

Robust virtual element methods for 3D stress-assisted diffusion problems

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Abstract

This article presents an initial exploration of stress-assisted diffusion problems in three dimensions within the framework of the Virtual Element Method. Hilbert spaces enriched with parameter-weighted norms, the extended Babuška–Brezzi–Braess theory for perturbed saddle-point problems, and Banach fixed-point theory play a crucial role in performing a robust analysis of the fully coupled non-linear system. The proposed virtual element formulations are provided with appropriate projection, interpolation, and stabilisation operators that ensures the well-posedness of the discrete problem. Numerical simulations are conducted to show the accuracy, performance, and applicability of the method.

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1 Introduction

Scope. Stress-assisted diffusion appears broadly in applications like lithium-ion battery cells, silicon rubber and hydrogen diffusion, polymer-based coatings, semiconductor fabrication, oxidation of silicon nanostructures, and enhancing of conductivity properties in soft living tissue. In these processes, the stress of the material involved affects the patterns of diffusion. This article addresses one of the simplest models for such an interaction, incorporating stress effects inside the diffusion coefficient, and recovering Fick's law in the absence of these phenomena [e.g., 2]. Moreover, we extend the analysis done by Khot et al. [6] such as the definition of the Virtual Element Method (VEM) spaces in 3D and the polynomial, interpolation, and stabilisation operators used in this framework.

Outline. The content of the article is organised as follows. The remainder of this section presents the strong form of the coupled fully coupled stress-assisted diffusion problem. Section 2 is devoted to presenting the weak formulation and well-posedness analysis using perturbed saddle-point theory and fixed-point arguments. In Section 3 we define the discrete problem, show the existence and uniqueness of a discrete solution, and outline the a priori error analysis. Finally, in Section 4 we provide numerical results that illustrate the theoretical results, and as an application of the model we present the lithiation of a perforated cylindrical anode particle.

Model statement. Let us consider the nonlinear formulation for stress-assisted diffusion of a solute that interacts with an elastic material in a domain Ω with boundary $\partial\Omega = \Gamma_D \cup \Gamma_N$:

$$-\operatorname{div}(2\mu\boldsymbol{\varepsilon}(\mathbf{u}) - \mathbf{p}\mathbb{I}) = \mathbf{f} \quad \text{in } \Omega, \quad \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_D, \quad (1a)$$

$$\mathbf{p} = -\lambda \operatorname{div} \mathbf{u} + \ell(\varphi) \quad \text{in } \Omega, \quad (2\mu\boldsymbol{\varepsilon}(\mathbf{u}) - \mathbf{p}\mathbb{I})\mathbf{n} = \mathbf{0} \quad \text{on } \Gamma_N, \quad (1b)$$

$$\boldsymbol{\zeta} = \mathbb{M}(\boldsymbol{\varepsilon}(\mathbf{u}), \mathbf{p})\nabla\varphi \quad \text{in } \Omega, \quad \varphi = \varphi_D \quad \text{on } \Gamma_D, \quad (1c)$$

$$\theta\varphi - \operatorname{div}(\boldsymbol{\zeta}) = \mathbf{g} \quad \text{in } \Omega, \quad \boldsymbol{\zeta} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N, \quad (1d)$$

where μ and λ are the Lamé parameters, ℓ is the active stress coefficient, \mathbf{f} is a vector of external body loads, $\boldsymbol{\zeta}$ is the diffusive flux, \mathbf{g} is a given net volumetric source of solute, θ is a positive model parameter, and $\mathbb{M}(\boldsymbol{\varepsilon}(\mathbf{u}), \mathbf{p})$ is the stress-assisted diffusion coefficient.

Equations (1a) and (1b) constitute a Herrmann-like mixed formulation for linear elasticity. The coupling between the displacement \mathbf{u} of the material, the pressure \mathbf{p} , and the solute concentration φ follows Hooke's law to express the Cauchy stress tensor as $2\mu\boldsymbol{\varepsilon}(\mathbf{u}) - \mathbf{p}\mathbb{I}$. Equations (1d) and (1c) correspond to the reaction-diffusion equation written in mixed form.

We adopt mixed loading boundary conditions for the coupled problem: the structure is clamped and has a given concentration φ_D on Γ_D , where the boundary subset $\Gamma_D \subset \partial\Omega$ is of positive surface measure. In addition, zero traction and solute flux are prescribed on $\Gamma_N := \partial\Omega \setminus \Gamma_D$, where \mathbf{n} denotes the outward unit normal vector to Γ_N .

