Semi-Implicit Finite Element Method and its Convergence of Single-Particle Reconstruction Using L^2-Gradient Flow *

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Abstract

In an earlier paper, we presented an iterative algorithm for reconstructing a three dimensional density function from a set of two dimensional electron microscopy images. By minimizing an energy functional consisting of a fidelity term and a regularization term, an L^2-gradient flow was derived. The flow was integrated by an explicit finite element method. In this paper, we present a semi-implicit finite element method for solving the same flow. Theoretical analysis for the convergence of the semi-implicit finite element method is presented.

1 Introduction

The reconstruction problem in computed tomography (CT), or some other application fields, for instance, electron tomography (ET), electron microscopy (EM), astronomy, geophysics, is to produce an image from a large number of its line-integral projections from different directions. In many applications of tomography, the reconstructed image reflects the X-ray attenuation coefficient when it travels though certain object, and the line integrals are obtained by measuring the attenuation of photons transmitted through the detected object. It is typically an inverse problem when we use the observed data though certain deterministic systems to inverse the degree of attenuation or some kind of physical quantity in actually applications.

The filtered back-projection (FBP) algorithm has been introduced in the medical field by [17], [19], and in the radio astronomy by [3]. The FBP, one pivotal component of commercial CT scanners, has remained popular for the past 25 years [15]. Main disadvantage of FBP lies in the highly computational complexity, particularly when the problem is extended to higher-resolution or higher-dimension. Great efforts on speed up the method have been made in the literatures [2], [4]. In addition, the direct Fourier reconstruction (DF) has been investigated, for instance, [13] and its further development [6], [16], [18]. Generally speaking, FBP is preferred to DF since the former provided images with better quality [11]. However, the back-projection

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part of FBP raises the computational complexity of the method to $O(n^3)$ arithmetic operations, while DF's complexity is just $O(n^2 \log n)$.

In [12], we presented an iterative algorithm for reconstructing a three dimensional density function from a set of two dimensional electron microscopy images. By minimizing an energy functional consisting of a fidelity term and a regularization term, an L^2-gradient flow was derived. The flow was integrated by an explicit finite element method. The method are compared with the weighted back projection, algebraic reconstruction technique and simultaneous iterative reconstructive technique. The numerical results show that the L^2-gradient flow method achieve a better resolution than the other three methods. However, the theoretical analysis on the convergence of the iterative method has not been considered.

In this paper, we present a semi-implicit finite element method for solving the same flow. An approximately optimal temporal step-size is determined which makes the semi-implicit more efficient than the explicit one. Theoretical analysis for the convergence of the semi-implicit finite element method is presented, which shows that the presented method is convergent.

The outline of this paper goes as follows. Section 2 sketches an overview of the mathematical background knowledge on image reconstruction. In Section 3, we first come up with a new computational method, then describe the detail derivation of our model, and finally give the concrete numerical computing procedures. The theory analysis of our numerical methods is given in Section 4.

2 Mathematical Preliminaries

The purpose of this section is to present various integral transforms and therein derive some their important properties. The material of this section serves as the theoretical basis for the rest of the paper. For detail derivation, we suggest the interested readers to refer to [8], [10], [14].

Let f be a function defined on $\mathbb{R}^3$, where $\mathbb{R}^3$ is the 3-dimensional real space consisting of 3-tuples of real numbers, usually denoted by single letters, $x = (x_1,\, x_2,\, x_3)^T,\ y = (y_1,\, y_2,\, y_3)^T$, etc. The inner product and norm in $\mathbb{R}^3$ are defined by $\langle x,\, y\rangle = x^T y = \sum_1^n x_i y_i$ and $\|x\| = \sqrt{\langle x,\, x\rangle}$, respectively. In addition, the gradient of f is denoted as $\nabla f = (f_{x_1}, f_{x_2}, f_{x_3})^T$. Let X be a real Banach space with norm $\|\cdot\|_X$.

Definition 2.1 *The space $L^p((0,T_0);X)$ consists of all measurable functions $u : [0,T_0] \to X$ with*

$$\|u\|_{L^p((0,T_0);X)} := \Big(\int_0^{T_0} \|u(t)\|_X^p \Big)^{\frac{1}{p}} < \infty,$$

for $1 \le q < \infty$, denoted as $\|u\|_{L^p(\mathbf{x})}$ for short, and

$$\|u\|_{L^\infty((0,T_0);X)} := \operatorname*{ess\,sup}_{0\le t\le T_0} \|u(t)\|_X < \infty,$$

abbreviated as $\|u\|_{L^\infty(\mathbf{x})}$.

The X-ray transform of a function $f \in \mathscr{L}_2(\mathbb{R}^3)$ is defined as

$$\mathbf{P}_\theta f(\mathbf{y}) = \int_{\mathbb{R}^1} f(s\theta + y)\mathrm{d}s, \quad y \in \Theta^\perp, \tag{2.1}$$

where $\Theta^\perp$ is the hyperplane passing through the origin and orthogonal to θ. From (2.1), we can see that the X-ray transform is the integral of $f \in \mathscr{L}_2(\mathbb{R}^3)$ over the straight line through point $y \in \Theta^\perp$ along the direction $\theta \in S^2$. Hence we can regard $\mathbf{P}f$ as a function defined on the tangent bundle $T = \{(\theta, y) : \theta \in S^2, y \in \Theta^\perp\}$.

The inner product in $\mathscr{L}_2(\mathbb{R}^3)$ can be defined as

$$\langle u(\mathbf{x}), v(\mathbf{x})\rangle = \int_{\mathbb{R}^3} u(\mathbf{x})v(\mathbf{x})\mathrm{d}\mathbf{x},$$

where $u(\mathbf{x}), v(\mathbf{x}) \in \mathscr{L}_2(\mathbb{R}^3)$. The analogous inner products in $\mathscr{L}_2(T)$ are given by

$$\langle h_1(\theta, y), h_2(\theta, y)\rangle = \int_T h_1(\theta, y)h_2(\theta, y)\mathrm{d}\theta\mathrm{d}\mathbf{y},$$

respectively, where

$$h_1(\theta, y), h_2(\theta, y) \in \mathscr{L}_2(T).$$

Using the definition $\mathbf{P}_\theta$, we obtain the following lemma.

