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AN IMMERSED EULERIAN-LAGRANGIAN LOCALIZED ADJOINT METHOD FOR TRANSIENT ADVECTION-DIFFUSION EQUATIONS WITH INTERFACES

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Abstract. We develop and analyze an immersed Eulerian-Lagrangian localized adjoint method (ImELLAM) for transient advection-diffusion equations with interfaces. The derived method possesses the combined advantages of the immersed finite element method and the Eulerian-Lagrangian method.

Key Words. advection-diffusion problem, Eulerian-Lagrangian method, error estimate, immersed finite element method, interfaces.

1. Introduction

Transient advection-diffusion equations arise in mathematical models for describing petroleum reservoir simulation, groundwater contaminant transport, geological storage of carbon dioxide and remediation, and many other applications [1, 13, 2, 7, 12, 13, 14, 20]. These equations admit solutions with moving steep fronts and complicated structures. Furthermore, subsurface porous medium matrix often contains a variety of faults and fractures of different magnitude. Those relatively large faults must be accurately incorporated into the corresponding mathematical models, in which the geological formations consist of several subdomains with different geological properties and salient physical interfaces. This also means that in the numerical discretization the computational meshes must align with the large faults in order to obtain a stable and accurate numerical solution. Note that the number of large faults is usually quite limited, so the modeling and numerical implementation is doable. On the other hand, there are numerous relatively small fractures which are very difficult, if not impossible at all, to describe in a deterministic manner geologically. As a matter of fact, these relatively tiny fractures are often described in a probability sense. The impact of these tiny fractures can be handled via the approach of upscaling or multiscale numerical techniques. As for those intermediate fractures, they are probably too big to be upscaled into the underlying numerical schemes in any reasonable manner. On the other hand, there are probably too many intermediate fractures such that the computational meshes of the underlying numerical scheme align with each of them. Based on these considerations we plan to adopt the approach of immersed numerical method to handle these intermediate fractures.

To expose the idea, in this paper we consider the one-dimensional transient linear advection-diffusion equation with interfaces

$$
\begin{aligned}
\phi u_t + (Vu - Du_x)_x &= f(x,t), \qquad && x \in (a,b), \quad 0 < t \le T, \\
u(x,0) &= u_0(x), && x \in [a,b].
\end{aligned} \tag{1}
$$

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In such areas as porous medium flow and transport, the geological formations may consist of several subdomains with different geological properties. Consequently, there exist physical interfaces between different subdomains. Across these interfaces, the concentration $u(x,t)$ and the Darcy flux $V(x)$ are continuous, but the porosity of the porous medium $\phi(x)$ and the diffusion coefficient $D(x)$ are discontinuous. Nevertheless, the diffusive flux is continuous across these interfaces. We assume that V is constant in the domain (a,b), ϕ and D are piecewise constants and $a < \alpha_1 < \cdots < \alpha_K < b$ are the interfaces. This leads to the following interface conditions for $k = 1, \cdots, K$,

$$[\![u]\!](\alpha_k, t) = 0, \qquad [\![Du_x]\!](\alpha_k, t) = 0, \qquad t \in [0,T], \tag{2}$$

where $[\![u]\!](\alpha_k, t) = u(\alpha_k^+, t) - u(\alpha_k^-, t)$ represents the jump of u across the interface $x = \alpha_k$. To focus on main idea for the development and the analysis of the ImELLAM scheme, we assume that the problem is closed by the periodic boundary condition.

In this paper we develop and analyze an immersed Eulerian-Lagrangian localized adjoint method (ImELLAM) for transient advection-diffusion equations with interfaces. The rest of the paper is organized as follows: In §2 we present some preliminaries that are needed in the development and analysis of the ImELLAM scheme. In §3 we derive the ImELLAM scheme. In §4 we prove an optimal-order error estimate for the ImELLAM scheme. §5 contains concluding remarks.

2. Preliminary

In this section we recall some preliminaries that are needed in the development and analysis of the ImELLAM scheme.

2.1. Sobolev Spaces. Let $W_p^k(a,b)$ consist of functions whose weak derivatives up to order-k are p-th Lebesgue integrable in (a,b), and $H^k(a,b) := W_2^k(a,b)$. Let $H_E^m(a,b)$ be the subspace of $H^m(a,b)$ with periodic boundary condition. For any Banach space X, we introduce Sobolev spaces involving time [6]

$$\begin{aligned}
W_p^k(t_1,t_2;X) \quad &:= \left\{ f : \left\| \frac{\partial^l f}{\partial t^l}(\cdot,t) \right\|_X \in L^p(t_1,t_2),\ 0 \le l \le k,\ 1 \le p \le \infty \right\}, \\
\|f\|_{W_p^k(t_1,t_2;X)} \quad &:= \begin{cases} \left(\displaystyle\sum_{l=0}^{k} \int_{t_1}^{t_2} \left\| \frac{\partial^l f}{\partial t^l}(\cdot,t) \right\|_X^p dt \right)^{1/p}, & 1 \le p < \infty, \\ \displaystyle\max_{0 \le l \le k} \operatorname*{esssup}_{t \in (t_1,t_2)} \left\| \frac{\partial^l f}{\partial t^l}(\cdot,t) \right\|_X, & p = \infty. \end{cases}
\end{aligned}$$

We also introduce piecewise-smooth Sobolev spaces incorporated with certain continuity conditions and the corresponding norms for the immersed finite element method [10, 15]

$$\begin{aligned}
PW_p^k(a,b) \quad &:= \Big\{ v : \ v|_{(\alpha_{k-1},\alpha_k)} \in W_p^k(\alpha_{k-1},\alpha_k), k = 1, \cdots, K+1 \Big\}, \\
PH_{int}^2(a,b) \quad &:= \Big\{ v : \ v \in C(a,b), \quad v|_{(\alpha_{k-1},\alpha_k)} \in H^2(\alpha_{k-1},\alpha_k), \\
&\qquad [\![Dv_x]\!](\alpha_k) = 0, \quad k = 1, \cdots, K+1 \Big\}.
\end{aligned}$$