The nonlinear terms. We assume that $\mathbb{M}(\cdot, \cdot)$ is symmetric, positive definite and uniformly bounded in $\mathbb{L}^\infty(\Omega)$, and likewise for its inverse $\mathbb{M}^{-1}(\cdot, \cdot)$. More explicitly, for all $\boldsymbol{w} \in \mathbf{H}^1(\Omega)$, $r \in L^2(\Omega)$ and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$ there exists $M \in \mathbb{R}$ such that $0 < M^{-1} \leq M$ with

$$M^{-1}\mathbf{x} \cdot \mathbf{x} \leq \mathbf{x} \cdot [\mathbb{M}^{-1}(\boldsymbol{\varepsilon}(\boldsymbol{w}), r)\mathbf{x}] \quad \text{and} \quad \mathbf{y} \cdot [\mathbb{M}^{-1}(\boldsymbol{\varepsilon}(\boldsymbol{w}), r)\mathbf{x}] \leq M\mathbf{x} \cdot \mathbf{y}. \quad (2)$$

In addition, we assume that $\ell : L^2(\Omega) \rightarrow L^2(\Omega)$ and satisfies $\|\ell(\vartheta)\|_{0,\Omega} \lesssim \|\vartheta\|_{0,\Omega}$ for all $\vartheta \in L^2(\Omega)$. Moreover, we assume that $\mathbb{M}^{-1}(\cdot, \cdot)$ and $\ell(\cdot)$ are

Lipschitz continuous with Lipschitz constants L_M and L_ℓ . Examples of these terms are given by Grigoreva et al. [5] for the stress-assisted diffusion and Taralov [8] for the active stress.

2 Weak formulation

In view of the boundary conditions, we define the Hilbert spaces

$$\begin{aligned}\mathbf{H}_D^1(\Omega) &:= \{\mathbf{v} \in \mathbf{H}^1(\Omega) : \mathbf{v} = \mathbf{0} \text{ on } \Gamma_D\}, \\ \mathbf{H}_N(\text{div}, \Omega) &:= \{\boldsymbol{\xi} \in \mathbf{H}(\text{div}, \Omega) : \boldsymbol{\xi} \cdot \mathbf{n} = 0 \text{ on } \Gamma_N\},\end{aligned}$$

with the boundary assignment understood as the trace of Sobolev functions (e.g., H^1 functions) onto the boundary, and consider the following weak formulation: for given $\mathbf{f} \in \mathbf{L}^2(\Omega)$, $\mathbf{g} \in L^2(\Omega)$, and $\varphi_D \in H^{1/2}(\Gamma_D)$, find $(\mathbf{u}, \mathbf{p}, \boldsymbol{\zeta}, \varphi) \in \mathbf{H}_D^1(\Omega) \times L^2(\Omega) \times \mathbf{H}_N(\text{div}, \Omega) \times L^2(\Omega)$ such that

$$2\mu \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) - \int_{\Omega} \mathbf{p} \text{div } \mathbf{v} = \int_{\Omega} \mathbf{f} \cdot \mathbf{v} \quad \forall \mathbf{v} \in \mathbf{H}_D^1(\Omega), \quad (3a)$$

$$- \int_{\Omega} \mathbf{q} \text{div } \mathbf{u} - \lambda^{-1} \int_{\Omega} \mathbf{p} \mathbf{q} = \lambda^{-1} \int_{\Omega} \ell(\varphi) \mathbf{q} \quad \forall \mathbf{q} \in L^2(\Omega), \quad (3b)$$

$$\int_{\Omega} \mathbb{M}(\boldsymbol{\varepsilon}(\mathbf{u}), \mathbf{p})^{-1} \boldsymbol{\zeta} \cdot \boldsymbol{\xi} + \int_{\Omega} \varphi \text{div } \boldsymbol{\xi} = \langle \varphi_D, \boldsymbol{\xi} \cdot \mathbf{n} \rangle_{\Gamma_D} \quad \forall \boldsymbol{\xi} \in \mathbf{H}_N(\text{div}, \Omega), \quad (3c)$$

$$\int_{\Omega} \psi \text{div } \boldsymbol{\zeta} - \theta \int_{\Omega} \varphi \psi = - \int_{\Omega} \mathbf{g} \psi \quad \forall \psi \in L^2(\Omega). \quad (3d)$$

