\Omega}=0,\ w_\tau^{(1)}(\cdot,0)=0,
\end{aligned}
$$

where $y_e:=x_e(X_e,t)$ and

$$
G_1(x_e) := -\frac{u_0^2(X_e)}{(\partial_X x_e)^2}\cdot\frac{1}{f}+\frac{u_0^3(X_e)}{(\partial_X x_e)^3}\frac{f'}{f^2}.
$$

The correction term $w_\tau^{(2)}\in C^\infty(\Omega;0,T)$ turns out to be the solution of the following linear equation:

$$
\begin{aligned}
&\frac{u_0^2(X_e)}{\partial_X x_e}\cdot\frac{1}{f\left(\frac{u_0(X_e)}{\partial_X x_e}\right)}\cdot\partial_t w_\tau^{(2)} + G_1(x_e)\cdot\partial_X w_\tau^{(2)}\cdot\partial_t x_e \\
&+ G_1(x_e)\cdot\partial_X w_\tau^{(1)}\cdot\partial_t w_\tau^{(1)} + \frac{1}{2}G_2(x_e)\cdot\partial_t x_e\cdot\left(\partial_X w_\tau^{(1)}\right)^2 \\
&= \partial_X\left[\frac{u_0^2(X_e)}{(\partial_X x_e)^3}\cdot H''\cdot\partial_X w_\tau^{(2)} + \frac{1}{2}\cdot G_3(x_e)\left(\partial_X w_\tau^{(1)}\right)^2\right] \\
&- u_0(X_e)\left(V_c''(x_e)+\int_\Omega W_c''(x_e-y_e)u_0(Y)dY\right)\cdot w_\tau^{(2)} \\
&- \frac{1}{2}u_0(X_e)\left(V_c'''(x_e)+\int_\Omega W_c'''(x_e-y_e)u_0(Y)dY\right)\cdot\left(w_\tau^{(1)}\right)^2 \\
&+ u_0(X_e)\left(V_e''(x_e)+\int_\Omega W_e''(x_e-y_e)u_0(Y)dY\right)\cdot w_\tau^{(2)} \\
&+ \frac{1}{2}u_0(X_e)\left(V_e'''(x_e)+\int_\Omega W_e'''(x_e-y_e)u_0(Y)dY\right)\cdot\left(w_\tau^{(1)}\right)^2 - l^{(2)}, \\
&\text{with } w_\tau^{(2)}|_{\partial\Omega}=0,\ w_\tau^{(2)}(\cdot,0)=0,
\end{aligned}
$$

where

$$G_2(x_e) := 2\frac{u_0^2(X_e)}{(\partial_X x_e)^3}\frac{1}{f} - 4\frac{u_0^3(X_e)}{(\partial_X x_e)^4}\frac{f'}{f^2} + 2\frac{u_0^4(X_e)}{(\partial_X x_e)^5}\frac{(f')^2}{f^3} - \frac{u_0^4(X_e)}{(\partial_X x_e)^5}\frac{f''}{f^2},$$
$$G_3(x_e) := -3\frac{u_0^2(X_e)}{(\partial_X x_e)^4}H'' - \frac{u_0^3(X_e)}{(\partial_X x_e)^5}H'''.$$

The correction term $w_h \in C^\infty(\Omega; 0, T)$ is the solution of the following linear equation:

$$\begin{aligned}
&\frac{u_0^2(X_e)}{\partial_X x_e} \cdot \frac{1}{f\left(\frac{u_0(X_e)}{\partial_X x_e}\right)} \cdot \partial_t w_h + G_1(x_e) \cdot \partial_X w_h \cdot \partial_t x_e \\
&= \partial_X\left[\frac{u_0^2(X_e)}{(\partial_X x_e)^3} \cdot H'' \cdot \partial_X w_h\right] - u_0(X)\left(V_c''(x_e) + \int_\Omega W_c''(x_e - y_e)u_0(Y)dY\right) \cdot w_h \\
&+ u_0(X)\left(V_e''(x_e) + \int_\Omega W_e''(x_e - y_e)u_0(Y)dY\right) \cdot w_h - g^{(1)}, \\
&w_h|_{\partial\Omega} = 0, \;\; w_h(\cdot, 0) = 0.
\end{aligned}$$

Since $w_\tau^{(1)}, w_\tau^{(2)}, w_h$ only depend on z and x_e, the following estimate is straightforward:

$$\|z - x_e\|_{H^m} = \tau\|w_\tau^{(1)}\|_{H^m} + \tau^2\|w_\tau^{(1)}\|_{H^m} + h^2\|w_h\|_{H^m} \le C'(\tau + h^2).$$

Instead of a direct comparison between the numerical and exact solutions, we evaluate the numerical error between the numerical solution and constructed solution z. The higher order truncation error enables us to obtain a discrete $W^{1,\infty}$ estimate of the numerical solution, which is required in the nonlinear convergence analysis.