Here $\alpha_0 = a$ and $\alpha_{K+1} = b$. We let $PW_2^k(a,b) = PH^k(a,b)$. For any function $v \in PW_p^k(a,b)$, we define

$$\|v\|^2_{W_p^m(a,b)} := \sum_{k=1}^{K+1} \|v\|^2_{W_p^m(\alpha_{k-1},\alpha_k)}.$$

2.2. The linear immersed finite element space. In this subsection we introduce the local linear immersed finite element basis functions and define the immersed finite element space. Let $a =: x_0 < x_1 < \cdots < x_I := b$ be a quasi-uniform space partition with $h_i = x_i - x_{i-1}$ for $i = 1, \cdots, I$ and $h = \max_{1\le i\le I} h_i$. For each interface α_k there exists one $j = j(k)$ such that the element (x_{j-1}, x_j) contains α_k. It is reasonable to assume that there is at most one interface in each spatial element. We require the basis function satisfy the natural jump condition:

$$\phi_i(x_j) = \begin{cases} 1, & \text{if} \quad i = j, \\ 0, & \text{otherwise}, \end{cases} \qquad [\![\phi_i]\!](\alpha_k) = 0, \qquad [\![D\phi_{ix}]\!](\alpha_k) = 0. \tag{3}$$

So ϕ_i is a standard hat function if no interface is located in (x_{i-1}, x_i). Otherwise, ϕ_{i-1} and ϕ_i are defined as follows [10, 15]:

$$\phi_{i-1}(x) = \begin{cases} \dfrac{x - x_{i-2}}{h_{i-1}}, & x_{i-2} \le x < x_{i-1}, \\ \dfrac{x_{i-1} - x}{\gamma_k} + 1, & x_{i-1} \le x < \alpha_k, \\ \dfrac{\beta_k(x_i - x)}{\gamma_k}, & \alpha_k \le x < x_i, \\ 0, & \text{otherwise}, \end{cases} \tag{4}$$

and

$$\phi_i(x) = \begin{cases} \dfrac{x - x_{i-1}}{\gamma_k}, & x_{i-1} \le x < \alpha_k, \\ \dfrac{\beta_k(x - x_i)}{\gamma_k} + 1, & \alpha_k \le x < x_i, \\ \dfrac{x_{i+1} - x}{h_{i+1}}, & x_i \le x \le x_{i+1}, \\ 0, & \text{otherwise}, \end{cases} \tag{5}$$

where β_k and γ_k are given by

$$\beta_k = \frac{D(\alpha_k^-)}{D(\alpha_k^+)}, \qquad \gamma_k = h_i - \frac{D(\alpha_k^+) - D(\alpha_k^-)}{D(\alpha_k^+)}(x_i - \alpha_k).$$

Let $S_h(a,b)$ be the immersed finite element space defined by

$$S_h(a,b) = \Big\{ v : v(x) = \sum_{i=1}^{I} v_i \phi_i(x) \Big\}$$

and $\Pi v \in S_h(a,b)$ be a interpolation of v for any $v \in PH^2_{int}(a,b)$. Then the following estimate holds [8, 9, 10, 11, 15, 16, 17].

$$\|\Pi v - v\|_{H^l(a,b)} \le C_1 h^{2-l} \|v\|_{H^2(a,b)}, \quad l = 0, 1. \tag{6}$$

3. An Immersed Eulerian-Lagrangian Localized Adjoint Method

Let $0 =: t_0 < t_1 < \ldots < t_n < \ldots < t_{N-1} < t_N := T$ be a quasi-uniform partition of the time interval $[0, T]$, with $\Delta t_n := t_n - t_{n-1}$ for $n = 1, 2, \ldots, N$ and $\Delta t = \max_{1 \le n \le N} \Delta t_n$. We develop the ImELLAM scheme within the framework of the Eulerian-Lagrangian localized adjoint method, which was originally proposed by Celia, Russell, Herrera, and Ewing [4]. In the ELLAM formulation, the space-time test functions $w \in H_E^1$ are chosen to be continuous and piecewise smooth and to vanish outside the space-time prism $[a, b] \times (t_{n-1}, t_n]$. We use the notation $w(x, t_{n-1}^+) = \lim_{t \to t_{n-1}+0} w(x, t)$ to account for the possible discontinuity of w in time at time t_{n-1}. We multiply (1) by w and integrate the resulting equation on $[a, b] \times (t_{n-1}, t_n]$ by parts to obtain

$$
\begin{aligned}
&\int_a^b \phi u(x, t_n) w(x, t_n) dx + \int_{t_{n-1}}^{t_n} \int_a^b (D u_x)(x, t) w_x(x, t) dx dt \\
&\quad - \int_{t_{n-1}}^{t_n} \int_a^b u(x, t)(\phi w_t + V w_x(x, t) dx dt \\
&= \int_a^b \phi u(x, t_{n-1}) w(x, t_{n-1}^+)\ dx + \int_{t_{n-1}}^{t_n} \int_a^b f(x, t) w(x, t) dx dt.
\end{aligned} \tag{7}
$$

In (7) we have used the interface conditions (2) and the periodic boundary condition to the advection-diffusion term

$$
\begin{aligned}
&\int_{t_{n-1}}^{t_n} \int_a^b (V u - D u_x)_x(x, t) w(x, t) dx dt \\
&= \sum_{k=1}^{K+1} \int_{t_{n-1}}^{t_n} \int_{\alpha_{k-1}}^{\alpha_k} (V u - D u_x)_x(x, t) w(x, t) dx dt \\
&= - \sum_{k=1}^{K+1} \int_{t_{n-1}}^{t_n} \int_{\alpha_{k-1}}^{\alpha_k} (V u - D u_x)(x, t) w_x(x, t) dx dt \\
&\quad + \sum_{k=1}^{K+1} \int_{t_{n-1}}^{t_n} (V u - D u_x)(\alpha_k, t) w(\alpha_k, t) dt \\
&\quad - \sum_{k=1}^{K+1} \int_{t_{n-1}}^{t_n} (V u - D u_x)(\alpha_{k-1}, t) w(\alpha_{k-1}, t) dt \\
&= - \int_{t_{n-1}}^{t_n} \int_a^b (V u - D u_x)(x, t) w_x(x, t) dx dt.
\end{aligned} \tag{8}
$$

