

A FAST PROXIMAL GRADIENT METHOD AND CONVERGENCE ANALYSIS FOR DYNAMIC MEAN FIELD PLANNING

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ABSTRACT. In this paper, we propose an efficient and flexible algorithm to solve dynamic mean-field planning problems based on an accelerated proximal gradient method. Besides an easy-to-implement gradient descent step in this algorithm, a crucial projection step becomes solving an elliptic equation whose solution can be obtained by conventional methods efficiently. By induction on iterations used in the algorithm, we theoretically show that the proposed discrete solution converges to the underlying continuous solution as the grid becomes finer. Furthermore, we generalize our algorithm to mean-field game problems and accelerate it using multilevel and multigrid strategies. We conduct comprehensive numerical experiments to confirm the convergence analysis of the proposed algorithm, to show its efficiency and mass preservation property by comparing it with state-of-the-art methods, and to illustrate its flexibility for handling various mean-field variational problems.

1. INTRODUCTION

Mean field planning (MFP) problems study how a large number of similar rational agents make strategic movements to minimize their cost in a process satisfying given initial and terminal density distributions [2, 20, 27–29, 40, 44, 45]. On the one hand, MFP can be viewed as a generalization of optimal transport (OT) [11, 12, 43, 48] where no interaction cost is considered in the process. On the other hand, MFP is also a special case of mean field game (MFG) problems where the terminal density is often provided implicitly [19, 21, 22, 29, 30, 32, 33, 35]. MFP, MFG and OT have wide applications in economics [1, 5, 25], engineering [24, 26, 50], quantum chemistry [18, 23], image processing [31, 41] as well as machine learning [8, 47, 49, 51].

More specifically, the dynamic MFP problem has the following optimization formulation:

$$(1.1) \quad \begin{aligned} & \min_{\rho, \mathbf{m}} \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \int_0^1 \mathcal{F}(\rho(t, \cdot)) dt \\ & \text{s.t. } \partial_t \rho + \operatorname{div}_{\mathbf{x}} \mathbf{m} = 0, \mathbf{m} \cdot \mathbf{n} = 0 \text{ for } \mathbf{x} \in \partial\Omega, \rho(0, \cdot) = \rho_0, \rho(1, \cdot) = \rho_1, \end{aligned}$$

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where $\rho(t, \mathbf{x}) \geq 0$ is the densities of agents, $\mathbf{m} := \rho \mathbf{v}$ with \mathbf{v} representing the strategy(control) of this agent, and any pair of feasible (ρ, \mathbf{m}) satisfies mass conservation and zero boundary flux conditions with initial and terminal densities of ρ being provided ρ_0, ρ_1 . In this variational problem, $L(\rho, \mathbf{m})$ denotes the dynamic cost, \mathcal{F} models the interaction cost. L is convex in ρ, \mathbf{m} , \mathcal{F} is convex in ρ and $\frac{\delta \mathcal{F}}{\delta \rho}$ exists. Especially, with $\mathcal{F} = 0$ and a specific choice of L , variational problem (1.1) reduces to the dynamic formulation of optimal transport (OT) proposed in [11, 12]. By relaxing the given terminal density as an implicit condition regularized by a convex functional \mathcal{G} with $\frac{\delta \mathcal{G}}{\delta \rho}$ existing, one can retrieve a class of MFG as the following formulation [16, 30, 35]:

$$(1.2) \quad \begin{aligned} & \min_{\rho, \mathbf{m}} \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \int_0^1 \mathcal{F}(\rho(t, \cdot)) dt + \mathcal{G}(\rho(1, \cdot)) \\ & \text{s.t. } \partial_t \rho + \operatorname{div}_{\mathbf{x}} \mathbf{m} = 0, \mathbf{m} \cdot \mathbf{n} = 0 \text{ for } \mathbf{x} \in \partial \Omega, \rho(0, \cdot) = \rho_0. \end{aligned}$$

The goal is to find the local minimizers and therefore solve the KKT system of (1.1) (or (1.2)).

Several numerical methods have been established to solve dynamic MFP, MFG and OT problems. One class of methods is based on solving partial differential equations (PDEs) corresponding to the KKT system of the variational problem [2, 4, 17], where conventional numerical methods in nonlinear PDEs can be applied. This class of methods can also be applied to handle general MFP and MFG problems that may not come from variational formulas. However, the nonlinearity of the PDE system limits the solvers to handle broader choices of the dynamic cost L and interaction cost \mathcal{F} .

Another class of methods focuses on the variational formulas of dynamic MFP, MFG and OT problems. By naturally combining with recent advances from optimization, existing methods include several first-order optimization algorithms to solve dynamic OT problems such as augmented Lagrangian [14, 15, 42], primal-dual [36] and G-prox [34], etc. These methods work on either the Lagrangian or the dual problem of the original optimization problem, particularly for dynamic OT where $\mathcal{F} \equiv 0$. These algorithms work very well since the involved sub-optimization problems have closed-form solutions.

We would like to propose a method that can efficiently compute the mean-field type of problems with mass preservation property and flexibility on a broad range of objective functions. Note that the mass conservation constraint in MFP is linear. A straightforward calculation shows that projection to the constraint set can be obtained from solving a linear equation, the standard Poisson equation. This motivates us to propose another algorithm to solve MFP problems based on the proximal gradient descent method [9, 46]. This method is composed of a gradient descent step and a projection step. For MFP problems with a smooth objective function, the gradient values can be evaluated in an element-wise manner. It also enjoys the flexibility to handle a broader range of L and \mathcal{F} . More importantly, the projection step leads to mass preservation in each iteration. The crucial part in the projection step is a fixed linear solver which can be computed efficiently by conventional fast algorithms. In this work, we use an accelerated version of the proximal gradient descent method, referred to as the fast iterative soft threshold algorithm (FISTA) [10], to solve the MFP problems. After that, we further generalize our algorithm to handle MFG problems. In addition, inspired by [7, 38, 39], we also

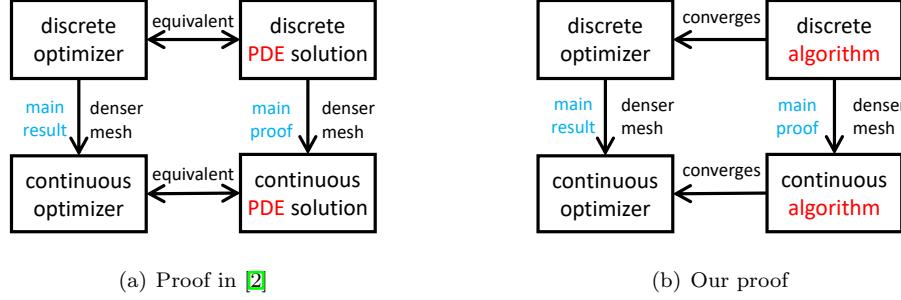


FIGURE 1. Sketch of two approaches of convergence proof

apply multigrid and multilevel methods to speed up the proposed algorithm. Our numerical experiments illustrate the efficiency, mass preservation and flexibility of the proposed algorithm for different MFP problems as well as MFG problems. The vanilla version of our algorithm performs comparably with state-of-the-art methods, while the multigrid and multilevel accelerated versions are more efficient than state-of-the-art methods.

Besides proposing a new algorithm for MFP problems, we analyze errors between the discrete solution and the continuous solution. Since MFP is a functional optimization problem, all numerical methods on a given mesh grid only provide approximated solutions to the continuous problem. It is important to understand how close the discrete numerical solution is to the continuous solution on a given mesh grid. Our analysis is from the algorithm perspective. We first derive an algorithm to optimize the variational problem and discretize each step of our algorithm. Our main effort is to prove that at each iteration, the discrete values are not far from the underlying continuous function values on grid points. Therefore we can show that the discrete algorithm converges to the continuous optimizer on grid points under certain smoothness conditions. Similar types of analysis may not be conveniently conducted in the existing methods including augmented Lagrangian, primal-dual and G-Prox since it could be difficult to have desired perturbation analysis of solving cubic equations involved in these three methods. We remark that [13,14] show the Γ -convergence for static problems by finite element methods, while they acknowledge that their assumptions for convergence to hold are more involved to check for dynamic problems. And we also notice that the convergence analysis for dynamic problems has been studied in [2,3,6] from the PDE perspective, where the authors argue solution of discrete KKT converges to the continuous solution based on the equivalence of continuous systems and discrete systems. To the best of our knowledge, this work is for the first time to examine the discretization error based on variational MFP and its optimization algorithm. We indicate the major difference between our error analysis based on optimization perspective and error analysis based on PDEs perspective in Figure 1.

Contributions. We summarize our contributions as follows:

- (1) We propose to use an accelerated proximal gradient method to solve the MFP problem (1.1).

- (2) We analyze the error between each iteration of discrete optimization and its continuous counterpart. We prove that the discrete solution converges to the continuous optimizer on grid points as the mesh size increases.
- (3) We apply multilevel and multigrid strategies to accelerate our algorithm. We also generalize our algorithm to solve MFG problems (1.2).
- (4) We conduct comprehensive numerical experiments to illustrate the efficiency and flexibility of our algorithms.

Organization. Our paper is organized as follows. In Section 2, we give a brief review of the MFP problem and provide several MFP examples and a MFG example. After that, we describe our algorithm and the implementation details in Section 3. In Section 4, we analyze the discretization error in our algorithm and prove the main theoretical result on the convergence of discrete solutions to the continuous solution as the grid size goes to zero. Furthermore, we generalize our algorithm to solve variational MFG problems and accelerate our algorithm by multilevel and multigrid methods in Section 5. Numerical experiments are provided in Section 6 to demonstrate the convergence order and to illustrate the efficiency and flexibility of our algorithm. At last we conclude this paper in Section 7.

2. REVIEW

In this section, we briefly review MFP problem and provide several examples which will be computed in the experiment section.

Consider the model on time interval $[0, 1]$ and space region $\Omega \in \mathbb{R}^D$. Let ρ be the density of agents through $t \in [0, 1]$, \mathbf{m} be the flux of the density which models strategies (control) of the agents, and $(\rho, \mathbf{m}) \in \mathcal{C}$:

$$(2.1) \quad \mathcal{C} := \left\{ \begin{array}{l} (\rho, \mathbf{m}) : \rho : [0, 1] \times \Omega \rightarrow \mathbb{R}^+, \|\rho\|_{L^1} < +\infty, \int_{\Omega} \rho(t, \mathbf{x}) d\mathbf{x} = 1, \forall t \in [0, 1], \\ \mathbf{m} : [0, 1] \times \Omega \rightarrow \mathbb{R}^D \text{ is Lebesgue measurable.} \end{array} \right\}$$

We are interested in ρ with given initial and terminal density ρ_0, ρ_1 and (ρ, \mathbf{m}) satisfying zero boundary flux and mass conservation law, which gives the constraint set $\mathcal{C}(\rho_0, \rho_1)$:

$$(2.2) \quad \mathcal{C}(\rho_0, \rho_1) := \mathcal{C} \cap \left\{ \begin{array}{l} (\rho, \mathbf{m}) : \partial_t \rho + \operatorname{div}_{\mathbf{x}} \mathbf{m} = 0, \\ \mathbf{m} \cdot \mathbf{n} = 0 \text{ for } \mathbf{x} \in \partial\Omega, \rho(0, \cdot) = \rho_0, \rho(1, \cdot) = \rho_1, \end{array} \right\}$$

where equations hold in the sense of distribution.

We denote $L : \mathbb{R}^+ \times \mathbb{R}^D \rightarrow \overline{\mathbb{R}} := \mathbb{R} \cup \{\infty\}$ as the dynamic cost function (e.g. (2.5) in this paper) and $\mathcal{F} : \mathcal{P}(\Omega) \rightarrow \overline{\mathbb{R}}$ as a functional modeling interaction cost. The goal of MFP is to minimize the total cost among all feasible $(\rho, \mathbf{m}) \in \mathcal{C}(\rho_0, \rho_1)$. Therefore the problem can be formulated as

$$(2.3) \quad \min_{(\rho, \mathbf{m}) \in \mathcal{C}(\rho_0, \rho_1)} \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \int_0^1 \mathcal{F}(\rho(t, \cdot)) dt.$$

It is clear to see $\mathcal{C}(\rho_0, \rho_1)$ is convex and compact. In addition, the mass conservation law $\partial_t \rho + \operatorname{div}_{\mathbf{x}} \mathbf{m} = 0$ and zero flux boundary condition $\mathbf{m} \cdot \mathbf{n} = 0, \mathbf{x} \in \partial\Omega$ imply that $\mathcal{C}(\rho_0, \rho_1) \neq \emptyset$ if and only if $\int_{\Omega} \rho_0 = \int_{\Omega} \rho_1$. Once $\mathcal{C}(\rho_0, \rho_1)$ is nonempty, the existence and uniqueness of the optimizer depend on L and \mathcal{F} .

There are many different choices of \mathcal{F} . In this paper, we consider

$$(2.4) \quad \mathcal{F}(\rho(t, \cdot)) := \lambda_E \int_{\Omega} F_E(\rho(t, \mathbf{x})) d\mathbf{x} + \lambda_Q \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x},$$

where $\lambda_E, \lambda_Q \geq 0$ are two parameters, $F_E : \mathbb{R}^+ \rightarrow \mathbb{R}$ serves as a function to regularize ρ , and $Q(\mathbf{x}) : \Omega \rightarrow \overline{\mathbb{R}}$ provides a moving preference for density ρ . Consider an illustrative example by choosing $\Omega_0 \subset \Omega$ and assuming $Q(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in \Omega_0 \\ +\infty, & \mathbf{x} \notin \Omega_0 \end{cases}$, then the mass has to move within Ω_0 in order to keep the cost finite. In a more general choice of Q , $\rho(t, \mathbf{x})$ tends to be smaller at the place where $Q(\mathbf{x})$ is larger and vice versa.

We then briefly discuss several concrete examples which will be considered in our numerical experiments.

Example 2.1 (Optimal transport [11]). In this paper, we consider a typical dynamic cost function L by

$$(2.5) \quad L(\beta_0, \boldsymbol{\beta}) := \begin{cases} \frac{\|\boldsymbol{\beta}\|^2}{2\beta_0} & \text{if } \beta_0 > 0 \\ 0 & \text{if } \beta_0 = 0, \boldsymbol{\beta} = \mathbf{0} \\ +\infty & \text{if } \beta_0 = 0, \boldsymbol{\beta} \neq \mathbf{0} \end{cases}.$$

If $\lambda_E = \lambda_Q = 0$, the MFP becomes the dynamic formulation of optimal transport problem:

$$(2.6) \quad (\text{OT}) \quad \min_{\rho, \mathbf{m} \in \mathcal{C}(\rho_0, \rho_1)} \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt.$$

Since $\mathbf{m} = \rho \mathbf{v}$, this definition of L makes sure that $\mathbf{m} = \mathbf{0}$ wherever $\rho = 0$. Because $\lambda_E = \lambda_Q = 0$, OT can be viewed as a special case of MFP where masses move freely in Ω through $t \in [0, 1]$.

Example 2.2 (Crowd motion [47]). Consider $F_E : \mathbb{R}^+ \rightarrow \mathbb{R}$, $\rho \mapsto \begin{cases} \rho \log(\rho), & \rho > 0 \\ 0, & \rho = 0 \end{cases}$,

and write $\Omega^+ := \Omega \cap \{\mathbf{x} \in \Omega : \rho(t, \mathbf{x}) > 0\}$, we have the crowd motion model

$$(2.7) \quad \min_{\rho, \mathbf{m} \in \mathcal{C}(\rho_0, \rho_1)} \left\{ \begin{array}{l} \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt \\ + \lambda_E \int_0^1 \int_{\Omega^+} \rho(t, \mathbf{x}) \log(\rho(t, \mathbf{x})) d\mathbf{x} dt + \lambda_Q \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x} dt \end{array} \right\}.$$

With F_E decreasing on $[0, e^{-1}]$ and increasing on $[e^{-1}, +\infty)$, $\rho(t, \mathbf{x})$ tends to be close to e^{-1} everywhere. So we expect to have the density $\rho(t, \mathbf{x})$ to be not sparse and not very large everywhere.

Example 2.3. If $F_E : \mathbb{R}^+ \rightarrow \mathbb{R}$, $\rho \mapsto \begin{cases} \frac{1}{|p|} \rho^p, & \rho > 0 \\ 0, & \rho = 0 \end{cases}$, where $p = 2$ or -1 , then we have the following two models.

$$(2.8) \quad \min_{\rho, \mathbf{m} \in \mathcal{C}(\rho_0, \rho_1)} \left\{ \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \lambda_E \int_0^1 \int_{\Omega} \frac{\rho^2(t, \mathbf{x})}{2} d\mathbf{x} dt + \lambda_Q \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x} dt \right\},$$

$$(2.9) \quad \min_{\rho, \mathbf{m} \in \mathcal{C}(\rho_0, \rho_1)} \left\{ \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \lambda_E \int_0^1 \int_{\Omega^+} \frac{1}{\rho(t, \mathbf{x})} d\mathbf{x} dt + \lambda_Q \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x} dt \right\}.$$

In (2.8), by Cauchy-Schwarz inequality, we have

$$(2.10) \quad \left(\int_{\Omega} \rho(t, \mathbf{x}) d\mathbf{x} \right)^2 \leq \int_{\Omega} \rho^2(t, \mathbf{x}) d\mathbf{x} \int_{\Omega} 1 d\mathbf{x},$$

therefore $\int_{\Omega} \rho^2(t, \mathbf{x}) d\mathbf{x}$ has a lower bound and achieves the lower bound when $\rho(t, \cdot)$ is a constant over Ω . Therefore, model (2.8) guides the solution density uniformly distributed over Ω . In (2.9), since the total mass $\int_{\Omega} \rho(t, \mathbf{x}) d\mathbf{x}$ is fixed and $\frac{1}{\rho}$ is larger when ρ is smaller, the value of regularization term $\lambda_E \int_{\Omega^+} \frac{1}{\rho(t, \mathbf{x})} d\mathbf{x}$ is smaller if $\rho(t, \mathbf{x})$ accumulates at several sites and vanishes at other regions. Therefore model (2.9) pursues a sparse optimizer $\rho(t, \mathbf{x})$.

