On Lagrangian schemes for the multidimensional porous medium equations by a discrete energetic variational approach

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Abstract

In this paper, we present a systematic framework to derive a Lagrangian scheme for general diffusion equations in multiple spatial dimensions by employing a discrete energetic variational approach. Such discrete energetic variational approaches are analogous to energetic variational approaches \([32, 21]\) in a semidiscrete level, which provide a basis of deriving the “semi-discrete equations” and can be applied to a large class of partial differential equations with energy-dissipation laws and kinematic relations. The numerical schemes derived by this framework can inherit various properties from the continuous energy-dissipation law, such as conservation of mass and the dissipation of the discrete energy. As an illustration, we develop two numerical schemes for the multidimensional porous medium equations (PME), based on two different energy-dissipation laws. We focus on the numerical scheme based on the energy-dissipation law with \(\frac{1}{2}\int_{\Omega}|u|^2\,dx\) as the dissipation. Several numerical experiments demonstrate the accuracy of this scheme as well as its ability in capturing the free boundary and estimating the waiting time for the PME in both 1D and 2D.

1. Introduction

The porous medium equation (PME) is an example of nonlinear evolution equations, which can be used in many physical and biological applications, such as the flow of an ideal gas through a porous medium \([29]\), radiative transfer theory \([30]\), biological aggregation \([51]\), population dynamics \([55]\), and tumor growth \([45]\). Besides its own applications in many diverse fields, the PME can be viewed as examples of general diffusions under the framework of energetic variational approaches (EnVarA) \([21]\).

One standard type of the initial-boundary problem of the PME can be written as

\[
\rho_t = c\Delta \rho^\alpha, \quad x \in \Omega \subset \mathbb{R}^d, \quad \alpha > 1, \quad t > 0, \\
\rho(x, 0) = \rho_0(x), \quad x \in \Omega, \\
\frac{\partial \rho}{\partial n} = 0, \quad x \in \partial\Omega, \quad t > 0,
\]

(1.1)

where \(\rho\) is a non-negative function, \(\Omega\) is a bounded domain and \(n\) is the external normal direction in \(\partial\Omega\). The constant \(c\) in (1.1) can be easily scaled out \([52]\), so we take \(c = 1\) in the following.

There are two important properties of the PME when the initial data has a compact support in \(\Omega\), known as the finite speed propagation and the waiting time phenomena, due to its degeneracy at \(\rho = 0\). Theoretical studies \([10, 27, 28, 55, 3, 52]\) have shown that the existence of the solutions
to the PME, which will have a compact support at any time \( t > 0 \) if the initial data has a compact support. The interface between the compact support and zero-region, called the free boundary, will move outward in a finite speed. Unlike the heat equation, the solution of the PME could become non-smooth even if the initial data is smooth. Moreover, for a certain initial data, the interface will not move until a finite positive time, called the \textit{waiting time} \cite{28, 3}.

From a numerical perspective, its lack of regularity and free boundary \cite{1, 3, 52} poses challenges for numerical simulations for the PME. For instance, numerical solutions by standard numerical approaches, such as PCSFE (Predictor-Correction Algorithm and Standard Finite Element) method, may contain oscillations near the free boundary, which cannot be removed by raising the degree of finite element space and/or by refining spatial meshes \cite{57}. On the other hand, it is difficult to track the movement of free boundary and estimate the waiting time of the PME in high accuracy. During the past, quite a number of numerical methods have been proposed for the PME \cite{50, 22, 16, 23, 6, 24, 36, 25, 12, 57, 63, 1, 5, 38, 39}, most of them are focus on the one-dimensional case.

A commonly used numerical approach is the interface tracking algorithm \cite{50, 22, 16, 23, 6, 24, 36}, in which the interface equation are solved in Lagrangian coordinate, while the solution inside the numerical support is updated in Eulerian coordinate. However, it is not easy to apply such method to the PME in high spatial dimensions and the case with complex support. In order to eliminate the oscillations around the free boundary, some numerical methods from hyperbolic conservation law, such as relaxation scheme \cite{25, 12}, locally discontinuous Galerkin (LDG) \cite{57} and WENO \cite{33}, have been applied to the PME successfully. Since the solution of the PME always steeper near the interface, some adaptive moving mesh methods have proved to be useful in solving the PME \cite{7, 5, 4, 38, 39}, especially in multiple space dimensions. A typical moving mesh method updates the computational mesh according to the monitor function defined by the numerical solution at current time, which might effect the dynamic of evolution. Hence, it might be difficult to track the free boundary and estimate the waiting time in high accuracy within the adaptive moving mesh methods.

While most of previous numerical approaches are Eulerian methods, there has been an increasing interesting in designing some Lagrangian methods for the equations like the PME \cite{8, 53, 9, 26, 11, 35, 10}. The Lagrangian methods is particularly suitable for the problem involving sharp interface and free boundary, especially for those with singularity. However, it is a common challenge to solve the Lagrangian scheme numerically, especially in high spatial dimensions. Moreover, most of Lagrangian methods start with the nonlinear PDEs for the Lagrangian maps \cite{9, 11, 17}, it might be difficult to choose the proper weak form to preserve the original variational structure. Our approach is quite close to the methods based on gradient flow structure in the \( L_2 \)-Wasserstein metric \cite{8, 53, 9, 26, 11, 35, 10}, but a different variational structure is used, which might be more natural from a physical point of view.

In this paper, we present a systematic framework to construct numerical schemes to general diffusion equations by a discrete energetic variational approach, which can be easily applied to multiple spatial dimensions. A discrete energy variational approach can be regarded as an analogue to the energetic variational approach \cite{32, 21} in a semidiscrete level, which provides a general framework to derive the “semi-discrete equations”, a system of ordinary differential equations in time, after introducing a proper discretization to the energy-dissipation law in space. As an illustration, we develop two numerical schemes for the multidimensional porous medium equations (PME), based on two different energy-dissipation laws. We focus on the numerical scheme based on the energy-dissipation law with \( \frac{1}{2} \int_\Omega |u|^2 \, dx \) as the dissipation. Several numerical experiments demonstrate the accuracy of this scheme as well as its ability in capturing the free boundary and estimating the waiting time for the PME in both 1D and 2D.

The rest of the paper is organized as follows. In section 2, we briefly review the energetic
variational approaches in a continuous level. In section 3, we introduce a discrete energetic variational approach for nonlinear diffusion equation and apply it to construct the numerical schemes for the PME. The numerical results for the PME in one and two spatial dimensions are presented in sections 4.

2. Energetic Variational Approaches

For a given energy-dissipation law and the kinematic (transport) relations, an energetic variational approach provides a general framework to determine the dynamics of system in a unique and well-defined way, through two distinct variational processes: Least Action Principle (LAP) and Maximum Dissipation Principle (MDP) [32, 21]. This approach is originated from pioneering work of Onsager [41, 42] and Rayleigh [48], and has been successfully applied to build up many mathematical models for complex fluids [32, 49, 18, 21].

The starting point of an energetic variational approach is the first and second laws of thermodynamics [21], which yields the following energy-dissipation law

$$\frac{d}{dt} E^{\text{total}}(t) = -2D(t),$$

for an isothermal closed system. $E^{\text{total}}$ is the total energy, which is the sum of the Helmholtz free energy $F$ and the kinetic energy $K$. $2D$ is the rate of energy dissipation, which is related to the entropy production in thermodynamics. The Least Action Principle states that the dynamics of a conservative system is determined as a critical point of the action functional

$$\delta A = \int_{T_0}^T \int_{\Omega(t)} \left( f_{\text{inertial force}} - f_{\text{conservative force}} \right) \cdot \delta \mathbf{x} \, d\mathbf{x} \, dt,$$

with respect to $\mathbf{x}$ (the trajectory in Lagrangian coordinates, if applicable) [2, 21], i.e.,

$$\delta A = \int_{T_0}^T \int_{\Omega(t)} \left( f_{\text{inertial force}} - f_{\text{conservative force}} \right) \cdot \delta \mathbf{x} \, d\mathbf{x} \, dt.$$

On the other hand, for a dissipative system ($D \geq 0$), according to Onsager [41, 42], the dissipative force can be obtained by minimization of the dissipation functional $D$ with respect to the “rate” $\mathbf{x}_t$, known as Maximum Dissipation Principle (MDP), i.e.,

$$\delta D = \int_{\Omega(t)} f_{\text{dissipative force}} \cdot \delta \mathbf{x}_t \, d\mathbf{x}.$$

Then, according to the force balance (Newton’s second law, in which the inertial force plays role of $ma$), we have

$$\frac{\delta A}{\delta \mathbf{x}} = \frac{\delta D}{\delta \mathbf{x}_t},$$

in Eulerian coordinates. We refer the reader to [21] for more detailed description of energetic variational approaches. Here we only focus on the derivation of the porous medium equations by an energetic variational approach.

From an energetic variational approach point of view, the PME can be viewed as a nonlinear diffusion [21], in which $\rho(\mathbf{x}, t)$ is a conserved quantity satisfying kinematic (transport) equation

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0.$$

For a given velocity field $\mathbf{u}(\mathbf{x}, t)$, one can define the corresponding flow map $\mathbf{x}(\mathbf{X}, t) : \Omega_0 \to \Omega_t$ as

$$\mathbf{x}_t = \mathbf{u}, \quad \mathbf{x}(\mathbf{X}, 0) = \mathbf{X}, \quad \mathbf{X} \in \Omega_0,$$
where $X$ are the Lagrangian coordinates and $x$ are Eulerian coordinates. The deformation matrix (the deformation gradient) $F(X, t)$ of the flow map $x(X, t)$ is defined by

$$F(X, t) = \nabla_X x(X, t),$$

(2.7)

which determines the kinematic relations of physical quantities in Lagrangian coordinates. For instance, the mass conservation (2.5) can be written equivalently as

$$\rho(x(X, t), t) = \rho_0(X)/\det F(X, t),$$

(2.8)

where $\rho_0(X)$ is the initial mass. One can view (2.8) as a composition of the flow map $x(X, t)$ and the initial density $\rho_0(X)$, i.e.,

$$\rho(x, t) = \rho_0 \circ X^{-1}(x, t),$$

(2.9)

where $X^{-1} : \Omega_t \to \Omega_0$ is the inverse of the flow map $x(X, t)$.