Lemma 2.1 *Let Ω^2 be a sphere with radius R in $\mathbb{R}^3$. R is sufficient large but finite. Then the projection operator*

$$\mathbf{P}_\theta : \mathscr{L}_2(\Omega^2) \longrightarrow \mathscr{L}_2(\Theta^\perp)$$

is linear and continuous.

See [**?**] for the proof.

3 Reconstruction Algorithm

In this paper, we concentrate on the 3-D image reconstruction from the parallel projections at different angles inasmuch as the reconstruction method proposed can be straightforwardly generalized to other projection geometries and higher dimensions.

3.1 Reconstruction Model

Let $f(\mathbf{x}) : \Omega \subset \mathbb{R}^3 \rightarrow \mathbb{R}$ represent an unknown density function of a biomedical image, which has a bounded support in a cube Ω, namely,

$$supp(f) \subseteq \Omega. \tag{3.1}$$

We want to find $f \in BV(\Omega)$ such that the following energy functional (see [12]) is minimized.

$$E(f) = E_1(f) \ + \ \lambda E_2(f), \tag{3.2}$$

where $E_1(f)$ stands for the fidelity term of estimate to the observed data, $E_2(f)$ stands for the regularized term obtained from some maximum a posterior estimation or some significant operations, and $\lambda \geq 0$ is a parameter, balancing the effects of the fidelity term and the regularized one, $BV(\Omega)$ stands for the bounded variation space. For the definition and properties of $BV(\Omega)$, we suggest the interested readers refer to [1], [7]. In this paper $E_1(f)$ and $E_2(f)$ are given as follows,

$$E_1(f) = \frac{1}{2}\sum_{i=1}^{p}\int_{\mathbb{R}^2}\Big(\mathbf{P}_{\theta_i} f(\mathbf{y}) - g_i(\mathbf{y})\Big)^2 \mathrm{d}\mathbf{y}, \tag{3.3}$$

$$E_2(f) = \int_{\mathbb{R}^3} \phi(\|\nabla f\|)\mathrm{d}\mathbf{x}, \tag{3.4}$$

where $\theta_i \in S^2$ is the given i-th projection direction, $g_i(\mathbf{y})$ is the corresponding i-th measured image. The way on how to choose the potential function ϕ can be found in [1], [5]. ϕ is the engine to remove interfered noise as well as to preserve geometric features.

To derive the reconstruction equations, we first need to variate the regularized model. Using formulas (3.2), (3.3) and (3.4) and then variating $E(f)$, we have

$$\delta(E(f), h) = \sum_{i=1}^{p}\int_{\mathbb{R}^2}\Big((\mathbf{P}_{\theta_i} f)(\mathbf{y}) - g_i(\mathbf{y})\Big)(\mathbf{P}_{\theta_i} h)(\mathbf{y})\mathrm{d}\mathbf{y} + \lambda\int_{\mathbb{R}^3}\frac{\phi'(\|\nabla f\|)\nabla f^T \nabla h}{\|\nabla f\|}\mathrm{d}\mathbf{x} \tag{3.5}$$

From a theoretical point of view, the model (3.2) is well-posed. We present this result in the following theorem.

Theorem 3.1 *Assuming ϕ is a convex, nondecreasing function from $\mathbb{R}^+$ to $\mathbb{R}^+$, $\lim_{s\to+\infty}\phi(s) = +\infty$. And there exists two constants $c > 0$ and $b \geq 0$ such that $cs - b \leq \phi(s) \leq cs + b$, $\forall s \geq 0$. Let $\mathbf{P} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^2)$ be a linear continuous operator and $\mathbf{P}1 \neq 0$. The minimization problem*

$$\min_{f\in BV(\Omega)} \Big(E_1(f) + \lambda E_2(f)\Big),$$

where E_1 and E_2 is given by (3.3) and (3.4), respectively, admits a unique solution.

The proof of existence and uniqueness of a solution for the minimization problem is similar to that of [21]. Hence, we do not give the proof because of nonessential difference.

3.2 Numerical Computing

The model introduced by us is a typical integro-differential equation. The formulas are highly nonlinear, so the Fourier analysis method is useless here. The frequently used solving manner is resort to gradient flow, i.e., converting the elliptic differential equation to a time-dependent parabolic one in the domain $[0,\, T_0] \;\times\; \Omega,\ T_0 \gg 0$. When the parabolic differential equation achieves its steady state solution, we obtain the solution of Euler-Lagrange equation. Therefore, in what follows our solving problem is

$$\int_{\mathbb{R}^3} \left[\frac{\partial f}{\partial t} h + \frac{\lambda \phi'(\|\nabla f\|)\nabla f}{\|\nabla f\|} \nabla h \right] \mathrm{d}\mathbf{x} + \sum_{i=1}^{p} \int_{\mathbb{R}^2} (\mathbf{P}_{\theta_i} f - g_i)\mathbf{P}_{\theta_i} h \mathrm{d}\mathbf{y} = 0, \tag{3.6}$$

with a given $f_0 = f(x, y, 0)$. To preserve the geometric features of the reconstructed image, we need to choose the regularization function $\phi(s)$.