Example 2.4 (A MFG model [16, 30, 35]). We provide an example of the MFG model (1.2) to complete this section. In the cases, the terminal density ρ_1 is not explicitly provided but it satisfies a given preference. This preference can be imposed by regularizing $\rho(1, \cdot)$ in the same spirit as $\int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x}$ and obtain the following MFG model,

$$(2.11) \quad \min_{(\rho, \mathbf{m}) \in \mathcal{C}(\rho_0)} \left\{ \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \lambda_E \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) \log(\rho(t, \mathbf{x})) d\mathbf{x} dt + \lambda_Q \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x} dt + \lambda_G \int_{\Omega} \rho(1, \mathbf{x}) G(\mathbf{x}) d\mathbf{x} \right\}$$

Here $\lambda_G > 0$ is a parameter, $G : \Omega \rightarrow \overline{\mathbb{R}}$ gives a preference of the distribution of $\rho(1, \mathbf{x})$ and the constraint set $\mathcal{C}(\rho_0)$ is similar to $\mathcal{C}(\rho_0, \rho_1)$:

$$(2.12) \quad \mathcal{C}(\rho_0) := \mathcal{C} \cap \left\{ \begin{array}{l} (\rho, \mathbf{m}) : \partial_t \rho + \operatorname{div}_{\mathbf{x}} \mathbf{m} = 0, \\ \mathbf{m} \cdot \mathbf{n} = 0 \text{ for } \mathbf{x} \in \partial \Omega, \rho(0, \cdot) = \rho_0. \end{array} \right\}$$

3. ALGORITHM

In this section, we first briefly review the FISTA algorithm proposed in [10]. Using a first-optimize-then-discretize approach, we describe the FISTA algorithm on variational problem (1.1). After that, we provide the details of our discretization

and implementation for the MFP. At the end of this section, we discuss a different approach based on a first-discretize-then-optimize strategy which turns out to lead to the same discrete algorithm.

To solve a general nonsmooth convex model

$$\min_{\mathbf{z}} u(\mathbf{z}) + v(\mathbf{z}),$$

where u is a smooth convex function and v is convex but possibly nonsmooth, one can apply the proximal gradient method [9,46]

$$\mathbf{z}^{(k+1)} := \text{Prox}_{\eta^{(k)} v} \left(\mathbf{z}^{(k)} - \eta^{(k)} \nabla u \left(\mathbf{z}^{(k)} \right) \right).$$

Here $\eta^{(k)} > 0$ is the step-size and the proximal operator is defined as:

$$(3.1) \quad \text{Prox}_{\eta v}(\mathbf{z}) := \underset{\mathbf{y}}{\operatorname{argmin}} \left\{ v(\mathbf{y}) + \frac{1}{2\eta} \|\mathbf{y} - \mathbf{z}\|_2^2 \right\}.$$

In particular, for an indicator function $\chi_{\mathcal{C}}(\mathbf{z}) = \begin{cases} 0, & \mathbf{z} \in \mathcal{C}, \\ +\infty, & \mathbf{z} \notin \mathcal{C} \end{cases}$ of a convex set \mathcal{C} , its proximal operator is exactly the projection operator to \mathcal{C} , i.e.

$$\text{Prox}_{\eta \chi_{\mathcal{C}}}(\mathbf{z}) = \text{Proj}_{\mathcal{C}}(\mathbf{z}) = \underset{\mathbf{y} \in \mathcal{C}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{y} - \mathbf{z}\|_2^2, \quad \forall \eta > 0.$$

FISTA is essentially an accelerated proximal gradient algorithm [10]. It introduces $\hat{\mathbf{z}}^{(k)}$ as a linear combination of $\mathbf{z}^{(k)}$ and $\mathbf{z}^{(k-1)}$ in each iteration, and conducts proximal gradient on $\hat{\mathbf{z}}^{(k)}$ to obtain $\mathbf{z}^{(k+1)}$. The algorithm is summarized in (3.2), where the step-sizes $\eta^{(k)}$ can either be a constant or be obtained by a backtracking line search.

$$(3.2) \quad \begin{cases} \mathbf{z}^{(k+1)} &= \text{Prox}_{\eta^{(k)} v} \left(\hat{\mathbf{z}}^{(k)} - \eta^{(k)} \nabla u(\hat{\mathbf{z}}^{(k)}) \right); \\ \tau^{(k+1)} &= \frac{1}{2} \left(1 + \sqrt{1 + 4 (\tau^{(k)})^2} \right); \\ \hat{\mathbf{z}}^{(k+1)} &= \mathbf{z}^{(k+1)} + \frac{\tau^{(k)} - 1}{\tau^{(k+1)}} (\mathbf{z}^{(k+1)} - \mathbf{z}^{(k)}). \end{cases}$$

As proved in [10], if $\mathbf{z}^* = \operatorname{argmin}_{\mathbf{z}} u(\mathbf{z}) + v(\mathbf{z})$, and $\{\mathbf{z}^{(k)}\}$ is generated by FISTA, then

$$\left[u \left(\mathbf{z}^{(k)} \right) + v \left(\mathbf{z}^{(k)} \right) \right] - [u(\mathbf{z}^*) + v(\mathbf{z}^*)] = \mathcal{O} \left(\frac{1}{(k+1)^2} \right).$$

3.1. FISTA for MFP. To apply the above FISTA method to problem (1.1), let us write

$$(3.3) \quad \min_{\rho, \mathbf{m} \in \mathcal{C}(\rho_0, \rho_1)} \mathcal{Y}(\rho, \mathbf{m}) := \int_0^1 \int_{\Omega} Y(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x}), \mathbf{x}) d\mathbf{x} dt,$$

where

$$(3.4) \quad Y(\beta_0, \boldsymbol{\beta}, \mathbf{x}) = L(\beta_0, \boldsymbol{\beta}) + \lambda_E F_E(\beta_0) + \lambda_Q \beta_0 Q(\mathbf{x}).$$

For convenience, we write $F'_E = \frac{d}{d\beta_0} F_E, Y_0 = \frac{\partial}{\partial\beta_0} Y, \nabla_{\beta} Y = \left(\frac{\partial}{\partial\beta_d} Y \right)_{d=1,\dots,D}$ and $L_0 = \frac{\partial}{\partial\beta_0} L, \nabla_{\beta} L = \left(\frac{\partial}{\partial\beta_d} L \right)_{d=1,\dots,D}$. This yields

$$(3.5) \quad \begin{cases} Y_0(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x}), \mathbf{x}) &= L_0(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) + \lambda_E F'_E(\rho(t, \mathbf{x})) + \lambda_Q Q(\mathbf{x}), \\ \nabla_{\beta} Y(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x}), \mathbf{x}) &= \nabla_{\beta} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})), \quad d = 1, \dots, D. \end{cases}$$

To apply FISTA to this problem, we need to compute the gradients $\delta_{\rho}\mathcal{Y}(\rho, \mathbf{m})$, $\delta_{\mathbf{m}}\mathcal{Y}(\rho, \mathbf{m})$ and the projection $\text{Proj}_{\mathcal{C}(\rho_0, \rho_1)}(\rho, \mathbf{m})$.

Gradient descent. Let the boundary values $\rho(0, \cdot) = \rho_0, \rho(1, \cdot) = \rho_1$ and $\mathbf{m}(t, \mathbf{x}) \cdot \mathbf{n} = 0$ for $\mathbf{x} \in \partial\Omega$ being fixed. By variational calculus, we have

$$(3.6) \quad \begin{aligned} \delta_{\rho}\mathcal{Y}(\rho, \mathbf{m})(t, \mathbf{x}) &= Y_0(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x}), \mathbf{x}), \\ \delta_{\mathbf{m}}\mathcal{Y}(\rho, \mathbf{m})(t, \mathbf{x}) &= \nabla_{\beta} Y(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x}), \mathbf{x}). \end{aligned}$$

Then with step-size $\eta^{(k)}$, the descent step can be written as

$$(3.7) \quad \left(\rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})} \right) = \left(\hat{\rho}^{(k)} - \eta^{(k)} \delta_{\rho}\mathcal{Y}(\hat{\rho}^{(k)}, \hat{\mathbf{m}}^{(k)}), \hat{\mathbf{m}}^{(k)} - \eta^{(k)} \delta_{\mathbf{m}}\mathcal{Y}(\hat{\rho}^{(k)}, \hat{\mathbf{m}}^{(k)}) \right).$$

Projection. The projection step solves the following minimization problem

$$(3.8) \quad \left(\rho^{(k+1)}, \mathbf{m}^{(k+1)} \right) = \underset{\rho, \mathbf{m} \in \mathcal{C}(\rho_0, \rho_1)}{\text{argmin}} \frac{1}{2} \left\| \rho - \rho^{(k+\frac{1}{2})} \right\|_{L^2}^2 + \frac{1}{2} \left\| \mathbf{m} - \mathbf{m}^{(k+\frac{1}{2})} \right\|_{L^2}^2.$$

Since the boundary values are fixed and boundary conditions are always satisfied, we only need to introduce dual variable $\phi^{(k+1)}(t, \mathbf{x})$, which is C^1 on $[0, 1] \times \Omega$, for mass conservation equation $\partial_t \rho + \text{div}_{\mathbf{x}} \mathbf{m} = 0$. Consider a Lagrangian function

$$(3.9) \quad \begin{aligned} \mathcal{L}(\rho, \mathbf{m}, \phi) &:= \frac{1}{2} \left\| \rho - \rho^{(k+\frac{1}{2})} \right\|_{L^2}^2 + \frac{1}{2} \left\| \mathbf{m} - \mathbf{m}^{(k+\frac{1}{2})} \right\|_{L^2}^2 + \langle \phi, \partial_t \rho + \text{div}_{\mathbf{x}} \mathbf{m} \rangle \\ &= \frac{1}{2} \left\| \rho - \rho^{(k+\frac{1}{2})} \right\|_{L^2}^2 + \frac{1}{2} \left\| \mathbf{m} - \mathbf{m}^{(k+\frac{1}{2})} \right\|_{L^2}^2 - \langle \partial_t \phi, \rho \rangle - \langle \nabla_{\mathbf{x}} \phi, \mathbf{m} \rangle \\ &\quad + \langle \phi(1, \cdot), \rho_1 \rangle - \langle \phi(0, \cdot), \rho_0 \rangle. \end{aligned}$$

$(\rho^{(k+1)}, \mathbf{m}^{(k+1)}, \phi^{(k+1)})$ is the saddle point of $\mathcal{L}(\rho, \mathbf{m}, \phi)$ if and only if

$$(3.10) \quad \begin{cases} \delta_{\rho} \mathcal{L}(\rho^{(k+1)}, \mathbf{m}^{(k+1)}, \phi^{(k+1)}) = 0, \\ \delta_{\mathbf{m}} \mathcal{L}(\rho^{(k+1)}, \mathbf{m}^{(k+1)}, \phi^{(k+1)}) = 0, \\ \delta_{\phi} \mathcal{L}(\rho^{(k+1)}, \mathbf{m}^{(k+1)}, \phi^{(k+1)}) = 0. \end{cases}$$

This yields

$$(3.11) \quad \begin{cases} \rho^{(k+1)} &= \rho^{(k+\frac{1}{2})} + \partial_t \phi^{(k+1)}, \\ \mathbf{m}^{(k+1)} &= \mathbf{m}^{(k+\frac{1}{2})} + \nabla_{\mathbf{x}} \phi^{(k+1)}, \end{cases}$$

and

$$(3.12) \quad \partial_t \rho^{(k+1)} + \text{div}_{\mathbf{x}} \mathbf{m}^{(k+1)} = 0.$$

Algorithm 1 FISTA for MFP

Parameters ρ_0, ρ_1
Initialization $\tau^{(1)} = 1$,

$$\begin{aligned} \rho^{(0)}(0, \cdot) &= \widehat{\rho}^{(0)}(0, \cdot) = \rho_0, \quad \rho^{(0)}(1, \cdot) = \widehat{\rho}^{(0)}(1, \cdot) = \rho_1, \\ \rho^{(0)}(t, \cdot) &= \widehat{\rho}^{(0)}(t, \cdot) = 1 \text{ for } 0 < t < 1, \\ \mathbf{m}^{(0)}(\cdot, \mathbf{x}) \cdot \mathbf{n} &= \widehat{\mathbf{m}}^{(0)}(\cdot, \mathbf{x}) \cdot \mathbf{n} = 0 \text{ for } \mathbf{x} \in \partial\Omega, \\ \mathbf{m}^{(0)}(\cdot, \mathbf{x}) &= \widehat{\mathbf{m}}^{(0)}(\cdot, \mathbf{x}) = \mathbf{1} \text{ for } \mathbf{x} \in \Omega \setminus \partial\Omega. \end{aligned}$$

for $k = 0, 1, 2, \dots$ **do**

gradient descent

(3.14)
$$\begin{cases} \rho^{(k+\frac{1}{2})}(t, \mathbf{x}) = \widehat{\rho}^{(k)}(t, \mathbf{x}) - \eta^{(k)} Y_0(\widehat{\rho}^{(k)}(t, \mathbf{x}), \widehat{\mathbf{m}}^{(k)}(t, \mathbf{x}), \mathbf{x}), \\ 0 < t < 1, \\ \mathbf{m}^{(k+\frac{1}{2})}(t, \mathbf{x}) = \widehat{\mathbf{m}}^{(k)}(t, \mathbf{x}) - \eta^{(k)} \nabla_{\mathbf{m}} Y(\widehat{\rho}^{(k)}(t, \mathbf{x}), \widehat{\mathbf{m}}^{(k)}(t, \mathbf{x}), \mathbf{x}), \\ 0 \leq t \leq 1, \end{cases} \begin{aligned} &\mathbf{x} \in \Omega, \\ &\mathbf{x} \in \Omega \setminus \partial\Omega. \end{aligned}$$

projection solve $\phi^{(k+1)}$ for

(3.15)
$$\begin{cases} -\Delta_{t, \mathbf{x}} \phi^{(k+1)}(t, \mathbf{x}) = \partial_t \rho^{(k+\frac{1}{2})}(t, \mathbf{x}) + \operatorname{div}_{\mathbf{x}} \mathbf{m}^{(k+\frac{1}{2})}(t, \mathbf{x}), & 0 \leq t \leq 1, \mathbf{x} \in \Omega \\ \partial_t \phi^{(k+1)}(t, \mathbf{x}) = 0, & t = 0, 1, \mathbf{x} \in \Omega \\ \nabla_{\mathbf{x}} \phi^{(k+1)}(t, \mathbf{x}) \cdot \mathbf{n} = 0, & 0 \leq t \leq 1, \mathbf{x} \in \partial\Omega, \end{cases}$$

and conduct

(3.16)
$$\begin{cases} \rho^{(k+1)} = \rho^{(k+\frac{1}{2})} + \partial_t \phi^{(k+1)}, \\ \mathbf{m}^{(k+1)} = \mathbf{m}^{(k+\frac{1}{2})} + \nabla_{\mathbf{x}} \phi^{(k+1)}. \end{cases}$$

update

(3.17)
$$\begin{aligned} \tau^{(k+1)} &= \frac{1 + \sqrt{1 + 4(\tau^{(k)})^2}}{2}, \\ \omega^{(k)} &= \frac{\tau^{(k)} - 1}{\tau^{(k+1)}}, \\ \left(\widehat{\rho}^{(k+1)}, \widehat{\mathbf{m}}^{(k+1)} \right) &= \left(1 + \omega^{(k)} \right) \left(\rho^{(k+1)}, \mathbf{m}^{(k+1)} \right) - \omega^{(k)} \left(\rho^{(k)}, \mathbf{m}^{(k)} \right). \end{aligned}$$

end for

Combining (3.11) and (3.12), it is clear that the dual variable $\phi^{(k+1)}$ solves the Poisson equation

(3.13)
$$\begin{cases} -\Delta_{t, \mathbf{x}} \phi^{(k+1)}(t, \mathbf{x}) = \partial_t \rho^{(k+\frac{1}{2})}(t, \mathbf{x}) + \operatorname{div}_{\mathbf{x}} \mathbf{m}^{(k+\frac{1}{2})}(t, \mathbf{x}), & 0 \leq t \leq 1, \mathbf{x} \in \Omega, \\ \partial_t \phi^{(k+1)}(t, \mathbf{x}) = 0, & t = 0, 1, \mathbf{x} \in \Omega, \\ \nabla_{\mathbf{x}} \phi^{(k+1)}(t, \mathbf{x}) \cdot \mathbf{n} = 0, & 0 \leq t \leq 1, \mathbf{x} \in \partial\Omega, \end{cases}$$

Therefore, we can obtain the projection (3.8) in two steps: solving the Poisson equation (3.13) and updating ρ, \mathbf{m} by (3.11).

The FISTA algorithm for MFP problem (3.3) is summarized in Algorithm 1.

Remark 3.1. To compute the projection, we need to solve a Poisson equation with Neumann boundary conditions (3.13). Since for any $\mathbf{x} \in \Omega$, $\rho^{(k+\frac{1}{2})}(0, \mathbf{x}) =$

$\rho_0(\mathbf{x}), \rho^{(k+\frac{1}{2})}(1, \mathbf{x}) = \rho_1(\mathbf{x})$ and for any $t \in [0, 1], \mathbf{x} \in \partial\Omega$, $\mathbf{m}^{(k+\frac{1}{2})}(t, \mathbf{x}) \cdot \mathbf{n} = 0$, we have

$$\begin{aligned} & \int_{[0,1] \times \Omega} \partial_t \rho^{(k+\frac{1}{2})}(t, \mathbf{x}) + \operatorname{div}_{\mathbf{x}} \mathbf{m}^{(k+\frac{1}{2})}(t, \mathbf{x}) d\mathbf{x} dt \\ &= \int_{\Omega} \left(\rho^{(k+\frac{1}{2})}(1, \mathbf{x}) - \rho^{(k+\frac{1}{2})}(0, \mathbf{x}) \right) d\mathbf{x} + \int_0^1 \int_{\partial\Omega} \mathbf{m}^{(k+\frac{1}{2})}(t, \mathbf{x}) \cdot \mathbf{n} ds dt \\ &= \int_{\Omega} \left(\rho_1^{(k+\frac{1}{2})}(\mathbf{x}) - \rho_0^{(k+\frac{1}{2})}(\mathbf{x}) \right) d\mathbf{x} \\ &= 0. \end{aligned}$$

This means (3.13) is solvable and the solution is unique up to a constant. In addition, the constant does not count in the projection step because in (3.11), we only need $\partial_t \phi^{(k+1)}$ and $\nabla_{\mathbf{x}} \phi^{(k+1)}$. Therefore the projection step is well-defined.