**Remark 2.1.** The scalar transport $\phi_t + (u \cdot \nabla)\phi = 0$ is equivalent to $\phi(x(X, t), t) = \phi_0(X)$ in the Lagrangian coordinates, which also can be viewed as a composition

$$\phi(x, t) = \phi_0 \circ X^{-1}(x, t).$$

(2.10)

**Remark 2.2.** The “initial data”, or “reference data”, $\rho_0(X)$ ($\phi_0(X)$) carries many information of the solutions, which may not be available for general problems. In practice, one may obtain $\rho_0(X)$ ($\phi_0(X)$) from other methods, such as those of Eulerian approaches.

In a diffusion, the kinetic energy $K$ is neglected, and the energy dissipation $D$ is taken to be $\frac{1}{2} \int_{\Omega_t} \eta(\rho)|u|^2$ like the Darcy’s law (the friction to the resting media) [21]. Hence, the overall energy-dissipation law for a diffusion is given by

$$\frac{d}{dt} \int_\Omega \omega(\rho) dx = -\int_\Omega \eta(\rho)|u|^2 dx,$$

(2.11)

where $\omega(\rho)$ is the free energy density, which is convex with respect to $\rho$, and $u$ is the velocity.

We first perform the LAP, i.e., compute a variation of $A = \int_0^T -F dt$ with respect to $x(X, t)$. Direct computation results in

$$\delta A = -\delta \int_0^T \int_{\Omega_0} \omega(\rho_0(X)/\det F) \det F dF dX$$

$$= -\int_0^T \int_{\Omega_0} \left( -\omega_\rho \left( \frac{\rho_0(X)}{\det F} \right) \frac{\rho_0(X)}{\det F} + \omega \left( \frac{\rho_0(X)}{\det F} \right) \right) (F^{-T} : \nabla_X \delta x) \det F dF dX,$$

(2.12)

where $\delta x$ is the test function. It can be noticed that even for this simple case, the variational result in Lagrangian coordinates is quite complicated, which involves $F^{-1}$ and det $F$.

Pull [2.12] back to Eulerian coordinates and apply the integration by parts, one can get

$$\delta A = -\int_0^T \int_\Omega (-\omega_\rho + \omega) (\nabla_x \cdot \delta x) dx dt = -\int_0^T \int_\Omega \nabla [\omega_\rho - \omega] \cdot \delta x dx dt,$$

(2.13)

where the boundary term vanishes due to the choice of $\delta x$.

The MDP can be done by taking variational of $D$ with respect to $x_t$, one can easily obtain
that
\[ \int \text{dissipative force} = \frac{\delta D}{\delta x_t} = \eta(\rho) x_t, \tag{2.14} \]

By the force balance \( \frac{\delta A}{\delta x} = \frac{\delta D}{\delta x_t} \), an energetic variational approach leads to
\[ \eta(\rho) u = -\nabla p, \tag{2.15} \]
where \( p = \omega \rho - \omega \). Combining with the mass conservation \( \text{(2.5)} \), we can get a generalized diffusion equation
\[ \rho_t = \nabla \cdot (\rho \eta(\rho) \nabla p(\rho)). \tag{2.16} \]

For the PME, a commonly used energy-dissipation law is to take \( \omega(\rho) = \frac{1}{\alpha-1} \rho^\alpha \) and \( \eta(\rho) = \rho \), i.e.
\[ \frac{d}{dt} \int \Omega \frac{1}{\alpha-1} \rho^\alpha = -\int \Omega \rho |u|^2 dx, \tag{2.17} \]
Then, the force balance gives
\[ \rho u = -\nabla \rho^\alpha, \tag{2.18} \]
which in turns yields the original PME \( \text{(1.1)} \) by \( \text{(2.16)} \).

It should be remarked that same governing equations can be obtained by using different \( \omega(\rho) \) and \( \eta(\rho) \) [see 17 for examples in the PME]. Correspondingly, different numerical schemes can be derived based on different energy-dissipation laws. Besides the classical energy-dissipation law \( \text{(2.17)} \) and the two used in \([17]\), we can employ another energy-dissipation law
\[ \frac{d}{dt} \int \Omega \omega(\rho) dx = -\int \Omega |u|^2 dx, \quad \omega(\rho) = \begin{cases} 2\rho \ln \rho, & \alpha = 2, \\ \frac{2\rho \ln \rho}{(\alpha-1)(\alpha-2)} \rho^{\alpha-1}, & \alpha > 2, \end{cases} \tag{2.19} \]
for the PME with \( \alpha \geq 2 \) to construct a numerical scheme. Following the above computation, one can verify that, under the energy-dissipation law \( \text{(2.19)} \), the force balance results in
\[ u = -\nabla \left( \frac{\alpha}{\alpha-1} \rho^{\alpha-1} \right), \tag{2.20} \]
which is equivalent to \( \text{(2.18)} \) on the compact support of \( \rho_0(X) \). We will show that in the following sections the numerical scheme derived from \( \text{(2.19)} \) has an advantage in tracking the free boundary in the PME, especially in multiple spatial dimensional situation.

**Remark 2.3.** Although the energy-dissipation law \( \text{(2.19)} \) is only defined for the PME with \( \alpha \geq 2 \), the force balance \( \text{(2.20)} \), i.e., the trajectory equation, is well defined for \( \alpha > 1 \). In the later section, we will show that the numerical scheme derived from \( \text{(2.19)} \) also works well for the case that \( 1 < \alpha < 2 \), although it can be interpreted through \( \text{(2.19)} \) in such cases.

3. A discrete energetic variational approach and numerical schemes

In this section, we introduce the abstract framework of a discrete energetic variational approach, and apply it to construct some Lagrangian schemes for the PME. Instead of numerically approximating \( \rho(x, t) \) in Eulerian coordinates, our numerical methods approximate the flow map \( x(X, t) \) directly, and the value of \( \rho(x, t) \) is determined by the kinematic relation (transport
equation)\textsuperscript{(2.8)}, i.e., a composition of the flow map $x(X, t)$ and the initial data $\rho_0(X)$:

$$
\rho(x, t) = \rho_0 \circ X^{-1}(x, t) = \frac{\rho_0(X)}{\det F(X, t)}.
$$

(3.1)

This is the main difference between our numerical approach and most of traditional approaches. Although we will focus on the PME in this section, one can apply this approach to construct a structure-preserving Lagrangian scheme for a large class of PDEs with an energy-dissipation law and a kinematic relation, especially those of general diffusions, such as Cahn-Hilliard and PNP\textsuperscript{[21]}. As mentioned in the beginning, a discrete energetic variational approach is an analogue to an energetic variational approach in a semidiscrete level. We first write down the energy-dissipation law in a semidiscrete level by discretization the flow map $x(X, t)$ in space. In current study, we will discretize $x(X, t)$ by a piecewise linear map. An advantage of a piecewise linear approximation to the flow map $x(X, t)$ is that the deformation matrix $F(X, t)$ is piecewise constant (matrix) for give $t$, so are the $\det F(X, t)$ and $F(X, t)^{-1}$.

One way to construct a piecewise linear approximation to the flow map $x(X, t)$ is to use a finite element method\textsuperscript{[10]}. To be more precise, let $T_h$ be triangulation of $\Omega_0 \subset \mathbb{R}^d$. $T_h$ consists of a set of simplexes $\{\tau_e \mid e = 1, \ldots, M\}$ and a set of nodal points $N_h = \{X_1, X_2, \ldots, X_N\}$. Define the finite element space by

$$
V_h = \{v \in C(\Omega_0) \mid v \text{ is linear on each element } \tau_e \in T_h\},
$$

(3.2)

which is a linear finite element space. Then the flow map $x(X, t)$ can be approximated by

$$
x_h(X, t) = \sum_{i=1}^{N} \xi_i(t) \phi_i(X) \in V_h,
$$

(3.3)

where $\phi_i(X) : \mathbb{R}^d \to \mathbb{R}$ is the hat function satisfies $\phi_i(X_j) = \delta_{ij}$, and $\xi_i(t) \in \mathbb{R}^d$ are coefficients to be determined later. We let

$$
\Xi(t) = \begin{pmatrix} \xi_1^{(1)}(t), \xi_2^{(1)}(t), \ldots, \xi_N^{(1)}(t), \ldots, \xi_1^{(d)}(t), \xi_2^{(d)}(t), \ldots, \xi_N^{(d)}(t) \end{pmatrix} \in \mathbb{R}^K,
$$

where $K = N \times d$.

Since $x_h(X, t) = \xi_i$, one can view $\xi_i(t)$ as coordinates in $\Omega_t$ and $x_h(X_i, t)$ as a trajectory of a “particle” $X_i$. The finite element method enables us to compute the deformation matrix $F_h(X) = \nabla_X x_h$ explicitly for given $\Xi$. We can write down the deformation matrix $F_h(X)$ as a $d \times d$-matrix-valued function of $\Xi$ on each element $\tau_e$, denoted by

$$
F_e(\Xi) = \nabla_X x_h \big|_{X \in \tau_e}.
$$

The admissible set of $\Xi$ is defined by

$$
F_{ad}^{\Xi} = \{\Xi \in \mathbb{R}^K \mid \det F_e(\Xi) > 0, \quad e = 1, \ldots, M\}.
$$

(3.4)

Correspondingly, the admissible set for $x_h$ is defined by

$$
F_{ad}^{x_h} = \left\{ x_h(X, t) = \sum_{i=1}^{N} \xi_i(t) \phi_i(X) \mid \Xi(t) \in F_{ad}^{\Xi} \right\}.
$$
The non-negativity of \( \rho(x_h(X, t), t) \) is naturally preserved as if \( x_h(X, t) \) is in the admissible set \( \mathcal{F}^{x_h} \).

For a given energy-dissipation law (2.11), in which \( \mathcal{K} = 0 \), by substituting (3.3) into the original action functional \( \mathcal{A} \) and the dissipation \( \mathcal{D} \), we can get a discrete action functional \( \mathcal{A}_h \) in terms of \( \Xi(t) \) and a discrete dissipation \( \mathcal{D}_h \) in terms of \( \Xi(t) \) and \( \Xi'(t) \). Similar to a continuous energetic variational approach stated in sect. 2, we can get the governing equation of terms of \( \Xi(t) \).

A discrete energetic variational approach follows the “discretize-then-variation” strategy [19, 14]. The idea of “discretize-then-variation”, or “discretize-then-minimize”, has been successfully applied to a large class of PDEs [19, 14, 8, 9, 15, 53]. In a recent published book [19], Furihata and Matsuo show that it is a systematic way to derive a structure-preserving numerical methods.