From a geometry point of view, the regularization term can remove the noise while preserving the geometric features very well, which is shown in [**?**]. In this paper, we choose

$$\phi_\epsilon(s) = \sqrt{s^2 + \epsilon^2}, \tag{3.7}$$

and use a semi-implicit finite element method to solve (3.6), where ϵ is a small positive constant. Let $\mathcal{T}_h$ be a pixel or voxel mesh of Ω with mesh size $h \in (0,\, 1)$. Let

$$V_h = \mathrm{span}\{\phi_0, \phi_1, \cdots, \phi_N\}$$

be the finite element space, where $\phi_i \in C^1(\mathbb{R}^3)$ are the basis functions with compact support Ω_i. We assume $\partial\Omega_i$ is regular (piecewise smooth). In this paper, we use tri-cubic B-spline function space defined on the uniform mesh $\mathcal{T}_h$. That is, ϕ_i is defined as follows:

$$\phi_{\alpha(n+1)^2+\beta(n+1)+\gamma}(\mathbf{x}) = N_\alpha(x) N_\beta(y) N_\gamma(z), \quad \mathbf{x} = [x, y, z]^T,$$

with $\alpha = 0, 1, \cdots, n,\ \ \beta = 0, 1, \cdots, n,\ \ \gamma_3 = 0, 1, \cdots, n$, where N_α are the one dimensional cubic B-spline basis function defined on the knots $[-2+\alpha, -1+\alpha, \alpha, 1+\alpha, 2+\alpha]$. It is easy to see that

$$N_\alpha(x) = N_0(x - \alpha). \tag{3.8}$$

Then Ω_i is a hypercube. Let

$$\Omega = \cup_{i=0}^{N} \Omega_i, \qquad N = (n+1)^3 - 1.$$

Then

$$f(\mathbf{x}) = \sum_{i=0}^{N} f_i \phi_i(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3,$$

has compact support Ω.

Let $\{t_m\}_{m=0}^{M}$ be a partition of $[0,\, T_0]$ with mesh sizes

$$\tau_m = t_m - t_{m-1} \in (0,\, 1), \quad k = \max_{1 \le m \le M} \tau_m.$$

We assume $\tau_m \ll 1$. In the following, we use the following notation

$$d_t f^m := \frac{f^m - f^{m-1}}{\tau_m},$$

namely, we use Euler forward scheme with respect to temporal variable t. Then the semi-implicit finite element discretization for the gradient flow (3.6) is given as follows: Find $F^m \in V^h$ for $m = 1, 2, \cdots, M$ such that

$$\int_{\mathbb{R}^3} \Big[d_t F^m v_h + \frac{\lambda \phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|} \nabla F^m \cdot \nabla v_h \Big] \mathrm{d}\mathbf{x} + \sum_{i=1}^{p} \int_{\mathbb{R}^2} (\mathbf{P}_{\theta_i} F^m - g_i) \mathbf{P}_{\theta_i} v_h \mathrm{d}\mathbf{y} = 0, \quad \forall v_h \in V^h, \tag{3.9}$$

with some initial value $F^0 \in V^h$ that approximates f_0.

Representing $F^m(\mathbf{x})$ as $\sum_{k=0}^{N} f_k^{(m)} \phi_k(\mathbf{x})$ and taking the test function $v_h(\mathbf{x}) = \phi_j(\mathbf{x})$, we can write (3.9) as a linear system of algebraic equations.

$$\sum_{k=0}^{N} (m_{jk} + \tau_m(q_{jk} + r_{jk}))\, f_k^{(m)} = \sum_{k=0}^{N} m_{jk} f_k^{(m-1)} + \tau_m b_j, \quad j = 0, \cdots, N, \tag{3.10}$$

where

$$m_{jk} = \int_{\mathbb{R}^3} \phi_j(\mathbf{x}) \phi_k(\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{3.11}$$

$$q_{jk} = \lambda \int_{\mathbb{R}^3} \Big[\frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|} \nabla \phi_k \cdot \nabla \phi_j \Big] \mathrm{d}\mathbf{x}, \tag{3.12}$$

$$r_{jk} = \sum_{i=1}^{p} \int_{\mathbb{R}^2} (\mathbf{P}_{\theta_i} \phi_k)(\mathbf{P}_{\theta_i} \phi_j) \mathrm{d}\mathbf{y}, \tag{3.13}$$

$$b_j = \sum_{i=1}^{p} \int_{\mathbb{R}^2} g_i(\mathbf{y})(\mathbf{P}_{\theta_i} \phi_j)(\mathbf{y}) \mathrm{d}\mathbf{y}. \tag{3.14}$$

Notice that since the basis functions are locally supported, the coefficient matrices $M := \{m_{jk}\}_{j,k=0}^{N}$, and $Q := \{q_{jk}\}_{j,k=0}^{N}$ of the systems are sparse. However, matrix $R := \{r_{jk}\}_{j,k=0}^{N}$ is not sparse. Also note that the matrices M, R and $B = [b_0, \cdots, b_N]^T$ do not depend on $F^{(m-1)}$. They can be previously computed.

3.3 Compute Temporal Step-size τ_m and Approximate Solution

In matrix form, equation (3.10) can be written as

$$(M + \tau_m(Q + R)) X^{(m)} = M X^{(m-1)} + \tau_m B, \tag{3.15}$$

where

$$X^{(m)} = [f_0^{(m)}, \cdots, f_N^{(m)}]^T, \quad m = 1, 2, \cdots, M.$$

Let

$$X^{(m)} = X^{(m-1)} + \tau_m Y + \tau_m^2 Z + O(\tau_m^3),$$

with

$$\begin{aligned} Y &= [y_0, y_1, \cdots, y_N]^T, \\ Z &= [z_0, z_1, \cdots, z_N]^T. \end{aligned}$$

Substitute $X^{(m)}$ into (3.15), we have

$$(M + \tau_m(Q+R))(Y + \tau_m Z + O(\tau_m^2)) = B - (Q+R)X^{(m-1)}.$$

Then

$$\begin{aligned} Y + \tau_m Z + O(\tau_m^2) &= \left(I + \tau_m M^{-1}(Q+R)\right)^{-1} M^{-1} \left(B - (Q+R)X^{(m-1)}\right) \\ &= \left(I - \tau_m M^{-1}(Q+R) + O(\tau_m^2)\right) M^{-1} \left(B - (Q+R)X^{(m-1)}\right). \quad (3.16) \end{aligned}$$