We follow the principle of the ELLAM framework to choose the test functions w satisfy the hyperbolic part of the adjoint equation of (1) [4]

$$
\phi w_t(x, t) + V w_x(x, t) = 0, \quad (x, t) \in (a, b) \times (t_{n-1}, t_n], \tag{9}
$$

with $w(x, t_n)$ being specified for $x \in (a, b)$. (9) implies that the last term on the left side of (7) vanishes and that the test functions w are constant along the trajectory $r(t; x, \bar{t})$ defined by

$$
\frac{dr}{dt} = \frac{V}{\phi(r)}, \quad r(t; x, \bar{t})|_{t = \bar{t}} = x. \tag{10}
$$

Without loss of generality, we assume $r(t; a, t_{n-1})$ and $r(t; b, t_n)$ do not intersect with any interfaces during the time interval $[t_{n-1}, t_n]$.

3.1. Evaluation of diffusion term. Now we evaluate the diffusion term in (7). Note that V is constant and $\phi(x)$ is a periodic function with respect to x of the period $b-a$. Thus, the curve $r(t;b,t_n)-(b-a)$ satisfies the initial-value problem

$$\begin{aligned}\frac{d(r(t;b,t_n)-(b-a))}{dt} &= \frac{dr(t;b,t_n)}{dt} = \frac{V}{\phi(r(t;b,t_n))} \\ &= \frac{V}{\phi(r(t;b,t_n)-(b-a))}, \\ r(t;b,t_n)-(b-a)\Big|_{t=t_n} &= b-(b-a) = a.\end{aligned}$$

Therefore, both $r(t;b,t_n)-(b-a)$ and $r(t;a,t_n)$ are the solutions of the same initial-value problem. The uniqueness of such problem concludes that

$$r(t;b,t_n) - r(t;a,t_n) = b-a \qquad \forall t \in [t_{n-1},t_n]. \tag{11}$$

For clarity of presentation, in the evaluation of diffusion term we reserve x for points in $[a,b]$ at time t_n representing the heads of characteristics. We use the variable y to represent the spatial coordinate of an arbitrary point at time $t \in (t_{n-1},t_n)$. We use the relation (11) and the periodicity of problem (1) to evaluate the diffusion term by the Euler quadrature as follows:

$$\begin{aligned}&\int_{t_{n-1}}^{t_n}\int_a^b D(y)u_y(y,t)w_y(y,t)dydt \\ &= \int_{t_{n-1}}^{t_n}\int_{r(t;a,t_n)}^{r(t;b,t_n)} D(y)u_y(y,t)w_y(y,t)dydt \\ &= \int_a^b\int_{t_{n-1}}^{t_n} D(r(t;x,t_n))u_y(r(t;x,t_n),t)w_x(x,t_n)dtdx \\ &= \Delta t_n\int_a^b D(x,t_n)u_x(x,t_n)w_x(x,t_n)dx + E_1(u,w),\end{aligned} \tag{12}$$

Here $E_1(u,w)$ is the local truncation error defined by

$$E_1(u,w) := \int_a^b\int_{t_{n-1}}^{t_n}\Big[(Du_x)(r(t;x,t_n),t) - (Du_x)(x,t_n)\Big]dt\ w_x(x,t_n)dx. \tag{13}$$

3.2. Evaluation of source and sink term. Before evaluation of the source and sink term, we introduce some notations. Let x^* denote the foot of characteristics at time t_{n-1} with head x at time step t_n, $\tilde{x}$ denote the head of characteristics at time t_n with foot x at time step t_{n-1}, and $t_k(x,t_n)$ denote the time when $r(t;x,t_n)$ intersects the interface α_k.

$$x^* = r(t_{n-1};x,t_n), \qquad \tilde{x} = r(t_n;x,t_{n-1}), \qquad \alpha_k = r(t_k(x,t_n);x,t_n).$$

Without loss of generality, we consider the case of $K=2$ and assume that $\tilde{\alpha}_1 \in (\alpha_1,\alpha_2)$, $\alpha_2^* \in (\alpha_1,\alpha_2)$, and $\tilde{\alpha}_2 \in (\alpha_2,b)$. We define a space-time prism Ω_k, which extends the cell $[\alpha_k,\tilde{\alpha}_k]$ backward along the characteristic curve $r(t;x,t_n)$ from $t=t_n$ to $t=t_{n-1}$, as follows:

$$\Omega_k = \{(x,t) : r(t;\alpha_k,t_n) < x < r(t;\tilde{\alpha}_k,t_n),\ t_{n-1}<t<t_n\}, \qquad k=1,2. \tag{14}$$