3.2. Discretization and implementation. For convenience, we here assume $\Omega = [0, 1]^D$. Then the boundary condition of $\mathbf{m} = (m_1, \dots, m_D)$ is provided as:

$$m_d(t, \mathbf{x}) = 0, \text{ if } x_d = 0, \text{ or } 1, \quad \text{for } d = 1, \dots, D.$$

Consider a uniform grid with n_0 segments on time interval $[0, 1]$ and n_d segments on the d -th space dimension. Namely, the mesh size on each dimension is $\Delta_d = \frac{1}{n_d}, d = 0, \dots, D$, and the staggered grid points are $t_j = (j - \frac{1}{2})\Delta_0, (x_d)_j = (j - \frac{1}{2})\Delta_d$. We use a multidimensional index vector $\mathbf{j} = (j_0, j_1, \dots, j_D)$ to indicate a grid point $(t_{j_0}, \mathbf{x}_{\mathbf{j}})$, where $\mathbf{x}_{\mathbf{j}} := ((x_1)_{j_1}, \dots, (x_D)_{j_D})$. We further write $u_{\mathbf{j}} := u(t_{j_0}, \mathbf{x}_{\mathbf{j}})$ the value of function u on the grid point and $U_{\mathbf{j}}$ the proposed numerical approximation of $u_{\mathbf{j}}$. Our discretization of ρ and \mathbf{m} is defined on different staggered grids. For convenience, we list the following index sets:

$$\begin{aligned} J_d &:= \left\{ \frac{3}{2}, \frac{5}{2}, \dots, n_d - \frac{1}{2} \right\}, \\ \overline{J}_d &:= \{1, 2, \dots, n_d\}, \\ \mathbf{J}_d &:= \overline{J}_0 \times \overline{J}_1 \times \dots \times \overline{J}_{d-1} \times J_d \times \overline{J}_{d+1} \times \dots \times \overline{J}_D, \\ \overline{\mathbf{J}} &:= \overline{J}_0 \times \overline{J}_1 \times \dots \times \overline{J}_D. \end{aligned}$$

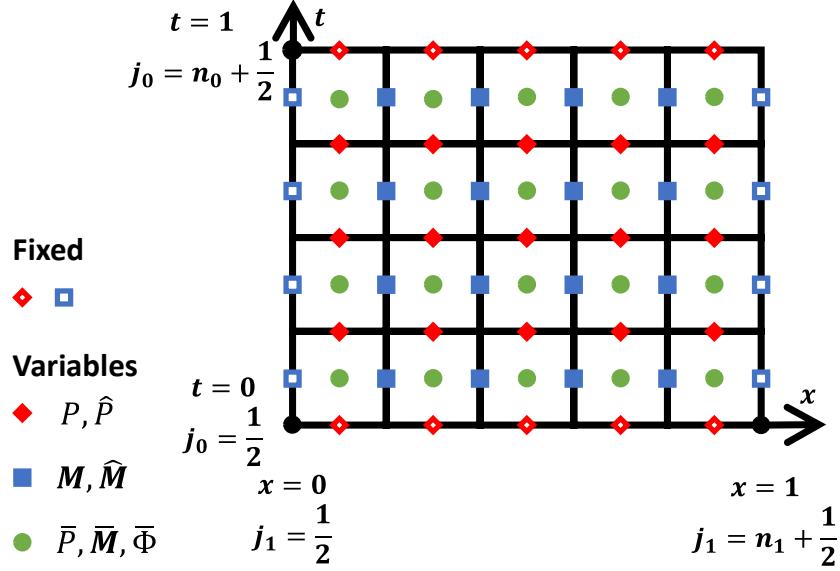
Figure 2 illustrates a 1D example, where $n_0 = 4, n_1 = 5$ and grid points related to $\mathbf{J}_0, \mathbf{J}_1$ and $\overline{\mathbf{J}}$ are annotated as red solid diamonds, blue solid squares and green solid dots, respectively.

We use P, \mathbf{M} and $\overline{\Phi}$ to denote the discretization of ρ, \mathbf{m} and ϕ , respectively. They are defined as:

$$\begin{aligned} P &:= \{P_{\mathbf{j}}\}_{\mathbf{j} \in \mathbf{J}_0} \in \mathbb{V}_0 := \mathbb{R}^{(n_0-1) \times n_1 \times \dots \times n_D}, \\ M_d &:= \{(M_d)_{\mathbf{j}}\}_{\mathbf{j} \in \mathbf{J}_d} \in \mathbb{V}_d := \mathbb{R}^{n_0 \times n_1 \times \dots \times n_{d-1} \times (n_d-1) \times n_{d+1} \times \dots \times n_D}, \\ \mathbf{M} &:= \{M_d\}_{d=1,2,\dots,D} \in \mathbb{V}_1 \times \dots \times \mathbb{V}_D, \\ \overline{\Phi} &:= \{\overline{\Phi}_{\mathbf{j}}\}_{\mathbf{j} \in \overline{\mathbf{J}}} \in \overline{\mathbb{V}} := \mathbb{R}^{n_0 \times n_1 \times \dots \times n_D}. \end{aligned}$$

Moreover, we also define:

$$\begin{aligned} \overline{P} &:= \{\overline{P}_{\mathbf{j}}\}_{\mathbf{j} \in \overline{\mathbf{J}}} \in \overline{\mathbb{V}} := \mathbb{R}^{n_0 \times n_1 \times \dots \times n_D}, \\ \overline{M}_d &:= \{(\overline{M}_d)_{\mathbf{j}}\}_{\mathbf{j} \in \overline{\mathbf{J}}} \in \overline{\mathbb{V}}, \\ \overline{\mathbf{M}} &:= \{\overline{M}_d\}_{d=1,2,\dots,D} \in \overline{\mathbb{V}}^D. \end{aligned}$$

FIGURE 2. Illustration of staggered grids for the case $d = 1$

Based on the above settings, we next discuss details of computing the objective value, implementing gradient descent and conducting the projection step.

Objective value. To compute the objective function, we need the value of $\rho(t, \mathbf{x})$ and $\mathbf{m}(t, \mathbf{x})$ on the same point (t, \mathbf{x}) . While P, M_d are defined on different grids, a natural idea is to transform them to the same central grid $\bar{\mathbf{J}}$ first. For convenience, let $M_0 \equiv P$. We can define the average operators as:

$$\mathcal{A}_d : \mathbb{V}_d \rightarrow \bar{\mathbb{V}}, \quad M_d \mapsto \bar{M}_d = \mathcal{A}_d(M_d), \quad \text{for } d = 0, 1, \dots, D,$$

$$(\bar{M}_d)_j := \begin{cases} \frac{1}{2}(M_d)_{j+\frac{e_d}{2}}, & j_d = 1, \\ \frac{1}{2} \left((M_d)_{j+\frac{e_d}{2}} + (M_d)_{j-\frac{e_d}{2}} \right), & j_d = 2, 3, \dots, n_d - 1, \\ \frac{1}{2}(M_d)_{j-\frac{e_d}{2}}, & j_d = n_d. \end{cases} \quad \forall j \in \bar{\mathbf{J}},$$

$$\mathcal{A} : \mathbb{V}_1 \times \dots \times \mathbb{V}_D \rightarrow \bar{\mathbb{V}}^D, \quad \mathbf{M} \mapsto \{\mathcal{A}_d(M_d)\}_{d=1, \dots, D},$$

where $e_d \in \mathbb{R}^{D+1}$ has 1 in the $(d+1)$ -th entry and 0 elsewhere, $d = 0, \dots, D$. The boundary conditions of \mathbf{M} are implicitly included in the average operator. We further define $\bar{P}_{\mathcal{A}} \in \bar{\mathbb{V}}$ to indicate density boundary conditions,

$$(\bar{P}_{\mathcal{A}})_j := \begin{cases} \frac{1}{2}\rho_0(\mathbf{x}_j), & j_0 = 1, \\ 0, & j_0 = 2, 3, \dots, n_0 - 1, \\ \frac{1}{2}\rho_1(\mathbf{x}_j), & j_0 = n_0. \end{cases} \quad \forall j \in \bar{\mathbf{J}},$$

As an example, in Figure 2, \mathcal{A}_0 maps P to \overline{P} . \mathcal{A}_1 maps M to \overline{M} , and the hollow diamonds on $t = 0, 1$ contribute to the nonzero entries of $\overline{P}_{\mathcal{A}}$.

Now, we are ready to evaluate the objective function by averaging P and M from their staggered grids to the central grid. Namely, we define $\overline{P}, \overline{M} \in \overline{\mathbb{V}}$ as

$$(3.18) \quad \overline{P} := \mathcal{A}_0(P) + \overline{P}_{\mathcal{A}}, \quad \overline{M} := \mathcal{A}(M),$$

then we approximate the objective value by

$$\left(\prod_{d=0}^D \Delta_d \right) \mathcal{Y}(P, M),$$

where

$$(3.19) \quad \mathcal{Y}(P, M) := \overline{\mathcal{Y}}(\overline{P}, \overline{M}) := \sum_{j \in \overline{J}} Y(\overline{P}_j, \overline{M}_j, \mathbf{x}_j).$$

Gradient descent. To fulfil gradient descent, we first average (P, M) from different grids \mathbf{J}_d to grid \overline{J} by (3.18) and pointwisely compute gradient values

$$(3.20) \quad \begin{aligned} \partial_{\overline{P}} \overline{\mathcal{Y}}(\overline{P}, \overline{M}) &:= \{Y_0(\overline{P}_j, \overline{M}_j, \mathbf{x}_j)\}_{j \in \overline{J}}, \\ \partial_{\overline{M}_d} \overline{\mathcal{Y}}(\overline{P}, \overline{M}) &:= \{Y_d(\overline{P}_j, \overline{M}_j, \mathbf{x}_j)\}_{j \in \overline{J}}, \quad d = 1, \dots, D, \\ \partial_{\overline{M}} \overline{\mathcal{Y}}(\overline{P}, \overline{M}) &:= \{\partial_{\overline{M}_d} \overline{\mathcal{Y}}(\overline{P}, \overline{M})\}_{d=1, \dots, D}. \end{aligned}$$

Then we average gradient values back to different grids \mathbf{J}_d . Defining another set of average operators as

$$\begin{aligned} \mathcal{A}_d^* : \overline{\mathbb{V}} \rightarrow \mathbb{V}_d, \overline{M}_d &\mapsto M_d, \quad (M_d)_j := \frac{1}{2} \left((\overline{M}_d)_{j+\frac{e_d}{2}} + (\overline{M}_d)_{j-\frac{e_d}{2}} \right), \\ \mathcal{A}^* : \overline{\mathbb{V}}^D &\rightarrow \mathbb{V}_1 \times \dots \times \mathbb{V}_D, \overline{M} \mapsto \{\mathcal{A}_d^*(\overline{M}_d)\}_{d=1, \dots, D}, \end{aligned}$$

we obtain desired gradient values:

$$(3.21) \quad \begin{aligned} \partial_P \mathcal{Y}(P, M) &= \mathcal{A}_0^* (\partial_{\overline{P}} \overline{\mathcal{Y}}(\overline{P}, \overline{M})), \\ \partial_M \mathcal{Y}(P, M) &= \mathcal{A}^* (\partial_{\overline{M}} \overline{\mathcal{Y}}(\overline{P}, \overline{M})). \end{aligned}$$

Combining (3.20), (3.21), we can implement gradient descent step (3.14) on discrete meshes by:

$$(3.22) \quad \left(P^{(k+\frac{1}{2})}, M^{(k+\frac{1}{2})} \right) = \left(\widehat{P}^{(k)}, \widehat{M}^{(k)} \right) - \eta^{(k)} \left(\partial_P \mathcal{Y}(\widehat{P}^{(k)}, \widehat{M}^{(k)}), \partial_M \mathcal{Y}(\widehat{P}^{(k)}, \widehat{M}^{(k)}) \right).$$

Projection. To compute the projection, we use a finite difference method to discretize the corresponding differential operators in the PDE constraint. We first define discrete partial derivative:

$$\mathcal{D}_d : \mathbb{V}_d \rightarrow \overline{\mathbb{V}}, \quad M_d \mapsto \mathcal{D}_d(M_d), \quad \text{for } d = 0, \dots, D.$$

$$(\mathcal{D}_d(M_d))_j := \begin{cases} \frac{1}{\Delta_d} (M_d)_{j+\frac{e_d}{2}}, & j_d = 1, \\ \frac{1}{\Delta_d} \left((M_d)_{j+\frac{e_d}{2}} - (M_d)_{j-\frac{e_d}{2}} \right), & j_d = 2, 3, \dots, n_d - 1, \\ -\frac{1}{\Delta_d} (M_d)_{j-\frac{e_d}{2}}, & j_d = n_d, \end{cases}$$

discrete divergence:

$$\text{Div} : \mathbb{V}_0 \times \mathbb{V}_1 \times \cdots \mathbb{V}_D \rightarrow \overline{\mathbb{V}}, \quad (P, \mathbf{M}) \mapsto \mathcal{D}_0(P) + \sum_{d=1}^D \mathcal{D}_d(M_d),$$

and the term $\overline{P}_{\mathcal{D}} \in \overline{\mathbb{V}}$ to impose boundary conditions:

$$(\overline{P}_{\mathcal{D}})_j := \begin{cases} -\frac{1}{\Delta_0} \rho_0(\mathbf{x}_j), & j_0 = 1, \\ 0, & j_0 = 2, 3, \dots, n_0 - 1, \\ \frac{1}{\Delta_0} \rho_1(\mathbf{x}_j), & j_0 = n_0. \end{cases}$$

Then the RHS of first equation in (3.15) can be approximated by

$$\text{Div} \left(P^{(k+\frac{1}{2})}, \mathbf{M}^{(k+\frac{1}{2})} \right) + \overline{P}_{\mathcal{D}}.$$

We approximate ∂_d with a central difference and ∂_{dd} with a three-point stencil finite difference. By homogeneous Neumann boundary condition, we have discrete second-order derivative operators

$$\begin{aligned} \mathcal{D}_{dd} : \overline{\mathbb{V}} &\rightarrow \overline{\mathbb{V}}, \quad \overline{\Phi} \mapsto \mathcal{D}_{dd}(\overline{\Phi}), \\ (\mathcal{D}_{dd}(\overline{\Phi}))_j &:= \begin{cases} \frac{1}{\Delta_d^2} (-\overline{\Phi}_j + \overline{\Phi}_{j+e_d}), & j_d = 1, \\ \frac{1}{\Delta_d^2} (\overline{\Phi}_{j-e_d} - 2\overline{\Phi}_j + \overline{\Phi}_{j+e_d}), & j_d = 2, 3, \dots, n_d - 1, \\ \frac{1}{\Delta_d^2} (\overline{\Phi}_{j-e_d} - \overline{\Phi}_j), & j_d = n_d, \end{cases} \\ \text{Lap} : \overline{\mathbb{V}} &\rightarrow \overline{\mathbb{V}}, \quad \overline{\Phi} \mapsto \mathcal{D}_{00}(\overline{\Phi}) + \sum_{d=1}^D \mathcal{D}_{dd}(\overline{\Phi}). \end{aligned}$$

The Poisson equation (3.15) on grids is therefore

$$(3.23) \quad -\text{Lap} \left(\overline{\Phi}^{(k+1)} \right) = \text{Div} \left(P^{(k+\frac{1}{2})}, \mathbf{M}^{(k+\frac{1}{2})} \right) + \overline{P}_{\mathcal{D}}.$$

Defining another set of derivative operators

$$\begin{aligned} \mathcal{D}_d^* : \overline{\mathbb{V}} &\rightarrow \mathbb{V}_d, \quad \overline{\Phi} \mapsto \mathcal{D}_d^*(\overline{\Phi}), \quad (\mathcal{D}_d^*(\overline{\Phi}))_j := \frac{1}{\Delta_d} \left((\overline{\Phi})_{j+\frac{e_d}{2}} - (\overline{\Phi})_{j-\frac{e_d}{2}} \right), \\ \text{Grad} : \overline{\mathbb{V}} &\rightarrow \mathbb{V}_0 \times \mathbb{V}_1 \times \cdots \mathbb{V}_D, \quad \overline{\Phi} \mapsto \{\mathcal{D}_d^*(\overline{\Phi})\}_{d=0,1,\dots,D}, \end{aligned}$$

we discretize the second step of projection (3.16) as

$$(3.24) \quad \left(P^{(k+1)}, \mathbf{M}^{(k+1)} \right) = \left(P^{(k+\frac{1}{2})}, \mathbf{M}^{(k+\frac{1}{2})} \right) + \text{Grad} \left(\overline{\Phi}^{(k+1)} \right).$$

Combining the above ingredients, we summarize FISTA for MFP on discrete mesh in Algorithm 2.

Algorithm 2 FISTA for MFP on discrete mesh

Parameters ρ_0, ρ_1
Initialization $\tau^{(1)} = 1$, $P^{(0)} = \widehat{P}^{(0)} = \mathbf{1}$, and $M_d^{(0)} = \widehat{M}_d^{(0)} = \mathbf{1}$.
for $k = 0, 1, 2, \dots$ **do**
 gradient descent
 (3.25)
$$\begin{cases} P^{(k+\frac{1}{2})} = \widehat{P}^{(k)} - \eta^{(k)} \partial_P \mathcal{Y}(\widehat{P}^{(k)}, \widehat{M}^{(k)}), \\ M^{(k+\frac{1}{2})} = \widehat{M}^{(k)} - \eta^{(k)} \partial_M \mathcal{Y}(\widehat{P}^{(k)}, \widehat{M}^{(k)}), \end{cases}$$

 projection solve $\overline{\Phi}^{(k+1)}$ for
 (3.26)
$$-\text{Lap}(\overline{\Phi}^{(k+1)}) = \text{Div}(P^{(k+\frac{1}{2})}, M^{(k+\frac{1}{2})}) + \overline{P}_{\mathcal{D}},$$

 and conduct
 (3.27)
$$(P^{(k+1)}, M^{(k+1)}) = (P^{(k+\frac{1}{2})}, M^{(k+\frac{1}{2})}) + \text{Grad}(\overline{\Phi}^{(k+1)}).$$

 update

$$\tau^{(k+1)} = \frac{1 + \sqrt{1 + 4(\tau^{(k)})^2}}{2},$$

$$\omega^{(k)} = \frac{\tau^{(k)} - 1}{\tau^{(k+1)}},$$

 (3.28)
$$(\widehat{P}^{(k+1)}, \widehat{M}^{(k+1)}) = (1 + \omega^{(k)}) (P^{(k+1)}, M^{(k+1)}) - \omega^{(k)} (P^{(k)}, M^{(k)}).$$

 end for

Remark 3.2. The discrete operators Div , Grad and Lap are consistent in the following sense. For space $\overline{\mathbb{V}}$ and $\mathbb{V}_0 \times \mathbb{V}_1 \times \dots \times \mathbb{V}_D$, if we view the elements $\overline{\Phi}$ and (P, M) as long vectors, we can define the inner product as

$$(3.29) \quad \begin{aligned} \langle \overline{\Phi}^1, \overline{\Phi}^2 \rangle &:= \sum_{j \in \overline{J}} \overline{\Phi}_j^1 \overline{\Phi}_j^2, \\ \langle (P^1, M^1), (P^2, M^2) \rangle &:= \sum_{j \in J_0} P_j^1 P_j^2 + \sum_{d=1}^D \sum_{j \in J_d} (M_d^1)_j (M_d^2)_j, \end{aligned}$$

and define the induced norm as $\|\cdot\|_F$. Then simple calculation shows that for any $\overline{\Phi} \in \overline{\mathbb{V}}$ and $(P, M) \in \mathbb{V}_0 \times \mathbb{V}_1 \times \dots \times \mathbb{V}_D$, the following equation holds

$$(3.30) \quad \begin{aligned} \text{Lap}(\overline{\Phi}) &= \text{Div} \circ \text{Grad}(\overline{\Phi}), \\ \langle -\text{Grad}(\overline{\Phi}), (P, M) \rangle &= \langle \overline{\Phi}, \text{Div}(P, M) \rangle. \end{aligned}$$

These match the relations between $\text{div}_{t,x}$, $\nabla_{t,x}$ and $\Delta_{t,x}$ on continuous spaces.