Define $\tilde{e}_i^n := z_i^n - x_i^n$ for $i = 0, 1, \dots, M$ and $n = 0, 1, \dots, N$. Notice that $\|\tilde{e}^0\| = 0$ at the initial time step t^0. We make an *a priori* assumption at the time step t^n that

$$\|\tilde{e}^n\| \le \tau^{\frac{11}{4}} + h^{\frac{7}{2}}. \tag{4.4}$$

Such an a priori assumption will be recovered by the convergence estimate at the next time step, as will be demonstrated later. With this a priori assumption at hand, we have the following estimates

$$\begin{aligned}
&\|D_h\tilde{e}^n\| \le C\left(\tau^{\frac{7}{4}} + h^{\frac{5}{2}}\right), \\
&\|D_h\tilde{e}^n\|_\infty \le CC_m\frac{\|D_h\tilde{e}^n\|}{h^{1/2}} \le C_mC\left(\tau^{\frac{5}{4}} + h^2\right), \text{ if } \; h = \mathcal{O}(\tau).
\end{aligned} \tag{4.5}$$

Let $C^* := \|D_h z^n\|_\infty$. Then, we get

$$\|D_h x^n\|_\infty = \|D_h z^n - D_h\tilde{e}^n\|_\infty \le C^* + 1 := C_0^*, \;\; \text{if} \;\; C_mC\left(\tau^{\frac{5}{4}} + h^2\right) \le 1. \tag{4.6}$$

Similarly, let $\tilde{C}_t^* := \left\|\frac{\tilde{D}_h z^n - \tilde{D}_h z^{n-1}}{\tau}\right\|_\infty$, and we obtain

$$\left\|\frac{\tilde{D}_h x^n - D_h x^{n-1}}{\tau}\right\|_\infty = \left\|\frac{\tilde{D}_h z^n - \tilde{D}_h z^{n-1}}{\tau} - \frac{\tilde{D}_h\tilde{e}^n - \tilde{D}_h\tilde{e}^{n-1}}{\tau}\right\|_\infty \le \tilde{C}_t^* + 1, \tag{4.7}$$

if

$$C_m C\left(\tau^{\frac{1}{4}}+h\right)\le 1.$$

Due to the fact that $\tilde{D}_h z\in\mathcal{Q}$, there exists $\delta_0>0$, such that $\tilde{D}_h z_i^n\ge\delta_0$. If $C_m C\left(\tau^{\frac{5}{4}}+h^2\right)\le\frac{\delta_0}{2}$, it is clear that $\tilde{D}_h x_i^n\ge\frac{\delta_0}{2}>0$, $0\le i\le M$, $n=0,\ \dots\ ,N$. We also notice that

$$\|\tilde{D}_h x^n\|\le\|D_h x^n\|,\ \text{and}\ \|\tilde{D}_h x^n\|_\infty\le\|D_h x^n\|_\infty.$$

Subtracting (4.3) from the fully discrete numerical scheme (3.7) yields

$$\begin{aligned}
&\frac{u_0^2(X_i)}{\tilde{D}_h x_i^n}\cdot\frac{1}{f\left(\frac{u_0(X_i)}{\tilde{D}_h x_i^n}\right)}\cdot\frac{\tilde{e}_i^{n+1}-\tilde{e}_i^n}{\tau}+R_i^n\tilde{D}_h\tilde{e}_i^n\\
&=d_h\left[\frac{u_0^2(X)}{(D_h\eta^{n+1})^3}H''\left(\frac{u_0(X)}{D_h\eta^{n+1}}\right)D_h\tilde{e}^{n+1}\right]_i-u_0(X_i)V_c''(\zeta_i^{n+1})\tilde{e}_i^{n+1}+u_0(X_i)V_e''(\zeta_i^n)\tilde{e}_i^n\\
&\quad-u_0(X_i)\left\langle W_c''(\zeta_i^{n+1}-\zeta^{n+1})\cdot(\tilde{e}_i^{n+1}-\tilde{e}^{n+1}),u_0(X)\right\rangle_{\mathcal{E}}\\
&\quad+u_0(X_i)\left\langle W_e''(\zeta_i^n-\zeta^n)\cdot(\tilde{e}_i^n-\tilde{e}^n),u_0(X)\right\rangle_{\mathcal{E}}+\tau^3 f_i^*+h^4 g_i^*,\ 1\le i\le M-1,
\end{aligned}\tag{4.8}$$

and $\tilde{e}_0^{n+1}=\tilde{e}_M^{n+1}=0$, where

$$R_i^n:=\frac{u_0^2(X_i)}{\tilde{D}_h x_i^n\cdot f\left(\frac{u_0(X_i)}{\tilde{D}_h x_i^n}\right)\cdot\tilde{D}_h z_i^n\cdot f\left(\frac{u_0(X_i)}{\tilde{D}_h z_i^n}\right)}\cdot\frac{z_i^{n+1}-z_i^n}{\tau}\cdot\left[f\left(\frac{u_0(X_i)}{\tilde{D}_h\xi_i^n}\right)-\frac{u_0(X_i)}{\tilde{D}_h\xi_i^n}f'\left(\frac{u_0(X_i)}{\tilde{D}_h\xi_i^n}\right)\right],$$

and ζ_i^n is between x_i^n and z_i^n, $\tilde{D}_h\xi_i^n$ is between $\tilde{D}_h x_i^n$ and $\tilde{D}_h z_i^n$, and $D_h\eta_i^n$ is between $D_h x_i^n$ and $D_h z_i^n$, $n=0,\ \dots\ ,N$.

To make the proof concise, we denote the following quantity

$$B:=\max_{x\in\Omega}\{\|V_c''(x)\|_\infty,\|V_e''(x)\|_\infty,\|W_c''(x)\|_\infty,\|W_e''(x)\|_\infty\}.$$