Unique solvability with parameter-weighted norms. Adopt the following notation for the functional spaces for displacement and total volumetric stress: $\mathbf{V}_1 := \mathbf{H}_D^1(\Omega)$ and $\mathbf{Q}_1 = \mathbf{Q}_{b_1} := L^2(\Omega)$, equipped with the scaled norms and semi-norms given by

$$\begin{aligned}\|\mathbf{u}\|_{\mathbf{V}_1}^2 &:= 2\mu \|\boldsymbol{\varepsilon}(\mathbf{u})\|_{0,\Omega}^2, & \|\mathbf{p}\|_{\mathbf{Q}_1}^2 &:= \left((2\mu)^{-1} + \lambda^{-1} \right) \|\mathbf{p}\|_{0,\Omega}^2, \\ |\mathbf{v}|_{s_1, \mathbf{V}_1}^2 &:= 2\mu |\mathbf{v}|_{s_1, \Omega}^2, & |\mathbf{q}|_{s_1, \mathbf{Q}_{b_1}}^2 &:= (2\mu)^{-1} |\mathbf{q}|_{s_1, \Omega}^2.\end{aligned}$$

Denote the functional spaces for diffusive flux and concentration as $\mathbf{V}_2 = \mathbf{H}_N(\text{div}, \Omega)$ and $\mathbf{Q}_2 = \mathbf{Q}_{b_2} := L^2(\Omega)$, furnished with norms and semi-norms:

$$\begin{aligned} \|\zeta\|_{\mathbb{M}, \Omega}^2 &:= \int_{\Omega} \mathbb{M}(\boldsymbol{\varepsilon}(\mathbf{u}), \mathbf{p})^{-1} \zeta \cdot \zeta, \\ \|\zeta\|_{\mathbf{V}_2}^2 &:= \|\zeta\|_{\mathbb{M}, \Omega}^2 + \mathbb{M} \|\text{div } \zeta\|_{0, \Omega}^2, \quad \|\varphi\|_{\mathbf{Q}_2}^2 := (\mathbb{M}^{-1} + \theta) \|\varphi\|_{0, \Omega}^2, \\ |\boldsymbol{\xi}|_{s_2, \mathbf{V}_2}^2 &:= \mathbb{M} |\boldsymbol{\xi}|_{s_2, \Omega}^2, \quad |\psi|_{s_2, \mathbf{Q}_{b_2}}^2 := \mathbb{M}^{-1} |\psi|_{s_2, \Omega}^2. \end{aligned}$$

Section 2 shows the robust unique solvability of our weak formulation when using the proposed spaces in conjunction with the extended Babuška–Brezzi–Braess theory for perturbed saddle-point problems and a fixed-point argument.

We finish this section by stating the continuous dependence on data [for further details: 6, Section 3].

Theorem 1. *Let $W = \{\mathbf{w} \in \mathbf{Q}_2: \|\mathbf{w}\|_{\mathbf{Q}_2} \leq C_2 \sqrt{\mathbb{M}} \|\varphi_D\|_{1/2, \Gamma_D} + \|\mathbf{g}\|_{0, \Omega}\}$. Under the assumptions over the non-linear terms (2), suppose further that $1 \leq \lambda$, $1 \leq \mu$, $\theta \leq \mathbb{M}^{-1}$, and $C_1 L_\ell \sqrt{2\mu} \mathbb{M}^2 C_2^2 L_{\mathbb{M}} (\|\varphi_D\|_{1/2, \Gamma_D} + \|\mathbf{g}\|_{0, \Omega}) < 1$. Then, for $\varphi \in W$ there is an unique solution $(\mathbf{u}, \mathbf{p}, \zeta, \varphi) \in \mathbf{V}_1 \times \mathbf{Q}_1 \times \mathbf{V}_2 \times \mathbf{Q}_2$ of (3) such that*

$$\|(\mathbf{u}, \mathbf{p})\|_{\mathbf{V}_1 \times \mathbf{Q}_1} \leq C_1 \left(\|\mathbf{F}_1\|_{\mathbf{V}'_1} + \|\mathbf{G}_1^\varphi\|_{\mathbf{Q}'_1} \right), \quad (4a)$$

$$\|(\zeta, \varphi)\|_{\mathbf{V}_2 \times \mathbf{Q}_2} \leq C_2 \left(\|\mathbf{F}_2\|_{\mathbf{V}'_2} + \|\mathbf{G}_2\|_{\mathbf{Q}'_2} \right), \quad (4b)$$

where the constants C_1 and C_2 do not depend on the physical parameters.