Remark 3.3. Directly solving the large linear system (3.26) could be very expensive. Thanks to the special structure of the operator Lap , there exist $\lambda^1 = 0$, $\lambda^i < 0$, $i \in \overline{J} \setminus \{\mathbf{1}\}$ and an orthonormal basis $\{\Psi^i\}_{i \in \overline{J}}$ of $(\overline{\mathbb{V}}, \|\cdot\|_F)$ such that

$$(3.31) \quad \text{Lap}(\overline{\Phi}) := \sum_{i \in \overline{J}} \lambda_i \langle \overline{\Phi}, \Psi^i \rangle \Psi^i.$$

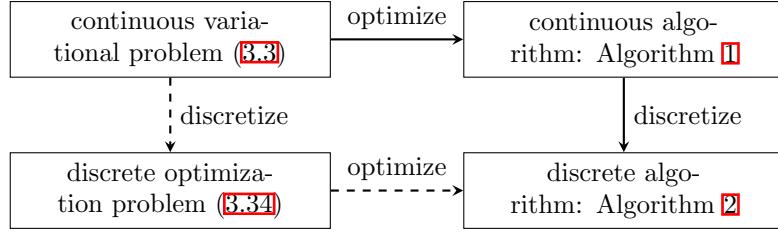


FIGURE 3. Equivalent approaches to obtain the discrete Algorithm 2

Therefore one way to define the inverse of Lap is

$$(3.32) \quad \text{Lap}^{-1}(\bar{\Phi}) := \sum_{i \in \bar{J} \setminus \{1\}} \frac{1}{\lambda_i} \langle \bar{\Phi}, \Psi^i \rangle \Psi^i.$$

This leads to a discrete cosine transform method to solve (3.26).

Remark 3.4. The Lipschitz smoothness of the objective function is important to the convergence of the algorithm. Recall that the dynamic cost $L(\beta_0, \beta)$ defined in (2.5) has a form of $\frac{\|\beta\|_2^2}{2\beta_0}$ when $\beta_0 > 0$, the objective function \mathcal{Y} is not Lipschitz smooth if P_j is only restricted to be nonnegative. However, if there exists $\rho > 0$, such that $P_j > \rho$ holds for all j , then the objective function is Lipschitz smooth, and the Lipschitz constant is smaller with larger ρ . In practice, when $\min_j P_j$ is close to 0, we need to pick the step-size η very carefully to avoid divergence. To improve the numerical stability of the algorithm and preserve the positivity of the density, one can add a small value ϵ uniformly to the initial and terminal densities ρ_0, ρ_1 to obtain an approximated solution to the original problem and/or add a safeguard step

$$(3.33) \quad \hat{P}^{(k+1)} = \max \left(\hat{P}^{(k+1)}, \epsilon' \right),$$

after the extrapolation step (3.28).

To derive the discrete Algorithm 2, we optimize the continuous problem (3.3) by Algorithm 1, then discretize the algorithm. This is a first-optimize-then-discretize approach. We can also consider a first-discretize-then-optimize approach. In fact, using our proposed discretization for MFP, the two approaches lead to the same algorithm, as illustrated in Figure 3. This is mainly because of the consistent relation of discrete operators discussed in Remark 3.2.

Based on previous notations, we discretize the original problem (3.3) to

$$(3.34) \quad \min_{(P, M) \in \mathcal{C}(\bar{P}_D)} \mathcal{Y}(P, M) := \sum_{j \in \bar{J}} Y \left((\mathcal{A}_0(P) + \bar{P}_A)_j, \mathcal{A}(M)_j, x_j \right),$$

where the constraints are linear and the constraint set is convex:

$$(3.35) \quad \mathcal{C}(\bar{P}_D) := \{(P, M) : \mathcal{D}_0(P) + \bar{P}_D + \text{Div}(M) = \mathbf{0}\}.$$

To optimize the problem with FISTA, we first compute the gradient. For any P, M , we define the corresponding values on \bar{J} by $\bar{P} := \mathcal{A}_0(P) + \bar{P}_A$, $\bar{M} := \mathcal{A}(M)$, then

$$(3.36) \quad \mathcal{Y}(P, M) = \sum_{j \in \bar{J}} Y(\bar{P}_j, \bar{M}_j, x_j).$$

We will have (3.20) by taking partial derivatives w.r.t. \bar{P}, \bar{M} , and then (3.21) by the chain rule. Therefore the gradient descent step is exactly (3.25). For projection, based on the inner product defined as (3.29) and induced norm, we can formulate the Lagrangian as

(3.37)

$$\mathcal{L}(P, M, \bar{\Phi}) := \frac{1}{2} \left\| (P, M) - \left(P^{(k+\frac{1}{2})}, M^{(k+\frac{1}{2})} \right) \right\|_F^2 + \left\langle \bar{\Phi}^{(k+1)}, \text{Div}(P, M) + \bar{P}_D \right\rangle.$$

Because of the consistency of the discrete operators (3.30), we know that (3.26), (3.27) compute the projection to $\mathcal{C}(\bar{P}_D)$. Therefore the FISTA algorithm to the discrete MFP problem (3.34) is exactly Algorithm 2.

4. CONVERGENCE

One major difference between Algorithm 1 and Algorithm 2 is that the former is for the continuous setup while the latter one is for a given discretized mesh grid, although both algorithms provide convergence sequences according to the FISTA theory. It is natural to ask if the discretized solution converges to the continuous solution when the mesh grid size Δ_d goes to zero. Specifically, with a given step-size sequence $\{\eta^{(k)}\}_k$, let the sequences $\{(\hat{\rho}^{(k)}, \hat{m}^{(k)})\}_k$, $\{(\rho^{(k)}, m^{(k)})\}_k$, $\{(\rho^{(k+\frac{1}{2})}, m^{(k+\frac{1}{2})})\}_k$ be obtained from Algorithm 1 and $\{(\hat{P}^{(k)}, \hat{M}^{(k)})\}_k$, $\{(P^{(k)}, M^{(k)}), (P^{(k+\frac{1}{2})}, M^{(k+\frac{1}{2})})\}_k$ from Algorithm 2. If $(\rho^{(k)}, m^{(k)}) \rightarrow (\rho^*, m^*)$ and $(P^{(k)}, M^{(k)}) \rightarrow (P^*, M^*)$ as $k \rightarrow \infty$, we would like to study whether (P^*, M^*) converge to (ρ^*, m^*) as the mesh grid size converges to zero. In this section, we theoretically analyze and provide a positive answer to this question under certain conditions.

We first introduce some notations. With given step-size sequence $\{\eta^{(k)}\}_k$, let $\{(\hat{\rho}^{(k)}, \hat{m}^{(k)})\}_k$, $\{(\rho^{(k)}, m^{(k)}), (\rho^{(k+\frac{1}{2})}, m^{(k+\frac{1}{2})})\}_k$ be obtained from Algorithm 1. With the same step-size sequence and initialization $P^{(0)} = \hat{P}^{(0)} = \rho_{J_0}^{(0)}$, $M^{(0)} = \hat{M}^{(0)} = m_J^{(0)}$, let $\{(\hat{P}^{(k)}, \hat{M}^{(k)})\}_k$, $\{(P^{(k)}, M^{(k)}), (P^{(k+\frac{1}{2})}, M^{(k+\frac{1}{2})})\}_k$ be obtained from Algorithm 2. For any index set J_d, \bar{J} , we write the continuous functions ρ and m evaluating on corresponding discrete grids as

$$\begin{aligned} \rho_{J_0} &:= \{\rho_j\}_{j \in J_0}, \quad (m_d)_{J_d} := \{(m_d)_j\}_{j \in J_d}, \quad m_J := \{(m_d)_{J_d}\}_{d=1,2,\dots,D}, \\ \rho_{\bar{J}} &:= \{\rho_j\}_{j \in \bar{J}}, \quad (m_d)_{\bar{J}} := \{(m_d)_j\}_{j \in \bar{J}}, \quad m_{\bar{J}} := \{(m_d)_{\bar{J}}\}_{d=1,2,\dots,D}. \end{aligned}$$

Let $m_0 \equiv \rho, M_0 \equiv P$. For any $k = 0, \frac{1}{2}, 1, 1 + \frac{1}{2}, \dots$, we define the error on grid points J_d by

$$\begin{aligned} E_d^{(k)} &:= M_d^{(k)} - \left(m_d^{(k)} \right)_{J_d}, \quad d = 0, \dots, D, \\ \mathbf{E}_m^{(k)} &:= \left\{ E_d^{(k)} \right\}_{d=1,\dots,D}, \\ \mathbf{E}^{(k)} &:= \left\{ E_0^{(k)}, \mathbf{E}_m^{(k)} \right\}. \end{aligned}$$

Similarly, for $k = 0, 1, 2, \dots$, we define

$$\begin{aligned}\widehat{E}_d^{(k)} &:= \widehat{M}_d^{(k)} - \left(\widehat{m}_d^{(k)} \right)_{\mathbf{J}_d}, \quad d = 0, \dots, D, \\ \widehat{E}_{\mathbf{m}}^{(k)} &:= \left\{ \widehat{E}_d^{(k)} \right\}_{d=1, \dots, D}, \\ \widehat{\mathbf{E}}^{(k)} &:= \left\{ \widehat{E}_0^{(k)}, \widehat{E}_{\mathbf{m}}^{(k)} \right\}, \\ E_{\phi}^{(k)} &:= \overline{\Phi}^{(k)} - \phi_{\mathbf{J}}^{(k)}.\end{aligned}$$

Recall that in Remark 3.2, we introduce induced norm $\|\cdot\|_F$ on space $\mathbb{V}_0 \times \mathbb{V}_1 \times \dots \times \mathbb{V}_D$ and $\overline{\mathbb{V}}$ as

$$\|\mathbf{E}\|_F := \left(\sum_{d=0}^D \sum_{\mathbf{j} \in \mathbf{J}_d} (E_d)_{\mathbf{j}}^2 \right)^{\frac{1}{2}}, \quad \|E_{\phi}\|_F := \left(\sum_{\mathbf{j} \in \overline{\mathbf{J}}} (E_{\phi})_{\mathbf{j}}^2 \right)^{\frac{1}{2}}.$$

We here define 2-norm $\|\cdot\|_2$ as

$$\|\cdot\|_2 := \left(\prod_{d=0}^D \Delta_d \right)^{\frac{1}{2}} \|\cdot\|_F.$$

Next, we propose several assumptions before stating the main theorem.

Assumption 1. Let ρ_0, ρ_1 be given initial and terminal densities. With the above notations, we assume the following conditions hold for any $k = 0, 1, \dots$,

- (1) $\rho_0, \rho_1, \rho^{(k)}, \mathbf{m}^{(k)}, \rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}, \widehat{\rho}^{(k)}, \widehat{\mathbf{m}}^{(k)}$, are C^2 , and $\phi^{(k)}$ are C^3 ,
- (2) There exist $\underline{\rho} \leq \overline{\rho}$, such that $\widehat{\rho}^{(k)}(t, \mathbf{x}), \widehat{P}_{\mathbf{j}}^{(k)} \in [\underline{\rho}, \overline{\rho}]$,
- (3) $\widehat{\mathbf{m}}^{(k)}(t, \mathbf{x}), \widehat{M}_{\mathbf{j}}^{(k)} \in \Omega_{\mathbf{m}} \subset \mathbb{R}^D$,
- (4) Y_d 's are C_Y -Lipschitz continuous on $[\underline{\rho}, \overline{\rho}] \times \Omega_{\mathbf{m}} \times [0, 1]^D$, i.e. for $d = 0, \dots, D$ and any $(\beta_0^1, \beta^1, \mathbf{x}^1), (\beta_0^2, \beta^2, \mathbf{x}^2) \in [\underline{\rho}, \overline{\rho}] \times \Omega_{\mathbf{m}} \times [0, 1]^D$,

$$(4.1) \quad |Y_d(\beta_0^1, \beta^1, \mathbf{x}^1) - Y_d(\beta_0^2, \beta^2, \mathbf{x}^2)| \leq C_Y \|(\beta_0^1, \beta^1, \mathbf{x}^1) - (\beta_0^2, \beta^2, \mathbf{x}^2)\|_1.$$

Remark 4.1. Assumption 1 is accessible for very general cases. In fact, when $\rho_0, \rho_1, \rho^{(0)}, \mathbf{m}^{(0)}$ are C^2 and Y is C^1 , one can show that Assumption 1 holds by induction on k . And Assumption 1(2) and (3) are true as long as $\{\rho^{(k)}, \mathbf{m}^{(k)}\}$ and $\{P^{(k)}, \mathbf{M}^{(k)}\}$ converges. With a typical choice $Y(\beta_0, \beta, \mathbf{x}) = L(\beta_0, \beta)$ where L is defined in (2.5), we retrieve the optimal transport problem. Both (3.3) and (3.34) have unique minimizers $\{\rho^*, \mathbf{m}^*\}$ and $\{P^*, \mathbf{M}^*\}$ and both algorithms converge. If in addition ρ_0, ρ_1 are C^2 and $\min_{\mathbf{x}} \{\rho_0(\mathbf{x}), \rho_1(\mathbf{x})\} \geq \underline{\rho} > 0$, then Assumption 1 holds with continuous initialization and carefully chosen step-sizes. We also would like to point out that the current analysis is based on smoothness assumptions. We admit that for ρ_0, ρ_1 that are only Lebesgue measurable, our proof is not applicable. The convergence under weaker assumptions and more general spaces is an interesting topic to be explored in the future.

We now state our main theorem which characterizes the error bound with respect to the grid size.

Theorem 4.2. *If Assumption I holds for $k = 0, 1, \dots$, then*

$$(4.2) \quad \left\| \mathbf{E}^{(k)} \right\|_2 \leq C \left(\sum_{d=0}^D \Delta_d \right) = \mathcal{O} \left(\sum_{d=0}^D \Delta_d \right).$$

Here C is a constant depending on dimension D , Lipschitz constant C_Y , step-sizes $\{\eta^{(s)}\}_{s=1,\dots,k}$ and sequences $\{\widehat{\rho}^{(s)}, \widehat{\mathbf{m}}^{(s)}\}_{s=1,\dots,k}$ but it is independent of $\{\Delta_d\}_{d=0,\dots,D}$.

Remark 4.3. This theoretical bound is not sharp as the constant C in the worst case is not bounded in terms of k . This suggests that we may have to choose an extremely fine grid to accommodate the size of C . However, our numerical results will show that a reasonably fine mesh is good enough to achieve satisfactory accuracy.

Note that Theorem 4.2 analyzes error bounds at each iteration along optimization paths from the continuous setup and its discretized counterpart. Consequently, we can have the following convergence analysis if both sequences from the continuous and discretized optimization converge (i.e. choice of the step-size satisfies convergence conditions used in FISTA [10]).

Corollary 4.4. *Suppose that $\{(P^{(k)}, \mathbf{M}^{(k)})\}_k$ and $\{(\rho^{(k)}, \mathbf{m}^{(k)})\}_k$ satisfy all conditions in Theorem 4.2. If in addition, there exist (P^*, \mathbf{M}^*) , (ρ^*, \mathbf{m}^*) such that $\rho^* \in C^1$, $\mathbf{m}_d^* \in C^1$ and*

$$(4.3) \quad \begin{aligned} \lim_{k \rightarrow \infty} \left\| (P^{(k)}, \mathbf{M}^{(k)}) - (P^*, \mathbf{M}^*) \right\|_2 &= 0, \\ \lim_{k \rightarrow \infty} \left\| (\rho^{(k)}, \mathbf{m}^{(k)}) - (\rho^*, \mathbf{m}^*) \right\|_{L_2} &= 0, \end{aligned}$$

where $\|\cdot\|_{L_2}$ denotes the standard L_2 -norm in the function space. Let $\Delta = \max_{d=0,\dots,D} \Delta_d$, then

$$(4.4) \quad \lim_{\Delta \rightarrow 0} \left\| \mathbf{E}^* \right\|_2 := \lim_{\Delta \rightarrow 0} \left\| (P^*, \mathbf{M}^*) - (\rho_{J_0}^*, \mathbf{m}_J^*) \right\|_2 = 0.$$

Proof. By triangular inequality,

$$\begin{aligned} &\left\| (P^*, \mathbf{M}^*) - (\rho_{J_0}^*, \mathbf{m}_J^*) \right\|_2 \\ &\leq \left\| (P^{(k)}, \mathbf{M}^{(k)}) - (P^*, \mathbf{M}^*) \right\|_2 + \left\| \mathbf{E}^{(k)} \right\|_2 + \left\| (\rho_{J_0}^{(k)}, \mathbf{m}_J^{(k)}) - (\rho_{J_0}^*, \mathbf{m}_J^*) \right\|_2. \end{aligned}$$

For any $\epsilon > 0$, there exists k_ϵ such that

$$(4.5) \quad \begin{aligned} \left\| (P^{(k_\epsilon)}, \mathbf{M}^{(k_\epsilon)}) - (P^*, \mathbf{M}^*) \right\|_2 &\leq \frac{\epsilon}{4}, \\ \left\| (\rho^{(k_\epsilon)}, \mathbf{m}^{(k_\epsilon)}) - (\rho^*, \mathbf{m}^*) \right\|_{L_2} &\leq \frac{\epsilon}{4}. \end{aligned}$$

By numerical integration, there exists a constant C_1 depending on $d, \rho^{(k_\epsilon)}, \mathbf{m}^{(k_\epsilon)}$, ρ^*, \mathbf{m}^* and independent of Δ_d such that

$$(4.6) \quad \begin{aligned} &\left\| (\rho_{J_0}^{(k_\epsilon)}, \mathbf{m}_J^{(k_\epsilon)}) - (\rho_{J_0}^*, \mathbf{m}_J^*) \right\|_2^2 \\ &\leq \int_0^1 \int_{\Omega} \left\| (\rho^{(k_\epsilon)}, \mathbf{m}^{(k_\epsilon)}) - (\rho^*, \mathbf{m}^*) \right\|_2^2 dx dt + C_1 \sum_{d=0}^D \Delta_d. \end{aligned}$$

By Theorem 4.2, there exists a constant C_2 independent of Δ_d such that

$$\left\| \mathbf{E}^{(k_\epsilon)} \right\|_2 \leq C_2 \sum_{d=0}^D \Delta_d.$$

Let $\delta = \frac{\epsilon}{(D+1)(|C_1| + |C_2|)}$. Then for any Δ_d satisfying $\max_{d=0, \dots, D} \Delta_d \leq \delta$, we have

$$(4.7) \quad \left| C_1 \sum_{d=0}^D \Delta_d \right| + \left| C_2 \sum_{d=0}^D \Delta_d \right| \leq \frac{\epsilon}{2}.$$

Combining (4.5), (4.6) and (4.7), we conclude that for any $\epsilon > 0$, there exists δ with all $\{\Delta_d\}_d$ satisfying $\Delta \leq \delta$ such that $\|\mathbf{E}^*\|_2 \leq \epsilon$. \square

To prove Theorem 4.2, we need to establish three lemmas to analyze the error introduced in each main step of the algorithm. After that, the proof of Theorem 4.2 can be obtained by induction.