Taking a discrete inner product with (4.8) by $2\tilde{e}^{n+1}$ gives

$$\begin{aligned}
&2\left\langle\alpha_n(\tilde{e}^{n+1}-\tilde{e}^n),\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}-2\tau\left\langle d_h\left[\frac{u_0^2(X)}{(D_h\eta^{n+1})^3}H''\left(\frac{u_0(X)}{D_h\eta^{n+1}}\right)D_h\tilde{e}^{n+1}\right],\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}\\
&=-2\tau\left\langle R_i^n\tilde{D}_h\tilde{e}^n,\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}-2\tau\left\langle u_0(X)V_c''(\zeta^{n+1})\tilde{e}^{n+1},\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}\\
&\quad+2\tau\left\langle u_0(X)V_e''(\zeta^n)\tilde{e}^n,\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}-2\tau\left\langle u_0(X)\left\langle W_c''(\zeta^{n+1}-\tilde{\zeta}^{n+1}),u_0(X)\right\rangle_{\mathcal{E}}\tilde{e}^{n+1},\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}\\
&\quad+2\tau\left\langle u_0(X)\left\langle W_c''(\zeta^{n+1}-\tilde{\zeta}^{n+1})\tilde{e}^{n+1},u_0(X)\right\rangle_{\mathcal{E}},\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}\\
&\quad+2\tau\left\langle u_0(X)\left\langle W_e''(\zeta^n-\tilde{\zeta}^n),u_0(X)\right\rangle_{\mathcal{E}}\tilde{e}^n,\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}\\
&\quad-2\tau\left\langle u_0(X)\left\langle W_e''(\zeta^n-\tilde{\zeta}^n)\tilde{e}^n,u_0(X)\right\rangle_{\mathcal{E}},\tilde{e}^{n+1}\right\rangle_{\mathcal{E}}+2\tau\left\langle\tau^3 f^*+h^4 g^*,\tilde{e}^{n+1}\right\rangle_{\mathcal{E}},
\end{aligned}\tag{4.9}$$

where $\tilde{\zeta}^n:=\zeta(X,t^n)$ and

$$\alpha_n:=\frac{u_0^2(X)}{\tilde{D}_h x^n}\cdot\frac{1}{f\left(\frac{u_0(X)}{\tilde{D}_h x^n}\right)},\ C_\alpha:=\frac{b_{u_0}^2}{C_0^*}\cdot\frac{1}{B_f}\le\|\alpha_n\|_\infty\le\frac{B_{u_0}^2}{\delta_0/2}\cdot\frac{1}{b_f}:=\bar{C}_\alpha,\tag{4.10}$$

with $0<b_f\le f(\cdot)$ and $B_f:=\|f(\cdot)\|_{W^{1,\infty}}$.

For the first term on the left-hand side of (4.9), we see that

$$2\left\langle \alpha_n(\tilde{e}^{n+1}-\tilde{e}^n), \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} = \alpha_n\|\tilde{e}^{n+1}\|^2 + \alpha_n\|\tilde{e}^{n+1}-\tilde{e}^n\|^2 - \alpha_n\|\tilde{e}^n\|^2 \\ \geq \alpha_n\|\tilde{e}^{n+1}\|^2 - \alpha_n\|\tilde{e}^n\|^2. \tag{4.11}$$

For the second term on the left-hand side, the following inequality is valid:

$$\begin{aligned} &-2\tau\left\langle d_h\left[\frac{u_0^2(X)}{(D_h\eta^{n+1})^3}H''\left(\frac{u_0(X)}{D_h\eta^{n+1}}\right)D_h\tilde{e}^{n+1}\right], \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \\ &= 2\tau\left\langle \frac{u_0^2(X)}{(D_h\eta^{n+1})^3}H''\left(\frac{u_0(X)}{D_h\eta^{n+1}}\right)D_h\tilde{e}^{n+1}, D_h\tilde{e}^{n+1}\right\rangle_{C} \geq 0, \end{aligned} \tag{4.12}$$

in which the summation by parts formula and $\tilde{e}_0^{n+1} = \tilde{e}_N^{n+1} = 0$ have been used.
For the first term on the right side, the Cauchy inequality is applied:

$$-2\tau\left\langle R_i^n\tilde{D}_h\tilde{e}^n, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \leq \tau C_1\|\tilde{D}_h\tilde{e}^n\|^2 + \tau C_1\|\tilde{e}^{n+1}\|^2, \tag{4.13}$$

in which $C_1 := \frac{B_{u_0}^2}{(\delta_0\cdot b_f)^2}\cdot C_t^*\cdot\left(B_f + \frac{B_{u_0}}{\delta_0}B_f\right)$ with $C_t^* = \|z_t\|_\infty$. For the second term on the right-hand side, the following bound is obvious:

$$-2\tau\left\langle u_0(X)V_c''(\zeta^{n+1})\tilde{e}^{n+1}, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \leq 2\tau C_2\|\tilde{e}^{n+1}\|^2, \tag{4.14}$$

where $C_2 := BB_{u_0}$. A similar bound could be derived for the third term on the right-hand side:

$$2\tau\left\langle u_0(X)V_e''(\zeta^n)\tilde{e}^n, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \leq \tau C_2\|\tilde{e}^n\|^2 + \tau C_2\|\tilde{e}^{n+1}\|^2. \tag{4.15}$$

For the forth and fifth terms on the right-hand side, we see that

$$\begin{aligned} &-2\tau\left\langle u_0(X)\left\langle W_c''(\zeta^{n+1}-\tilde{\zeta}^{n+1}), u_0(X)\right\rangle_{\mathcal{E}}\tilde{e}^{n+1}, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \\ &+2\tau\left\langle u_0(X)\left\langle W_c''(\zeta^{n+1}-\tilde{\zeta}^{n+1})\tilde{e}^{n+1}, u_0(X)\right\rangle_{\mathcal{E}}, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \\ &\leq 4\tau C_3\|\tilde{e}^{n+1}\|^2, \end{aligned} \tag{4.16}$$

with $C_3 := BB_{u_0}^2L$ $(L := |\Omega|)$, in which the results follow from the definition of the discrete L^2 norm and simple estimates. A similar estimate is available for the sixth and seventh terms:

$$\begin{aligned} &2\tau\left\langle u_0(X)\left\langle W_e''(\zeta^n-\tilde{\zeta}^n), u_0(X)\right\rangle_{\mathcal{E}}\tilde{e}^n, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \\ &-2\tau\left\langle u_0(X)\left\langle W_e''(\zeta^n-\tilde{\zeta}^n)\tilde{e}^n u_0(X)\right\rangle_{\mathcal{E}}, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} \\ &\leq 3\tau C_3\|\tilde{e}^n\|^2 + 3\tau C_3\|\tilde{e}^{n+1}\|^2. \end{aligned} \tag{4.17}$$