In the following, we apply a discrete energetic variational approach to derive numerical schemes for a general diffusion with energy-dissipation law (2.11), especially the PME, in 2D. The numerical schemes in other spatial dimensions follow easily from this. In order to simplify the notation, we let \( \xi(t) = (a_1(t), b_1(t)) \), and denote

\[
a(t) = (a_1(t), a_2(t), \ldots a_N(t)), \quad b(t) = (b_1(t), b_2(t), \ldots, b_N(t)).
\]

Hence, \( \Xi(t) = (a(t), b(t)) \). Let \( N(e) \) be all the indices \( e \) such that \( X_i \) is contained in \( \tau_e \) for given \( X_i \in \mathcal{N}_h \). The support of \( \phi_i \) is denote by

\[
G(i) = \cup_{e \in N(i)} \tau_e.
\]
For each element \( \tau_e \), the nodes of \( \tau_e \) are denoted by \( X^0_i, X^1_i, X^2_i \), the global index of the nodes of \( \tau_e \) are denoted by \( e_n(c,l) \) \((l = 1, 2, 3)\).

Substituting (3.3) into (2.11), we get a discrete action functional

\[
A_h(a(t), b(t)) = - \int_0^T \int_{\Omega} \omega \left( \frac{\rho_0(X)}{\det F(X, t)} \right) \det F(X, t) dX dt
\]

and the discrete dissipation

\[
D_h(\alpha'(t), \beta(t), \alpha(t), \beta(t)) = \frac{1}{2} \int_{\Omega} \eta(\rho) |x|^2 \det F(X, t) dX,
\]

where

\[
F_e(t) := F_e(a(t), b(t)) = \nabla_X x_h |_{X \in \tau_e}
\]
is the deformation matrix \( F(X, t) \) on each element \( \tau_e \) at \( t \), which can be written down as a function of \( a_{en(c,l)}(t) \) and \( b_{en(c,l)}(t) \) \((l = 1, 2, 3)\) explicitly [see Appendix].

By taking the variation of (3.8) with respect to \( a_i(t) \) and \( b_i(t) \), we have

\[
\frac{\delta A_h}{\delta a_i}(a(t), b(t)) = -\sum_{e=1}^{N} \sum_{\tau_e} \frac{\partial}{\partial a_i} \int_{\tau_e} \omega \left( \frac{\rho_0(X)}{\det F_e(t)} \right) \det F_e(t) dX,
\]

\[
\frac{\delta A_h}{\delta b_i}(a(t), b(t)) = -\sum_{e=1}^{N} \sum_{\tau_e} \frac{\partial}{\partial b_i} \int_{\tau_e} \omega \left( \frac{\rho_0(X)}{\det F_e(t)} \right) \det F_e(t) dX,
\]

where

\[
\frac{\partial}{\partial \chi} \int_{\tau_e} \omega \left( \frac{\phi_0(X)}{\det F_e} \right) \det F_e dX = \int_{\tau_e} (-\omega \rho + \omega) \left( F_e^{-T} : \frac{\partial F_e}{\partial \chi} \right) \det F_e dX,
\]
on each element \( \tau_e \), \( \chi = a_{en(c,l)} \) or \( b_{en(c,l)} \).

On the meantime, taking variations of (3.14) with respect to \( a'_i(t) \) and \( b'_i(t) \) results in

\[
\frac{\delta D_h}{\delta a'_i} = \sum_{i=1}^{N} \sum_{\tau_e} \eta(\rho) \left( \sum_{j=1}^{N} a'_j(t) \phi_j(X) \right) \phi_i(X) \det F_e(t) dX = M_{ij}(a(t), b(t)) a'_j(t),
\]

\[
\frac{\delta D_h}{\delta b'_i} = \sum_{i=1}^{N} \sum_{\tau_e} \eta(\rho) \left( \sum_{j=1}^{N} b'_j(t) \phi_j(X) \right) \phi_i(X) \det F_e(t) dX = M_{ij}(a(t), b(t)) b'_j(t),
\]

where Einstein summation notation is used, \( \eta(\rho) = \eta(\rho_0(X)/\det F_e(t)) \), and \( M_{ij}(a(t), b(t)) \) is
defined by
\[ M_{ij}(a(t), b(t)) = \sum_{i=1}^{N} \sum_{e \in N(i)} \int_{\tau_e} \eta(\rho) \phi_j(X) \phi_i(X) \det F_e(t) \, dX. \] (3.13)

Hence, the force balance (3.5) results in the “semi-discrete equations”
\[
M_{ij}(a(t), b(t)) a_i'(t) = \delta A_h \delta a_i(a(t), b(t)),
\]
\[
M_{ij}(a(t), b(t)) b_j'(t) = \delta A_h \delta b_i(a(t), b(t)),
\] (3.14)
for \( i = 1, 2, \ldots, N \), which can be discretized in time by using some numerical method for systems of ordinary differential equations. It can be noticed that there exist crossing terms in both sides of (3.14).

Remark 3.2. In this special case, \( D(\Xi(t), \Xi'(t)) \) in (3.6) doesn’t depend on \( \Xi'(t) \), and
\[
D(\Xi(t), \Xi'(t)) = \begin{pmatrix} M(a(t), b(t)) & 0 \\ 0 & M(a(t), b(t)) \end{pmatrix},
\] (3.15)
which is a symmetric matrix.

Although both (3.10) and (3.12) involve the numerical integration over each element, they can be computed out by centroid method (known as midpoint method in 1D). As \( F(X, t) \), \( \det F(X, t) \) and \( F(X, t)^{-1} \) are approximated in a piecewise constant manner, using high-accuracy numerical quadrature over each element cannot improve the numerical accuracy. This is another advantage of the piecewise linear approximation to the flow map, which is actually quadrature-free and can be applied to a high spatial dimensional case. The computational cost is roughly proportional to the number of nodes (“particle”). One can view our numerical approach as a type of cell-centered Lagrangian scheme, where the momentum is defined at the nodes and the other variables (density, pressure, and specific internal energy) are cell-centered [34]. In the following, we denote
\[
\rho_0^e = \rho_0(X_c^e), \quad \rho_c(t) = \rho_0(X_c^e) / \det F_e(t),
\]
where \( X_c^e \) is the centroid of \( \tau_e \).

Remark 3.3. In general, we cannot have an explicit form for the “semi-discrete equation” (3.14) in high dimensional situations, as (3.10) and (3.13) depend on the triangulation \( T_h \). In practice, \( M_{ij}(a(t), b(t)) \) and \( \delta A_h \delta a_i(a(t), b(t)) \) can be assembled using the standard technique in the finite element methods, that is, summing the results on each element over the mesh [31].

In order to get a numerical scheme, we need to introduce a proper temporal discretization to the “semi-discrete equation” (3.14). One can use explicit Euler scheme, and the numerical scheme can be written as
\[
M_{ij}^n(a^n, b^n) \frac{a_i^{n+1} - a_i^n}{\tau} = \delta A_h \delta a_i(a^n, b^n),
\]
\[
M_{ij}^n(a^n, b^n) \frac{b_j^{n+1} - b_j^n}{\tau} = \delta A_h \delta b_i(a^n, b^n),
\] (3.16)
where
\[ M_{ij}^n(a^n, b^n) = \sum_{e \in N(i)} \int_{\tau} \eta(\rho^n) \phi_j(X) \phi_i(X) \text{det} F^{-1}_n dX. \] (3.17)

Although the explicit Euler scheme is simple in the numerical implementation, one have to choose \( \tau \) to be significantly small to ensure \( \Xi_{n+1} \in F_{n+1} \) and the dissipation of the discrete energy.

A better approach is to adopt a backward Euler scheme for the temporal discretization, i.e.,
\[ M_{ij}^*(a^n, b^n) = \frac{a_i^{n+1} - a_i^n}{\tau}, \]
\[ M_{ij}^*(a^n, b^n) = \frac{b_j^{n+1} - b_j^n}{\tau}, \] (3.18)

where \( M_{ij}^*(a^n, b^n) \) is defined by
\[ M_{ij}^*(a^n, b^n) = \sum_{e \in N(i)} \int_{\tau} \eta(\rho^n) \phi_j(X) \phi_i(X) \text{det} F^{-1}_n dX, \] (3.19)

and \( \gamma_i = n \) or \( n + 1 \). In practice, we have the choice of taking \( \eta(\rho(t)) \) and \( \text{det} F(t) \) in (3.13) explicitly or implicitly, such that \( M^* \) depends on \( a^n, b^n \), but is independent with \( a^{n+1}, b^{n+1} \). The theoretical analysis of the choice are in the progress.

**Remark 3.4.** One can also adopt some high-order temporal discretization to the “semi-discrete equations” (3.14). However, the resulting numerical scheme might be difficult to deal with. We will study the high-order temporal discretization in the future work.

**Remark 3.5.** In general, discrete-then-variation and variation-then-discrete may give us different numerical scheme. In order to get the numerical schemes (3.16) and (3.18), one should substitute (3.3) into a particular weak form of the force balance (2.15) (strong form of the variations results), and introduce a proper approximation and temporal discretization. A weak form of (2.13) can be written as
\[ \int_{\Omega} \eta(\rho) x_1 \cdot y \text{det} F dX = - \int_{\Omega} (\omega \rho + \omega) (F^{-T} : \nabla x y) \text{det} F dX, \] (3.20)

where \( y \) is a test function, \( F = \nabla x x \). One can get (3.18) by taking the test function \( y = \phi_i \) \((i = 1, \ldots N)\) and approximating (3.20) by
\[ \int_{\Omega} \eta(\rho^n) x_i^{n+1} - x_i^n \cdot y \text{det} F^{-1} dX = - \int_{\Omega} (\omega \rho + \omega) (F^{-T} : \nabla x y) \text{det} F^{n+1} dX. \] (3.21)

It should be remarked that we might need to approximate \( \text{det} F \) in both side of (3.20) in different manners (explicitly or implicitly) to get back to (3.18). From an energetic variational approach point of view, the test functions may be in different space for the LAP and the MDP. Hence, starting with the force balance (2.13) may not give us a structure-preserving Lagrangian scheme without using a proper weak form.

The above framework works for any general diffusions has the energy-dissipation law (2.11) and the kinematic relation (2.5). Next, we apply such framework to develop two numerical schemes for the PME based on energy-dissipation law (2.17) and (2.19). The RHS of (3.18) can
be computed from (3.10) and (3.11) for a given $\omega(\rho)$. For the LHS in (3.18), we take
\[
M^e_{ij}(a^n, b^n) = \sum_{e \in N(i)} \int_{\tau_e} \rho_0(X) \phi_j(X) \phi_i(X) dX.
\] (3.22)
for the PME with energy-dissipation law (2.17), while for the energy-dissipation law (2.19), we take
\[
M^e_{ij}(a^n, b^n) = \sum_{e \in N(i)} \int_{\tau_e} \phi_j(X) \phi_i(X) dF^n dX.
\] (3.23)
We call the numerical scheme (3.18) with (3.22) as the scheme 1, which is based on energy-dissipation law (2.17), while (3.18) with (3.23) is called the scheme 2, which is based on energy-dissipation law (2.19). One can develop other numerical schemes for the PME by other different energy-dissipation laws, such as two used in Ref. [17].