Lemma 4.5. *If Assumption 1 holds for $k = 0, 1, \dots$, then*

$$(4.8) \quad \left\| \mathbf{E}^{(k+\frac{1}{2})} \right\|_2 \leq C(D, C_Y, \eta^{(k)}) \left\| \widehat{\mathbf{E}}^{(k)} \right\|_2 + C \left(\widehat{\rho}^{(k)}, \widehat{\mathbf{m}}^{(k)} \right) \left(\sum_{d=0}^D \Delta_d \right) + \mathcal{O} \left(\sum_{d=0}^D \Delta_d^2 \right).$$

Proof. By definition of $E_d^{(k+\frac{1}{2})}$, we substitute discrete variables in (3.25) by the sum of error and continuous variables. This leads to

$$\left(E_d^{(k+\frac{1}{2})} \right)_j + \left(m_d^{(k+\frac{1}{2})} \right)_j = \left(\widehat{E}_d^{(k)} \right)_j + \left(\widehat{m}_d^{(k)} \right)_j - \eta^{(k)} \left(\partial_{M_d} \mathcal{Y}(\widehat{P}^{(k)}, \widehat{\mathbf{M}}^{(k)}) \right)_j.$$

From (3.14), we have

$$\left(m_d^{(k+\frac{1}{2})} \right)_j = \left(\widehat{m}_d^{(k)} \right)_j - \eta^{(k)} Y_d \left(\widehat{\rho}_j^{(k)}, \widehat{\mathbf{m}}_j^{(k)}, \mathbf{x}_j \right).$$

Combining the above gives us

$$\left(E_d^{(k+\frac{1}{2})} \right)_j = \left(\widehat{E}_d^{(k)} \right)_j - \eta^{(k)} \left[\left(\partial_{M_d} \mathcal{Y}(\widehat{P}^{(k)}, \widehat{\mathbf{M}}^{(k)}) \right)_j - Y_d \left(\widehat{\rho}_j^{(k)}, \widehat{\mathbf{m}}_j^{(k)}, \mathbf{x}_j \right) \right].$$

Therefore we have the norm estimation

$$(4.9) \quad \begin{aligned} \left\| \mathbf{E}^{(k+\frac{1}{2})} \right\|_F &\leq \left\| \widehat{\mathbf{E}}^{(k)} \right\|_F \\ &+ \eta^{(k)} \left[\sum_{d=0}^D \sum_{j \in J_d} \left| \left(\partial_{M_d} \mathcal{Y}(\widehat{P}^{(k)}, \widehat{\mathbf{M}}^{(k)}) \right)_j - Y_d \left(\widehat{\rho}_j^{(k)}, \widehat{\mathbf{m}}_j^{(k)}, \mathbf{x}_j \right) \right|^2 \right]^{\frac{1}{2}}. \end{aligned}$$

For any $\mathbf{j} \in \mathbf{J}_d$, the definition of $\left(\partial_{M_d} \mathcal{Y}(\widehat{P}^{(k)}, \widehat{\mathbf{M}}^{(k)})\right)_{\mathbf{j}}$ in (3.21) yield,

$$\begin{aligned}
& \left| \left(\partial_{M_d} \mathcal{Y} \left(\widehat{P}^{(k)}, \widehat{\mathbf{M}}^{(k)} \right) \right)_{\mathbf{j}} - Y_d \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right| \\
& \leq \frac{1}{2} \left| \left(\partial_{\overline{M}_d} \overline{\mathcal{Y}} \left(\overline{\widehat{P}}^{(k)}, \overline{\widehat{\mathbf{M}}}^{(k)} \right) \right)_{\mathbf{j} + \frac{\mathbf{e}_d}{2}} - Y_d \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right| \\
& \quad + \frac{1}{2} \left| \left(\partial_{\overline{M}_d} \overline{\mathcal{Y}} \left(\overline{\widehat{P}}^{(k)}, \overline{\widehat{\mathbf{M}}}^{(k)} \right) \right)_{\mathbf{j} - \frac{\mathbf{e}_d}{2}} - Y_d \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right| \\
(4.10) \quad & = \frac{1}{2} \left| Y_d \left(\overline{\widehat{P}}_{\mathbf{j} + \frac{\mathbf{e}_d}{2}}^{(k)}, \overline{\widehat{\mathbf{M}}}_{\mathbf{j} + \frac{\mathbf{e}_d}{2}}^{(k)}, \mathbf{x}_{\mathbf{j} + \frac{\mathbf{e}_d}{2}} \right) - Y_d \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right| \\
& \quad + \frac{1}{2} \left| Y_d \left(\overline{\widehat{P}}_{\mathbf{j} - \frac{\mathbf{e}_d}{2}}^{(k)}, \overline{\widehat{\mathbf{M}}}_{\mathbf{j} - \frac{\mathbf{e}_d}{2}}^{(k)}, \mathbf{x}_{\mathbf{j} - \frac{\mathbf{e}_d}{2}} \right) - Y_d \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right| \\
& \leq \frac{C_Y}{2} \left\| \left(\overline{\widehat{P}}_{\mathbf{j} + \frac{\mathbf{e}_d}{2}}^{(k)}, \overline{\widehat{\mathbf{M}}}_{\mathbf{j} + \frac{\mathbf{e}_d}{2}}^{(k)}, \mathbf{x}_{\mathbf{j} + \frac{\mathbf{e}_d}{2}} \right) - \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right\|_1 \\
& \quad + \frac{C_Y}{2} \left\| \left(\overline{\widehat{P}}_{\mathbf{j} - \frac{\mathbf{e}_d}{2}}^{(k)}, \overline{\widehat{\mathbf{M}}}_{\mathbf{j} - \frac{\mathbf{e}_d}{2}}^{(k)}, \mathbf{x}_{\mathbf{j} - \frac{\mathbf{e}_d}{2}} \right) - \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right\|_1.
\end{aligned}$$

Note that $\overline{\widehat{P}}_{\mathbf{j}}^{(k)}, \left(\overline{\widehat{\mathbf{M}}}_d^{(k)} \right)_{\mathbf{j}}$ can be written as the sum of errors and continuous values:

$$\begin{aligned}
\overline{\widehat{P}}_{\mathbf{j}}^{(k)} &= \left(\mathcal{A}_0 \left(\widehat{E}_0^{(k)} + \widehat{\rho}_{\mathbf{j}_0}^{(k)} \right) + \overline{P}_{\mathcal{A}} \right)_{\mathbf{j}} \\
&= \left(\mathcal{A}_0 \left(\widehat{E}_0^{(k)} \right) \right)_{\mathbf{j}} + \left(\mathcal{A}_0 \left(\widehat{\rho}_{\mathbf{j}_0}^{(k)} \right) + \overline{P}_{\mathcal{A}} \right)_{\mathbf{j}} \\
&= \left(\mathcal{A}_0 \left(\widehat{E}_0^{(k)} \right) \right)_{\mathbf{j}} + \widehat{\rho}_{\mathbf{j}}^{(k)} + \mathcal{O}(\Delta_0^2), \\
\left(\overline{\widehat{\mathbf{M}}}_d^{(k)} \right)_{\mathbf{j}} &= \left(\mathcal{A}_d \left(\widehat{E}_d^{(k)} \right) \right)_{\mathbf{j}} + \left(\widehat{\mathbf{m}}_d^{(k)} \right)_{\mathbf{j}} + \mathcal{O}(\Delta_d^2),
\end{aligned}$$

where the last equality in the above two equations is obtained from using Taylor expansion to $\widehat{\rho}^{(k)}$ and $\widehat{\mathbf{m}}_d^{(k)}$. We further have:

$$\begin{aligned}
& \left\| \left(\overline{\widehat{P}}_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}}^{(k)}, \overline{\widehat{\mathbf{M}}}_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}}^{(k)}, \mathbf{x}_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}} \right) - \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right\|_1 \\
& \leq \left\| \left(\left(\mathcal{A}_0 \left(\widehat{E}_0^{(k)} \right) \right)_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}}, \left(\mathcal{A} \left(\widehat{E}_{\mathbf{m}}^{(k)} \right) \right)_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}}, \mathbf{0} \right) \right\|_1 \\
(4.11) \quad & \quad + \left\| \left(\widehat{\rho}_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}}^{(k)}, \mathbf{x}_{\mathbf{j} \pm \frac{\mathbf{e}_d}{2}} \right) - \left(\widehat{\rho}_{\mathbf{j}}^{(k)}, \widehat{\mathbf{m}}_{\mathbf{j}}^{(k)}, \mathbf{x}_{\mathbf{j}} \right) \right\|_1 + \mathcal{O}(\Delta_d^2) \\
& \leq \frac{1}{2} \sum_{d'=0}^D \left| \left(\widehat{E}_{d'}^{(k)} \right)_{\mathbf{j}} + \left(\widehat{E}_{d'}^{(k)} \right)_{\mathbf{j} + \mathbf{e}_d} \right| + \frac{1}{2} \sum_{d'=0}^D \left| \left(\widehat{E}_{d'}^{(k)} \right)_{\mathbf{j}} + \left(\widehat{E}_{d'}^{(k)} \right)_{\mathbf{j} - \mathbf{e}_d} \right| \\
& \quad + C \left(\widehat{\rho}^{(k)}, \widehat{\mathbf{m}}^{(k)} \right) \Delta_d + \mathcal{O}(\Delta_d^2),
\end{aligned}$$

where $C(\hat{\rho}^{(k)}, \hat{\mathbf{m}}^{(k)}) = \max \left\{ \frac{\partial}{\partial x_d} \hat{m}_{d'}^{(k)}(t, \mathbf{x}) : d' = 0, \dots, D \right\}$. Combining (4.10) and (4.11) provides:

$$\begin{aligned} & \left| \left(\partial_{M_d} \mathcal{Y}(\hat{P}^{(k)}, \hat{\mathbf{M}}^{(k)}) \right)_{\mathbf{j}} - Y_d(\hat{\rho}_j^{(k)}, \hat{\mathbf{m}}_j^{(k)}, \mathbf{x}_j) \right| \\ & \leq \frac{C_Y}{4} \sum_{d'=0}^D \left| \left(\hat{E}_{d'}^{(k)} \right)_{\mathbf{j}} + \left(\hat{E}_{d'}^{(k)} \right)_{\mathbf{j}+e_d} \right| + \frac{C_Y}{4} \sum_{d'=0}^D \left| \left(\hat{E}_{d'}^{(k)} \right)_{\mathbf{j}} + \left(\hat{E}_{d'}^{(k)} \right)_{\mathbf{j}-e_d} \right| \\ & \quad + C(\hat{\rho}^{(k)}, \hat{\mathbf{m}}^{(k)}) \Delta_d + \mathcal{O}(\Delta_d^2), \end{aligned}$$

and applying the triangle inequality yields:

$$\begin{aligned} & \left[\sum_{d=0}^D \sum_{\mathbf{j} \in \mathbf{J}_d} \left| \left(\partial_{M_d} \mathcal{Y}(\hat{P}^{(k)}, \hat{\mathbf{M}}^{(k)}) \right)_{\mathbf{j}} - Y_d(\hat{\rho}_j^{(k)}, \hat{\mathbf{m}}_j^{(k)}, \mathbf{x}_j) \right|^2 \right]^{\frac{1}{2}} \\ & \leq \left[\sum_{d=0}^D \sum_{\mathbf{j} \in \mathbf{J}_d} \sum_{d'=0}^D \frac{C_Y^2}{8} \left(\left(\hat{E}_{d'}^{(k)} \right)_{\mathbf{j}-e_d}^2 + 2 \left(\hat{E}_{d'}^{(k)} \right)_{\mathbf{j}}^2 + \left(\hat{E}_{d'}^{(k)} \right)_{\mathbf{j}+e_d}^2 \right) \right]^{\frac{1}{2}} \\ & \quad + \left[\sum_{d=0}^D \sum_{\mathbf{j} \in \mathbf{J}_d} C^2(\hat{\rho}^{(k)}, \hat{\mathbf{m}}^{(k)}) \Delta_d^2 \right]^{\frac{1}{2}} + \left(\prod_{d=0}^D n_d \right)^{\frac{1}{2}} \mathcal{O} \left(\sum_{d=0}^D \Delta_d^2 \right) \\ & \leq C(D, C_Y) \left\| \hat{\mathbf{E}}^{(k)} \right\|_F \\ & \quad + \left(\prod_{d=0}^D n_d \right)^{\frac{1}{2}} C(\hat{\rho}^{(k)}, \hat{\mathbf{m}}^{(k)}) \left(\sum_{d=0}^D \Delta_d \right) + \left(\prod_{d=0}^D n_d \right)^{\frac{1}{2}} \mathcal{O} \left(\sum_{d=0}^D \Delta_d^2 \right). \end{aligned}$$

Together with estimation (4.9), we have

$$\begin{aligned} (4.12) \quad & \left\| \mathbf{E}^{(k+\frac{1}{2})} \right\|_2 \leq \left(1 + C(D, C_Y, \eta^{(k)}) \right) \left\| \hat{\mathbf{E}}^{(k)} \right\|_2 \\ & \quad + C(\hat{\rho}^{(k)}, \hat{\mathbf{m}}^{(k)}) \left(\sum_{d=0}^D \Delta_d \right) + \mathcal{O} \left(\sum_{d=0}^D \Delta_d^2 \right). \end{aligned}$$

Therefore we prove the lemma. \square

Next, we examine the error introduced in the projection step.

Lemma 4.6. *Suppose that $\rho_0, \rho_1, \rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}$ are C^2 , and $\phi^{(k+1)}$ is C^3 , then*

$$\left\| \mathbf{E}^{(k+1)} \right\|_2 \leq 2 \left\| \mathbf{E}^{(k+\frac{1}{2})} \right\|_2 + C(\rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}, \phi^{(k+1)}) \left(\sum_{d=0}^D \Delta_d \right).$$

Proof. By definition of error terms and (3.26), we have

$$(4.13) \quad -\text{Lap} \left(E_{\phi}^{(k+1)} + \phi_{\mathbf{J}}^{(k+1)} \right) = \text{Div} \left(\mathbf{E}^{(k+\frac{1}{2})} + \left(\rho_{\mathbf{J}_0}^{(k+\frac{1}{2})}, \mathbf{m}_{\mathbf{J}}^{(k+\frac{1}{2})} \right) \right) + \overline{P}_{\mathcal{D}}.$$

Since $(\phi^{(k+1)}, \rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})})$ satisfies (3.15), and $\rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}$ are C^2 , by Taylor expansions, we have

$$(4.14) \quad -\text{Lap}(\phi_{\bar{\mathbf{J}}}^{(k+1)}) = \text{Div}(\rho_{\mathbf{J}_0}^{(k+\frac{1}{2})}, \mathbf{m}_{\mathbf{J}}^{(k+\frac{1}{2})}) + \bar{P}_D + \mathbf{C}_1 \left(\sum_{d=0}^D \Delta_d \right).$$

Here $\mathbf{C}_1 = \mathbf{C}_1(\rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}, \phi^{(k+1)}) \in \bar{\mathbb{V}}$ indicates its entries are constants depending on $\rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}, \phi^{(k+1)}$. Combining (4.13) and (4.14) gives us

$$(4.15) \quad -\text{Lap}(E_{\phi}^{(k+1)}) = \text{Div}(\mathbf{E}^{(k+\frac{1}{2})}) + \mathbf{C}_1 \left(\sum_{d=0}^D \Delta_d \right).$$

Similarly, the second step on discrete mesh (3.27) gives

$$(4.16) \quad \begin{aligned} \mathbf{E}^{(k+1)} + (\rho_{\mathbf{J}_0}^{(k+1)}, \mathbf{m}_{\mathbf{J}}^{(k+1)}) &= \mathbf{E}^{(k+\frac{1}{2})} + \text{Grad}(E_{\phi}^{(k+1)}) \\ &\quad + (\rho_{\mathbf{J}_0}^{(k+\frac{1}{2})}, \mathbf{m}_{\mathbf{J}}^{(k+\frac{1}{2})}) + \text{Grad}(\phi_{\bar{\mathbf{J}}}^{(k+1)}), \end{aligned}$$

and on continuous setting (3.16) gives

$$(4.17) \quad (\rho_{\mathbf{J}_0}^{(k+1)}, \mathbf{m}_{\mathbf{J}}^{(k+1)}) = (\rho_{\mathbf{J}_0}^{(k+\frac{1}{2})}, \mathbf{m}_{\mathbf{J}}^{(k+\frac{1}{2})}) + \text{Grad}(\phi_{\bar{\mathbf{J}}}^{(k+1)}) + \mathbf{C}_2 \left(\sum_{d=0}^D \Delta_d \right).$$

Thus we have:

$$(4.18) \quad \mathbf{E}^{(k+1)} = \mathbf{E}^{(k+\frac{1}{2})} + \text{Grad}(E_{\phi}^{(k+1)}) + \mathbf{C}_2 \left(\sum_{d=0}^D \Delta_d \right),$$

where $\mathbf{C}_2 = \mathbf{C}_2(\phi^{(k+1)}) \in \bar{\mathbb{V}}$.

Combining (4.15) and (4.18), we obtain

$$(4.19) \quad \begin{aligned} \mathbf{E}^{(k+1)} &= (\text{Id} - \text{Grad} \circ \text{Lap}^{-1} \circ \text{Div}) \mathbf{E}^{(k+\frac{1}{2})} \\ &\quad - \text{Grad} \circ \text{Lap}^{-1} \mathbf{C}_1 \left(\sum_{d=0}^D \Delta_d \right) + \mathbf{C}_2 \left(\sum_{d=0}^D \Delta_d \right). \end{aligned}$$

Claim. $\|\text{Grad} \circ \text{Lap}^{-1} \circ \text{Div}\|_2 \leq 1$, $\|\text{Grad} \circ \text{Lap}^{-1}\|_2 \leq \frac{1}{4}$.