Also we let $\bar{\Omega}$ denote $[a,b]\times(t_{n-1},t_n)\setminus(\Omega_1\cup\Omega_2)$. We then evaluate the source and sink term as follows

$$
\begin{aligned}
&\int_{\Omega_k} f(y,t)w(y,t)dydt \\
&\quad = \int_{\alpha_k}^{\tilde{\alpha}_k} \int_{t(x,t_n)}^{t_n} f(r(t;x,t_n),t)w(r(t;x,t_n),t)r_x(t;x,t_n)dtdx \\
&\qquad + \int_{\alpha_k^*}^{\alpha_k} \int_{t_{n-1}}^{t_k(\tilde{x},t_n)} f(r(t;x,t_{n-1}),t)w(r(t;x,t_{n-1}),t)r_x(t;x,t_{n-1})dtdx \\
&\quad = \int_{\alpha_k}^{\tilde{\alpha}_k} \int_{t_k(x,t_n)}^{t_n} f(r(t;x,t_n),t)w(x,t_n)dtdx \\
&\qquad - \int_{t_{n-1}}^{t_n} \int_{t_{n-1}}^{\theta} f(r(t;\alpha_k,\theta),t)w(\alpha_k,\theta)r_\theta(t;\alpha_k,\theta)dtd\theta \\
&\quad = \int_{\alpha_k}^{\tilde{\alpha}_k} (t_n - t_k(x,t_n))f(x,t_n)w(x,t_n)dx \\
&\qquad + \int_{t_{n-1}}^{t_n} \frac{V}{\phi(\alpha_k^-)}(\theta - t_{n-1})f(\alpha_k,\theta)w(\alpha_k,\theta)d\theta + E_2(k,f,w).
\end{aligned}
$$

Here $E_2(k,f,w)$ is the local truncation error defined by

$$
\begin{aligned}
&E_2(k,f,w) \\
&\quad = -\int_{\alpha_k}^{\tilde{\alpha}_k} \int_{t_k(x,t_n)}^{t_n} (f(x,t_n) - f(r(t;x,t_n),t))w(x,t_n)dtdx \\
&\qquad - \int_{t_{n-1}}^{t_n} \int_{t_{n-1}}^{\theta} \frac{V}{\phi(\alpha_k^-)}(f(\alpha_k,\theta) - f(r(t;\alpha_k,\theta),t))w(\alpha_k,\theta)dtd\theta.
\end{aligned}
$$

On the other hand, we evaluate the source and sink term on $\bar{\Omega}$ as follows

$$
\begin{aligned}
&\int_{t_{n-1}}^{t_n} \int_a^b f(y,t)w(y,t)dydt \\
&\quad = \int_{(a,\alpha_1)\cup(\tilde{\alpha}_1,\alpha_2)\cup(\alpha_2,b)} \int_{t_{n-1}}^{t_n} f(r(t;x,t_n),t)w(r(t;x,t_n),t)r_x(t;x,t_n)dtdx \\
&\quad = \int_{(a,\alpha_1)\cup(\tilde{\alpha}_1,\alpha_2)\cup(\alpha_2,b)} \int_{t_{n-1}}^{t_n} f(r(t;x,t_n),t)w(x,t_n)dtdx \\
&\quad = \Delta t_n \int_{(a,\alpha_1)\cup(\tilde{\alpha}_1,\alpha_2)\cup(\alpha_2,b)} f(x,t_n)w(x,t_n)dx + E_3(f,w).
\end{aligned}
$$

Here $E_3(f,w)$ is the local truncation error defined by

$$
\begin{aligned}
&E_3(f,w) \\
&\quad = -\Delta t_n \int_{(a,\alpha_1)\cup(\tilde{\alpha}_1,\alpha_2)\cup(\alpha_2,b)} \int_{t_{n-1}}^{t_n} (f(x,t_n) - f(r(t;x,t_n),t))w(x,t_n)dtdx.
\end{aligned}
$$

We combine the preceding equations to obtain the following equation in the presence of K interfaces

$$
\begin{aligned}
&\int_{t_{n-1}}^{t_n}\int_a^b f(y,t)w(y,t)dydt \\
&\quad= \Delta t_n \int_{\bigcup_{k=1}^{K-1}(\tilde{\alpha}_k,\alpha_{k+1})\cup(a,\alpha_1)\cup(\alpha_K,b)} f(x,t_n)w(x,t_n)dx \\
&\qquad+\sum_{k=1}^{K}\int_{\alpha_k}^{\tilde{\alpha}_k}(t_n-t_k(x,t_n))f(x,t_n)w(x,t_n)dx \\
&\qquad+\sum_{k=1}^{K}\int_{t_{n-1}}^{t_n}\frac{V}{\phi(\alpha_k^-)}(\theta-t_{n-1})f(\alpha_k,\theta)w(\alpha_k,\theta)d\theta \\
&\qquad+\sum_{k=1}^{K}E_2(k,f,w)+E_3(f,w).
\end{aligned} \tag{15}
$$

3.3. An ImELLAM scheme. We substitute (12) and (15) into (7) to obtain an ImELLAM reference equation for problem (1)

$$
\begin{aligned}
&\int_a^b \phi(x)u(x,t_n)w(x,t_n)dx+\Delta t_n\int_a^b D(x)u_x(x,t_n)w_x(x,t_n)dx \\
&\quad=\int_a^b \phi(x)u(x,t_{n-1})w(x,t_{n-1}^+)\,dx \\
&\qquad+\Delta t_n \int_{\bigcup_{k=1}^{K-1}(\tilde{\alpha}_k,\alpha_{k+1})\cup(a,\alpha_1)\cup(\alpha_K,b)} f(x,t_n)w(x,t_n)dx \\
&\qquad+\sum_{k=1}^{K}\int_{\alpha_k}^{\tilde{\alpha}_k}(t_n-t_k(x,t_n))f(x,t_n)w(x,t_n)dx \\
&\qquad+\sum_{k=1}^{K}\int_{t_{n-1}}^{t_n}\frac{V}{\phi(\alpha_k^-)}(\theta-t_{n-1})f(\alpha_k,\theta)w(\alpha_k,\theta)d\theta \\
&\qquad-E_1(u,w)+\sum_{k=1}^{K}E_2(k,f,w)+E_3(f,w).
\end{aligned} \tag{16}
$$