We obtain

$$Y = M^{-1}\left(B - (Q+R)X^{(m-1)}\right), \quad (3.17)$$

$$\begin{aligned} Z &= -M^{-1}(Q+R)M^{-1}\left(B - (Q+R)X^{(m-1)}\right) \\ &= -M^{-1}(Q+R)Y. \quad (3.18) \end{aligned}$$

Let

$$y(\mathbf{x}) = \sum_{j=0}^{N} y_j \phi_j(\mathbf{x}), \quad z(\mathbf{x}) = \sum_{j=0}^{N} z_j \phi_j(\mathbf{x}).$$

Then

$$F^m(\mathbf{x}) = F^{m-1}(\mathbf{x}) + \tau_m\, y(\mathbf{x}) + \tau_m^2\, z(\mathbf{x}) + O(\tau_m^3).$$

Substitute $F^m(\mathbf{x})$ into (3.2), we have

$$e(\tau_m) := E\left(F^{m-1} + \tau_m y(\mathbf{x}) + \tau_m^2 z(\mathbf{x}) + O(\tau_m^3)\right)$$

Compute the power series expansion of $e(\tau_m)$ with respect to τ_m,

$$e(\tau_m) = e_0 + e_1\tau_m + \frac{1}{2}e_2\tau_m^2 + \cdots,$$

where

$$e_1 = \sum_{i=1}^{p} \int_{\mathbb{R}^2} (\mathbf{P}_{\theta_i} F^{m-1} - g_i)(\mathbf{P}_{\theta_i} y) \mathrm{d}\mathbf{y} + \lambda \int_{\mathbb{R}^3} \phi'(\|\nabla F^{m-1}\|) \frac{\nabla F^{m-1} \cdot \nabla y}{\|\nabla F^{m-1}\|} \mathrm{d}\mathbf{x}, \tag{3.19}$$

$$\begin{aligned} e_2 = & \sum_{i=1}^{p} \int_{\mathbb{R}^2} (\mathbf{P}_{\theta_i} y)^2 + 2(\mathbf{P}_{\theta_i} F^{m-1} - g_i)(\mathbf{P}_{\theta_i} z) \mathrm{d}\mathbf{y} \\ & + \lambda \int_{\mathbb{R}^3} \phi''(\|\nabla F^{m-1}\|) \frac{(\nabla F^{m-1} \cdot \nabla y)^2}{\|\nabla F^{m-1}\|^2} \mathrm{d}\mathbf{x} \\ & + \lambda \int_{\mathbb{R}^3} \phi'(\|\nabla F^{m-1}\|) \left[\frac{\|\nabla y\|^2 + 2\nabla F^{m-1} \cdot \nabla z}{\|\nabla F^{m-1}\|} - \frac{(\nabla F^{m-1} \cdot \nabla y)^2}{\|\nabla F^{m-1}\|^3} \right] \mathrm{d}\mathbf{x}. \end{aligned} \tag{3.20}$$

Then from

$$e'(\tau_m) = 0,$$

we obtain a linear equation. Solving the equation, we obtain τ_m as follows.

$$\tau_m = -\frac{e_1}{e_2}. \tag{3.21}$$

Having τ_m, Y and Z, $X^{(m)}$ can be approximated as

$$X^{(m)} \approx X^{(m-1)} + \tau_m Y + \tau_m^2 Z. \tag{3.22}$$

Now we summarize the iteration scheme as the following algorithm.

Algorithm 3.1 *Semi-implicit Finite Element Method*

1. Set $m = 0$, set the initial B-spline coefficients $X^{(0)} = \mathbf{0}$.
2. Compute $M = \{m_{jk}\}$ and $B = \{b_j\}$ using (3.11) and (3.14), respectively.
3. Compute $Q = \{q_{jk}\}$ using (3.12).
4. Compute Y and Z using (3.17) and (3.18), respectively.
5. Compute e_1 and e_2 using (3.19) and (3.20) and then compute τ_m using (3.21).
6. Compute $X^{(m)}$ using (3.22).
7. Check the terminate condition, if it is satisfied, stop the iteration, otherwise, set m to be $m + 1$, return to step 3.

Remark 3.1 *In (3.22), if we take $Z = \mathbf{0}$, then the obtained $X^{(m)}$ is the same as the one obtained from the explicit finite element method for the given τ_m. Hence our method can be regarded as a correction of the explicit finite element method by adding a second order term $\tau_m^2 Z$. Even higher order terms can be computed from (3.16). But since τ_m in general is small, these terms are negligible.*

3.4 The Computation of RX

In the above algorithm, we need to compute the multiplication of R and a vector X. In general, matrix R is not sparse. Hence if the size of N is large, for instance $N = 512^3$, the required space for storing R, which is $N^2 = 512^6$, may beyond the capacity of the used computer. Hence, it is impractical to compute directly the multiplication of R and a vector $X = [x_0, \cdots, x_N]^T$. What we suggest is to represent RX as follows

$$RX = \sum_{i=1}^{p} \int_{\mathbb{R}^2} \sum_{k=0}^{N} x_k (\mathbf{P}_{\theta_i}\phi_k)(\mathbf{y})(\mathbf{P}_{\theta_i}\phi_j)(\mathbf{y})\mathrm{d}\mathbf{y}.$$

Hence, we first compute

$$X_i(\mathbf{y}) := \sum_{k=0}^{N} x_k (\mathbf{P}_{\theta_i}\phi_k)(\mathbf{y}), \quad i = 1, \cdots, p, \tag{3.23}$$

then compute

$$y_{ij} := \int_{\mathbb{R}^2} X_i(\mathbf{y})(\mathbf{P}_{\theta_i}\phi_j)(\mathbf{y})\mathrm{d}\mathbf{y}, \text{ for } i = 1, \cdots, p, \quad j = 0, \cdots, N. \tag{3.24}$$

Finally, RX is computed as

$$RX = \left[\sum_{i=1}^{p} y_{i0}, \cdots, \sum_{i=1}^{p} y_{iN} \right]^T. \tag{3.25}$$

3.5 Algorithm Details and Analysis of Computational Complexity

We present algorithm details and analyze the computational complexity for Algorithm 3.1 from step 2 to step 6. The costs for the first and last step is relatively small.