Therefore

$$\begin{aligned} \|\mathbf{E}^{(k+1)}\|_2 &\leq 2 \|\mathbf{E}^{(k+\frac{1}{2})}\|_2 + \frac{1}{4} \left\| \mathbf{C}_1 \left(\sum_{d=0}^D \Delta_d \right) \right\|_2 + \left\| \mathbf{C}_2 \left(\sum_{d=0}^D \Delta_d \right) \right\|_2 \\ &\leq 2 \|\mathbf{E}^{(k+\frac{1}{2})}\|_2 + C \left(\sum_{d=0}^D \Delta_d \right), \end{aligned}$$

and C depends on $\rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}, \phi^{(k+1)}$.

Proof of claim. It is easy to check that with

$$\begin{aligned} \lambda^i &= -4 \sum_{d=0}^D n_d^2 \sin^2 \left(\frac{(i_d - 1)\pi}{2n_d} \right), \\ \Psi_{\mathbf{j}}^i &= \prod_{d=0}^D \sqrt{\frac{1 + \delta_{1i_d}}{n_d}} \cos \left(\left(j_d - \frac{1}{2} \right) \frac{(i_d - 1)\pi}{n_d} \right), \end{aligned}$$

$\{\Psi^i\}_{i \in \overline{J}}$ forms an orthonormal basis of $(\overline{\mathbb{V}}, \|\cdot\|_F)$, and for any $\overline{\Phi} \in \overline{\mathbb{V}}$,

$$(4.20) \quad \text{Lap}(\overline{\Phi}) := \sum_{i \in \overline{J}} \lambda_i \langle \overline{\Phi}, \Psi^i \rangle \Psi^i.$$

For $d = 0, 1, \dots, D$, and $\mathbf{i} \in \overline{J}$, $i_d \neq 1$, let $\sigma^{d,i} \in \mathbb{R}$ and $\Psi^{d,i} \in \mathbb{V}_0 \times \mathbb{V}_1 \times \dots \times \mathbb{V}_D$ be:

$$\begin{aligned} \sigma^{d,i} &= -2n_d \sin \left(\frac{(i_d - 1)\pi}{2n_d} \right), \\ \Psi^{d,i} &= \left\{ \Psi^{d,i}_{d'} \right\}_{d'=0,1,\dots,D}, \\ \text{where } \Psi^{d,i}_{d'} &= \frac{1}{\sigma^{d,i}} \mathcal{D}_d^*(\Psi^i), \quad \Psi^{d,i}_{d'} = \mathbf{0}, d' \neq d, \end{aligned}$$

then $\{\Psi^{d,i}\}$ forms an orthonormal basis of $(\mathbb{V}_0 \times \mathbb{V}_1 \times \dots \times \mathbb{V}_D, \|\cdot\|_F)$.

Since $\|\cdot\|_2 = \left(\prod_{d=0}^D \Delta_d \right)^{\frac{1}{2}} \|\cdot\|_F$, we next compute the $\|\text{Grad} \circ \text{Lap}^{-1} \circ \text{Div}\|_2$, $\|\text{Grad} \circ \text{Lap}^{-1}\|_2$ with basis of $(\overline{\mathbb{V}}, \|\cdot\|_F)$ and $(\mathbb{V}_0 \times \mathbb{V}_1 \times \dots \times \mathbb{V}_D, \|\cdot\|_F)$. For any basis $\Psi^i \in \overline{\mathbb{V}}$,

$$\text{Grad} \circ \text{Lap}^{-1}(\Psi^1) = \mathbf{0},$$

$$\text{Grad} \circ \text{Lap}^{-1}(\Psi^i) = \sum_{\substack{d=0, \\ i_d \neq 1}}^D \frac{\sigma^{d,i}}{\lambda^i} \Psi^{d,i}, \quad \mathbf{i} \neq \mathbf{1},$$

thus when $n_d > 1$ for $d = 0, \dots, D$, we have

$$\|\text{Grad} \circ \text{Lap}^{-1}\|_2 \leq \max_{\mathbf{i} \in \overline{J} \setminus \{\mathbf{1}\}} \left(\frac{1}{(\lambda^i)^2} \sum_{\substack{d=0, \\ i_d \neq 1}}^D (\sigma^{d,i})^2 \right)^{\frac{1}{2}} = \max_{\mathbf{i} \in \overline{J} \setminus \{\mathbf{1}\}} \frac{1}{|\lambda^i|} \leq \frac{1}{4}.$$

And for any basis $\Psi^{d,i} \in \mathbb{V}_0 \times \mathbb{V}_1 \times \dots \times \mathbb{V}_D$,

$$\begin{aligned} &\text{Grad} \circ \text{Lap}^{-1} \circ \text{Div}(\Psi^{d,i}) \\ &= \text{Grad} \circ \text{Lap}^{-1} \left(\frac{1}{\sigma^{d,i}} \mathcal{D}_d \circ \mathcal{D}_d^*(\Psi^i) \right) = \text{Grad} \circ \text{Lap}^{-1}(-\sigma^{d,i} \Psi^i) \\ &= \text{Grad} \left(-\frac{\sigma^{d,i}}{\lambda^i} \Psi^i \right) = -\sum_{\substack{d'=0, \\ i_{d'} \neq 1}}^D \frac{\sigma^{d,i} \sigma^{d',i}}{\lambda^i} \Psi^{d',i}, \end{aligned}$$

therefore

$$\begin{aligned} \|\text{Grad} \circ \text{Lap}^{-1} \circ \text{Div}\|_2 &\leq \max_{d=0,1,\dots,D} \max_{\mathbf{i} \in \overline{J}, i_d \neq 1} \left(\left(\frac{\sigma^{d,i}}{\lambda^i} \right)^2 \sum_{\substack{d'=0, \\ i_{d'} \neq 1}}^D (\sigma^{d',i})^2 \right)^{\frac{1}{2}} \\ &= \max_{d=0,1,\dots,D} \max_{\mathbf{i} \in \overline{J}, i_d \neq 1} \left(\frac{(\sigma^{d,i})^2}{|\lambda^i|} \right)^{\frac{1}{2}} \leq 1. \end{aligned}$$

The claim and thus the lemma is proved. \square

The last step is to estimate the error introduced in linear interpolation step (3.17), (3.28).

Lemma 4.7.

$$\|\widehat{\mathbf{E}}^{(k+1)}\|_2 \leq |1 + \omega^{(k)}| \|\mathbf{E}^{(k+1)}\|_2 + |\omega^{(k)}| \|\mathbf{E}^{(k)}\|_2.$$

Proof. By definition of error terms and (3.28)

$$\begin{aligned} & \widehat{E}_d^{(k+1)} + \left(\widehat{m}_d^{(k+1)}\right)_{J_d} \\ &= \left(1 + \omega^{(k)}\right) \left(E_d^{(k+1)} + \left(m_d^{(k+1)}\right)_{J_d}\right) - \omega^{(k)} \left(E_d^{(k)} + \left(m_d^{(k)}\right)_{J_d}\right), \end{aligned}$$

and by (3.17)

$$\left(\widehat{m}_d^{(k+1)}\right)_{J_d} = \left(1 + \omega^{(k)}\right) \left(m_d^{(k+1)}\right)_{J_d} - \omega^{(k)} \left(m_d^{(k)}\right)_{J_d}.$$

Therefore we have

$$\widehat{\mathbf{E}}^{(k+1)} = \left(1 + \omega^{(k)}\right) \mathbf{E}^{(k+1)} - \omega^{(k)} \mathbf{E}^{(k)}.$$

By triangular inequality, the lemma is proved. \square

With Lemma 4.5-Lemma 4.7, we can show Theorem 4.2 by induction.

Proof of Theorem 4.2.

Proof. We first restate results from Lemma 4.5-Lemma 4.7

$$\begin{aligned} \|\mathbf{E}^{(k+1)}\|_2 &\leq 2 \|\mathbf{E}^{(k+\frac{1}{2})}\|_2 + C \left(\rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}, \phi^{(k+1)}\right) \left(\sum_{d=0}^D \Delta_d\right), \\ \|\mathbf{E}^{(k+\frac{1}{2})}\|_2 &\leq C(D, C_Y, \eta^{(k)}) \|\widehat{\mathbf{E}}^{(k)}\|_2 + C \left(\widehat{\rho}^{(k)}, \widehat{\mathbf{m}}^{(k)}\right) \left(\sum_{d=0}^D \Delta_d\right) + \mathcal{O} \left(\sum_{d=0}^D \Delta_d^2\right), \\ \|\widehat{\mathbf{E}}^{(k)}\|_2 &\leq |1 + \omega^{(k-1)}| \|\mathbf{E}^{(k)}\|_2 + |\omega^{(k-1)}| \|\mathbf{E}^{(k-1)}\|_2. \end{aligned}$$

From these, we obtain

$$(4.21) \quad \|\mathbf{E}^{(1)}\|_2 \leq C \|\widehat{\mathbf{E}}^{(0)}\|_2 + C \sum_{d=0}^D \Delta_d + \mathcal{O} \left(\sum_{d=0}^D \Delta_d^2\right),$$

$$(4.22) \quad \|\mathbf{E}^{(k+1)}\|_2 \leq C \|\mathbf{E}^{(k)}\|_2 + C \|\mathbf{E}^{(k-1)}\|_2 + C \sum_{d=0}^D \Delta_d + \mathcal{O} \left(\sum_{d=0}^D \Delta_d^2\right), \quad k \geq 1,$$

where C depends on $D, C_Y, \eta^{(k)}, \rho^{(k+\frac{1}{2})}, \mathbf{m}^{(k+\frac{1}{2})}, \widehat{\rho}^{(k)}, \widehat{\mathbf{m}}^{(k)}, \phi^{(k+1)}$.

The initialization gives us

$$\|\mathbf{E}^{(0)}\|_2 = 0, \|\widehat{\mathbf{E}}^{(0)}\|_2 = 0.$$

Then based on (4.22), it is straightforward to show (4.2) by applying induction on k directly. \square

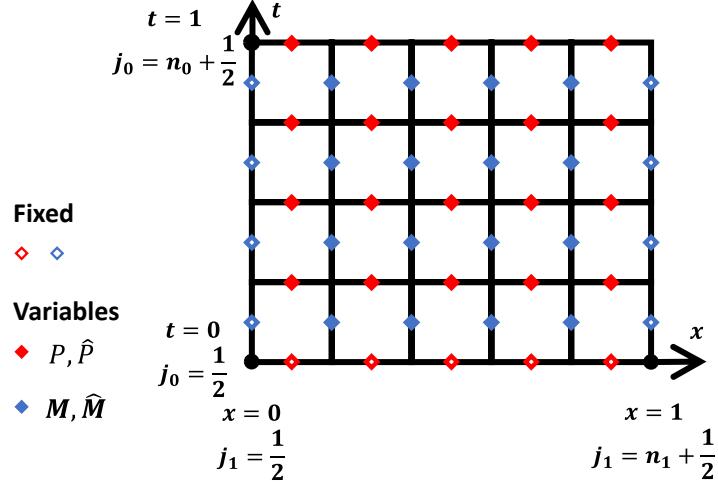


FIGURE 4. Illustration of discretization (MFG)

5. GENERALIZATION AND ACCELERATION

In this section, we generalize the proposed algorithm to solve potential MFG problems. Moreover, we also discuss how to use multilevel and multigrid strategies to speed up our algorithm.

5.1. Generalization to potential MFG. To apply FISTA to the MFG problem (1.2), we follow a first-discretize-then-optimize approach. One crucial difference between MFG and MFP is whether $\rho(1, \cdot)$ is provided explicitly. For MFG, we consider a discretization in Figure 4 and modify our previous notations related to ρ .

The index set and discrete variable are now

$$J_0 := \left\{ \frac{3}{2}, \frac{5}{2}, \dots, n_0 + \frac{1}{2} \right\}, \quad P := \{P_j\}_{j \in J_0} \in \mathbb{V}_0 := \mathbb{R}^{n_0 \times n_1 \times \dots \times n_D},$$

and the discrete operators are

$$\mathcal{A}_0 : \mathbb{V}_0 \rightarrow \overline{\mathbb{V}}, P \mapsto \overline{P},$$

$$\overline{P}_j := \begin{cases} \frac{1}{2} P_{j+\frac{e_0}{2}}, & j_0 = 1, \\ \frac{1}{2} (P_{j+\frac{e_0}{2}} + P_{j-\frac{e_0}{2}}), & j_0 = 2, 3, \dots, n_0, \end{cases}$$

$$\mathcal{D}_0 : \mathbb{V}_0 \rightarrow \overline{\mathbb{V}}, P \mapsto \mathcal{D}_0(P),$$

$$(\mathcal{D}_0(P))_j := \begin{cases} \frac{1}{\Delta_0} P_{j+\frac{e_0}{2}}, & j_0 = 1, \\ \frac{1}{\Delta_0} (P_{j+\frac{e_0}{2}} - P_{j-\frac{e_0}{2}}), & j_0 = 2, 3, \dots, n_0. \end{cases}$$

Since the boundary condition is only at $t = 0$, we modify $\bar{P}_{\mathcal{A}}, \bar{P}_{\mathcal{D}} \in \bar{\mathbb{V}}$ to

$$(\bar{P}_{\mathcal{A}})_j := \begin{cases} \frac{1}{2}\rho_0(\mathbf{x}_j), & j_0 = 1, \\ 0, & j_0 = 2, 3, \dots, n_0, \end{cases}$$

$$(\bar{P}_{\mathcal{D}})_j := \begin{cases} -\frac{1}{\Delta_0}\rho_0(\mathbf{x}_j), & j_0 = 1, \\ 0, & j_0 = 2, 3, \dots, n_0. \end{cases}$$

Take model (2.11) in Section 2 as an example, the discrete problem can be formulated as

$$(5.1) \quad \begin{aligned} \min_{(P, \mathbf{M}) \in \mathcal{C}_{MFG}(\bar{P}_{\mathcal{D}})} \mathcal{Y}_{MFG}(P, \mathbf{M}) := & \Delta_0 \sum_{d=0}^D \sum_{j_d=1}^{n_d} J_{MFG}((\mathcal{A}_0(P) + \bar{P}_{\mathcal{A}})_j, \mathcal{A}(\mathbf{M})_j, \mathbf{x}_j) \\ & + \lambda_G \sum_{\substack{j \in \mathbf{J}_0, \\ j_0=n_0+\frac{1}{2}}} P_j G(\mathbf{x}_j), \end{aligned}$$

where

$$(5.2) \quad J_{MFG}(\beta_0, \boldsymbol{\beta}, \mathbf{x}) := L(\beta_0, \boldsymbol{\beta}) + \lambda_E \beta_0 \log(\beta_0) + \lambda_Q \beta_0 Q(\mathbf{x}),$$

$$(5.3) \quad \mathcal{C}_{MFG}(\bar{P}_{\mathcal{D}}) := \{(P, \mathbf{M}) : \mathcal{D}_0(P) + \bar{P}_{\mathcal{D}} + \text{Div}(\mathbf{M}) = \mathbf{0}\}.$$

Since this is an optimization problem with linear constraints, we apply FISTA to it as detailed in Algorithm 3. In the algorithm, $\mathcal{A}_0^\top, \mathcal{A}^\top, \mathcal{D}_0^\top, \text{Div}^\top$ are conjugate operators of $\mathcal{A}_0, \mathcal{A}, \mathcal{D}_0, \text{Div}$ in norm $\|\cdot\|_F$. Similar to what we discussed before, one can have:

$$\begin{cases} \partial_{\bar{P}} \mathcal{Y}_{MFG}(P, \mathbf{M}) := \{\Delta_0(J_{MFG})_{\beta_0}((\mathcal{A}_0(P) + \bar{P}_{\mathcal{A}})_j, \mathcal{A}(\mathbf{M})_j, \mathbf{x}_j)\}_{j \in \bar{\mathbf{J}}}, \\ \partial_{\bar{\mathbf{M}}} \mathcal{Y}_{MFG}(P, \mathbf{M}) := \{\Delta_0(J_{MFG})_{\boldsymbol{\beta}}((\mathcal{A}_0(P) + \bar{P}_{\mathcal{A}})_j, \mathcal{A}(\mathbf{M})_j, \mathbf{x}_j)\}_{j \in \bar{\mathbf{J}}}, \end{cases}$$

and

$$\begin{cases} (\partial_P \mathcal{Y}_{MFG}(P, \mathbf{M}))_j := (\mathcal{A}_0^\top (\partial_{\bar{P}} \mathcal{Y}_{MFG}(P, \mathbf{M})))_j, & j_0 \neq n_0 + \frac{1}{2}, \\ (\partial_P \mathcal{Y}_{MFG}(P, \mathbf{M}))_j := (\mathcal{A}_0^\top (\partial_{\bar{P}} \mathcal{Y}_{MFG}(P, \mathbf{M})))_j + \lambda_G G(\mathbf{x}_j), & j_0 = n_0 + \frac{1}{2}, \\ \partial_{\mathbf{M}} \mathcal{Y}_{MFG}(P, \mathbf{M}) := \mathcal{A}^\top (\partial_{\bar{\mathbf{M}}} \mathcal{Y}_{MFG}(P, \mathbf{M})). \end{cases}$$

Remark 5.1. In Algorithm 3, we also need to solve a discrete Poisson equation (5.4) and the approach is similar as presented in Remark 3.3.

5.2. Multilevel and multigrid FISTA. Inspired by [37, 39], we borrow ideas from multigrid and multilevel methods in numerical PDEs to our variational problem. We first restrict our initialization to coarser meshes and solve the optimization problem to a certain accuracy. Then we successively refine the mesh and solve the problem until we obtain the solution on a desired fine mesh. According to [37, 39], the solution on the coarse mesh approximates that on the finer mesh and gives a better initialization when solving the problem on the finer mesh. Therefore, these methods can reduce computational cost on the finest level and thus accelerate the proposed algorithm. This section presents the implementation details.