**Remark 3.6.** For the two dimensional case, we cannot have an explicit form for the numerical scheme (3.18) in a general mesh, as $\frac{\delta A_h}{\delta a_{en(e,l)}(a^{n+1}, b^{n+1})}$ and $M^e(a^n, b^n)$ depend on the triangulation $T_h$. But during the computer implementation, since we have the explicit form of $F$, as a function of $a_{en(e,l)}$ and $b_{en(e,l)}$ on each element $\tau_e$ (shown in the Appendix), we can compute $\frac{\delta A_h}{\delta a_{en(e,l)}}(a^{n+1}, b^{n+1})$ and $M^e(a^n, b^n)$ by using the standard technique in finite element methods, that is, summing the results on each element over the mesh [31]. For instance, $\frac{\delta A_h}{\delta a_{en(e,l)}}(a^{n+1}, b^{n+1})$ and $M^e(a^n, b^n)$ in our scheme 2 [scheme (3.18)] can be computed by Algorithm 1 and Algorithm 2. We can have an explicit form of

```
Algorithm 1: Assembly of $\frac{\delta A_h}{\delta a_{en(e,l)}}(a^{n+1}, b^{n+1})$ or $\frac{\delta A_h}{\delta b_{en(e,l)}}(a^{n+1}, b^{n+1})$

1 for $e = 1, 2, \ldots, \#M$ do
2
3 for $l = 1, 2, 3$ do
4
5 end

Algorithm 2: Assembly of $M^e(a^n, b^n)$

1 for $e = 1, 2, \ldots, \#M$ do
2
3 for $m = 1, 2, 3$ do
4
5 end
6
7 end
```
\[ \frac{\delta A_h}{\delta a_i} (a^{n+1}, b^{n+1}) \] and \( M^*(a^n, b^n) \) in a uniform triangulation in a rectangular domain by applying Algorithm 1 and Algorithm 2.

**Remark 3.7.** Due to the degeneracy of the PME at \( \rho = 0 \), the semi-discrete equation (3.3), corresponding to the energy-dissipation law (2.17), is also degenerate at the region that \( \rho_0(X) = 0 \), that is to say, if \( X_k \in \mathbb{R}^2 \setminus \Omega \), where \( \Omega \) is the support of \( \rho_0(X) \), then

\[
M_{kj}(a(t), b(t)) = 0, \quad \frac{\delta A_h}{\delta a_k} (a(t), b(t)) = 0, \quad \frac{\delta A_h}{\delta b_k} (a(t), b(t)) = 0,
\] (3.24)

which means the nodes (“particle”) in such region have no well-defined velocity. In the meantime, we can only derive the PME from the energy-dissipation law (2.17) on the compact support of \( \rho_0(X) \), hence, both numerical schemes can only be used in the compact support of \( \rho_0(X) \). It is a commonly used strategy that solving the PME only within the solution support \([50, 16, 23, 6, 7, 5, 39, 17]\), known as the non-embedding approach. The main challenge of this approach is that the evolution of free boundary has to be tracked explicitly \([39]\). Our cell-centered Lagrangian schemes enable us to treat the movement of free boundary in a uniform way, as the velocity of the free boundary is also well-defined, which is a major advantage in high dimensional situations.

In later sections, we will show that our schemes, especially the scheme based on energy-dissipation law (3.24), can capture the free boundary of the PME, in both 1D and 2D, without explicitly track the movement of the free boundary.

**Remark 3.8.** Since the corresponding trajectory equation (2.20) of (2.19) is exactly the equation for the movement of free boundary, we expect the numerical scheme based on the energy-dissipation law (2.17) has an advantage in tracking the movement of the free boundary. Although the energy-dissipation law (2.17) is only valid for the PME with \( \alpha \geq 2 \), our numerical tests show that the scheme 2 also works well for \( 1 < \alpha < 2 \).

For the above discretization, we can prove the following theorem (3.18):

**Theorem 3.1.** Let \( \Omega_0 \) be the compact support of \( \rho_0(X) \), for given \( \Xi^n \in F_{ad}^\Xi \), there exists a solution \( \Xi^{n+1} \) to numerical scheme (3.18) such that the following discrete energy dissipation law holds, i.e.,

\[
\frac{E_h(\Xi^{n+1}) - E_h(\Xi^n)}{\tau} \leq -C \frac{1}{\tau^2} D_0^\tau(\Xi^n - \Xi^{n+1}) \cdot (\Xi^n - \Xi^{n+1}) \leq 0,
\] (3.25)

for some constant \( C \in (\frac{1}{2}, 1) \), where the discrete energy is defined by

\[
E_h(\Xi) = \sum_{e=1}^M \int_{\tau_e} \omega \left( \frac{\rho_e^0}{\det F_e(\Xi)} \right) \det F_e(\Xi) dX, \quad \Xi \in F_{ad}^\Xi,
\] (3.26)

\( \rho_e^0 \) is the initial density in the centroid of \( \tau_e \), and \( D_0^\tau(\Xi^n) \) is defined by (3.13) with \( M = M^* \).

**Proof.** The numerical scheme (3.18) can be written as

\[
D_0^\tau(\Xi^{n+1} - \Xi^n) = \frac{\delta E}{\delta \Xi}(\Xi^{n+1}),
\] (3.27)

where \( \frac{\delta E}{\delta \Xi} = -\frac{\delta A_h}{\delta \Xi} \) is used, and \( D_0^\tau(\Xi^n) \) is a symmetric matrix.

Note that if \( \Xi^{n+1} \) is a minimizer of the following minimization problem for given \( \Xi^n \):

\[
\Xi^{n+1} := \text{argmin}_{\Xi \in F_{ad}^\Xi} J(\Xi),
\] (3.28)

\[
E_h(\Xi^{n+1}) = E_h(\Xi^n),
\]

\[
\text{for some constant } C \in (\frac{1}{2}, 1),
\]

\[
\frac{E_h(\Xi^{n+1}) - E_h(\Xi^n)}{\tau} \leq -C \frac{1}{\tau^2} D_0^\tau(\Xi^n - \Xi^{n+1}) \cdot (\Xi^n - \Xi^{n+1}) \leq 0,
\] (3.25)

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\[
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\[
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\] (3.25)

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\[
E_h(\Xi) = \sum_{e=1}^M \int_{\tau_e} \omega \left( \frac{\rho_e^0}{\det F_e(\Xi)} \right) \det F_e(\Xi) dX, \quad \Xi \in F_{ad}^\Xi,
\] (3.26)

\( \rho_e^0 \) is the initial density in the centroid of \( \tau_e \), and \( D_0^\tau(\Xi^n) \) is defined by (3.13) with \( M = M^* \).

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\[
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\] (3.27)

where \( \frac{\delta E}{\delta \Xi} = -\frac{\delta A_h}{\delta \Xi} \) is used, and \( D_0^\tau(\Xi^n) \) is a symmetric matrix.

Note that if \( \Xi^{n+1} \) is a minimizer of the following minimization problem for given \( \Xi^n \):

\[
\Xi^{n+1} := \text{argmin}_{\Xi \in F_{ad}^\Xi} J(\Xi),
\] (3.28)
where

\[ J(\Xi) = \frac{1}{2\tau} D_\tau^* (\Xi - \Xi^n) \cdot (\Xi - \Xi^n) + E(\Xi), \]  

(3.29)

then \( \Xi^{n+1} \) is a solution of (3.18). Hence, we only need to prove that there exists a minimizer of (3.29) in \( F_{ad}^\Xi \).

Note \( \forall \Xi \in \partial F_{ad}^\Xi \) (there exists some \( e \) such that \( \det F_\tau(\Xi) = 0 \)), \( J(\Xi) = \infty \), so \( J(\Xi) \) is coercive on \( F_{ad}^\Xi \). In the meantime, \( J(\Xi) \) is a continuous function of \( \Xi \) in the closed convex set \( F_{ad}^\Xi \), so \( J(\Xi) \) at least has a minimizer in \( F_{ad}^\Xi \).

Since \( \Xi^{n+1} \) is a (local) minimizer of \( J(\Xi) \), we have

\[ \left( \frac{1}{\tau} D_\tau^* + \frac{\delta^2 E}{\delta \Xi^2} (\Xi^{n+1}) \right) (\Xi - \Xi^{n+1}) \cdot (\Xi - \Xi^{n+1}) \geq 0 \]

(3.30)

for \( \Xi \in F_{ad}^\Xi \). By Taylor’s theorem, we get

\[
E_h(\Xi^n) = E_h(\Xi^{n+1}) + \frac{\delta E}{\delta \Xi} (\Xi^{n+1})(\Xi^n - \Xi^{n+1}) + \frac{1}{2} \frac{\delta^2 E}{\delta \Xi^2} (\Xi^{n+1})(\Xi^n - \Xi^{n+1}) \cdot (\Xi^n - \Xi^{n+1}) \]

\[
\geq E_h(\Xi^{n+1}) + \frac{\delta E}{\delta \Xi} (\Xi^{n+1}) \cdot (\Xi^n - \Xi^{n+1}) - \frac{1}{2} D_\tau^* (\Xi^n - \Xi^{n+1}) \cdot (\Xi^n - \Xi^{n+1}) \]

for some \( \Xi^c = (1-c)\Xi^{n+1} + c\Xi^n \in F_{ad}^\Xi \).