3 Virtual element discretisation

Mesh assumptions. Let \mathcal{T}^h be a decomposition of Ω into polyhedral elements P with diameter h_P , let \mathcal{F}^h be the set of faces f with length h_f , and let \mathcal{E}^h be the set of edges e of \mathcal{T}^h with length h_e . Throughout this article we assume that there exists a universal constant $\rho > 0$ such that the following mesh assumptions hold.

- (M1) Each polyhedral element \mathbf{P} is star-shaped with respect to a ball of radius $\geq \rho \mathbf{h}_{\mathbf{P}}$.
- (M2) Every face f of \mathbf{P} is of diameter \mathbf{h}_f and is star-shaped with respect to a disk of radius $\geq \rho \mathbf{h}_{\mathbf{P}}$.
- (M3) Every edge e of \mathbf{P} has length $\geq \rho \mathbf{h}_{\mathbf{P}}$.

Polynomial spaces. Given an integer $k \geq 0$ the space of polynomials of degree $\leq k$ on \mathbf{P} is denoted by $\mathcal{P}_k(\mathbf{P})$ (resp. for faces f). The space of the gradients of polynomials of grade $\leq k+1$ on \mathbf{P} is denoted as $\mathcal{G}_k(\mathbf{P}) := \nabla(\mathcal{P}_{k+1}(\mathbf{P}))$ with standard notation $\mathcal{P}_{-1}(\mathbf{P}) = \{\mathbf{0}\}$ for $k = -1$. Let $\mathcal{G}_k^\oplus(\mathbf{P}) \subseteq (\mathcal{P}_k(\mathbf{P}))^3$ be any space that satisfies the property $(\mathcal{P}_k(\mathbf{P}))^3 = \mathcal{G}_k(\mathbf{P}) \oplus \mathcal{G}_k^\oplus(\mathbf{P})$. In particular, following Beirão da Veiga et al. [12], we set $\mathcal{G}_k^\oplus(\mathbf{P}) := \mathbf{x} \wedge (\mathcal{P}_{k-1}(\mathbf{P}))^3$ with $\mathbf{x} = (x_1, x_2, x_3)^t$, and \wedge denoting the usual cross product. Likewise, the space that defines the rotational of polynomials with degree $\leq k+1$ is denoted as $\mathcal{R}_k(\mathbf{P}) := \text{curl}(\mathcal{P}_{k+1}(\mathbf{P}))$, and $\mathcal{R}_k^\oplus(\mathbf{P}) \subseteq (\mathcal{P}_k(\mathbf{P}))^3$ satisfies the property $(\mathcal{P}_k(\mathbf{P}))^3 = \mathcal{R}_k(\mathbf{P}) \oplus \mathcal{R}_k^\oplus(\mathbf{P})$ with $\mathcal{R}_k^\oplus(\mathbf{P}) = \mathbf{x} \mathcal{P}_{k-1}(\mathbf{P})$.

Let $\mathbf{x}_{\mathbf{P}} = (x_{1,\mathbf{P}}, x_{2,\mathbf{P}}, x_{3,\mathbf{P}})^t$ denote the barycentre of \mathbf{P} and let $\mathcal{M}_k(\mathbf{P})$ be the set of scaled monomials

$$\mathcal{M}_k(\mathbf{P}) := \left\{ \left(\frac{\mathbf{x} - \mathbf{x}_{\mathbf{P}}}{\mathbf{h}_{\mathbf{P}}} \right)^\alpha, 0 \leq |\alpha| \leq k \right\},$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)^t$ is a non-negative multi-index with $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$ and $\mathbf{x}^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3}$. In particular, a basis of $\mathcal{G}_k(\mathbf{P})$ and $\mathcal{G}_k^\oplus(\mathbf{P})$ is $\mathcal{M}_k^\nabla(\mathbf{P}) := \nabla \mathcal{M}_{k+1}(\mathbf{P}) \setminus \{\mathbf{0}\}$ and $\mathcal{M}_k^\oplus(\mathbf{P}) := \mathbf{x}_{\mathbf{P}} \wedge (\mathcal{M}_{k-1}(\mathbf{P}))^3$, where $(\mathcal{M}_k(\mathbf{P}))^3 = \mathcal{M}_k^\nabla(\mathbf{P}) \oplus \mathcal{M}_k^\oplus(\mathbf{P})$ holds. In addition, we introduce the notation $\mathcal{M}_{k \setminus k-1}(\mathbf{P}) := \mathcal{M}_k(\mathbf{P}) \setminus \mathcal{M}_{k-1}(\mathbf{P})$.