For notation simplicity, we assume $h = \Delta_0 = \Delta_1 = \dots = \Delta_D$ in this section. Let ${}^h\Omega$ be a grid with $h = \Delta_d$, ${}^h\mathbf{J}_d$ be the certain \mathbf{J}_d on the grid. Then index ${}^h\mathbf{j} \in {}^h\mathbf{J}_d$

Algorithm 3 FISTA for MFGParameters ρ_0, ρ_1 Initialization $\tau^{(1)} = 1$, $P^{(0)} = \widehat{P}^{(0)} = \mathbf{1}$, and $M_d^{(0)} = \widehat{M}_d^{(0)} = \mathbf{1}$.**for** $k = 0, 1, 2, \dots$ **do** **gradient descent:**

$$\begin{cases} P^{(k+\frac{1}{2})} = P^{(k)} - \eta^{(k)} \partial_P \mathcal{Y}_{MFG}(P^{(k)}, \mathbf{M}^{(k)}), \\ \mathbf{M}^{(k+\frac{1}{2})} = \mathbf{M}^{(k)} - \eta^{(k)} \partial_M \mathcal{Y}_{MFG}(P^{(k)}, \mathbf{M}^{(k)}) \end{cases}$$

projection: solve $\overline{\Phi}^{(k+1)}$ for

$$(5.4) \quad \left(\mathcal{D}_0 \mathcal{D}_0^\top + \text{Div} \text{Div}^\top \right) \overline{\Phi}^{(k+1)} = \mathcal{D}_0 \left(P^{(k+\frac{1}{2})} \right) + \overline{P}_\mathcal{D} + \text{Div} \left(\mathbf{M}^{(k+\frac{1}{2})} \right),$$

 and project $\left(P^{(k+\frac{1}{2})}, \mathbf{M}^{(k+\frac{1}{2})} \right)$ to $\mathcal{C}_{MFG}(\overline{P}_\mathcal{D})$ by

$$\begin{cases} P^{(k+1)} = P^{(k+\frac{1}{2})} - \mathcal{D}_0^\top \left(\overline{\Phi}^{(k+1)} \right), \\ \mathbf{M}^{(k+1)} = \mathbf{M}^{(k+\frac{1}{2})} - \text{Div}^\top \left(\overline{\Phi}^{(k+1)} \right). \end{cases}$$

update

$$\tau^{(k+1)} = \frac{1 + \sqrt{1 + 4 (\tau^{(k)})^2}}{2},$$

$$\omega^{(k)} = \frac{\tau^{(k)} - 1}{\tau^{(k+1)}},$$

$$\left(\widehat{P}^{(k+1)}, \widehat{\mathbf{M}}^{(k+1)} \right) = \left(1 + \omega^{(k)} \right) \left(P^{(k+1)}, \mathbf{M}^{(k+1)} \right) - \omega^{(k)} \left(P^{(k)}, \mathbf{M}^{(k)} \right).$$

end for

stands for the point $h\mathbf{j}$. If there is no ambiguity, we can omit the prescript of \mathbf{j} . For example, we define ${}^h u_{\mathbf{j}} = u \left(h \left(\mathbf{j} - \frac{1}{2} \right) \right)$ for any function u and approximate the value by ${}^h U_{\mathbf{j}}$.

Consider L levels of grids ${}^{h_1} \Omega, \dots, {}^{h_L} \Omega$ where the finest level is ${}^{h_1} \Omega$, and $h_l := 2^{l-1} h_1$. We first define how to prolongate values on a coarser grid into a finer grid. Assume that ${}^h \mathbf{j} \in {}^h \mathbf{J}_d$ stands for point $h \left(\mathbf{j} - \frac{1}{2} \right)$ on the finer grid ${}^h \Omega$, we define its neighbourhood on the coarser grid ${}^{2h} \Omega$ as

$$(5.5) \quad \begin{aligned} {}^{2h} {}_h \mathcal{N}_{\mathbf{j}} := & \left\{ {}^{2h} \mathbf{i} \in {}^{2h} \mathbf{J}_d : \left\| 2h \left({}^{2h} \mathbf{i} - \frac{1}{2} \right) - h \left({}^h \mathbf{j} - \frac{1}{2} \right) \right\|_2 \right. \\ & \left. = \min_{{}^{2h} \mathbf{i}' \in {}^{2h} \mathbf{J}_d} \left\| 2h \left({}^{2h} \mathbf{i}' - \frac{1}{2} \right) - h \left({}^h \mathbf{j} - \frac{1}{2} \right) \right\|_2 \right\}. \end{aligned}$$

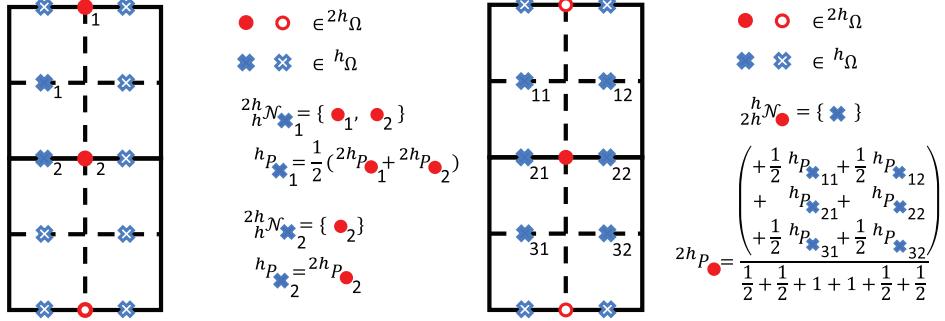


FIGURE 5. Illustration of Prolongation (left) and Restriction (right) for 1D case

Then with boundary values

$$\begin{aligned} {}^{2h}P_i &= {}^{2h}(\rho_0)_i, \quad i_0 = \frac{1}{2}, \\ {}^{2h}P_i &= {}^{2h}(\rho_1)_i, \quad i_0 = \frac{1}{2h} + \frac{1}{2}, \\ {}^{2h}(M_d)_i &= 0, \quad i_d = \frac{1}{2}, \frac{1}{2h} + \frac{1}{2}, \end{aligned}$$

we define the prolongation $({}^hP, {}^hM) = \text{Pro}({}^{2h}P, {}^{2h}M)$ by averaging values in neighbourhoods:

$$(5.6) \quad \begin{cases} {}^hP_j := \frac{1}{|{}^{2h}\mathcal{N}_j|} \sum_{{}^{2h}i \in {}^{2h}\mathcal{N}_j} {}^{2h}P_i, & \forall {}^hj \in {}^h\mathbf{J}_0, \\ {}^h(M_d)_j := \frac{1}{|{}^{2h}\mathcal{N}_j|} \sum_{{}^{2h}i \in {}^{2h}\mathcal{N}_j} {}^{2h}(M_d)_i, & \forall {}^hj \in {}^h\mathbf{J}_d. \end{cases}$$

An example of prolongation in 1D is shown in the left panel of Figure 5.

From a finer grid to a coarser grid, the neighbourhood is defined inversely. Suppose ${}^{2h}i \in {}^{2h}\mathbf{J}_d$, its neighbourhood is the set of all ${}^hj \in {}^h\mathbf{J}_d$ whose neighbourhood includes ${}^{2h}i$:

$$(5.7) \quad {}^{2h}\mathcal{N}_i := \left\{ {}^hj \in {}^h\mathbf{J}_d : {}^{2h}i \in {}^{2h}\mathcal{N}_j \right\},$$

and the restriction from finer level to coarser level $({}^hP, {}^hM) = \text{Res}({}^{2h}P, {}^{2h}M)$ is defined by a weighted average over neighbourhoods:

$$(5.8) \quad \begin{cases} {}^{2h}P_i := \sum_{{}^hj \in {}^{2h}\mathcal{N}_i} \frac{1}{|{}^{2h}\mathcal{N}_j|} {}^hP_j / \sum_{{}^hj \in {}^{2h}\mathcal{N}_i} \frac{1}{|{}^{2h}\mathcal{N}_j|}, & \forall {}^{2h}i \in {}^{2h}\mathbf{J}_0, \\ {}^{2h}(M_d)_i := \sum_{{}^hj \in {}^{2h}\mathcal{N}_i} \frac{1}{|{}^{2h}\mathcal{N}_j|} {}^h(M_d)_j / \sum_{{}^hj \in {}^{2h}\mathcal{N}_i} \frac{1}{|{}^{2h}\mathcal{N}_j|}, & \forall {}^{2h}i \in {}^{2h}\mathbf{J}_d. \end{cases}$$

An example of the restriction is shown in the right panel of Figure 5.

We describe our multigrid FISTA in Algorithm 4, in which Algorithm $\mathcal{D}_K(\cdot)$ means to run Algorithm 2 for K iterations and Algorithm $\mathcal{D}(\cdot)$ means to run the algorithm till convergence. The first two inputs of Algorithm $\mathcal{D}(\cdot)$ are initial and terminal densities ρ_0, ρ_1 , and the last two inputs are initialization $P^{(0)} = \hat{P}^{(0)}$, $\mathbf{M}^{(0)} = \hat{\mathbf{M}}^{(0)}$.

Algorithm 4 Multigrid FISTA for MFP

Parameters $L, h_l = 2^{l-1}h, K, {}^{h_l}\rho_0, {}^{h_l}\rho_1 (l = 1, \dots, L)$
Initialization ${}^{h_1}P^{(0)} = \mathbf{1}, {}^{h_1}M^{(0)} = \mathbf{1}$ **pre-smoothing**

$$\left({}^{h_1}P, {}^{h_1}M \right) = \text{Algorithm 2}_K \left(\rho_0, \rho_1, {}^{h_1}P^{(0)}, {}^{h_1}M^{(0)} \right)$$

for $l = 2, 3, \dots, L$ **do**

$$\left({}^{h_l}P, {}^{h_l}M \right) = \text{Algorithm 2}_K \left(\rho_0, \rho_1, \text{Res} \left({}^{h_{l-1}}P, {}^{h_{l-1}}M \right) \right)$$

end for**correction and post-smoothing**

$$\left({}^{h_L}P, {}^{h_L}M \right) = \text{Algorithm 2} \left(\rho_0, \rho_1, {}^{h_L}P, {}^{h_L}M \right)$$

for $l = L-1, L-2, \dots, 1$ **do**

$$\begin{aligned} \left({}^{h_l}P, {}^{h_l}M \right) &= \left({}^{h_l}P, {}^{h_l}M \right) + \text{Algorithm 2} \left(\rho_0, \rho_1, \text{Pro} \left({}^{h_{l+1}}P, {}^{h_{l+1}}M \right) \right) \\ &\quad - \text{Pro} \left({}^{h_{l+1}}P, {}^{h_{l+1}}M \right) \end{aligned}$$

end for

Note that to keep the cost of Algorithm 4 low, we need to choose a K not very large. Motivated by [39], we remove the pre-smoothing steps by setting $K = 0$ and this leads to our Algorithm 5 multilevel FISTA.

Algorithm 5 Multilevel FISTA for MFP

Parameters $L, h_l = 2^{l-1}h, {}^{h_l}\rho_0, {}^{h_l}\rho_1 (l = 1, \dots, L)$
Initialization ${}^{h_L}P^{(0)} = \mathbf{1}, {}^{h_L}M^{(0)} = \mathbf{1}$

$$\left({}^{h_L}P, {}^{h_L}M \right) = \text{Algorithm 2} \left(\rho_0, \rho_1, {}^{h_L}P^{(0)}, {}^{h_L}M^{(0)} \right)$$

for $l = L-1, L-2, \dots, 1$ **do**

$$\left({}^{h_l}P, {}^{h_l}M \right) = \text{Algorithm 2} \left(\rho_0, \rho_1, \text{Pro} \left({}^{h_{l+1}}P, {}^{h_{l+1}}M \right) \right)$$

end for

6. NUMERICAL EXPERIMENTS

In this section, we conduct comprehensive experiments to show the efficiency and effectiveness of the proposed numerical algorithms. We first numerically verify the convergence of rate of the algorithm with respect to the mesh size. After that, our computation efficiency tests demonstrate that the proposed Algorithm 2 has comparable efficiency with the state-of-the-art methods. Interestingly, the proposed multilevel method performs around 10 times faster than existing methods. We further illustrate the flexibility of our algorithms on different MFP problems. In

TABLE 1. Convergence rate of Algorithm 2 applied to 1D OT problem ($k = 50000$)

Δ_0	Δ_1	$\ E^{(k,*)}\ _2$	order	$\ E^{(k,*)}\ _\infty$	order	W_2^2 error	order
1/16	1/64	3.19E-04		2.88E-03		4.88E-06	
1/32	1/128	1.08E-04	1.56	1.47E-03	0.97	1.22E-06	2.00
1/64	1/256	3.76E-05	1.53	7.44E-04	0.98	3.05E-07	2.00
1/128	1/512	1.37E-05	1.46	3.62E-04	1.04	7.63E-08	2.00

all the numerical experiments, we use the dynamic cost function L defined in (2.5). All of our numerical experiments are implemented in Matlab on a PC with an Intel(R) i7-8550U 1.80GHz CPU and 16 GB memory. The codes to reproduce the numerical results in this paper are available in https://github.com/Jiajia-Yu/FISTA_MFP_euc.

6.1. Convergence rate. To numerically verify the theoretical convergence analysis discussed in Section 4, we first apply the proposed numerical algorithm to a simple 1D OT example with the exact solution as follows.

Let $\Omega = [0, 1]$, $\rho_0(x) = x + \frac{1}{2}$, $\rho_1(x) = 1$. Then we can have the following theoretical solution of the OT between ρ_0 and ρ_1 .

$$(6.1) \quad \rho^*(t, x) = \begin{cases} x + \frac{1}{2}, & t = 0, \\ \frac{\sqrt{2tx + (\frac{t}{2} - 1)^2} + t - 1}{t\sqrt{2tx + (\frac{t}{2} - 1)^2}}, & 0 < t \leq 1. \end{cases}$$

$$(6.2) \quad m^*(t, x) = \begin{cases} \frac{1}{4}x(x-1)(2x+1), & t = 0, \\ \frac{x}{t^2} - \frac{3-t}{2t^3}\sqrt{2tx + \left(\frac{t}{2} - 1\right)^2} \\ - \frac{(t-1)(t^2-4)}{8t^3}\frac{1}{\sqrt{2tx + (\frac{t}{2} - 1)^2}} - \frac{3t-4}{2t^3}, & 0 < t \leq 1. \end{cases}$$

We also know $W_2^2(\rho_0, \rho_1) = \frac{1}{120}$.

Note that it would be quite difficult to check $E^{(k)}$ as we do not have the evolution path, $\rho^{(k)}$ and $m^{(k)}$, in the continuous Algorithm 1. Instead, we compute the following values:

$$\begin{aligned} \|E^{(k,*)}\|_2 &:= \sqrt{\Delta_0 \Delta_1} \left[\sum_{j \in J_0} \left| P_j^{(k)} - \rho_j^* \right|^2 + \sum_{j \in J_1} \left| M_j^{(k)} - m_j^* \right|^2 \right]^{\frac{1}{2}}, \\ \|E^{(k,*)}\|_\infty &:= \max \left\{ \max_{j \in J_0} \left| P_j^{(k)} - \rho_j^* \right|, \max_{j \in J_1} \left| M_j^{(k)} - m_j^* \right| \right\}, \\ W_2^2 \text{ error: } & \left| \Delta_0 \Delta_1 \mathcal{Y} \left(P^{(k)}, M^{(k)} \right) - W_2^2(\rho_0, \rho_1) \right|. \end{aligned}$$

Here $\|E^{(k,*)}\|_2$ is related to $\|E^{(k)}\|_2$ by:

$$\|E^{(k,*)}\|_2 \leq \|E^{(k)}\|_2 + \left\| \left(\rho_{J_0}^{(k)}, m_{J_0}^{(k)} \right) - \left(\rho_{J_0}^*, m_{J_0}^* \right) \right\|_2.$$

TABLE 2. Time comparison of OT in 1D for different grid sizes ($n_0 = 64$, $tol = 10^{-4}$, F=FISTA, A=ALG, G=G-prox) with the best performance highlighted in red

n_1	Iter			Time (s)			Time(s)/Iter		
	F	A	G	F	A	G	F	A	G
256	611	435	426	1.74	2.99	2.93	2.85E-03	6.86E-03	6.88E-03
512	611	435	429	3.06	5.91	6.92	5.00E-03	1.36E-02	1.61E-02
1024	611	435	430	7.60	12.93	12.85	1.24E-02	2.97E-02	2.99E-02
2048	611	435	431	24.84	36.15	32.72	4.07E-02	8.31E-02	7.59E-02
4096	611	435	431	51.79	69.99	68.09	8.48E-02	1.61E-01	1.58E-01

TABLE 3. Time comparison of OT in 2D for different grid sizes ($n_0 = 64$, F=FISTA, A=ALG, G=G-prox) with the best performance highlighted in red

n_1, n_2	Iter			Time (s)			Time(s)/Iter		
	F	A	G	F	A	G	F	A	G
128	116	64	66	46.20	46.07	46.49	3.98E-01	7.20E-01	7.04E-01
256	116	64	66	212.31	201.52	190.31	1.83E+00	3.15E+00	2.88E+00
512	116	64	66	810.86	761.65	752.59	6.99E+00	1.19E+01	1.14E+01

For given Δ_0, Δ_1 , we can choose very large k such that

$$\left\| \mathbf{E}^{(k,*)} \right\|_2 \leq \left\| \mathbf{E}^{(k)} \right\|_2 + \epsilon^{(k)}$$

and $\epsilon^{(k)} \ll \Delta_0 + \Delta_1$. Fixing k , according to our theoretical analysis, we expect to observe at least

$$\left\| \mathbf{E}^{(k,*)} \right\|_2 = \mathcal{O}(\Delta_0 + \Delta_1),$$

and

$$\left\| \mathbf{E}^{(k,*)} \right\|_\infty \leq \left\| \mathbf{E}^{(k,*)} \right\|_F = (\Delta_0 \Delta_1)^{-\frac{1}{2}} \left\| \mathbf{E}^{(k,*)} \right\|_2 = \mathcal{O}(1).$$

Numerical results are shown in Table 1 where we observe

$$\left\| \mathbf{E}^{(k,*)} \right\|_2 = \mathcal{O}(\Delta_0^{1.5} + \Delta_1^{1.5}), \quad \left\| \mathbf{E}^{(k,*)} \right\|_\infty = \mathcal{O}(\Delta_0 + \Delta_1).$$

This indicates that the convergence rate of our numerical experiments performs better than theoretical prediction. This is not surprising as our theoretical analysis may not be sharp.