The ImELLAM scheme states as follows: Find $u_h(x,t_n)\in S_h(a,b)$ for $n=1,\cdots,N$ such that for any $w_h(x,t_n)\in S_h(a,b)$

$$
\begin{aligned}
&\int_a^b \phi(x)u_h(x,t_n)w_h(x,t_n)dx+\Delta t_n\int_a^b D(x)u_{hx}(x,t_n)w_{hx}(x,t_n)dx \\
&\quad=\int_a^b \phi(x)u_h(x,t_{n-1})w_h(x,t_{n-1}^+)\,dx \\
&\qquad+\Delta t_n \int_{\bigcup_{k=1}^{K-1}(\tilde{\alpha}_k,\alpha_{k+1})\cup(a,\alpha_1)\cup(\alpha_K,b)} f(x,t_n)w_h(x,t_n)dx \\
&\qquad+\sum_{k=1}^{K}\int_{\alpha_k}^{\tilde{\alpha}_k}(t_n-t_k(x,t_n))f(x,t_n)w_h(x,t_n)dx \\
&\qquad+\sum_{k=1}^{K}\int_{t_{n-1}}^{t_n}\frac{V}{\phi(\alpha_k^-)}(\theta-t_{n-1})f(\alpha_k,\theta)w_h(\alpha_k,\theta)d\theta.
\end{aligned} \tag{17}
$$

4. An optimal-order error estimate for the ImELLAM scheme

In this section we prove the main theorem of this paper.

Theorem 4.1. *Assume $u \in L^\infty(0,T;H^2)\bigcap H^1(0,T;H^2)$, $f \in H^1(0,T;L^2)$, then the following optimal-order error estimate holds for the ImELLAM scheme (17).*

$$\begin{aligned}
&\|u_h - u\|_{L^\infty(0,T;L^2)} \\
&\quad \le C\Delta t\Big(\Big\|\frac{du}{dt}\Big\|_{L^2(0,T;H^1)} + \|u\|_{L^2(0,T;H^1)} + \Big\|\frac{df}{dt}\Big\|_{L^2(0,T;L^2)} \\
&\quad\quad + \|f\|_{L^2(0,T;L^2)}\Big) + Ch^2\big(\|u\|_{L^\infty(0,T;H^2)} + \|u\|_{H^1(0,T;H^2)}\big).
\end{aligned}$$

Here the constant C is independent of u, h, or Δt.

Proof. Without loss of generality, we assume $K = 2$ in the proof, e.g. there are two interfaces in the domain (a,b). In this case, the combination of piecewise diffusion coefficients and porosity and the periodicity of the problem concludes that

$$\phi(x) = \begin{cases} \phi_-, & x \in [a,\alpha_1), \\ \phi_+, & x \in (\alpha_1,\alpha_2), \\ \phi_-, & x \in (\alpha_2, b], \end{cases} \qquad D(x) = \begin{cases} D_-, & x \in [a,\alpha_1), \\ D_+, & x \in (\alpha_1,\alpha_2), \\ D_-, & x \in (\alpha_2, b]. \end{cases} \tag{18}$$

Let $e = u_h - u$ and choose $w(x,t_n)$ in the reference equation (16) to be $w_h(x,t_n) \in S_h(a,b)$. We then subtract (16) from (17) to get an error equation for any $w_h(x,t_n) \in S_h(a,b)$.

$$\begin{aligned}
&\int_a^b \phi(x)e(x,t_n)w_h(x,t_n)dx + \Delta t_n \int_a^b D(x)e_x(x,t_n)w_{hx}(x,t_n)dx \\
&\quad = \int_a^b \phi(x)e(x,t_{n-1})w_h(x,t_{n-1}^+)\,dx + E_1(u,w_h) \\
&\quad\quad - \sum_{k=1}^K E_2(k,f,w_h) - E_3(f,w_h).
\end{aligned} \tag{19}$$

Let $\xi = u_h - \Pi u$ and $\eta = \Pi u - u$. The estimate for η is given in (6), so we need only to estimate ξ. We choose $w_h(x,t_n)$ to be $\xi(x,t_n)$ and rewrite the error equation (19) in terms of ξ and η as follows:

$$\begin{aligned}
&\int_a^b \phi(x)\xi^2(x,t_n)dx + \Delta t_n \int_a^b D(x)\xi_x^2(x,t_n)dx \\
&\quad = \int_a^b \phi(x)\xi(x,t_{n-1})\xi(x,t_{n-1}^+)dx + \int_a^b \phi(x)\eta(x,t_{n-1})\xi(x,t_{n-1}^+)dx \\
&\quad\quad - \int_a^b \phi(x)\eta(x,t_n)\xi(x,t_n)dx - \Delta t_n \int_a^b D(x)\eta_x(x,t_n)\xi_x(x,t_n)dx \\
&\quad\quad + E_1(u,\xi) - \sum_{k=1}^K E_2(k,f,\xi) - E_3(f,\xi).
\end{aligned} \tag{20}$$

The left side of (20) is in the form we need, so we need only to estimate the right side term by term. The first term on the right side of (20), which can be bounded in a standard way when no interface is present, now requires careful analysis. The standard estimate gives

$$
\begin{aligned}
&\int_a^b \phi(x)\xi(x,t_{n-1})\xi(x,t_{n-1}^+)dx \\
&\quad \le \frac{1}{2}\int_a^b \phi(x)\xi^2(x,t_{n-1})dx + \frac{1}{2}\int_a^b \phi(x)\xi^2(\tilde{x},t_n)dx \\
&\quad = \frac{1}{2}\int_a^b \phi(x)\xi^2(x,t_{n-1})dx + \frac{1}{2}\int_a^b \phi(\tilde{x})\xi^2(\tilde{x},t_n)dx \\
&\qquad + \frac{1}{2}\int_a^b (\phi(x)-\phi(\tilde{x}))\xi^2(\tilde{x},t_n)dx.
\end{aligned} \tag{21}
$$