Discrete formulation for the elasticity problem. The definition of the enhanced 3D Virtual Element (VE) space follows the approach for Stokes-like problems given by Beirão da Veiga et al. [11]. Given $k_1 \geq 2$, first, we define

an extended enhance local space as

$$\begin{aligned} \mathbf{V}_1^{h,k_1}(\mathbf{P}) &:= \{\mathbf{v}_h \in \mathbf{H}^1(\mathbf{P}) : \mathbf{v}_h|_{\partial\mathbf{P}} \in (\tilde{\mathcal{B}}_1^{h,k_1}(\partial\mathbf{P}))^3 \text{ for } \operatorname{div} \mathbf{v}_h \in \mathcal{P}_{k_1-1}(\mathbf{P}), \\ &\quad -2\mu \operatorname{div} \boldsymbol{\varepsilon}(\mathbf{v}_h) - \nabla s \in \mathcal{G}_{k_1}^\oplus(\mathbf{P}) \text{ for some } s \in L_0^2(\mathbf{P}), \\ &\quad \int_{\mathbf{P}} (\mathbf{v}_h - \Pi_1^{\varepsilon,k_1} \mathbf{v}_h) \cdot \mathbf{m}_{k_1}^\oplus = 0 \quad \forall \mathbf{m}_{k_1}^\oplus \in \mathcal{M}_{k_1 \setminus k_1-2}^\oplus(\mathbf{P})\}. \end{aligned}$$

The boundary space of VE functions, along the boundary $\partial\mathbf{P}$ of \mathbf{P} , is defined as

$$\tilde{\mathcal{B}}_1^{h,k_1}(\partial\mathbf{P}) := \{\mathbf{v}_h \in \mathbf{C}^0(\partial\mathbf{P}) : \mathbf{v}_h|_f \in \tilde{\mathcal{B}}_1^{h,k_1}(f), \forall f \subset \partial\mathbf{P}\}.$$

For each face $f \in \partial\mathbf{P}$, the enhanced VE space $\tilde{\mathcal{B}}_1^{h,k_1}(f)$ locally solves the Poisson equation with Dirichlet boundary conditions and is defined by

$$\begin{aligned} \tilde{\mathcal{B}}_1^{h,k_1}(f) &:= \{\mathbf{v}_h \in \mathbf{H}^1(f) : \mathbf{v}_h|_{\partial f} \in \mathbf{C}^0(\partial f) \text{ for } \mathbf{v}|_e \in \mathcal{P}_{k_1}(e), \quad \Delta_f \mathbf{v}_h \in \mathcal{P}_{k_1+1}(f), \\ &\quad \int_f (\mathbf{v}_h - \Pi_1^{\varepsilon,k_1,f} \mathbf{v}_h) \mathbf{m}_{k_1+1} = 0 \quad \forall e \subset \partial f, \forall \mathbf{m}_{k_1+1} \in \mathcal{M}_{k_1+1 \setminus k_1-2}(f)\}, \end{aligned}$$

where Δ_f denotes the tangential differential operator on f , and $\Pi_1^{\varepsilon,k_1,f}$ is the restriction to the face f of the energy projection operator for scalar functions defined in (5). The global discrete spaces are set defined as

$$\begin{aligned} \mathbf{V}_1^{h,k_1} &:= \{\mathbf{v}_h \in \mathbf{V}_1 : \mathbf{v}_h|_{\mathbf{P}} \in \mathbf{V}_1^{h,k_1}(\mathbf{P}), \forall \mathbf{P} \in \mathcal{T}^h\}, \\ \mathbf{Q}_1^{h,k_1} &:= \{\mathbf{q}_h \in \mathbf{Q}_1 : \mathbf{q}_h|_{\mathbf{P}} \in \mathcal{P}_{k_1-1}(\mathbf{P}), \forall \mathbf{P} \in \mathcal{T}^h\}. \end{aligned}$$

Discrete formulation for the reaction-diffusion problem. The construction of $\mathbf{H}(\operatorname{div}, \Omega)$ conforming 3D VE space naturally follows the same approach as its 2D counterpart. Further details, are given by Beirão da Veiga et al. [10]. In this case, we differ from the 2D version by setting $k_2 \geq 1$. The discrete VE space locally solves the $\nabla(\operatorname{div}) - \operatorname{curl}$ problem:

$$\begin{aligned} \mathbf{V}_2^{h,k_2}(\mathbf{P}) &:= \{\boldsymbol{\xi}_h \in \mathbf{H}(\operatorname{div}, \mathbf{P}) \cap \mathbf{H}(\operatorname{curl}, \mathbf{P}) : \boldsymbol{\xi}_h \cdot \mathbf{n}_p^f|_f \in \mathcal{P}_{k_2}(f), \forall f \in \partial\mathbf{P}, \\ &\quad \nabla(\operatorname{div} \boldsymbol{\xi}_h) \in \mathcal{G}_{k_2-2}(\mathbf{P}), \operatorname{curl} \boldsymbol{\xi}_h \in \mathcal{R}_{k_2-1}(\mathbf{P})\}. \end{aligned}$$