The local truncation error term can be controlled by the standard Cauchy inequality:

$$\begin{aligned} 2\tau\left\langle \tau^3 f^* + h^4 g^*, \tilde{e}^{n+1}\right\rangle_{\mathcal{E}} &\leq \tau\|\tau^3 f^* + h^4 g^*\|^2 + \tau\|\tilde{e}^{n+1}\|^2 \\ &\leq \tau C(\tau^3+h^4)^2 + \tau\|\tilde{e}^{n+1}\|^2. \end{aligned} \tag{4.18}$$

We now perform a preliminary estimate on $\|D_h x^{n+1}\|_\infty$. Substituting (4.11)–(4.18) into (4.9) leads to

$$\|\tilde{e}^{n+1}\| \leq \tilde{C}\tau^{\frac{1}{2}}\left(\tau^{\frac{7}{4}} + h^{\frac{5}{2}}\right),$$

where $\tilde{C}$ is a constant depending on $\bar{C}_\alpha$, C_1, C_2, C_3. By choosing $h = \mathcal{O}(\tau)$, we see that

$$\|\tilde{e}^{n+1}\|_\infty \leq \frac{C_m\|\tilde{e}^{n+1}\|}{h^{\frac{1}{2}}} \leq C_m\tilde{C}\left(\tau^{\frac{7}{4}} + h^{\frac{5}{2}}\right).$$

Then, we arrive at

$$\|D_h x^{n+1}\|_\infty = \|D_h z^{n+1} - D_h\tilde{e}^{n+1}\|_\infty \leq C^* + C_m\tilde{C}(\tau^{\frac{3}{4}} + h^{\frac{3}{2}}) \leq C^* + 1 := C_0^*,$$

if $C_m\tilde{C}\left(\tau^{\frac{3}{4}} + h^{\frac{3}{2}}\right) \leq 1$. Since $H(\cdot)$ is a strictly convex functional, there exists a positive constant b_H, such that $H'' \geq b_H > 0$. Subsequently, (4.12) could be rewritten as follows

$$2\tau\left\langle \frac{u_0^2(X)}{(D_h\xi^{n+1})^3}H''\left(\frac{u_0(X)}{D_h\xi^{n+1}}\right)D_h\tilde{e}^{n+1}, D_h\tilde{e}^{n+1}\right\rangle_C \geq 2\tau C_4\|D_h\tilde{e}^{n+1}\|^2,\ C_4 := \frac{b_{u_0}^2}{(C_0^*)^3}b_H. \tag{4.19}$$

As a consequence, a substitution of (4.11)–(4.18) and (4.19) into (4.9) leads to

$$\begin{aligned}
&\alpha_n\|\tilde{e}^{n+1}\|^2 - \alpha_n\|\tilde{e}^n\|^2 + \tau C_4\|\tilde{D}_h\tilde{e}^{n+1}\|^2 \\
&\leq \tau\left(1 + \frac{C_1^2}{C_4} + 3C_2 + 7C_3\right)\|\tilde{e}^{n+1}\|^2 + \tau(C_2 + 3C_3)\|\tilde{e}^n\|^2 + C\tau(\tau^3 + h^4)^2,
\end{aligned}$$

where the fact $\|\tilde{D}_h x^n\| \leq \|D_h x^n\|$ has been used, as well as the following inequality:

$$2C_1\tau\|\tilde{D}_h\tilde{e}^n\| \cdot \|\tilde{e}^{n+1}\| \leq \frac{C_1^2}{C_4}\tau\|\tilde{e}^{n+1}\|^2 + C_4\tau\|\tilde{D}_h\tilde{e}^n\|^2.$$

Let $C_5 := 1 + \frac{C_1^2}{C_4} + 3C_2 + 7C_3$. Summing in time leads to

$$\begin{aligned}
\alpha_n\|\tilde{e}^{n+1}\|^2 + \tau C_4\sum_{k=1}^{n+1}||\tilde{D}_h\tilde{e}^k||^2 \leq \quad & \tau\sum_{k=1}^{n}\frac{(\alpha_k - \alpha_{k-1})}{\tau}\|\tilde{e}^k\|^2 + \tau(C_2 + 3C_3)\sum_{k=1}^{n}\|\tilde{e}^k\|^2 \\
& + \tau C_5\sum_{k=1}^{n+1}\|\tilde{e}^k\|^2 + CT(\tau^3 + h^4)^2,
\end{aligned}$$

where we have used the bound (4.7) and the fact that

$$\begin{aligned}
\left\|\frac{\alpha_k - \alpha_{k-1}}{\tau}\right\|_\infty &= \left\|\left[-\frac{u_0^2(X)}{(\tilde{D}_h\vartheta)^2}\cdot\frac{1}{f} + \frac{u_0^3(X)}{(\tilde{D}_h\vartheta)^3}\cdot\frac{f'}{f^2}\right]\frac{\tilde{D}_h x^k - \tilde{D}_h x^{k-1}}{\tau}\right\|_\infty \\
&\leq \frac{B_{u_0}^3}{(\delta_0/2)^3}\cdot\frac{B_f}{(b_f)^2}\cdot(\tilde{C}_t^* + 1) := \tilde{C}_\alpha,
\end{aligned}$$

where $[0, T]$ is the time interval under consideration and $\tilde{D}_h\vartheta$ is between $\tilde{D}_h x^k$ and $\tilde{D}_h x^{k-1}$ with $\|\tilde{D}_h\vartheta\|_\infty \geq \frac{\delta_0}{2}$. Furthermore, we get

$$\|\tilde{e}^{n+1}\|^2 + \tau\frac{C_4}{C_\alpha}\sum_{k=1}^{n+1}\|\tilde{D}_h\tilde{e}^k\|^2 \leq \quad \frac{\tau}{C_\alpha}(C_5 + C_2 + 3C_3 + \tilde{C}_\alpha)\sum_{k=1}^{n+1}\|\tilde{e}^k\|^2 + \frac{CT}{C_\alpha}(\tau^3 + h^4)^2.$$