Hence,

\[
E_h(\Xi^n) - E_h(\Xi^{n+1}) \geq \frac{\delta E_h}{\delta \Xi} (\Xi^{n+1}) \cdot \frac{\Xi^n - \Xi^{n+1}}{\tau} - \frac{1}{2\tau^2} D_\tau^* (\Xi^n - \Xi^{n+1}) \cdot (\Xi^n - \Xi^{n+1}) \]

\[
= \frac{1}{\tau^2} \left( D_\tau^* (\Xi^{n+1} - \Xi^n) \cdot (\Xi^{n+1} - \Xi^n) - \frac{1}{2} D_\tau^* (\Xi^n - \Xi^{n+1}) \cdot (\Xi^n - \Xi^{n+1}) \right) \]

\[
= \left( 1 - \frac{1}{2c^2} \right) \frac{1}{\tau^2} D_\tau^* (\Xi^{n+1} - \Xi^n) \cdot (\Xi^{n+1} - \Xi^n) \geq 0 \]

(3.32)

\[ \tag*{\Box} \]

Remark 3.9. In one-dimensional case, due to \( \det F = F \), it is easy to show that \( E(\Xi) \) is convex. Hence, we can have a stronger result similar to that in [17]:

\[
E_h(\Xi^n) - E_h(\Xi^{n+1}) \geq \frac{\delta E_h}{\delta \Xi} (\Xi^{n+1}) \cdot \frac{\Xi^n - \Xi^{n+1}}{\tau} \]

\[
= \frac{1}{\tau^2} D_\tau^* (\Xi^{n+1} - \Xi^n) \cdot (\Xi^{n+1} - \Xi^n) \geq 0, \]

(3.33)

where the first inequality follows the convexity of \( E(\Xi) \). And since \( J(\Xi) \) is also convex, we can have a uniquely solvable result of numerical scheme (3.27).

In high dimensional situation \((d \geq 2)\), we can not get a uniquely solvable result of numerical scheme (3.27) due to the lack of convexity of \( J(\Xi) \) and \( E(\Xi) \), which inherits from continuous energy-dissipation law [See remark 3.1].

Remark 3.10. Although there exists a (local) minimizer in the admissible class \( F_{ad}^\Xi \) for (3.38), which is a solution of numerical scheme (3.18), we still need to choose a proper optimization methods to find a minimizer \( \Xi^{n+1} \) in \( F_{ad}^\Xi \). For the PME in 1D or 2D, numerical tests show that a standard damped Newton’s method with fixed step-size is adequate to this purpose. Since
we may only find a local minimizer of $J(\Xi)$ due to lack of convexity for the general problem, in
general case, the dynamical evolution of a flow-map based Lagrangian methods may be different
from Eulerian methods.

Remark 3.11. The above approach start with the spatial discretization to the flow map (3.3),
we can also begin with introducing a temporal discretization to the continuous energy-dissipation
law (2.11) by

$$\frac{E(x^{n+1}) - E(x^n)}{\tau} = -\int_\Omega \eta(\rho) \frac{|x^{n+1}_h - x^n_h|^2}{\tau} \det F_h^{\gamma_2} dX. \tag{3.34}$$

where $x^n = x(X, t_n)$, and $\gamma_i = n$ or $n+1$, as in (3.19). The RHS of (3.34) can be viewed as an
approximation to $\frac{d}{dt} E(x(X, t^*))$ for some $t^* \in [t^n, t^{n+1}]$, i.e.,

$$-\int_\Omega \eta(\rho(t^*)) |x(t^*)|^2 \det F_h dX \approx -\int_\Omega \eta(\rho) \frac{|x^{n+1} - x^n|^2}{\tau} \det F_h^{\gamma_2} dX. \tag{3.35}$$

Using the spatial discretization (3.3), we will have the following discrete energy-dissipation law:

$$\frac{E(\Xi^{n+1}) - E(\Xi^n)}{\tau} = -D^{n+1}_n \Xi^{n+1} - \Xi^n \cdot \frac{\Xi^{n+1} - \Xi^n}{\tau}, \tag{3.36}$$

where $D^n_n = D(\Xi^n)$ is same to that in (3.27). Note that

$$E(\Xi^{n+1}) - E(\Xi^n) = \nabla_\Xi E(\Xi_c) \cdot (\Xi^{n+1} - \Xi^n) \tag{3.37}$$

for some $\Xi_c = \mathbf{1} - c \Xi^{n+1} + c \Xi^n$. It is straightforward to show that if $\Xi^{n+1} \in F^\Xi_{ad}$ satisfies

$$D^n_n \frac{\Xi^{n+1} - \Xi^n}{\tau} = -\nabla_\Xi E(\Xi_c), \tag{3.38}$$

then $\Xi^{n+1}$ satisfies (3.36).

In our scheme (3.27), we approximate $\nabla E_\Xi(\Xi_c)$ by $\nabla_\Xi E(\Xi^{n+1})$, which causes the difference
between (3.25) and (3.36).

Remark 3.12. We can design a numerical scheme that satisfies (3.36) exactly. Let

$$\Xi^n = \sum_{i=1}^K \kappa^n_i e_i, \quad \Xi^{n+1} = \sum_{i=1}^K \kappa^{n+1}_i e_i, \tag{3.39}$$

where $e_i$ is the standard orthonormal basis in $\mathbb{R}^K$. Note the RHS of (3.36) can be written as

$$-\frac{1}{\tau^2} \sum_{i=1}^K \left( \sum_{j=1}^K D^i_j(\Xi^n)(\kappa^{n+1}_j - \kappa^n_j) \right) (\kappa^{n+1}_i - \kappa^n_i). \tag{3.40}$$

On the other hand, the LHS of (3.36) can be written as

$$\frac{1}{\tau} \sum_{i=1}^K E(\Xi^n_{(i)}) - E(\Xi^n_{(i-1)}). \tag{3.41}$$
where
\[
\Xi^n_0 = \Xi^n, \quad \Xi^n_i = \Xi^n + \sum_{l=1}^i (\kappa_l^{n+1} - \kappa_l^n) e_l.
\] (3.42)

Hence, direct computation shows that \( \Xi^{n+1} = \Xi^n_0 \) satisfies (3.36) if
\[
E(\Xi^n_i) - E(\Xi^n_{i-1}) = -\frac{1}{\tau} \sum_{j=1}^K (\sum_{i=1}^K D_{ij}(\Xi^n)(\kappa_j^{n+1} - \kappa_j^n)) (\kappa_i^{n+1} - \kappa_i^n), \quad i = 1, \ldots, K, \] (3.43)
which give us a numerical scheme
\[
\frac{1}{\tau} \sum_{j=1}^K D_{ij}(\Xi^n)(\kappa_j^{n+1} - \kappa_j^n) = -\frac{E(\Xi^n_i) - E(\Xi^n_{i-1})}{\kappa_i^{n+1} - \kappa_i^n}, \quad i = 1, \ldots, K. \] (3.44)

The scheme (3.44) preserves the discrete energy-dissipation law (3.36), and might be useful when the variation of \( E(\Xi) (A(\Xi)) \) cannot be computed efficiently. However, to our knowledge, the numerical analysis and experiments for such type of scheme is lacking. We will explore this type of scheme in the future work.

Next we will briefly talk about the post-process after we obtain \( x_h \). According to the kinematic relation, \( \rho(x) \) can be computed by
\[
\rho(x(X, t), t) = \rho_0(X)/\det F(X, t).
\] (3.45)

Hence, we can compute the density of each element, i.e, the density in the centroid of each element is by
\[
\rho_h(x^e_c, t) = \rho_0(X^e_c)/\det F^e_c(t),
\] (3.46)
where \( x^e_c \) is the centroid of \( x_h(\tau_e) \), while \( X^e_c \) is the centroid of \( \tau_e \). For each node \( X_i \), since the determinant of the deformation matrix \( F \) may be different in different elements contain \( X_i \), we can compute the \( \rho_h(x_h(X_i), t) \) in each nodes by
\[
\rho_h(x_h(X_i), t) = \rho_0(X_i) \frac{\sum_{e \in G(i)} |\tau_e|}{\sum_{e \in G(i)} |\tau_e| \det F^e(t)}.
\] (3.47)

**Numerical scheme in 1D:** At the end of this section, we write down our two numerical schemes, based on energy-dissipation law (2.17) and (2.19), explicitly in one-dimensional case. Let \( \Omega_0 = [\xi_l, \xi_r] \) be the compact support of \( \rho_0(X) \), and \( \xi_l = X_1 < X_2 < \ldots < X_N = \xi_r \) be nodes in \( \Omega_0 \). We can approximate the flow map \( x(X, t) \) by
\[
x_h(X, t) = \sum_{i=1}^N a_i(t)\phi_i(X),
\] (3.48)
where \( \phi_i(X) \) is a hat function satisfies \( \phi_i(X_j) = \delta_{ij} \). Let \( a(t) = (a_1(t), a_2(t), \ldots, a_N(t))' \) and \( h_i = X_{i+1} - X_i \), in one-dimensional case, the admissible set of \( a \) is simply as
\[
F^a_{ad} = \{ a = (a_1, a_2, \ldots, a_N)' \mid a_1 < a_2 < \ldots < a_N \}.
\] (3.49)
The discrete action functional and the discrete dissipation can be written as
\[
A_h(a(t)) = -\int_0^T \sum_{i=1}^{N-1} \int_{X_i}^{X_{i+1}} \omega \left( \frac{\rho_0(X)}{\det F_i(t)} \right) \det F_i(t) dX dt, \\
D_h(a'(t), a(t)) = \frac{1}{2} \sum_{i=1}^{N-1} \int_{X_i}^{X_{i+1}} \eta \left( \frac{\rho_0(X)}{\det F_i(t)} \right) \left( \sum_{j=1}^N a'_j(t) \phi_j(X) \right)^2 \det F_i(t) dX,
\]
where
\[
\det F_i = (a_{i+1} - a_i)/h_i, \quad i = 1, 2, \ldots, N - 1.
\]
For the energy-dissipation law \((2.17)\), direct computation results in
\[
\frac{\delta A_h}{\delta a_i}(a) = -\frac{1}{h} \left( \int_{X_i}^{X_{i+1}} \left( \frac{\rho_0(X)}{(a_{i+1} - a_i)/h_i} \right)^\alpha dX - \int_{X_{i-1}}^{X_i} \left( \frac{\rho_0(X)}{(a_i - a_{i-1})/h_{i-1}} \right)^\alpha dX \right)
\]
\[
\approx - \left( \frac{\rho_0(X_{i+1/2})}{(a_{i+1} - a_i)/h_i} \right)^\alpha - \left( \frac{\rho_0(X_{i-1/2})}{(a_i - a_{i-1})/h_{i-1}} \right)^\alpha,
\]
and
\[
\frac{\delta D_h}{\delta a'_i}(a(t), a'(t)) = \int_{X_i}^{X_{i+1}} \rho_0(X) \left( \sum_{j=1}^N a'_j(t) \phi_j(X) \right) \phi_i(X) dX
\]
\[
+ \int_{X_i}^{X_{i+1}} \rho_0(X) \left( \sum_{j=1}^N a'_j(t) \phi_j(X) \right) \phi_i(X) dX.
\]
Hence, in the one-dimensional case, our scheme 1 based on energy-dissipation law \((2.17)\) can be written as
\[
M_{ij} \frac{a^{n+1}_j - a^n_i}{\tau} = - \left( \frac{\rho_0(X_{i+1/2})}{(a_{i+1}^{n+1} - a_i^{n+1})/h_i} \right)^\alpha - \left( \frac{\rho_0(X_{i-1/2})}{(a_i^{n+1} - a_{i-1}^{n+1})/h_{i-1}} \right)^\alpha
\]
where \(M\) is a triangular matrix, given by
\[
M_{ij} = \begin{cases} 
\rho_0(X_{i-1/2})h_{i-1}/6, & j = i - 1, \\
\rho_0(X_{i-1/2})h_{i-1}/3 + \rho_0(X_{i+1/2})h_i/3, & j = i, \\
\rho_0(X_{i+1/2})h_i/6, & j = i + 1, \\
0, & \text{otherwise},
\end{cases} \quad 1 \leq i, j \leq N,
\]
where we define \(X_{1/2} = 0, X_{N+1/2} = 0\) and \(h_0 = h_N = h\) to simplify the notation.