Then, the discrete global spaces are defined by

$$\begin{aligned} \mathbf{V}_2^{h,k_2} &:= \{\boldsymbol{\xi}_h \in \mathbf{V}_2: \boldsymbol{\xi}_h|_P \in \mathbf{V}_2^{h,k_2}(P), \forall P \in \mathcal{T}^h\}, \\ \mathbf{Q}_2^{h,k_2} &:= \{\boldsymbol{\psi}_h \in \mathbf{Q}_2: \boldsymbol{\psi}_h|_P \in \mathcal{P}_{k_2-1}(P), \forall P \in \mathcal{T}^h\}. \end{aligned}$$

Polynomial projections. The energy projection operator given by $\Pi_1^{\varepsilon,k_1} : \mathbf{H}^1(P) \rightarrow (\mathcal{P}_{k_1}(P))^3$, and the L^2 -projections operators defined as $\Pi_j^{0,k_j} : \mathbf{L}^2(P) \rightarrow (\mathcal{P}_{k_j}(P))^3$ with $j = 1, 2$ ensure that

$$\bullet \begin{cases} \int_P \boldsymbol{\varepsilon}(\mathbf{v}_h - \Pi_1^{\varepsilon,k_1} \mathbf{v}_h) : \boldsymbol{\varepsilon}(\mathbf{m}_{k_1}) = 0 \quad \forall \mathbf{m}_{k_1} \in (\mathcal{M}_{k_1}(P))^3, \\ \int_{\partial P} (\Pi_1^{\varepsilon,k_1} \mathbf{v}_h - \mathbf{v}_h) \cdot \mathbf{m}_{\text{RBM}} = 0 \quad \forall \mathbf{m}_{\text{RBM}} \in \text{RBM}(P), \end{cases} \quad (5)$$

$$\bullet \int_P (\mathbf{v}_h - \Pi_j^{0,k_j} \mathbf{v}_h) \cdot \mathbf{m}_{k_j} = 0 \quad \forall \mathbf{m}_{k_j} \in (\mathcal{M}_{k_j}(P))^3, \quad (6)$$

where $\text{RBM}(P)$ denotes the set of scaled rigid body motions. We recall that the definition for scalar functions is analogous with the usual notation Π_1^{ε,k_1} and Π_j^{0,k_j} for $j = 1, 2$. Finally, we refer the reader to Beirão da Veiga et al. [11, Proposition 5.1] for the computability of projection operators Π_1^{ε,k_1} and Π_1^{0,k_1} , pointing out that the enhance the property plays a key role (resp. [10, Theorem 3.2] for Π_2^{0,k_2}).

Interpolation operators. Let $1/2 < s_1 \leq k_1$ and $0 \leq s_2 \leq k_2$. The Fortin-like [7, 3] interpolation operators $\Pi_1^{F,k_1} : \mathbf{H}^{s_1+1}(P) \rightarrow \mathbf{V}_1^{h,k_1}(P)$, and $\Pi_2^{F,k_2} : \mathbf{H}^{s_2+1}(P) \rightarrow \mathbf{V}_2^{h,k_2}(P)$ are defined via the degrees of freedom:

$$\text{DoF}_j(\mathbf{v} - \Pi_i^{F,k_i} \mathbf{v}) = 0 \quad \forall \mathbf{v} \in \mathbf{H}^{s_i+1}(P), j = 1, \dots, \dim(\mathbf{V}_i^{h,k_i}(P)), i = 1, 2,$$

where the operator DoF_j indicates the application of the j th degree of freedom [11, 10]. Note that the associated commutative property is given as $\text{div} \Pi_j^{F,k_j}(\cdot) = \Pi_j^{0,k_j-1} \text{div}(\cdot)$.

Approximation and interpolation estimates. The following two Lemmas collect all the results involving approximation and interpolation estimates needed for the discrete formulation. We recall that these estimates arise as consequence of classical estimates and the robust version are given by Khot et al. [6, Section 4]. The extension to the 3D estimates follow similarly.