An application of the discrete Gronwall inequality yields the desired convergence result

$$\|\tilde{e}^{n+1}\|^2 + \tau\frac{C_4}{C_\alpha}\sum_{k=1}^{n+1}\|\tilde{D}_h\tilde{e}^k\|^2 \leq e^{C_0T}\frac{CT}{C_\alpha}(\tau^3 + h^4)^2,$$

where $C_0 := \frac{1}{C_\alpha}(C_2 + 3C_3 + C_5 + \tilde{C}_\alpha)$. This estimate in turn implies that

$$\|\tilde{e}^{n+1}\| \leq \gamma(\tau^3 + h^4), \text{ with } \gamma := \left(\frac{CT}{C_\alpha}\right)^{\frac{1}{2}} e^{\frac{C_0T}{2}}.$$

Therefore, the a priori assumption (4.4) is valid at t^{n+1}:

$$\|\tilde{e}^{n+1}\| \leq \gamma(\tau^3 + h^4) \leq \left(\tau^{\frac{11}{4}} + h^{\frac{7}{2}}\right),$$

provided that $\tau \leq \gamma^{-4}$ and $h \leq \gamma^{-2}$. Since

$$\|\tilde{D}_h\tilde{e}^{n+1}\| = \|\tilde{D}_h z^{n+1} - \tilde{D}_h x^{n+1}\| \leq C\gamma(\tau^2 + h^3),$$

we obtain

$$\|e^{n+1}\| = \|x_e^{n+1} - x^{n+1}\| \leq C(\tau + h^2),$$

and

$$\|\tilde{D}_h e^{n+1}\| = \|\tilde{D}_h x_e^{n+1} - \tilde{D}_h x^{n+1}\| \leq C(\tau + h^2).$$

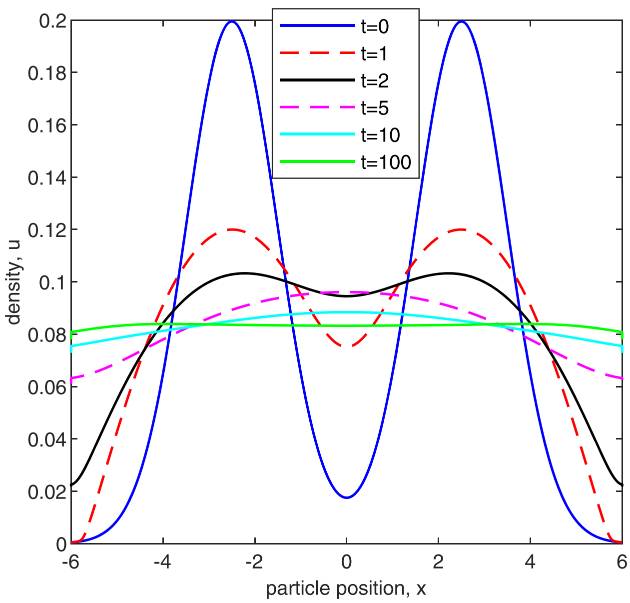


FIGURE 1 The evolution of the numerical density u with $h = 1/50$, $\tau = 1/50$ [Colour figure can be viewed at wileyonlinelibrary.com]

Finally, we consider the estimate on the error between the numerical solution u^{n+1} and the exact solution u_e^{n+1}. Due to the boundedness of both u^{n+1} and u_e^{n+1}, we can obtain

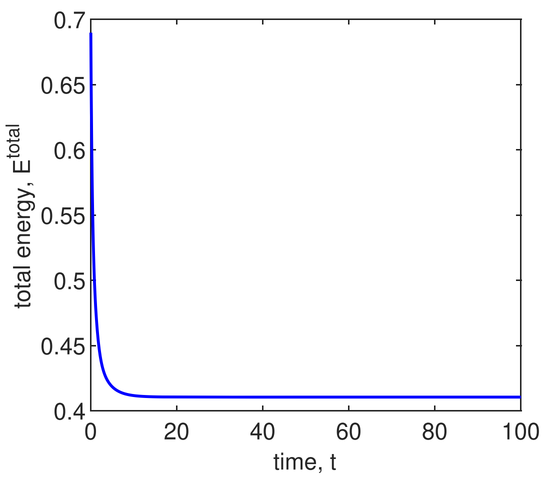
$$\begin{aligned}\|u_e^{n+1}-u^{n+1}\| &= \left\| \frac{u_0(X)}{\partial_X x_e^{n+1}} - \frac{u_0(X)}{\tilde{D}_h x^{n+1}} \right\| \\ &= \left\| \frac{u_0(X)}{\partial_X x_e^{n+1}} - \frac{u_0(X)}{\tilde{D}_h x_e^{n+1}} + \frac{u_0(X)}{\tilde{D}_h x_e^{n+1}} - \frac{u_0(X)}{\tilde{D}_h x^{n+1}} \right\| \le C(\tau + h^2).\end{aligned}$$