Remark 3.13. In Ref. [27], the authors develop several numerical schemes for the one-dimensional PME based on different energy-dissipation laws. For the energy-dissipation law \((2.17)\), their numerical scheme can be written as (scheme 0 in [27])
\[
\rho_0(X_i) \frac{a^{n+1}_i - a^n_i}{\tau} = -\frac{1}{h} \left( \left( \frac{\rho_0(X_{i+1/2})}{(a_i^{n+1} + a_{i+1}^{n+1})/h} \right)^\alpha - \left( \frac{\rho_0(X_{i-1/2})}{(a_i^{n+1} - a_{i-1}^{n+1})/h} \right)^\alpha \right).
\]
Formally, with the equidistant node, our scheme \((3.53)\) only differs from theirs in the temporal
discretization for all inner points. A drawback of their temporal discretization is that, in order to prevent the solution to escape from the admissible set, they should use a specific and inefficient damped Newton methods, in which the step-size is roughly proportional to $\min(\rho_0(X_i))$. Our temporal discretization follow the maximum dissipation principle, in which $M(a)$ control the movement of each nodes. A standard damped Newton with a fixed step-size can prevent the solution to escape from the admissible set in our scheme. Their scheme can only be applied to the region in which $\rho_0 > 0$ (a different scheme is used for the movement of free boundary). Moreover, the starting point of the numerical approach in Ref. [17] is the force balance (2.18) in strong form, it is difficult to extend their approach to a high dimensional situation. Strictly speaking, their numerical schemes may not preserve the original energy-dissipation law in general.

Similarly, in the one-dimensional case, our scheme 2, which is based on energy-dissipation law (2.19), can be written as

$$M_{ij}(a^n) \frac{x_j^{n+1} - x_j^n}{\tau} = -\frac{\alpha}{\alpha - 1} \left( \frac{\rho_0(X_{i+1/2})}{(a_i^{n+1} - a_i^{n+1})/h} \right)^{\alpha - 1} - \left( \frac{\rho_0(X_{i-1/2})}{(a_i^{n+1} - a_i^{n+1})/h} \right)^{\alpha - 1},$$  \hspace{1cm} (3.56)

where

$$M_{ij}(a^n) = \begin{cases} (a_i^n - a_{i-1}^n)/6, & j = i - 1, \\ (1 - \delta_1)(a_i^n - a_{i-1}^n)/3 + (1 - \delta_{N_1})(a_{i+1} - a_i)/3, & j = i, \\ (a_i^{n+1} - a_i^n)/6, & j = i + 1, \\ 0, & \text{otherwise}, \end{cases} \hspace{1cm} 1 \leq i, j \leq N. \hspace{1cm} (3.57)$$

where we define $X_{i/2} = 0$, $X_{N+1/2} = 0$ and $h_0 = h_N = h$ to simplify the notation.

4. Numerical Experiments

In this section, we present some numerical results to demonstrate the accuracy of our numerical methods. We’ll focus on our scheme 2, which is based on the energy-dissipation law (2.19). The error of a numerical solution is measured in $L^2$-norms defined by

$$||e_h||^2_L = \left( \int_{\Omega} e_h^2(x)dx \right)^{1/2},$$  \hspace{1cm} (4.1)

where $e_h(x)$ is the difference between the numerical solution $\rho_h(x)$ and the exact solution $\rho(x)$. We compute the numerical integration in (4.1) by the centroid method (known as midpoint method in 1D), which defines the discrete $L^2$-norm, i.e.,

$$||e_h||^2_L = \left( \sum_{c=1}^M e_h(x_c^e)^2 |\tau_c| \det F_c \right)^{1/2},$$  \hspace{1cm} (4.2)

where $x_c^e$ is the centroid of $x_h(\tau_c)$, $\rho_h(x_c^e)$ is computed by (3.46).

4.1. One-dimensional problems

4.1.1. Barenblatt-Pattle solution

To verify the accuracy of our numerical methods, we first consider a benchmark solution, the Barenblatt-Pattle solution, which is an exact weak solution for the PME established by Barenblatt...
and Pattle [13]. The one-dimensional Barenblatt-Pattle solution is given by,

\[ B_\alpha(x, t) = t^{-k} \left[ 1 - \frac{k(\alpha - 1)}{2\alpha} \frac{|x|^2}{t^{2\alpha}} \right]^{1/(\alpha - 1)}, \quad t > 0, \]  

(4.3)

where \( k = (\alpha + 1)^{-1} \) and \( u_+ = \max(u, 0) \). For any time \( t > 0 \), this solution has a compact support \([ -\xi_\alpha(t), \xi_\alpha(t) ]\) with the interface \(|x| = \xi_\alpha \) moving outward at a finite speed, where

\[ \xi_\alpha(t) = \sqrt{\frac{2\alpha}{k(\alpha - 1)}} t^k. \]  

(4.4)

We take the Barenblatt solution at \( t = 1 \), i.e., \( B_\alpha(x, 1) \), as the initial data, and compare our numerical solution at time \( T \) with \( B_\alpha(x, T + 1) \). Fig. 4.1 shows the numerical and exact solutions for \( \alpha = 4 \) at \( T = 1 \) and \( T = 10 \), where the numerical solutions are computed by scheme 1 \((3.53) \) [shown by blue-square] and scheme 2 \((3.56) \) [shown by red-circle] with \( \Omega_0 \) to be the compact support of the initial data. The results demonstrate that both our numerical schemes can approximate the exact solutions well without oscillation. The numerical solutions by scheme 2 \((3.56) \) approximate the exact solutions better near the interface.

![Figure 4.1: Solution for the PME for \( \alpha = 4 \), with \( \rho_0(X) = B_\alpha(x, 1) \) at different time: (a) \( T = 1 \), (b) \( T = 10 \) \( (N = 51, h \approx 0.14, \tau = 0.01) \). [Exact: dark line, scheme 1: blue square, scheme 2 : red circle].](image)

The converge rate of Barenblatt solutions with \( \alpha = 3 \) and 4 for both numerical schemes is shown in Table 4.1. The error at \( X = 0 \) and the error in \( L^2 \)-norm is presented. For both schemes, the converge rate of the error at \( X = 0 \) is second order since the solution is smooth far away from the interface. The scheme 1 has a first-order converge rate, while the scheme 2 can achieve second-order in \( L^2 \)-norm. When \( \alpha \) becomes larger, the converge rate of scheme 2 in \( L^2 \)-norm can keep in second order. As expected, the numerical error of scheme 2 is smaller than that of scheme 1, as it track the movement of free boundary better. We can reduce the numerical error of our scheme 1 by tracking the movement of the free boundary explicitly, i.e., replacing the equations of \( X_b \in \partial\Omega_0 \) with the equation of free boundary. In the following, we’ll focus on our scheme 2, which based on energy-dissipation law \((2.19) \). All the following numerical solutions are computed by scheme 2.

Fig. 4.2(a) shows the trajectory of each node for Barenblatt solution with \( \alpha = 4 \) \([N = 51, \tau = 0.01, \text{scheme 2} \)\]. It can be noticed that the final grid is almost uniform. This is because
\[ \alpha = 3 \]

| \( N \) | \( \tau \) | \( \text{Error at } X(0) \) | \( L^2\)-error | Order | \( \text{Error at } X(0) \) | \( L^2\)-error | Order |
|---|---|---|---|---|---|---|---|
| 51 | 1/100 | 2.6421e-04 | 0.0036 | 9.0421e-05 | 3.5109e-04 | 1.8784 |
| 101 | 1/400 | 1.9301e-05 | 0.0071 | 5.7058e-06 | 1.9917 | 3.5109e-04 | 1.8784 |
| 201 | 1/1600 | 1.9301e-05 | 0.0071 | 5.7058e-06 | 1.9917 | 3.5109e-04 | 1.8784 |

\[ \alpha = 4 \]

| \( N \) | \( \tau \) | \( \text{Error at } X(0) \) | \( L^2\)-error | Order | \( \text{Error at } X(0) \) | \( L^2\)-error | Order |
|---|---|---|---|---|---|---|---|
| 51 | 1/100 | 2.6925e-04 | 0.0051 | 2.3969e-04 | 5.0786e-04 | 1.8784 |
| 101 | 1/400 | 7.6531e-05 | 0.0027 | 6.0120e-05 | 1.9953 | 1.7697 |
| 201 | 1/1600 | 2.2855e-05 | 0.0014 | 1.5073e-05 | 1.9959 | 1.7697 |

Table 4.1: The convergence rate of numerical solutions for \( \rho_0(X) = B_\alpha(X,1) \) at the finite time \( T = 1 \) for \( \alpha = 2 \) and \( \alpha = 4 \).

The solution doesn’t become steeper during the time evolution. We plot in Fig. (4.2) (b) the evolution of the numerical interface for the Barenblatt solution \( [N = 51, \tau = 0.01, \text{scheme 2}] \), with four different parameters \( \alpha = 4, 5, 6, \text{and 8} \), from \( T = 0 \) to 1, in which the solid line is the position of the exact interface, and the circle indicates the position of the numerical interface. The results show that the exact interface can be approximated in high accuracy.

**Figure 4.2:** (a) The trajectory of the nodes for Barenblatt solution with \( \alpha = 4 \). (b) Movement of the interface for the Barenblatt solution: \( \alpha = 4, 5, 6, \text{and 8} \) [Exact: blue line; Numerical: red circle].