Lemma 2. *For any $\mathbf{v} \in \mathbf{H}^{s_1+1}(\mathbb{P}) \cap \mathbf{V}_1(\mathbb{P})$, $\mathbf{q} \in \mathbf{H}^{s_1}(\mathbb{P}) \cap \mathbf{Q}_{b_1}(\mathbb{P})$, $\boldsymbol{\xi} \in \mathbf{H}^{s_2}(\mathbb{P}) \cap \mathbf{V}_2(\mathbb{P})$ and $\boldsymbol{\psi} \in \mathbf{H}^{s_2}(\mathbb{P}) \cap \mathbf{Q}_{b_2}(\mathbb{P})$, the projections $\Pi_1^{\varepsilon, k_1} \mathbf{v}$, $\Pi_1^{0, k_1} \mathbf{q}$, $\Pi_2^{0, k_2} \boldsymbol{\xi}$ and $\Pi_2^{0, k_2} \boldsymbol{\psi}$ satisfy the estimates*

$$\begin{aligned} \|\mathbf{v} - \Pi_1^{\varepsilon, k_1} \mathbf{v}\|_{\mathbf{V}_1(\mathbb{P})} &\lesssim h_{\mathbb{P}}^{s_1} |\mathbf{v}|_{s_1+1, \mathbf{V}_1(\mathbb{P})}, & \|\mathbf{q} - \Pi_1^{0, k_1} \mathbf{q}\|_{\mathbf{Q}_{b_1}(\mathbb{P})} &\lesssim h_{\mathbb{P}}^{s_1} |\mathbf{q}|_{s_1, \mathbf{Q}_{b_1}(\mathbb{P})}, \\ \|\boldsymbol{\xi} - \Pi_2^{0, k_2} \boldsymbol{\xi}\|_{\mathbb{M}, \mathbb{P}} &\lesssim h_{\mathbb{P}}^{s_2} |\boldsymbol{\xi}|_{s_2, \mathbf{V}_2(\mathbb{P})}, & \|\boldsymbol{\psi} - \Pi_2^{0, k_2} \boldsymbol{\psi}\|_{\mathbf{Q}_{b_2}(\mathbb{P})} &\lesssim h_{\mathbb{P}}^{s_2} |\boldsymbol{\psi}|_{s_2, \mathbf{Q}_{b_2}(\mathbb{P})}. \end{aligned}$$

Lemma 3. *Given $\mathbf{v} \in \mathbf{H}^{s_1+1}(\mathbb{P}) \cap \mathbf{V}_1(\mathbb{P})$ and $\boldsymbol{\xi} \in \mathbf{H}^{s_2}(\mathbb{P}) \cap \mathbf{V}_2(\mathbb{P})$, the Fortin interpolation operators Π_1^{F, k_1} and Π_2^{F, k_2} satisfy*

$$\|\mathbf{v} - \Pi_1^{F, k_1} \mathbf{v}\|_{\mathbf{V}_1(\mathbb{P})} \lesssim h_{\mathbb{P}}^{s_1} |\mathbf{v}|_{s_1+1, \mathbf{V}_1(\mathbb{P})}, \quad \|\boldsymbol{\xi} - \Pi_2^{F, k_2} \boldsymbol{\xi}\|_{\mathbb{M}, \mathbb{P}} \lesssim h_{\mathbb{P}}^{s_2} |\boldsymbol{\xi}|_{s_2, \mathbf{V}_2(\mathbb{P})}.$$

The virtual element formulation for the stress-assisted diffusion problem. The discrete formulation for the fully-coupled problem reads:

For given $\mathbf{f} \in \mathbf{L}^2(\Omega)$, $\mathbf{g} \in \mathbf{L}^2(\Omega)$, and $\varphi_D \in H^{1/2}(\Gamma_D)$, find $(\mathbf{u}_h, \mathbf{p}_h, \boldsymbol{\zeta}_h, \varphi_h) \in \mathbf{V}_1^{h, k_1} \times \mathbf{Q}_1^{h, k_1} \times \mathbf{V}_2^{h, k_2} \times \mathbf{Q}_2^{h, k_2}$ such that