1. Matrix M is sparse, its elements has close form representation. Utilizing the the tensor product structure of the basis functions, we only need to store and inverse a $n \times n$ matrix. Hence, the computational cost of the inversion of M is $O(n^3)$. Let p be the number of projections, then using the translation property (3.8) of the basis functions, we know that $\mathbf{P}_{\theta_i}\phi_j$ can be computed from $\mathbf{P}_{\theta_i}\phi_0$. Since $\mathbf{P}_{\theta_i}\phi_j$ has compact support, the computational cost for b_j is $O(p)$. Hence, the computational complexity for B is $O(pn^3)$. All these computations in step 2 are out of the m-iteration loop in Algorithm 3.1. They can be previously computed.

2. The cost for computing Q in step 3 is in the same order as computing M. It is $O(n^3)$. Since q_{jk} depends on F^{m-1}, it needs to be recomputed in each of the m-iterations.

3. To compute Y and Z in step 4, we need to first compute $QX^{(m-1)}$ and $RX^{(m-1)}$. Since Q is a sparse matrix, the cost for computing $QX^{(m-1)}$ is $O(n^3)$. $RX^{(m-1)}$ is computed using (3.23)–(3.25). The cost for computing one $X_i(\mathbf{y})$ using (3.23) is $O(n^3)$. For computing all $X_i(\mathbf{y})$, $i = 1, \cdots, p$, the cost is $O(pn^3)$. Since $\mathbf{P}_{\theta_i}\phi_j$ is local supported, the cost for computing y_{ij} is $O(1)$. Hence the total cost for computing $\{y_{ij}\}$ is $O(pn^3)$. Finally, computing RX using (3.25) requires $O(pn^3)$ arithmetic operations. Adding these together, the total cost for computing RX is $O(pn^3)$. The cost for computing the multiplication M^{-1} with a vector is $O(n^3)$ using the property that M^{-1} is approximately a band matrix. In summary, Y can be computed with the complexity $O(pn^3)$. After Y is computed, Z is similarly computed via (3.18). Again, the cost is $O(pn^3)$.

4. Now we consider the computations of e_1 and e_2 in step 5. The cost for computing all the $\mathbf{P}_{\theta_i}y$ is $O(pn^3)$. The cost for computing ∇F^{m-1} and ∇y is $O(n^3)$. Hence the order for computing e_1 and e_2 using (3.19) and (3.20) is $O(pn^3)$.

5. The cost for computing $X^{(m)}$ in step 6 using (3.22) is $O(n^3)$. Hence, for one m-iteration, the total cost is in the order of $O(pn^3)$.

Remark 3.2 *The analysis above shows that the computational complexity of the semi-implicit scheme is $O(pn^3)$ for one iteration. This is in the same order as the explicit finite element method presented in [12]. However, since the semi-implicit scheme requires less iterations in general than the explicit scheme, the presented method is more efficient.*

4 Convergence of semi-implicit finite element discretization

In this section, we give the convergent analysis of finite element discretization for semi-implicit scheme.

Lemma 4.1 *Assume that $f_0 \in L^2(\mathbb{R}^3)$ with support Ω, $g_i \in L^2(\mathbb{R}^2)$ and $\partial\Omega$ is sufficiently regular. Then, for each fixed $\epsilon > 0$, $\{F^m\}$ derived from semi-implicit scheme (3.9) satisfies*

$$\sum_{m=1}^{l}\Big[\tau_m\|d_tF^m\|^2_{L^2(\mathbb{R}^3)}+\frac{\tau_m^2}{2}\sum_{i=1}^{p}\|d_t(\mathbf{P}_{\theta_i}F^m-g_i)\|^2_{L^2(\mathbb{R}^2)}\Big]+J_{\lambda,\epsilon}(F^l)\leq J_{\lambda,\epsilon}(F^0),\quad 1\leq l\leq M. \tag{4.1}$$

Proof. To verify (4.1), testing (3.9) with d_tF^m yields

$$\|d_tF^m\|^2_{L^2(\mathbb{R}^3)}+\int_{\mathbb{R}^3}\lambda\Big[\frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}\nabla F^m\cdot\nabla d_tF^m\Big]\mathrm{d}\mathbf{x}+\sum_{i=1}^{p}\int_{\mathbb{R}^2}(\mathbf{P}_{\theta_i}F^m-g_i)d_t\mathbf{P}_{\theta_i}F^m\mathrm{d}\mathbf{y}=0. \tag{4.2}$$

Considering the last term on the left-hand of (4.2), we derive

$$\int_{\mathbb{R}^2}(\mathbf{P}_{\theta_i}F^m-g_i)d_t\mathbf{P}_{\theta_i}F^m\mathrm{d}\mathbf{y}=\frac{d_t\|\mathbf{P}_{\theta_i}F^m-g_i\|^2_{L^2(\mathbb{R}^2)}}{2}+\frac{\tau_m\|d_t(\mathbf{P}_{\theta_i}F^m-g_i)\|^2_{L^2(\mathbb{R}^2)}}{2}, \tag{4.3}$$

and similarly,

$$\nabla F^m \cdot \nabla d_t F^m = \frac{d_t\|\nabla F^m\|^2 + \tau_m \|\nabla d_t F^m\|^2}{2}. \tag{4.4}$$