□

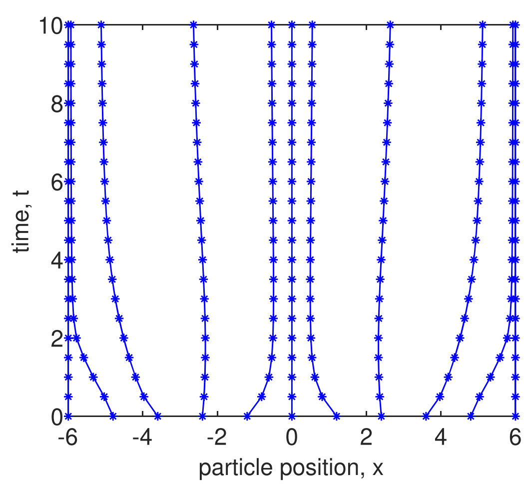
Remark 4.2. A theoretical justification of the numerical convergence for the nonlinear FP equation has been very limited in the existing literature. Among the existing works, it is worthy of mentioning,[47] in which the convergence of a semi-discrete scheme was proven. Meanwhile, only the convergence is theoretically justified, while an optimal convergence analysis has not been available yet. In addition, the nonlocal interaction has not been involved in the PDE formulation. To the authors' knowledge, our work is the first such result to theoretically justify an optimal rate convergence analysis for the nonlinear FP equation.

5 | THE NUMERICAL RESULTS

In this section, we present a numerical example to verify the optimal convergence order, even at a steady state. We first solve the trajectory Equation (2.4) with the initial and boundary conditions (2.5) and (2.6) using the fully discrete scheme (3.7), and then approximate the density function u in (2.3) by (3.10) and (3.11).



(A) Total Energy



(B) Particle positions

FIGURE 2 The evolution of the total energy and particle positions with $h = 1/50$, $\tau = 1/50$ [Colour figure can be viewed at wileyonlinelibrary.com]

The discrete L^2 and L^∞ norm of the numerical error is defined as follows:

$$\|e_h\|_2^2 := \left(\frac{1}{2}e_{h_0}^2 h + \sum_{i=1}^{M-1} e_{h_i}^2 h + \frac{1}{2}e_{h_M}^2 h\right), \ \|e_h\|_\infty := \max_{0\le i\le M}\{|e_{h_i}|\},$$

where $e_h = (e_{h_0}, e_{h_1}, \dots, e_{h_M})$ and h is a uniform grid spacing. We denote the error of the numerical trajectory and the density by $e_h^x := x_e - x$ and $e_h^u := u_e - u$, respectively.

Let $\Omega = (-l, l)$. In the following example, the FP equation (1.1) with porous medium type diffusion is considered with $H(u) = \frac{\gamma}{m}u^m$ ($\gamma = 12$ and $m = 2$), $V(x) = -\frac{\sigma}{2}x^2$ ($\sigma = 0.001$), and Gaussian kernel $W(x) = -\frac{1}{\sqrt{2\pi}}e^{-\frac{|x|^2}{2}}$, which is nonconvex, nonconcave. Hence, we split W by $W = W_c - W_e$, where $W_c = ax^2$ and

$$W_e = \frac{1}{\sqrt{2\pi}}e^{-\frac{|x|^2}{2}} + ax^2, \ a := \frac{1}{\sqrt{2\pi}}\max\left\{1, e^{-\frac{l^2}{2}}(1-l^2)\right\}.$$

The initial state is set as

$$u(x,0) = \frac{1}{2\sqrt{2\pi}}\left[e^{-\frac{\left(x-\frac{5}{2}\right)^2}{2}} + e^{-\frac{\left(x+\frac{5}{2}\right)^2}{2}}\right], x \in \Omega := (-6, 6).$$

Figure 1 displays the evolution of density u, which remains positive and does not have a support, mainly because the force of diffusion and external potential is bigger than the attractive force. The movement of particles in Figure 2B presents the relationship of $H(\cdot)$, $V(\cdot)$ and $\mathcal{K}$. In Figure 2A, the total energy evolution is shown, indicating free-energy dissipation as time evolves. The discrete L^∞ and L^2 numerical errors for x and u are displayed in Table 1, at $t = 1$, which implies first-order temporal convergence rate and second order spatial convergence rate. Notice that the reference exact solution is obtained numerically on a rather refined mesh with $h = 1/1{,}000$ and $\tau = 1/1{,}000$. These results have verified the analysis presented in Theorem 4.2. In addition, as demonstrated in Table 2, such an optimal rate convergence is also valid at $t = 100$, where the system is almost in an equilibrium state. The reference exact solution at the steady state is computed by (4.10) in Duan et al[12] on a rather refined mesh with $h = 1/100$ and $\tau = 1/100$. This result confirms that the numerical scheme of the trajectory x can preserve the equilibria, whose theoretical description (theorem 4.4) has been given in Duan et al.[12] The convergence order of u in the discrete L^∞ norm decreases for the steady state, due to the first-order accurate approximation of u at the boundary points; cf. (3.11).