Quantitatively, we show the error of the right interface of our scheme 2 with different \( \alpha \) \( (\alpha = 4, 5, 6 \text{ and 8}) \) at \( T = 1 \) in Table. 4.2, which shows that our scheme 2 can track the movement of the free boundary in second-order, even for large \( \alpha \).

| \( \alpha \) | \( N = 51, \tau = 1/100 \) | \( N = 101, \tau = 1/400 \) | Order |
|---|---|---|---|
| 4 | 3.7241e-04 | 8.9717e-05 | 2.0534 |
| 5 | 4.4021e-04 | 1.0629e-04 | 2.0502 |
| 6 | 4.6867e-04 | 1.1329e-04 | 2.0486 |
| 8 | 4.8008e-04 | 1.1619e-04 | 2.0468 |

Table 4.2: Numerical Error of right interface at \( T = 1 \) for initial data \( \rho_0(X) = B_\alpha(X,1) \) with different \( \alpha \) \( (\alpha = 4, 5, 6 \text{ and 8}) \) at \( T = 1 \). The numerical solutions are computed by scheme 2.

**Remark 4.1.** Although the scheme 2 is derived by the energy-dissipation law (2.19), which is valid for \( \alpha \geq 2 \), numerical tests show that this scheme also works well for the case with
$1 < \alpha < 2$. Fig. 4.3 shows the numerical and exact solutions for $\alpha = 5/3$ and $\alpha = 1.1$ at $T = 1$ with $\rho_0(X) = B_\alpha(x,1)$.

**Figure 4.3:** Solution for the PME with $\rho_0(X) = B_\alpha(x,1)$ at $T = 1$ for (a) $\alpha = 5/3$, (b) $\alpha = 1.1$. The exact solutions are shown by solid line, while the numerical solutions computed by scheme 2 are shown by red-circle.

### 4.1.2. Waiting Time

Now, we study the waiting time phenomenon of the PME by our numerical methods. The waiting time phenomenon occurs for a certain type of initial data. For instance, if $\rho_0(X)$ satisfies

$$
\frac{\alpha}{\alpha - 1} \rho_0^{-1}(X) = \begin{cases}
(1 - \theta) \sin^2 X + \theta \sin^4 X, & \text{if } -\pi \leq X \leq 0, \\
0, & \text{otherwise},
\end{cases}
$$

(4.5)

**Figure 4.4:** Numerical solution for the initial condition (4.5) with $\theta = 0$ and $\alpha = 4$ at various time: (a) $t = 0$, (b) $t = 0.05$, (c) $t = 0.1$, (d) $t = 0.2$, in which the first and last element are manually refined ($N = 107, \tau = 10^{-4}$).
then there exist a positive waiting time for $0 \leq \theta \leq 1$. According to the theoretical result, for $0 \leq \theta \leq 1/4$, the waiting time for the initial data (4.5) is $t = \frac{2(\alpha + 1)(1-\theta)}{\theta}$.

Most of previous studies estimate the waiting time from the trajectory of numerical interface, but the numerical waiting time may not be clearly estimated in some cases. As an alternative approach, Nakaki and Tomoeda estimate the waiting time for the one-dimensional PME by transforming the original equation into another equation whose solution will blow up at the waiting time of the original PME. Recently, Duan et al. proposed an elegant criterion to determine the waiting time in one-dimensional case, and they manually set the velocity of interface to be zero before the numerical waiting time. We can easily adopt the criterion proposed in [17] into our numerical scheme in one-dimensional case. Fig. 4.4 shows the numerical solutions for the initial data (4.5) with $\theta = 0$ and $\alpha = 4$ at various time, in which we manually refine the first and last element to improve the numerical accuracy ($N = 107$, $\tau = 10^{-4}$). The numerical waiting time we obtained is $t = 0.1054$, which is consistent with theoretical results ($t = 0.1$).

![Figure 4.5: (a) Numerical right interface computed by our numerical scheme with [red dashed-line] and without [blue solid-line] manually setting the velocity of interface to be zero before the numerical waiting time for the initial data (4.5) with $\theta = 0$ and $\alpha = 4$. (b) Numerical right interface computed by our numerical scheme with [red dashed-line] and without [blue solid-line] manually setting the velocity of interface to be zero before the numerical waiting time for the initial data (4.5) with $\theta = \frac{1}{2}$ and $\alpha = 7$.](image)

A natural question is whether we can estimate the waiting time from our numerical interface without manually setting the velocity of interface to be zero, as it is difficult to apply similar criterion to the PME in high spatial dimensions. Fig. 4.5 (a) shows the right numerical interface computed by our numerical method with and without manually setting the velocity of interface to be zero before the numerical waiting time for the initial data (4.5) with $\theta = 0$ and $\alpha = 4$. Surprisingly, these two line almost coincide with each other after the numerical waiting time. Moreover, we noticed that the compact support will shrink at beginning due to the numerical approximation. These motivate us to define the numerical waiting time by the time when the numerical support begins to expand, i.e.,

$$t^*_N = \inf \left\{ t \mid |\xi_b(t)| > \xi_0^b, b = 1 \text{ and } N \right\},$$  \hspace{1cm} (4.6)

where $\xi_b(t)$ is the position of left and right interface at time $t$ and $\xi_0^b$ is the initial position of left and right interface. Although no theoretical justification is available at this point, numerical experiments show that this criterion give a clear estimation to the waiting time for all cases that
we tested. Fig. 4.5 (b) shows another example for the initial data (4.5) with $\theta = \frac{1}{2}$ and $\alpha = 7$, in which the numerical interface for both approaches are shown. Both approaches indicate that the waiting time in this case is about $t^* \approx 0.124$.

4.2. 2D Simulations

We now apply our numerical scheme 2, which is based on the energy-dissipation law (2.19), to the PME in two dimensions. Although the explicit form of the numerical scheme cannot be given in a general mesh, using the explicit form of $F_e$ as a function of $a_{en(e,l)}$ and $b_{en(e,l)}$ on each element $\tau_e$ (shown in the Appendix), we can compute $\delta A_h \delta a_i(a_{n+1}, b_{n+1})$ and $M^*(a^n, b^n)$ by Algorithm 1 and Algorithm 2 in remark 3.6, during the computer implementation.

4.2.1. Barenblatt-Pattle solution

We first validate our numerical scheme by studying the 2D Barenblatt-Pattle solution. The Barenblatt-Pattle solution in $d$-dimensions is given by

$$B_\alpha(x, t) = t^{-k} \left( C_0 - \frac{k(\alpha - 1)}{2d} \frac{|x|^2}{t^{2k/d}} \right)^{1/(\alpha - 1)},$$

(4.7)

where $k = (\alpha - 1 + 2/d)^{-1}$, $C_0$ is a constant, related to the initial mass. This solution is radially symmetric, self-similar, and has compact support $|x| \leq \xi_\alpha(t)$ for any finite time, where

$$\xi_\alpha = \sqrt{\frac{2dC_0}{k(\alpha - 1)}} t^{k/d}. \quad (4.8)$$

We take Barenblatt solution (4.7) for $C_0 = 0.1$ at $t = 1$ as the initial data, and compare the numerical solution at $T = 1$ with the exact solution $B_\alpha(x, T + 1)$. Since the Barenblatt solution is steeper near the interface, we use the non-uniform mesh in $\Omega_0$ in our 2D simulation, which can largely reduce computational cost. The initial non-uniform mesh in $\Omega_0$ is generated by DistMesh [44].

Fig. 4.6 shows the numerical solutions for $\alpha = 4$ at $T = 1$ in a non-uniform mesh with $N = 516$. The numerical error at $T = 1$ are plot in Fig. 4.6(b), which indicates that the $L^\infty$-norm of the numerical solution is $O(10^{-4})$ for $N = 516$. The numerical and exact interfaces at $T = 1$ are shown in Fig. 4.6(c), which demonstrated that our numerical scheme can track the movement of free boundary in 2D in high accuracy with a small $N$.

We now test the converge rate of 2D Barenblatt solution. The error for numerical solutions with $\rho_0(X) = B_\alpha(X, 1)$ at $T = 0.1$ in $L^2$-norm for both $\alpha = 2$ and $\alpha = 4$ is shown in Table 4.3. It shows that we can achieve a second-order convergence rate for both $\alpha = 2$ and $\alpha = 4$ in $L^2$-norm.

| $\alpha = 2$ | Order | $L^\infty$-error |
|------------|-------|-----------------|
| $\tau = 1/100$ | 6.6358e-04 | 0.0090 |
| $\tau = 1/400$ | 1.6065e-04 | 2.0262 |
| $\tau = 1/1000$ | 3.9867e-05 | 2.0096 |

| $\alpha = 4$ | Order | $L^\infty$-error |
|------------|-------|-----------------|
| $\tau = 1/100$ | 6.6358e-04 | 0.0090 |
| $\tau = 1/400$ | 1.6065e-04 | 2.0262 |
| $\tau = 1/1000$ | 3.9867e-05 | 2.0096 |

Table 4.3: The convergence rate of numerical solutions with $\rho_0(X) = B_\alpha(X, 1)$ at $T = 0.1$ for the PME with $\alpha = 2$ and $\alpha = 4$. 

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4.2.2. Waiting time

Now, we apply our numerical scheme (scheme 2) to the PME with the initial data has a waiting-time phenomenon in two-dimensional situations. We take the initial value as:

$$\rho_0(X, Y) = \begin{cases} 
\cos(\frac{\pi}{2} \sqrt{X^2 + Y^2}), & \text{for } \sqrt{X^2 + Y^2} \leq 1, \\
0, & \text{otherwise},
\end{cases} \quad (4.9)$$

which has a positive waiting time.

The numerical solutions for this initial data at various time are shown in Fig. 4.7 [N = 2105 and \(\tau = 10^{-3}\)]. We use the non-uniform mesh in \(\Omega_0\), which is dense around the free boundary. In order to validate our numerical results, we also compute the same initial date within the axisymmetric assumption, which can reduce the problem into a one-dimensional problem and enable us to apply the criterion in [17] to estimate the waiting time. The numerical solutions
Figure 4.7: Numerical results for the initial data (4.7) obtained by the 2D simulation [(a)-(c)] and 1D simulation with the axisymmetric assumption [(d)-(f)] at $t = 0.05, 0.1$ and $t = 0.15$.

obtained within the axisymmetric assumption for $N = 201$ and $\tau = 10^{-4}$ are shown in Fig. 4.7 (d)-(f).