Hence, using (4.3) and (4.4), (4.2) becomes

$$\begin{aligned}\|d_t F^m\|^2_{L^2(\mathbb{R}^3)} \;&+\; \frac{\sum_{i=1}^p d_t\|\mathbf{P}_{\theta_i} F^m - g_i\|^2_{L^2(\mathbb{R}^2)}}{2} + \frac{\tau_m \sum_{i=1}^p \|d_t(\mathbf{P}_{\theta_i} F^m - g_i)\|^2_{L^2(\mathbb{R}^2)}}{2} \\ &+\; \frac{1}{2}\int_{\mathbb{R}^3} \frac{\lambda \phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|} \left(d_t\|\nabla F^m\|^2 + \tau_m\|\nabla d_t F^m\|^2\right) \mathrm{d}\mathbf{x} = 0. \end{aligned} \tag{4.5}$$

Noting that the forth term on the left-hand side of (4.5), we have (using the formula $a^2 - b^2 = 2b(a-b) + (a-b)^2$)

$$\begin{aligned}\frac{1}{2}\int_{\mathbb{R}^3} \frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|} d_t\|\nabla F^m\|^2 \mathrm{d}\mathbf{x} \;&=\; \frac{1}{\tau_m}\int_{\mathbb{R}^3} \phi'_\epsilon(\|\nabla F^{m-1}\|)(\|\nabla F^m\| - \|\nabla F^{m-1}\|)\mathrm{d}\mathbf{x} \\ &+ \frac{1}{2\tau_m}\int_{\mathbb{R}^3} \frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}(\|\nabla F^m\| - \|\nabla F^{m-1}\|)^2 \mathrm{d}\mathbf{x}. \end{aligned} \tag{4.6}$$

Using Cauchy inequality $\nabla F^m \cdot \nabla F^{m-1} \le \|\nabla F^m\|\|\nabla F^{m-1}\|$ and $\phi'_\epsilon(s) \ge 0$, we obtain

$$\frac{1}{2\tau_m}\int_{\mathbb{R}^3} \frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}(\|\nabla F^m\| - \|\nabla F^{m-1}\|)^2 \mathrm{d}\mathbf{x} \le \frac{1}{2}\int_{\mathbb{R}^3} \frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|} \tau_m \|\nabla d_t F^m\|^2 \mathrm{d}\mathbf{x}. \tag{4.7}$$

Substituting (4.6)-(4.7) into (4.5), we obtain

$$\begin{aligned}\|d_t F^m\|^2_{L^2(\mathbb{R}^3)} \;&+\; \frac{\sum_{i=1}^p d_t\|\mathbf{P}_{\theta_i} F^m - g_i\|^2_{L^2(\mathbb{R}^2)}}{2} + \frac{\tau_m \sum_{i=1}^p \|d_t(\mathbf{P}_{\theta_i} F^m - g_i)\|^2_{L^2(\mathbb{R}^2)}}{2} \\ &+\; \frac{\lambda}{\tau_m}\int_{\mathbb{R}^3} \phi'_\epsilon(\|\nabla F^{m-1}\|)(\|\nabla F^m\| - \|\nabla F^{m-1}\|)\mathrm{d}\mathbf{x} \\ &+\; \frac{\lambda}{\tau_m}\int_{\mathbb{R}^3} \frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}(\|\nabla F^m\| - \|\nabla F^{m-1}\|)^2 \mathrm{d}\mathbf{x} \le 0. \end{aligned} \tag{4.8}$$

We can show that (see [?] for details of this derivation)

$$\begin{aligned}\int_{\mathbb{R}^3} \phi'_\epsilon(\|\nabla F^{m-1}\|)(\|\nabla F^m\| \;-\; \|\nabla F^{m-1}\|)\mathrm{d}\mathbf{x} + \int_{\mathbb{R}^3} \frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}(\|\nabla F^m\| - \|\nabla F^{m-1}\|)^2 \mathrm{d}\mathbf{x} \\ \ge \int_{\mathbb{R}^3} \phi'_\epsilon(\|\nabla F^m\|)(\|\nabla F^m\| - \|\nabla F^{m-1}\|)\mathrm{d}\mathbf{x} \end{aligned} \tag{4.9}$$

Using the convexity of $\phi_\epsilon(s)$, the term on the right-hand side of (4.9) is bounded by

$$\int_{\mathbb{R}^3} \phi'_\epsilon(\|\nabla F^m\|)(\|\nabla F^m\| - \|\nabla F^{m-1}\|)\mathrm{d}\mathbf{x} \ge \tau_m\, d_t \int_{\mathbb{R}^3} \phi_\epsilon(\|\nabla F^m\|)\mathrm{d}\mathbf{x}. \tag{4.10}$$

According to (4.8), (4.9) and (4.10), we get

$$\|d_t F^m\|^2_{L^2(\mathbb{R}^3)} + \frac{\sum_{i=1}^p d_t\|\mathbf{P}_{\theta_i}F^m - g_i\|^2_{L^2(\mathbb{R}^2)}}{2} + \frac{\tau_m \sum_{i=1}^p \|d_t(\mathbf{P}_{\theta_i}F^m - g_i)\|^2_{L^2(\mathbb{R}^2)}}{2}$$
$$+ \lambda d_t \int_{\mathbb{R}^3} \phi_\epsilon(\|\nabla F^m\|)\mathrm{d}\mathbf{x} \le 0. \tag{4.11}$$

Applying the summation operator $\sum_{m=1}^l \tau_m$ to the above inequality, we get (4.1).