TABLE 1 Numerical error and convergence order of the density u and the numerical trajectory x at time $t = 1$

h	τ	$\|e_h^u\|$	Order	$\|e_h^u\|_\infty$	Order
1/10	1/10	1.059e-02		6.156e-03	
1/20	1/40	2.700e-03	1.972	1.636e-03	1.994
1/40	1/160	6.000e-04	2.170	3.626e-04	2.174
h	τ	$\|e_h^x\|$	Order	$\|e_h^x\|_\infty$	Order
1/10	1/10	5.429e-02		5.632e-02	
1/20	1/40	1.410e-02	1.977	1.465e-02	1.943
1/40	1/160	3.139e-03	2.166	3.262e-03	2.167

TABLE 2 Numerical error and convergence order of the density u and the numerical trajectory x at steady state $t = 100$

h	τ	$\|e_h^u\|$	Order	$\|e_h^u\|_\infty$	Order
1/2	1/2	1.276e-02		7.410e-03	
1/4	1/8	4.833e-03	1.400	3.331e-03	1.154
1/8	1/32	1.371e-03	1.817	1.033e-03	1.689
h	τ	$\|e_h^x\|$	Order	$\|e_h^x\|_\infty$	Order
1/2	1/2	1.393e-02		3.262e-02	
1/4	1/8	3.451e-03	1.883	8.067e-03	2.016
1/8	1/32	8.531e-04	1.954	2.002e-03	2.010

6 | CONCLUDING REMARKS

Based on an energetic variational approach, a structure-preserving scheme for the nonlinear FP equation with the nonlocal interaction has been established and studied in a recent work,[12] while a theoretical justification for optimal convergence analysis has not been available and a numerical evidence for the preservation of equilibria has not be involved. In this work, we provide an optimal rate convergence analysis for the proposed numerical scheme, which gives the second order spatial convergence and the first-order temporal convergence for the nonlinear numerical scheme. A careful asymptotic expansion for the exact solution in terms of the numerical scheme is applied to obtain higher order consistency. Furthermore, we use two-step error estimates: a rough estimate to control a discrete $W^{1,\infty}$ bound of the numerical solution and a refined estimate to derive the desired convergence results. Numerical simulations have verified the convergence order, even at the steady state.

Although an optimal rate convergence analysis has been derived for the proposed numerical method, it is desirable but challenging to develop second-order accurate temporal discretization that is also able to preserve unconditional energy dissipation in the discrete sense. Another challenge is that the trajectory equation will be a very complicated nonlinear parabolic system with the Jacobian of the flow map in higher dimensions. The development of numerical schemes with structure-preserving properties for higher dimensional cases deserves further investigations.

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CONFLICT OF INTEREST

This work does not have any conflicts of interest

ORCID

Wenbin Chen https://orcid.org/0000-0001-8305-0764
Cheng Wang https://orcid.org/0000-0003-4220-8080

REFERENCES

1. Benedetto D, Caglioti E, Carrillo JA, Pulvirenti M. A non-Maxwellian steady distribution for one-dimensional granular media. *J Stat Phys*. 1998;91:979-990.
2. Burger M, Capasso V, Morale D. On an aggregation model with long and short range interactions. *Nonlinear Anal Real World Appl*. 2007;8(3):939-958.
3. Carrillo JA, Craig K, Yao Y. Aggregation-diffusion equations: dynamics, asymptotics, and singular limits. arXiv preprint arXiv:1810.03634; 2018.
4. Carrillo JA, Fornasier M, Toscani G, Vecil F. Particle, Kinetic, and Hydrodynamic Models of Swarming. In *:Mathematical Modeling of Collective Behavior in Socio-Economic and Life Sciences*. Boston, MA: Birkhäuser Boston, Inc.; 2010:297-336.
5. Carrillo JA, McCann RJ, Villani C. Kinetic equilibration rates for granular media and related equations: entropy dissipation and mass transportation estimates. *Rev Mat Iberoam*. 2003;19(3):971-1018.
6. Kolokolnikov T, Carrillo JA, Bertozzi A, Fetecau R, Lewis M. Emergent behaviour in multi-particle systems with non-local interactions [Editorial]. *Phys D*. 2013;260:1-4.
7. Lushnikov PM, Chen N, Alber M. Macroscopic dynamics of biological cells interacting via chemotaxis and direct contact. *Phys Rev E*. 2008;78:061904.
8. Topaz CM, Bertozzi AL, Lewis MA. A nonlocal continuum model for biological aggregation. *Bull Math Biol*. 2006;68:1601-1623.
9. Villani C. Topics in Optimal Transportation. *Am Math Soc*. Providence, Rhode Island; 2003.
10. Carrillo JA, Chertock A, Huang Y. A finite-volume method for nonlinear nonlocal equations with a gradient flow structure. *Commun Comput Phys*. 2015;17:233-258.