The location of free boundary by the 2D simulation [blue solid line] and 1D simulation with the axisymmetric assumption [red dashed line] is plotted in Fig. 4.8(a), where we define the location of free boundary in 2D simulation results by

$$|\xi| = \max(\min\{|x_h(X_b)| \mid X_b \in \partial \Omega_0\}, \xi_0),$$

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where $\xi_0$ is the radius of the initial support. Both results indicate the wait time is around 0.128. Fig. 4.8(b) plots the numerical interface at $t = 0.5$ for both approaches, in which the free boundary in the 2D simulation result is shown by blue square and the result obtained by 1D simulation is shown in red solid line. It can be concluded that the numerical solutions obtained by both approaches are consistent, which validates our numerical scheme 2 in 2D, and we can have a clear estimation to the waiting time in 2D from the numerical interface obtained by the scheme 2.

### 4.2.3 Complex Support

Next we consider examples with complex compact supports in 2D. We first take the initial data as

$$
\rho_0(X)^{\alpha-1} = \begin{cases} 
25(0.25^2 - (\sqrt{X^2 + Y^2} - 0.75)^2)^{\frac{1}{2}}, & \sqrt{X^2 + Y^2} \in [0.5, 1] \text{ and } (X < 0 \text{ or } Y < 0), \\
25(0.25^2 - X^2 - (Y - 0.75)^2)^{\frac{1}{2}}, & X^2 + (Y - 0.75)^2 \leq 0.25^2 \text{ and } X \geq 0, \\
25(0.25^2 - (X - 0.75)^2 - Y^2)^{\frac{1}{2}}, & (X - 0.75)^2 + Y^2 \leq 0.25^2 \text{ and } Y \geq 0, \\
0, & \text{otherwise,} 
\end{cases}
$$

which has a partial donut-shaped support. Similar examples are studied in [5, 39].

Fig. 4.9 shows the numerical solutions of the PME with $\alpha = 3$ for the initial condition (4.10) at various time, which are computed by scheme 2 with $N = 910$ and $\tau = 10^{-2}$. One can see that our method works well for the concave domain. However, as pointed out in [5], a Lagrangian method can not handle the topological change automatically, which is also a limitation of our numerical approach. For this example, since the domain will evolve to reach a point where two ends of the “horseshoe” intersecting each other, the tangling of mesh cannot be avoided after this point. In order to get solutions beyond this point, one can manually interpolate the solution on to a new mesh, which can be viewed as an update to $\rho_0(X)$ (along with the mesh).

In our last numerical example, we study a peaks merge problem for the PME with $\alpha = 4$, in which the initial data has two peaks, connected by a thin layer of mass. Similar numerical experiments are studied in [38, 10].
Figure 4.9: Numerical solutions of the PME with $\alpha = 3$ for the initial condition (4.10) by scheme 2 at various time $[N = 910, \tau = 10^{-2}]$: (a) $t = 0$, (b) $t = 0.1$, (c) $t = 0.2$.

Let $\Omega = [-1,1]^2$, consider the initial data

$$\rho_0(X,Y) = e^{-20((X-0.3)^2+(Y-0.3)^2)} + e^{-20((X+0.3)^2+(Y+0.3)^2)} + 0.001.$$  \hspace{1cm} (4.11)
Figure 4.10: Numerical solutions for the PME with $\alpha = 4$ for the initial condition (4.10) at various time by scheme 2: (a) $t = 0.1$, (b) $t = 1$, (c) $t = 5$. The initial mesh is a uniform mesh on $\Omega = [-1,1]^2$ [N = 841, $\tau = 10^{-2}$].

The boundary condition on $\partial \Omega$ is the Neumann boundary condition. In our numerical simulation, we take $\Omega_0 = \Omega$ and manually set the velocity of the nodes on $\partial \Omega_0$ to be zero for the Neumann boundary condition. Fig. 4.10 shows the numerical solutions by scheme 2 at various time.
(t = 0.1, 1 and 5) with a uniform initial mesh in Ω0 [N = 841, τ = 10^{-2}]. It can be seen that the mesh is concentrated around the “interface”, in which the solution is steep, during the evolution. One can view our approach as a kind of moving mesh method. Unlike most of traditional moving mesh approach, in which both updating the mesh and solving the equation in the new mesh are required, we only need to solve the equation of the flow map, i.e., the equation of the mesh, the numerical solutions are determined by the kinematic relation. Similar to [10], it is a surprise that our numerical method can handle the situation of “peaks merge”, although local coarsening and remeshing is still needed in order to get better numerical solutions.

5. Summary

Structure-preserving and adaptive are two important aspects in designing efficient numerical methods for PDEs arising in numerous physical and biological modeling. It is usually a difficult task to construct a numerical scheme to a conservative or dissipative PDE that retain the conservation/dissipation properties in a discrete sense [19]. In this paper, we proposed a general framework to derive an efficient structure-preserving numerical scheme by employing a discrete energetic variational approach. A discrete energetic variational approach provides basis of deriving the “semi-discrete equations” after introducing a proper spatial discretization to the given energy-dissipation law, and can be applied to a large class of partial differential equations with energy-dissipation laws and kinematic relations, such as general diffusion equations, phase-field equations, and equations of liquid crystal. Within a piecewise linear approximation to the flow map, our approach is capable of handling high spatial dimensional situations. As an application, we develop two numerical schemes for the PME based on different energy-dissipation laws. By performing numerical experiments in both 1D and 2D, we show that the numerical scheme based on the energy-dissipation law (2.19) can better capture the free boundary and estimate the waiting time for the PME, without explicitly tracking the movement of the free boundary.

On the notion of our numerical approach, large deformations and topological changes can be difficult to handle by the dynamics of the flow map, usually with higher nonlinearity, degeneracy, or possible singularities. Furthermore, for general problems, a proper “initial data” may not be available. In order to solve these problems, we will employ a hybrid method, which solves the original equation in Eulerian and Lagrangian coordinates alternatively, in the ongoing work. In other word, during the evolution of the flow map, we can update the “initial data” (“reference data”) and the mesh, where the “initial data” is obtained by some Eulerian methods.

Finally, in the current approach, our piecewise linear approximation to the flow map is based on a finite element method, which provides us a simple framework to compute the deformation matrix F on each element explicitly, but it is not obvious to incorporate the local coarsening and remeshing into it. One possible idea is to incorporate the particle methods [13] into our framework, in which remeshing for particle distortion can be easily dealt with, although how to compute the deformation matrix F might still be a challenge.

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Appendix A. Explicit form of \( F_e \) in 2D

In the appendix, we give the explicit form of \( F_e \) as a function of \( a_{en(l,e)} \) and \( b_{en(l,e)} \) \((l = 1, 2, 3)\) on each element \( \tau_e \).

For a given element \( \tau_e \), we denote the nodes of it by \( X_i^e \), and we let \( \xi_i^e = (a_i^e, b_i^e) \triangleq \xi_{en(l,e)} \) \((l = 1, 2, 3)\). The discrete flow map on \( \tau_e \) can be written as

\[
x_h(X) = \sum_{i=1}^{3} \xi_i^e \lambda_i^e(X), \quad X \in \tau_e,
\]

(A.1)

where \( \lambda_i^e \in P_1(\tau_e) \) is a nodal basis on \( \tau_e \), which satisfies \( \lambda_i^e(X_m^e) = \delta_{im} \) \((l, m = 1, 2, 3)\).

We can compute \( \lambda_i^e(X) \) by mapping \( \tau_e \) into the reference triangle \( \tau_s = \{X = (\hat{X}, \hat{Y}) \in \mathbb{R}^2 : \hat{X} \geq 0, \hat{X} + \hat{Y} \leq 1\} \) with nodes \( \hat{X}_1 = (0, 0), \hat{X}_2 = (1, 0), \) and \( \hat{X}_3 = (0, 1) \). The map between \( \tau_s \) to \( \tau_e \) is given by

\[
X = L_e(\hat{X}) = A_e \hat{X} + b_e,
\]

(A.2)

where

\[
A_e = \begin{pmatrix}
X_1^e - X_1^f & X_2^e - X_1^f \\
Y_2^e - Y_1^e & Y_3^e - Y_1^e
\end{pmatrix}, \quad b_e = X_1^e.
\]

(A.3)

Hence,

\[
\lambda_i^e(X) = \lambda_i^e(L_e^{-1}(X)), \quad l = 1, 2, 3.
\]

(A.4)

Since the nodal basis on \( \tau_s \) is given by

\[
\lambda_1^s(\hat{X}, \hat{Y}) = 1 - \hat{X} - \hat{Y}, \quad \lambda_2^s(\hat{X}, \hat{Y}) = \hat{X}, \quad \lambda_3^s(\hat{X}, \hat{Y}) = \hat{Y},
\]

we have

\[
\nabla X \lambda_i^s(X) = A_e^{-T} \nabla \xi \lambda_i^e(\hat{X}),
\]

(A.5)

where

\[
\nabla \xi \lambda_1^e = \begin{pmatrix}
-1 \\
-1
\end{pmatrix}, \quad \nabla \xi \lambda_2^e = \begin{pmatrix}
1 \\
0
\end{pmatrix}, \quad \nabla \xi \lambda_3^e = \begin{pmatrix}
0 \\
1
\end{pmatrix}, \quad A_e^{-1} = \frac{1}{\det A_e} \begin{pmatrix}
Y_3^e - Y_1^e & X_1^e - X_3^e \\
Y_1^e - Y_2^e & X_2^e - X_1^e
\end{pmatrix}.
\]

Then, we can compute \( F_e \) as a function of \( a_i^e \) and \( b_i^e \) on \( \tau_e \) directly by (A.1), which is

\[
F_e(a_i^e, b_i^e) = \sum_{l=1}^{3} \xi_{en(l,e)} \otimes \nabla X \lambda_i^e(X)
\]

\[
= \begin{pmatrix}
a_1^e & a_2^e & a_3^e \\
b_1^e & b_2^e & b_3^e
\end{pmatrix} \nabla \xi \lambda_i^e(\xi) A_e^{-1}
\]

\[
= \frac{1}{\det A_e} \begin{pmatrix}
a_1^e Y_3^e - a_2^e Y_1^e + a_3^e Y_2^e - a_2^e X_3^e - a_3^e X_1^e + a_3^e X_2^e \\
b_1^e Y_2^e - b_2^e Y_3^e + b_3^e Y_1^e - b_2^e X_3^e - b_3^e X_1^e + b_3^e X_2^e
\end{pmatrix},
\]

where \( X_i^e - m = X_i^e - X_m^e, Y_i^e - m = Y_i^e - Y_m^e \) \((l, m = 1, 2, 3)\).

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