This does not work here. We should be careful to the second term after the first inequality. We again assume $\tilde{\alpha}_1 \in (\alpha_1,\alpha_2)$, $\alpha_2^* \in (\alpha_1,\alpha_2)$, and $\tilde{\alpha}_2 \in (\alpha_2, b)$. Note that for $x \in [a,\alpha_1^*) \cup (\alpha_1,\alpha_2^*) \cup x \in (\alpha_2, b]$, $\tilde{x} \in [\tilde{a},\alpha_1) \cup (\tilde{\alpha}_1,\alpha_2) \cup (\tilde{\alpha}_2,\tilde{b}]$ and $\phi(x) = \phi(\tilde{x})$. More specifically, $\tilde{x}$ can be specified as follows

$$
\begin{aligned}
&\tilde{x} = x + \frac{V}{\phi_-}\Delta t_n,\ x \in [a,\alpha_1^*] \cup [\alpha_2, b], \\
&\tilde{x} = x + \frac{V}{\phi_+}\Delta t_n,\ x \in [\alpha_1,\alpha_2^*], \\
&\alpha_1 = x + \frac{V}{\phi_-}(t(x,t_{n-1}) - t_{n-1}), \\
&\tilde{x} = \alpha_1 + \frac{V}{\phi_+}(t_n - t(x,t_{n-1})), \quad x \in (\alpha_1^*,\alpha_1), \\
&\alpha_2 = x + \frac{V}{\phi_+}(t(x,t_{n-1}) - t_{n-1}), \\
&\tilde{x} = \alpha_2 + \frac{V}{\phi_-}(t_n - t(x,t_{n-1})), \quad x \in (\alpha_2^*,\alpha_2).
\end{aligned}
$$

With these expressions we directly get

$$
\frac{d\tilde{x}}{dx} = \begin{cases} 1, & x \in [a,\alpha_1^*] \cup [\alpha_1,\alpha_2^*] \cup [\alpha_2,b], \\ \dfrac{\phi_-}{\phi_+}, & x \in (\alpha_1^*,\alpha_1), \\ \dfrac{\phi_+}{\phi_-}, & x \in (\alpha_2^*,\alpha_2). \end{cases} \tag{22}
$$

We can now do a better job than we did in (21) and evaluate the second term on its right-hand side precisely

$$
\begin{aligned}
&\int_a^b \phi(x)\xi^2(\tilde{x},t_n)dx \\
&\quad = \int_a^{\alpha_1^*} \phi(\tilde{x})\xi^2(\tilde{x},t_n)dx + \int_{\alpha_1^*}^{\alpha_1} \phi_-\xi^2(\tilde{x},t_n)dx + \int_{\alpha_1}^{\alpha_2^*} \phi(\tilde{x})\xi^2(\tilde{x},t_n)dx \\
&\qquad + \int_{\alpha_2^*}^{\alpha_2} \phi_+\xi^2(\tilde{x},t_n)dx + \int_{\alpha_2}^{b} \phi(\tilde{x})\xi^2(\tilde{x},t_n)dx =
\end{aligned} \tag{23}
$$

$$
\begin{aligned}
&= \int_{\tilde a}^{\alpha_1} \phi(\tilde x)\xi^2(\tilde x,t_n)d\tilde x + \int_{\alpha_1}^{\tilde\alpha_1} \phi_-\xi^2(\tilde x,t_n)\frac{\phi_+}{\phi_-}d\tilde x \\
&\quad + \int_{\tilde\alpha_1}^{\alpha_2} \phi(\tilde x)\xi^2(\tilde x,t_n)d\tilde x + \int_{\alpha_2}^{\tilde\alpha_2} \phi_+\xi^2(\tilde x,t_n)\frac{\phi_-}{\phi_+}d\tilde x \\
&\quad + \int_{\tilde\alpha_2}^{\tilde b} \phi(\tilde x)\xi^2(\tilde x,t_n)d\tilde x \\
&= \int_{\tilde a}^{\tilde b} \phi(\tilde x)\xi^2(\tilde x,t_n)d\tilde x = \int_a^b \phi(x)\xi^2(x,t_n)dx.
\end{aligned}
$$

This allows us to bound the first term on the right side of (20) by

$$
\begin{aligned}
&\int_a^b \phi(x)\xi(x,t_{n-1})\xi(x,t_{n-1}^+)dx \\
&\quad \le \frac12\int_a^b \phi(x)\xi^2(x,t_{n-1})dx + \frac12\int_a^b \phi(x)\xi^2(x,t_n)dx.
\end{aligned}
$$

We decompose the second and the third terms as follows:

$$
\begin{aligned}
&\int_a^b \phi(x)\eta(x,t_{n-1})\xi(x,t_{n-1}^+)dx - \int_a^b \phi(x)\eta(x,t_n)\xi(x,t_n)dx \\
&\quad = -\int_a^b\int_{t_{n-1}}^{t_n} \phi(x)\eta_t(x,t)dt\xi(x,t_n)dx \\
&\qquad + \int_a^b \phi(x)\eta(x,t_{n-1})(\xi(\tilde x,t_n)-\xi(x,t_n))dx.
\end{aligned}
\tag{24}
$$

The first term on the right side is bounded by

$$
\begin{aligned}
&\Big|\int_a^b\int_{t_{n-1}}^{t_n} \eta_t(x,t)dt\xi(x,t_n)dx\Big| \\
&\quad \le C\Delta t_n\|\xi(\cdot,t_n)\|_{L^2}^2 + C\|\eta\|_{H^1(t_{n-1},t_n;L^2)}^2 \\
&\quad \le C\Delta t_n\|\xi(\cdot,t_n)\|_{L^2}^2 + Ch^4\|u\|_{H^1(t_{n-1},t_n;H^2)}.
\end{aligned}
$$