11. Carrillo JA, Toscani G. Asymptotic L^1-decay of solutions of the porous medium equation to self-similarity. *Indiana Univ Math J*. 2000;49(1):113-142.
12. Duan C, Chen W, Liu C, Yue X, Zhou S. Structure-preserving numerical methods for nonlinear Fokker-Planck equations with nonlocal interactions by an energetic variational approach. *SIAM J Sci Comput*. 2021;43(1):B82-B107.
13. Liu H, Wang Z. An entropy satisfying discontinuous Galerkin method for nonlinear Fokker-Planck equations. *J Sci Comput*. 2016;68(3):1217-1240.
14. Qian Y, Wang Z, Zhou S. A conservative, free energy dissipating , and positivity preserving finite difference scheme for multi-dimensional nonlocal Fokker-Planck equation. *J Comput Phys*. 2019;386(1):22-36.
15. Carrillo JA, Jüngel A, Markowich PA, Toscani G, Unterreiter A. Entropy dissipation methods for degenerate parabolic problems and generalized Sobolev inequalities. *Monatshefte Math*. 2001;133(1):1-82.
16. Sun Z, Carrillo JA, Shu C-W. A discontinuous Galerkin method for nonlinear parabolic equations and gradient flow problems with interaction potentials. *J Comput Phys*. 2018;352:76-104.
17. Bailo R, Carrillo JA, Hu J. Fully discrete positivity-preserving and energy-dissipating schemes for aggregation-diffusion equations with a gradient-flow structure. *Commun Math Sci.* 2020;18(5):1259-1303. https://doi.org/10.4310/CMS.2020.v18.n5.a5
18. Bessemoulin-Chatard M, Filbet F. A finite volume scheme for nonlinear degenerate parabolic equations, SIAM. *J Sci Comput*. 2012;34(5):559-583.
19. Liu H, Maimaitiyiming W. Positive and free energy satisfying schemes for diffusion with interaction potentials. *J Comput Phys*. 2020;419:109483.
20. Liu H, Yu H. The entropy satisfying discontinuous Galerkin method for Fokker-Planck equations. *J Sci Comput*. 2015;62:803-830.
21. Liu H, Yu H. Maximum-principle-satisfying third order discontinuous Galerkin schemes for Fokker-Planck equations. *SIAM J Sci Comput*. 2014;36(5):A2296-A2325.
22. Carrillo JA, Huang Y, Patacchini FS, Wolansky G. Numerical study of a particle method for gradient flows. *Kinet Relat Models*. 2017;10(3):613-641.
23. Carrillo JA, Ranetbauer H, Wolfram MT. Numerical simulation of nonlinear continuity equations by evolving diffeomorphisms.*J Comput Phys*. 2016;327:186-202.
24. Ding J, Wang Z, Zhou S. Positivity preserving finite difference methods for Poisson–Nernst–Planck equations with steric interactions: Application to slit-shaped nanopore conductance. *J Comput Phys*. 2019;397:108864.
25. Ding J, Wang Z, Zhou S. Structure-preserving and efficient numerical methods for ion transport. *J Comput Phys*. 2020;418:109597.
26. Hu J, Huang X. A fully discrete positivity-preserving and energy-dissipative finite difference scheme for Poisson–Nernst–Planck equations. *Numer Math*. 2020;145:77-115.
27. Liu H, Wang Z. A free energy satisfying discontinuous Galerkin method for one-dimensional Poisson-Nernst-Planck systems. *J Comput Phys*. 2017;328:413-437.
28. Liu C, Wang C, Wise S, Yue X, Zhou S. A positivity-preserving, energy stable and convergent numerical scheme for the Poisson-Nernst-Planck system. *Math Comp*. 2021;90:2071-2106.
29. Qian Y, Wang C, Zhou S. A positive and energy stable numerical scheme for the Poisson–Nernst–Planck–Cahn–Hilliard equations with steric interactions. *J Comput Phys*. 2021;426:109908.
30. Metti MS, Xu J, Liu C. Energetically stable discretizations for charge transport and electrokinetic models. *J Comput Phys*. 2016;306:1-18.
31. Weinan E, Liu JG. Projection method I: convergence and numerical boundary layers. *SIAM J Numer Anal*. 1995;32:1017-1057.
32. Liu JG. Projection method. III. Spatial discretization on the staggered grid. *Math Comp*. 2002;71:27-47.
33. Samelson R, Temam R, Wang C, Wang S. Surface pressure Poisson equation formulation of the primitive equations: Numerical schemes. *SIAM J Numer Anal*. 2003;41:1163-1194.
34. Wang C, Liu JG. Convergence of gauge method for incompressible flow. *Math Comp*. 2000;69:1385-1407.
35. Duan C, Chen W, Liu C, Wang C, Yue X. A second order accurate, energy stable numerical scheme for porous medium equation by an Energetic Variational approach. *Commun Math Sci*. 2021. Accepted and in press.
36. Duan C, Liu C, Wang C, Yue X. Convergence analysis of a numerical scheme for the porous medium equation by an energetic variational approach. *Numer Math Theor Meth Appl*. 2020;13:63-80.
37. Li X, Qiao Z, Wang C. Convergence analysis for a stabilized linear semi-implicit numerical scheme for the nonlocal Cahn-Hilliard equation. *Math Comp*. 2021;90:171-188.
38. Eyre DJ. Unconditionally gradient stable time marching the Cahn-Hilliard equation. In: *MRS Proceedings*. Vol. 529. Cambridge Univ Press; 1998:39.
39. Duan C, Liu C, Wang C, Yue X. Numerical complete solution for random genetic drift by energetic variational approach. *ESAIM Math Model Num*. 2019;53(2):615-634.
40. Baskaran A, Lowengrub JL, Wang C, Wise SM. Convergence analysis of a second order convex splitting scheme for the modified phase field crystal equation. *SIAM J Numer Anal*. 2013;51:2851-2873.
41. Guan Z, Lowengrub JL, Wang C. Convergence analysis for second order accurate schemes for the periodic nonlocal Allen-Cahn and Cahn-Hilliard equations. *Math Model Appl Sci*. 2017;40:6836-6863.
42. Guan Z, Wang C, Wise SM. A convergent convex splitting scheme for the periodic nonlocal Cahn-Hilliard equation. *Numer Math*. 2014;128:377-406.

43. Wang C, Liu JG. Analysis of finite difference schemes for unsteady Navier-Stokes equations in vorticity formulation. *Numer Math*. 2002;91:543-576.
44. Wang C, Liu JG, Johnston H. Analysis of a fourth order finite difference method for incompressible Boussinesq equations. *Numer Math*. 2004;97:555-594.
45. Wang L, Chen W, Wang C. An energy-conserving second order numerical scheme for nonlinear hyperbolic equation with an exponential nonlinear term. *J Comput Appl Math*. 2015;280:347-366.
46. Duan C, Liu C, Wang C, Yue X. Numerical methods for porous medium equation by an energetic variational approach. *J Comput Phys*. 2019;385:13-32.
47. Carrillo JA, Gualdani MP, Jüngel A. Convergence of an entropic semi-discretization for nonlinear Fokker-Planck equations in R^d. *Publ Mat*. 2008;52:413-433.

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