For finite element solution $\{F^m\}$, in what follows we give its constant and linear interpolation in temporal direction t [9]

$$\overline{F}^{\epsilon,h,k}(\mathbf{x},\, t) := F^{m-1}(\mathbf{x}), \quad \forall t \in [t_{m-1}, t_m), \quad 1 \le m \le M, \tag{4.12}$$
$$\overline{\overline{F}}^{\epsilon,h,k}(\mathbf{x},\, t) := \frac{t - t_{m-1}}{\tau_m} F^m(\mathbf{x}) + \frac{t_m - t}{\tau_m} F^{m-1}(\mathbf{x}), \quad \forall t \in [t_{m-1},\, t_m], \quad 1 \le m \le M. \tag{4.13}$$

Obviously, $\overline{F}^{\epsilon,h,k}$ is continuous in spatial x but discontinuous in t. However, $\overline{\overline{F}}^{\epsilon,h,k}$ is continuous in both x and t.

Theorem 4.1 *Assume that $f_0 \in L^2(\mathbb{R}^3)$ with support Ω and sufficiently regular boundary $\partial\Omega$, $g_i \in L^2(\mathbb{R}^2)$. Then under the following initial value constraint*

$$\lim_{h\to 0} \|f_0 - F^0\|_{L^2(\mathbb{R}^3)} = 0,$$

there exits $f^\epsilon \in L^\infty((0,T); BV(\Omega)) \cap H^1((0,T); L^2(\mathbb{R}^3))$ such that

$$\lim_{h,k\to 0} \|f^\epsilon - \overline{F}^{\epsilon,h,k}\|_{L^\infty((0,T_0);L^p(\mathbb{R}^3))} = 0, \tag{4.14}$$
$$\lim_{h,k\to 0} \|f^\epsilon - \overline{\overline{F}}^{\epsilon,h,k}\|_{L^\infty((0,T_0);L^p(\mathbb{R}^3))} = 0, \tag{4.15}$$

uniformly in ϵ for any $p \in [1,\, \frac{n}{n-1})$.

Proof. To show (4.14)-(4.15), we first notice that (4.1) implies the following (uniform in both h, k and ϵ) estimates

$$\|\overline{\overline{F}}_t^{\epsilon,h,k}\|_{L^2(L^2(\mathbb{R}^3))} = \Big(\sum_{m=1}^M \tau_m \|d_t F^m\|^2_{L^2(\mathbb{R}^3)}\Big)^{\frac{1}{2}} \le C, \tag{4.16}$$

$$\begin{aligned} \|\mathbf{P}_{\theta_i}\overline{F}^{\epsilon,h,k}\|_{L^\infty(L^2(\mathbb{R}^2))} &\le \|\mathbf{P}_{\theta_i}\overline{\overline{F}}^{\epsilon,h,k}\|_{L^\infty(L^2(\mathbb{R}^2))} \\ &= \max_{0\le m\le M} \|\mathbf{P}_{\theta_i}F^m\|_{L^2(\mathbb{R}^2)} \\ &\le \max_{0\le m\le M} \|\mathbf{P}_{\theta_i}F^m - g_i\|_{L^2(\mathbb{R}^2)} + \|g_i\|_{L^2(\mathbb{R}^2)} \le C, \end{aligned} \tag{4.17}$$

$$\begin{aligned}\|\nabla\overline{F}^{\epsilon,h,k}\|_{L^\infty(L^1(\mathbb{R}^3))} &\le \|\nabla\overline{\overline{F}}^{\epsilon,h,k}\|_{L^\infty(L^1(\mathbb{R}^3))} = \max_{0\le m\le M}\|\nabla F^m\|_{L^1(\mathbb{R}^3)} \\ &\le \max_{0\le m\le M}\int_{\mathbb{R}^3}\phi_\epsilon(\|\nabla F^m\|)\mathrm{d}\mathbf{x}\le C, \end{aligned}\tag{4.18}$$

$$\begin{aligned}&\sum_{m=1}^{M}\sum_{i=1}^{p}\|\mathbf{P}_{\theta_i}F^m-\mathbf{P}_{\theta_i}F^{m-1}\|^2_{L^2(\mathbb{R}^2)}\\ &=\sum_{m=1}^{M}\tau_m^2\sum_{i=1}^{p}\|d_t(\mathbf{P}_{\theta_i}F^m-g_i)\|^2_{L^2(\mathbb{R}^2)}\le C,\quad if\quad \lambda\neq 0,\end{aligned}\tag{4.19}$$

where C is a sufficiently large constant.

Then, testing (3.9) with F^m yields

$$\int_{\mathbb{R}^3}\Big[d_tF^m\cdot F^m+\frac{\lambda\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}\nabla F^m\cdot\nabla F^m\Big]\mathrm{d}\mathbf{x}+\sum_{i=1}^{p}\int_{\mathbb{R}^2}(\mathbf{P}_{\theta_i}F^m-g_i)\mathbf{P}_{\theta_i}F^m\mathrm{d}\mathbf{y}=0.\tag{4.20}$$

Noting the first and the last terms in the integration of (4.20), we derive

$$d_tF^m\cdot F^m=\frac{F^m-F^{m-1}}{\tau_m}F^m=\frac{d_t|F^m|^2}{2}+\frac{\tau_m|d_tF^m|^2}{2},\tag{4.21}$$

and

$$\int_{\mathbb{R}^2}(\mathbf{P}_{\theta_i}F^m-g_i)\mathbf{P}_{\theta_i}F^m\mathrm{d}\mathbf{y}=\frac{\|\mathbf{P}_{\theta_i}F^m-g_i\|^2_{L^2(\mathbb{R}^2)}+\|\mathbf{P}_{\theta_i}F^m\|^2_{L^2(\mathbb{R}^2)}-\|g_i\|^2_{L^2(\mathbb{R}^2)}}{2},\tag{4.22}$$