We substitute the the following expression

$$
\begin{aligned}
\xi(\tilde x,t_n)-\xi(x,t_n) &= \int_0^1 \frac{d\xi}{ds}(x+s(\tilde x-x),t_n)ds \\
&= \int_0^1 \xi_x(x+s(\tilde x-x),t_n)ds(\tilde x-x)
\end{aligned}
$$

into the second term on the right side of (24) to get

$$
\begin{aligned}
&\Big|\int_a^b \phi(x)\eta(x,t_{n-1})(\xi(\tilde x,t_n)-\xi(x,t_n))dx\Big| \\
&\quad = \Big|\int_a^b \phi(x)\eta(x,t_{n-1})\int_0^1 \xi_x(x+s(\tilde x-x),t_n)ds(\tilde x-x)dx\Big| \\
&\quad \le C\Delta t_n\big\|\xi_x(\cdot,t_n)\big\|\ \big\|\eta(\cdot,t_n)\big\| \\
&\quad \le \varepsilon\Delta t_n\int_a^b D(x)\xi_x^2(x,t_n)dx + C\Delta t h^4\|u\|_{L^\infty(0,T;H^2)}^2.
\end{aligned}
$$

Note that there must be elements $[x_{j_1-1},x_{j_1}]$ and $[x_{j_2-1},x_{j_2}]$, such that the interfaces α_1 and α_2 locate in, respectively, and so $D(x)$ and $\xi_x(x,t_n)$ are constant on each element $[x_{i-1}, x_i]$ for $i \neq j_1, j_2$, but they are not constant on $[x_{j_1-1}, x_{j_1}]$ and $[x_{j_2-1}, x_{j_2}]$. Then we decompose the fourth term on the right side of (20) as

$$\begin{aligned}
&\Delta t_n \int_a^b D(x)\eta_x(x,t_n)\xi_x(x,t_n)dx \\
&= \Delta t_n \sum_{i=1, i\neq j_1, j_2}^{I} \int_{x_{i-1}}^{x_i} D(x)\eta_x(x,t_n)\xi_x(x,t_n)dx \\
&\quad + \Delta t_n \sum_{i=j_1,j_2} \int_{x_{i-1}}^{x_i} D(x)\eta_x(x,t_n)\xi_x(x,t_n)dx.
\end{aligned} \tag{25}$$

We use the interpolation property $\eta(x_i, t_n) = 0$ for $i = 0, 1, \cdots, I$ to obtain that the first term on the right side vanishes directly.

Now we consider the second term on the right side of (25). $\xi_x(x, t_n)$ is not constant on $[x_{j_k-1}, x_{j_k}]$, but it is constant on both $[x_{j_k-1}, \alpha_k]$ and $[\alpha_k, x_{j_k}]$, respectively, for $k = 1, 2$. Then we use $[\![\eta]\!](\alpha_k, t_n) = 0$, $[\![D\xi_x]\!](\alpha_k, t_n) = 0$, and $\eta(x_i, t_n) = 0$ for $i = j_k - 1, j_k$ to get

$$\begin{aligned}
&\int_{x_{j_k-1}}^{\alpha_k} D(\alpha_k^-)\eta_x(x,t_n)\xi_x(x,t_n)dx \\
&\qquad + \int_{\alpha_k}^{x_{j_k}} D(\alpha_k^+)\eta_x(x,t_n)\xi_x(x,t_n)dx = 0.
\end{aligned}$$

Therefore,

$$\int_{x_{j_k-1}}^{x_{j_k}} D(x)\eta_x(x,t_n)\xi_x(x,t_n)dx = 0.$$

We bound the fifth term on the right-hand side of (20) by

$$\begin{aligned}
&\Big|\int_a^b \int_{t_{n-1}}^{t_n} \Big[(D\ u_x)(x,t_n) - (D\ u_x)(r(t;x,t_n),t)\Big] dt\ \xi_x(x,t_n)dx\Big| \\
&= \Big|\int_a^b \xi_x(x,t_n)\Big[\int_{t_{n-1}}^{t_n}\int_t^{t_n} \frac{d}{d\theta}(D\ u_x)(r(\theta;x,t_n),\theta)d\theta dt\Big]dx \\
&\le \varepsilon\Delta t_n \int_a^b D(x,t_n)\xi_x^2(x,t_n)dx \\
&\quad + C(\Delta t_n)^2\Big(\Big\|\frac{du}{dt}\Big\|^2_{L^2(t_{n-1},t_n;H^1)} + \|u\|^2_{L^2(t_{n-1},t_n;H^1)}\Big).
\end{aligned}$$

We similarly bound the local truncation term $E_3(f, \xi)$ by

$$\begin{aligned}
\big|E_3(f,\xi)\big| \le\ & C\Delta t_n\|\xi(\cdot,t_n)\|^2 \\
& + C(\Delta t)^2\Big(\Big\|\frac{df}{dt}\Big\|^2_{L^2(t_{n-1},t_n;L^2)} + \|f\|^2_{L^2(t_{n-1},t_n;L^2)}\Big).
\end{aligned}$$

Using the definitions of the test function (9) and the characteristic (10), the truncation error $|E_2(k, f, \xi)|$ can be bounded by