6.2. Computation efficiency. In this part, we demonstrate the efficiency of our algorithms by comparing them with state-of-the-art methods for dynamic OT problems. We apply our algorithms to OT problems with ρ_0, ρ_1 being Gaussian distribution densities with mean $\frac{1}{3}, \frac{2}{3}$ for the 1D example and $(\frac{1}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{1}{3})$ for the 2D example, and compare the results and computation time with those using ALG(augmented Lagrangian) [11, 12] and G-prox [34]. For all approaches, the stopping criteria are

$$\left\| \left(P^{(k+1)}, \mathbf{M}^{(k+1)} \right) - \left(P^{(k)}, \mathbf{M}^{(k)} \right) \right\|_2 \leq tol.$$

TABLE 4. Efficiency and accuracy comparisons of OT in 1D ($n_0 = 64, n_1 = 256$) with the best performance highlighted in red

	Num Iter	Time (s)	Stationarity Residue	Feasibility Residue	Mass Residue
FISTA	611	1.723	3.27E-05	2.28E-13	1.33E-15
ALG	435	2.840	9.43E-05	2.41E-04	1.64E-08
G-prox	426	2.761	1.93E-04	1.88E-04	2.96E-08
MLFISTA	882	0.422	7.97E-05	2.28E-13	1.11E-15
MGFISTA ($K = 5$)	1448	1.195	4.79E-05	2.33E-13	1.77E-15
MGFISTA ($K = 10$)	1517	1.341	3.95E-05	2.28E-13	2.22E-15

TABLE 5. Efficiency and accuracy comparison of OT in 2D ($n_0 = 64, n_1 = n_2 = 256$) with the best performance highlighted in red

	Num Iter	Time (s)	Stationarity Residue	Feasibility Residue	Mass Residue
FISTA	116	232.560	9.22E-04	6.01E-13	1.42E-14
ALG	64	211.043	8.75E-04	4.99E-03	3.10E-03
G-prox	66	208.696	9.29E-04	6.88E-03	3.10E-03
MLFISTA	162	12.853	3.43E-03	2.95E-13	2.07E-14
MGFISTA ($K = 5$)	315	134.226	1.07E-03	5.99E-13	1.67E-14
MGFISTA ($K = 10$)	315	170.580	9.86E-04	6.00E-13	2.02E-14

To enhance the algorithm stability, we use $\rho_0 + 0.1, \rho_1 + 0.1$ as the initial and terminal densities in the numerical experiment.

In Table 2 and Table 3, we report computation time and the number of iterations for each algorithm on different grid sizes in 1D and 2D. From the tables, the proposed Algorithm 2 outperforms ALG and G-prox in 1D and achieves similar efficiency in 2D. Interestingly, CPU time per iteration in our algorithm is the least among these three algorithms. This is because, at each iteration, solving a Poisson equation is required for all three algorithms while our method does not need to solve $\prod_{d=0}^D n_d$ cubic equations required in ALG and G-prox. Therefore our method needs less time in the 1D experiment although it needs more iterations to achieve the given stopping criteria. But this computation save is marginal compared with the cost of solving the Poisson equation in 2D. Thus, our method spends comparable time instead of less time in the 2D experiment.

Moreover, as shown in Table 4 and Table 5, we further accelerate the proposed algorithm by at most 10 times with the help of multilevel and multigrid strategies. We also compute the residue of being a stationary point, residue of feasibility constraint (2.2), and residue of mass conservation to check the accuracy of the solutions. From the residue comparisons listed in the tables, it is clear to see that all of our algorithms provide solutions with far better mass preservation property than results from ALG and G-prox methods due to the nature of the projection step in our method. Qualitatively, Figure 6 also shows that all 6 algorithms in our experiments provide satisfactory results in accuracy.

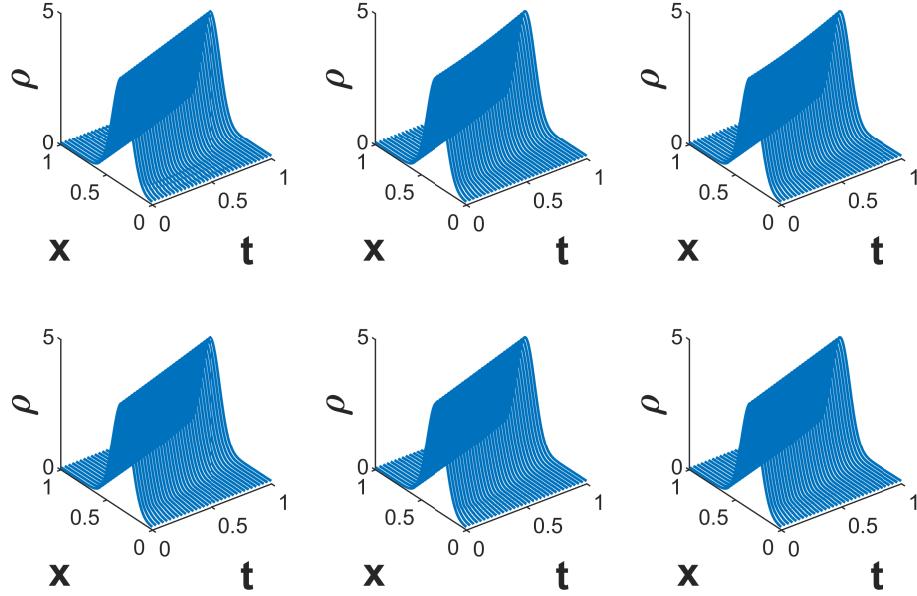


FIGURE 6. Qualitative comparisons of $\rho(t, \cdot)$ in 1D. Row 1 from left to right: FISTA, ALG, G-Prox. Row 2 from left to right: MLFISTA, MGFISTA($K = 5$), MGFISTA($K = 10$).

Remark 6.1. From Table 4 and Table 5, we observe that with multilevel and multigrid strategies, the algorithms take more iterations to converge. This is because we need more iterations on the coarser mesh to obtain a good initialization on the finer mesh. But since each iteration on the coarser mesh is less expensive, schemes with multilevel and multigrid strategies take much less time to complete.

Remark 6.2. As we point out in Remark 3.4, adding a constant to initial and terminal densities improves the numerical stability, but it also changes the original problem and gives an approximation to the original problem. This example shows that the approximation is good if the constant is not too large. In the 1D example of this part, with initial and terminal densities being Gaussian, the exact W_2^2 value is $\frac{1}{9} \approx 0.111111$. Numerically, we truncate the domain to $[0, 1]$ and add a shift of 0.1 to initial and terminal densities. And the approximated W_2^2 value is 0.104710 with a relative error of 0.057.

6.3. MFP with obstacles. Most numerical examples of MFP in the literature consider Ω to be a regular region, i.e. $\Omega = [0, 1] \times [0, 1]$. However, in real applications, problems defined in irregular regions might make the implementation very complicated. One potential way of handling irregular domain is to set Q to be an indicator function of obstacles which leads to solutions staying in the irregular domain. In a different example, [42] provides an interesting optimal transport example where the region is a maze with many “walls”. Here we consider several illustrative cases where there are one or two pieces of obstacles in our square domain and show

that our algorithm can deal with this case without modification of implementation. More detailed studies in this direction will be explored in our future work.

To be precise, letting $\Omega = [-\frac{1}{2}, \frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}]$, we consider MFP problem with objective function

$$\int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \lambda_Q \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x}.$$

Different choices of ρ_0, ρ_1, Q are shown in the first row of Figure 7 and $Q(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in \Omega_0, \\ 0, & \mathbf{x} \notin \Omega_0 \end{cases}$ where Ω_0 is the white region. By setting λ_Q to be a very large number (e.g. $\lambda_Q = 8 \times 10^4$ in our implementation), we expect the set Ω_0 to be viewed as an obstacle and the density evolution to circumvent the region. The snapshots of the evolution shown in Figure 7 demonstrate the success of our algorithm since the mass circumvents the obstacles very well.

6.4. Flexibility. As one of the greatest advantages, our method enjoys the flexibility to handle different types of objective functions in variational MFP problems. To show the effectiveness of our algorithm, we apply Algorithm 2 to the five models listed in Section 2. We can also observe how different objective functions affect density evolutions.

Let $\Omega = [0, 1] \times [0, 1]$, ρ_0, ρ_1 to be two images shown in Figure 8, $G(\mathbf{x}) = -\rho_1(\mathbf{x})$ and $Q(\mathbf{x}) = \begin{cases} 0, & \rho_0(\mathbf{x}) \neq 0 \text{ or } \rho_1(\mathbf{x}) \neq 0, \\ 1, & \text{otherwise} \end{cases}$. We consider MFP problems of the following form

$$\min_{(\rho, \mathbf{m}) \in \mathcal{C}(\rho_0, \rho_1)} \left\{ \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt + \lambda_E \int_0^1 \int_{\Omega} F_E(\rho(t, \mathbf{x})) d\mathbf{x} dt + \lambda_Q \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x} dt \right\}.$$

We apply the proposed algorithm to the following four MFP models discussed in Examples 2.1–2.3:

$$(6.3) \quad (\text{OT}) \quad \lambda_E = \lambda_Q = 0,$$

$$(6.4) \quad (\text{Model 1}) \quad \lambda_E = 0.01, \lambda_Q = 0.1, F_E : \mathbb{R}^+ \rightarrow \mathbb{R}, \rho \mapsto \begin{cases} \rho \log(\rho), & \rho > 0, \\ 0, & \rho = 0, \end{cases}$$

$$(6.5) \quad (\text{Model 2}) \quad \lambda_E = 0.01, \lambda_Q = 0.1, F_E : \mathbb{R}^+ \rightarrow \mathbb{R}, \rho \mapsto \frac{\rho^2}{2},$$

$$(6.6) \quad (\text{Model 3}) \quad \lambda_E = 0.01, \lambda_Q = 0.1, F_E : \mathbb{R}^+ \rightarrow \mathbb{R}, \rho \mapsto \begin{cases} \frac{1}{\rho}, & \rho > 0, \\ 0, & \rho = 0, \end{cases}$$

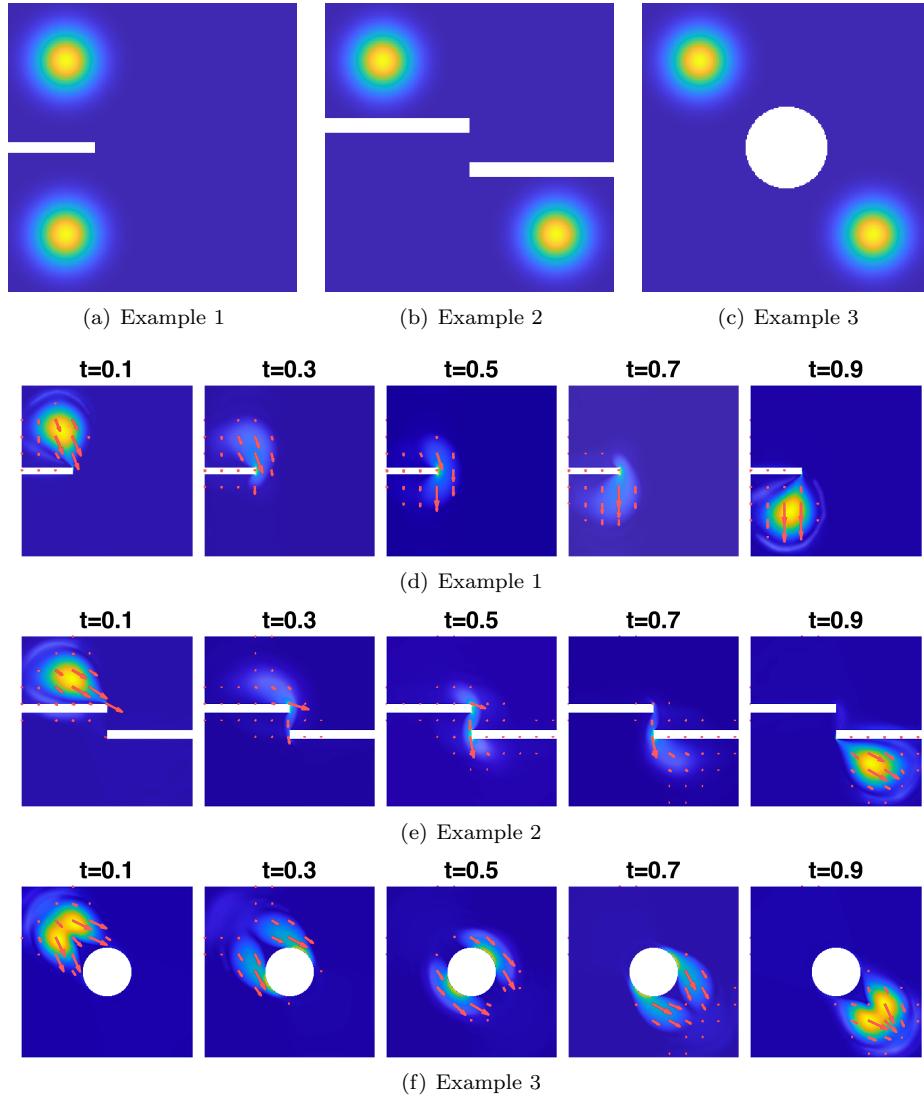


FIGURE 7. (a-c) Initial density ρ_0 , terminal density ρ_1 and obstacle region Ω_0 highlighted as white regions. (d-f) Snapshots of ρ at $t = 0.1, 0.3, 0.5, 0.7, 0.9$.

and a MFG model shown in Example 2.4
(6.7)

$$\min_{(\rho, \mathbf{m}) \in \mathcal{C}(\rho_0)} \left\{ \begin{array}{l} \int_0^1 \int_{\Omega} L(\rho(t, \mathbf{x}), \mathbf{m}(t, \mathbf{x})) d\mathbf{x} dt \\ + \lambda_E \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) \log(\rho(t, \mathbf{x})) d\mathbf{x} dt + \lambda_Q \int_0^1 \int_{\Omega} \rho(t, \mathbf{x}) Q(\mathbf{x}) d\mathbf{x} dt \\ + \lambda_G \int_{\Omega} \rho(1, \mathbf{x}) G(\mathbf{x}) d\mathbf{x} \end{array} \right\}$$

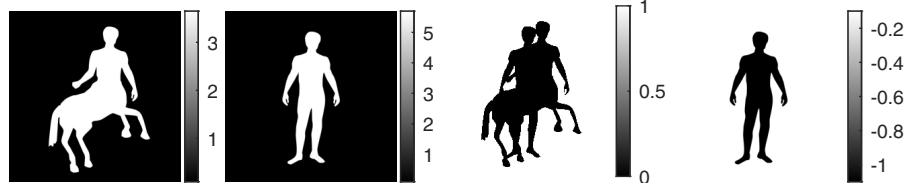


FIGURE 8. From left to right: Initial density ρ_0 , final ρ_1 , interaction penalty $Q(\mathbf{x})$ and terminal density regularizer $G(\mathbf{x})$

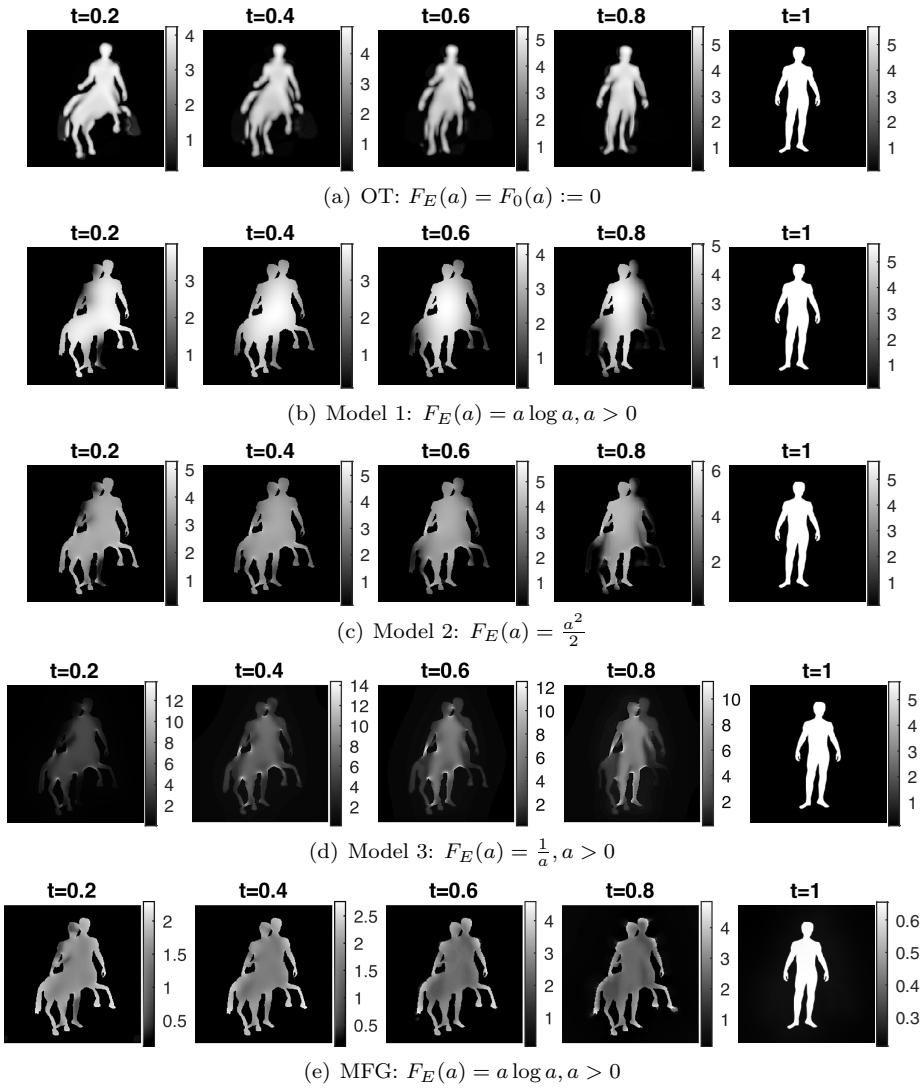


FIGURE 9. Snapshot of ρ at $t = 0.2, 0.4, 0.6, 0.8, 1$ (from left to right)

with $\lambda_E = 0.01, \lambda_Q = 0.1, \lambda_G = 1$. It is worth mentioning that to solve model (6.3)-(6.6), we must rescale ρ_1, ρ_1 such that $\int_{\Omega} \rho_0 = \int_{\Omega} \rho_1$ but we do not have to rescale $G(\mathbf{x})$ for ρ_0 in (6.7).

Figure 9 shows the snapshots of the density evolutions. Since (6.5)-(6.7) set the space preference to the evolution, the mass evolutions are within the dark region and the optimal transport model (6.3) has a more free evolution style.

Comparing model (6.4), (6.5) with (6.6), we observe that the mass evolution of model (6.4), (6.5) is dense, while that of (6.6) experiences a congest-flatten process and tends to be sparse. This is compatible with our discussions in Section 2.

7. CONCLUSION

In this paper, we propose an efficient and flexible algorithm to solve potential MFP problems based on an accelerated proximal gradient algorithm. In the optimal transport setting, we can converge faster or nearly as fast as G-prox and approach optimizer with the same accuracy. With multilevel and multigrid strategies, our algorithm can be accelerated up to 10 times without sacrificing accuracy. In broader settings of MFP and MFG, our method is more flexible than primal-dual or dual algorithms as it enjoys the flexibility to handle differentiable objective functions. Theoretically, we, for the first time, analyze the error introduced by discretizing ρ, \mathbf{m} based on an optimization point of view, and show that under some mild assumptions, our algorithm converges to the optimizer. In the future, we expect to extend the proposed algorithms for nonpotential mean field games, which have vast applications in mathematical finance, communications, and data science.

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