Using (4.21) and (4.22), (4.20) becomes

$$\begin{aligned}&\frac{d_t\|F^m\|^2_{L^2(\mathbb{R}^3)}}{2}+\frac{\tau_m\|d_tF^m\|^2_{L^2(\mathbb{R}^3)}}{2}+\lambda\int_{\mathbb{R}^3}\frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}\|\nabla F^m\|^2\mathrm{d}\mathbf{x}\\ &\qquad+\frac{\sum_{i=1}^p\|\mathbf{P}_{\theta_i}F^m-g_i\|^2_{L^2(\mathbb{R}^2)}}{2}+\frac{\sum_{i=1}^p\|\mathbf{P}_{\theta}F^m\|^2_{L^2(\mathbb{R}^2)}}{2}=\frac{\sum_{i=1}^p\|g_i\|^2_{L^2(\mathbb{R}^2)}}{2}.\end{aligned}\tag{4.23}$$

Therefore, applying the summation operator $2\sum_{m=1}^{l}\tau_m$ to the resulting equality (4.23), we obtain

$$\begin{aligned}&\|F^l\|^2_{L^2(\mathbb{R}^3)}+\sum_{m=1}^{l}\tau_m^2\|d_tF^m\|^2_{L^2(\mathbb{R}^3)}+\lambda\sum_{m=1}^{l}\tau_m\int_{\mathbb{R}^3}\frac{\phi'_\epsilon(\|\nabla F^{m-1}\|)}{\|\nabla F^{m-1}\|}\|\nabla F^m\|^2\mathrm{d}\mathbf{x}\\ &+\sum_{m=1}^{l}\tau_m\sum_{i=1}^{p}\|\mathbf{P}_{\theta_i}F^m-g_i\|^2_{L^2(\mathbb{R}^2)}+\sum_{m=1}^{l}\tau_m\sum_{i=1}^{p}\|\mathbf{P}_{\theta}F^m\|^2_{L^2(\mathbb{R}^2)}\\ &\quad\le\left(\sum_{m=1}^{l}\tau_m\right)\sum_{i=1}^{p}\|g_i\|^2_{L^2(\mathbb{R}^2)}+\|F^0\|^2_{L^2(\mathbb{R}^3)},\qquad\forall 1\le l\le M.\end{aligned}\tag{4.24}$$

Since $\sum_{m=1}^{l}\tau_m \le T_0$, we have

$$\left(\sum_{m=1}^{l}\tau_m\right)\sum_{i=1}^{p}\|g_i\|^2_{L^2(\mathbb{R}^2)}+\|F^0\|^2_{L^2(\mathbb{R}^3)} \le T_0\sum_{i=1}^{p}\|g_i\|^2_{L^2(\mathbb{R}^2)}+\|F^0\|^2_{L^2(\mathbb{R}^3)} \le C, \quad \forall 1\le l\le M. \tag{4.25}$$

Hence, according to (4.24) and (4.25), we get

$$\|\overline{F}^{\epsilon,h,k}\|_{L^\infty(L^2(\mathbb{R}^3))} \le \|\overline{\overline{F}}^{\epsilon,h,k}\|_{L^\infty(L^2(\mathbb{R}^3))} = \max_{0\le m\le M}\|F^m\|_{L^2(\mathbb{R}^3)} \le C, \tag{4.26}$$

$$\sum_{m=1}^{M}\|F^m-F^{m-1}\|^2_{L^2(\mathbb{R}^3)} = \sum_{m=1}^{M}\tau_m^2\|d_tF^m\|^2_{L^2(\mathbb{R}^3)} \le C. \tag{4.27}$$

Then, based on (4.16), (4.18), (4.26) and (4.27), there exists a convergent subsequence of $\{\overline{\overline{F}}^{\epsilon,h,k}\}$ (denoted by the same notation) [9][20] and a function $f^\epsilon \in L^\infty((0,T);BV(\Omega)) \cap H^1((0,T);L^2(\mathbb{R}^3))$ such that as $h,k\to 0$

$$\begin{aligned}\overline{\overline{F}}^{\epsilon,h,k} \longrightarrow f^\epsilon \quad & \textit{weakly} \star \ \ \textit{in} \quad L^\infty((0,\,T_0);\,L^2(\mathbb{R}^3)),\\ & \textit{weakly} \ \ \textit{in} \quad L^2((0,\,T_0);\,L^2(\mathbb{R}^3)),\\ & \textit{strongly} \ \ \textit{in} \quad L^p(\Omega), 1\le p<\frac{n}{n-1}, \textit{for} \ \ \textit{a.e.} \ \ t\in[0,\,T_0],\end{aligned} \tag{4.28}$$

and

$$\overline{\overline{F}}_t^{\epsilon,h,k} \longrightarrow f_t^\epsilon \quad \textit{weakly} \ \ \textit{in} \ \ L^2((0,\,T_0);\,L^2(\mathbb{R}^3)). \tag{4.29}$$

Here we have used the fact that $BV(\Omega)$ is compactly embedded in $L^p(\Omega)$ for $1\le p<\frac{n}{n-1}$. Notice that the assumption on F^0 implies that $f^\epsilon(0)=f_0$. Therefore, the proof of (4.14) is completed.

Using (4.1), we have

$$\sum_{m=1}^{M}\tau_m\|d_tF^m\|^2_{L^2(\mathbb{R}^3)} \le C.$$

According to above formula, it is easy to show that

$$\begin{aligned}\|\overline{\overline{F}}^{\epsilon,h,k}-\overline{F}^{\epsilon,h,k}\|^2_{L^2(L^2(\mathbb{R}^3))} &= \int_0^{T_0}\|\overline{\overline{F}}^{\epsilon,h,k}-\overline{F}^{\epsilon,h,k}\|^2_{L^2(\mathbb{R}^3)}\mathrm{d}t\\ &= \frac{1}{3}\sum_{m=1}^{M}\tau_m^3\|d_tF^m\|^2_{L^2(\mathbb{R}^3)}\\ &\le \frac{k^2}{3}\sum_{m=1}^{M}\tau_m\|d_tF^m\|^2_{L^2(\mathbb{R}^3)} \le Ck^2.\end{aligned} \tag{4.30}$$

Using (4.14) and (4.30), we obtain (4.15). Therefore, for semi-implicit scheme (3.9) the proof of convergence is completed.

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