$$
\begin{aligned}
&\big|E_2(k,f,\xi)\big| \\
&= \bigg| \int_{\alpha_k}^{\tilde\alpha_k} \int_{t_k(x,t_n)}^{t_n} \int_t^{t_n} \frac{d}{d\tau} f(r(\tau;x,t_n),\tau) d\tau dt \xi(x,t_n) dx \\
&\qquad + \int_{t_{n-1}}^{t_n} \int_{t_{n-1}}^{\theta} \frac{V}{\phi(\alpha_k^-)} \int_t^{\theta} \frac{d}{d\tau} f(r(\tau;\alpha_k,\theta),\tau) d\tau \xi(\alpha_k,\theta) dt d\theta \bigg| \\
&= \bigg| \int_{\alpha_k}^{\tilde\alpha_k} \int_{t_k(x,t_n)}^{t_n} \int_t^{t_n} \frac{d}{d\tau} f(r(\tau;x,t_n),\tau) d\tau dt \ \xi(x,t_n) dx \\
&\qquad + \int_{t_{n-1}}^{t_n} \int_{t_{n-1}}^{\theta} \frac{V}{\phi(\alpha_k^-)} \int_t^{\theta} \frac{d}{d\tau} f\Big(r\Big(\tau;\alpha_k + \frac{V}{\phi(\alpha_k^+)}(t_n-\theta),t_n\Big),\tau\Big) d\tau \\
&\qquad\quad \xi\Big(\alpha_k + \frac{V}{\phi(\alpha_k^+)}(t_n-\theta),t_n\Big) dt d\theta \bigg| \\
&= \bigg| \int_{\alpha_k}^{\tilde\alpha_k} \int_{t_k(x,t_n)}^{t_n} \int_t^{t_n} \frac{d}{d\tau} f(r(\tau;x,t_n),\tau) d\tau dt \xi(x,t_n) dx \\
&\qquad + \int_{\alpha_k}^{\tilde\alpha_k} \int_{t_{n-1}}^{t_k(x,t_n)} \int_t^{t_k(x,t_n)} \frac{d}{d\tau} f(r(\tau;x,t_n),\tau) d\tau dt \xi(x,t_n) dx \bigg| \\
&\le C\Delta t_n \|\xi(\cdot,t_n)\|^2 + C(\Delta t)^2 \Big(\Big\| \frac{df}{dt} \Big\|^2_{L^2(t_{n-1},t_n;L^2)} + \|f\|^2_{L^2(t_{n-1},t_n;L^2)} \Big).
\end{aligned}
$$

We combine the preceding estimates to get

$$
\begin{aligned}
&\|\xi(\cdot,t_n)\|^2_{L^2} + \Delta t_n \int_a^b D(x) \xi_x^2(x,t_n) dx \\
&\le \frac{1+C\Delta t_n}{2} (\|\xi(\cdot,t_n)\|^2_{L^2} + \|\xi(\cdot,t_{n-1})\|^2_{L^2}) + \varepsilon \Delta t_n \int_a^b D(x) \xi_x^2(x,t_n) dx \\
&\quad + C(\Delta t_n)^2 \Big(\Big\| \frac{du}{dt} \Big\|^2_{L^2(t_{n-1},t_n;H^1)} + \|u\|^2_{L^2(t_{n-1},t_n;H^1)} + \Big\| \frac{df}{dt} \Big\|^2_{L^2(t_{n-1},t_n;L^2)} \\
&\quad + \|f\|^2_{L^2(t_{n-1},t_n;L^2)} \Big) + Ch^4 (\|u\|^2_{H^1(t_{n-1},t_n;H^2)} + \Delta t_n \|u\|^2_{L^\infty(0,T;H^2)}).
\end{aligned}
$$

We choose $\varepsilon = \frac{1}{2}$, sum the estimate for $n = 1, \ldots, N_1 (\le N)$, and cancel like terms to obtain

$$
\begin{aligned}
&\|\xi(\cdot,t_{N_1})\|^2_{L^2} + \sum_{n=1}^{N_1} \Delta t_n \int_a^b D(x) \xi_x^2(x,t_n) dx \\
&\le C \sum_{n=0}^{N_1-1} \Delta t_n \|\xi(\cdot,t_n)\|^2_{L^2} + C(\Delta t)^2 \Big(\Big\| \frac{du}{dt} \Big\|^2_{L^2(0,T;H^1)} + \|u\|^2_{L^2(0,T;H^1)} \\
&\quad + \Big\| \frac{df}{dt} \Big\|^2_{L^2(0,T;L^2)} + \|f\|^2_{L^2(0,T;L^2)} \Big) + Ch^4 \big(\|u\|^2_{L^\infty(0,T;H^2)} + \|u\|^2_{H^1(0,T;H^2)} \big).
\end{aligned}
$$

We apply Gronwall inequality to conclude

$$
\begin{aligned}
\|\xi\|_{L^\infty(0,T;L^2)} \quad &\le C\Delta t \Big(\Big\| \frac{du}{dt} \Big\|_{L^2(0,T;H^1)} + \|u\|_{L^2(0,T;H^1)} + \Big\| \frac{df}{dt} \Big\|_{L^2(0,T;L^2)} \\
&\quad + \|f\|_{L^2(0,T;L^2)} \Big) + Ch^2 \big(\|u\|_{L^\infty(0,T;H^2)} + \|u\|_{H^1(0,T;H^2)} \big).
\end{aligned}
$$

We combine this estimate with (6) to finish the proof. □

5. Concluding Remark

In this paper we combine the immersed finite element method with the Eulerian-Lagrangian localized adjoint method to develop an immersed Eulerian-Lagrangian localized adjoint method (ImELLAM) for transient advection-diffusion equations with interfaces. This type of problems arises, e.g., in matheamtical and numerical modeling of subsurface flow and transport in fractured media. In practice, there are often too many fractures and faults of intermediate size to align the computational meshes with. On the other hand, these faults and fractures are often too large to be upscaled into the numerical model. The ImELLAM scheme developed in this paper provides a feasible solution technique for effectively simulating subsurface flow and transport in porous media with faults and fractures of intermediate size. The derived method possesses the combined advantages of the immersed finite element method and the Eulerian-Lagrangian method. The underlying Eulerian-Lagrangian framework is well suited for handling the Lagrangian nature of the transport problem, while the incorporation of the immersed finite element method in the method allows the method to effectively treat the physical interfaces.

The analysis of the ImELLAM scheme presents additional numerical difficulties to the already very technical analysis of Eulerian-Lagrangian methods [5, 18, 19] due to the introduction of the immerse finite element basis functions. Here the analysis technique of immerse finite element methods [8, 9, 10] has been utilized to aid the proof of the main theorem in this paper. The numerical implementation of ImELLAM scheme is also an important issue which is based upon the already very technical implementation of immersed finite element methods and Eulerian-Lagrangian methods. The numerical implementation of the ImELLAM scheme will be conducted in the near future and corresponding numerical results will be presented elsewhere.

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