$$\begin{aligned} &\sum_{\mathbb{P} \in \mathcal{T}^h} \left[2\mu \int_{\mathbb{P}} \boldsymbol{\varepsilon}(\bar{\mathbf{u}}_h) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}_h) + \mathbf{S}_1^{\mathbb{P}}(\mathbf{u}_h - \bar{\mathbf{u}}_h, \mathbf{v}_h - \bar{\mathbf{v}}_h) - \int_{\Omega} \mathbf{p}_h \operatorname{div} \mathbf{v}_h \right] \\ &= \sum_{\mathbb{P} \in \mathcal{T}^h} \int_{\mathbb{P}} \bar{\mathbf{f}} \cdot \mathbf{v}_h \quad \forall \mathbf{v}_h \in \mathbf{V}_1^{h, k_1}, \end{aligned} \tag{7a}$$

$$\sum_{\mathbb{P} \in \mathcal{T}^h} \left[- \int_{\mathbb{P}} \mathbf{q}_h \operatorname{div} \mathbf{u}_h - \lambda^{-1} \int_{\mathbb{P}} \mathbf{p}_h \mathbf{q}_h \right] = \sum_{\mathbb{P} \in \mathcal{T}^h} \lambda^{-1} \int_{\mathbb{P}} \ell(\varphi_h) \mathbf{q}_h \quad \forall \mathbf{q}_h \in \mathbf{Q}_1^{h, k_1}, \tag{7b}$$

$$\sum_{\mathbb{P} \in \mathcal{T}^h} \left[\int_{\mathbb{P}} \mathbb{M}(\bar{\mathbf{u}}_h, \mathbf{p}_h)^{-1} \bar{\boldsymbol{\zeta}}_h \cdot \bar{\boldsymbol{\xi}}_h + \mathbf{S}_2^{\bar{\mathbf{u}}_h, \mathbf{p}_h, \mathbb{P}}(\boldsymbol{\zeta}_h - \bar{\boldsymbol{\zeta}}_h, \boldsymbol{\xi}_h - \bar{\boldsymbol{\xi}}_h) + \int_{\mathbb{P}} \varphi_h \operatorname{div} \boldsymbol{\xi}_h \right]$$

$$= \sum_{P \in \mathcal{T}^h} \langle \varphi_D, \boldsymbol{\xi}_h \cdot \mathbf{n} \rangle_{\partial P \cap \Gamma_D} \quad \forall \boldsymbol{\xi}_h \in \mathbf{V}_2^{h,k_2}, \quad (7c)$$

$$\sum_{P \in \mathcal{T}^h} \left[\int_P \psi_h \operatorname{div} \boldsymbol{\zeta}_h - \theta \int_{\Omega} \varphi_h \psi_h \right] = - \sum_{P \in \mathcal{T}^h} \int_P \mathbf{g} \psi_h \quad \forall \psi_h \in Q_2^{h,k_2}, \quad (7d)$$

with $\bar{\mathbf{u}}_h := \Pi_1^{\varepsilon,k_1} \mathbf{u}_h$, $\bar{\mathbf{v}}_h := \Pi_1^{\varepsilon,k_1} \mathbf{v}_h$, $\bar{\mathbf{f}} := \Pi_1^{0,k_1-2} \mathbf{f}$, $\bar{\boldsymbol{\zeta}}_h := \Pi_2^{0,k_2} \boldsymbol{\zeta}_h$ and $\bar{\boldsymbol{\xi}}_h := \Pi_2^{0,k_2} \boldsymbol{\xi}_h$. The stabilisation terms are any symmetric and positive semi-definite bilinear forms such that in the kernel of Π_1^{ε,k_1} (resp. Π_2^{0,k_2}) we have $\|\mathbf{v}_h\|_{\mathbf{V}_1} \lesssim S_1^E(\mathbf{v}_h, \mathbf{v}_h) \lesssim \|\mathbf{v}_h\|_{\mathbf{V}_1(P)}$ and $\|\boldsymbol{\xi}_h\|_{\mathbb{M},\Omega} \lesssim S_2^{\bar{\mathbf{u}}_h, \mathbf{p}_h, E}(\boldsymbol{\xi}_h, \boldsymbol{\xi}_h) \lesssim \|\boldsymbol{\xi}_h\|_{\mathbb{M},\Omega}$.

Similarly to the continuous case, the continuous dependence on data for (7) follows as an extension of Theorem 1 of Khot et al. [6, Section 4]. This is a consequence of the stabilisation operators and the Fortin-like interpolation operators that lead to the discrete inf-sup condition [defined Lemma 3, 1]. Note the associated constants \bar{C}_1 and \bar{C}_2 that appear in the discrete well-posedness result of Rekha et al. [6, Theorem 4.11] (independent of the physical parameters) do not need to coincide with C_1 and C_2 in (4). We finalise by recalling the convergence result of the VE scheme.

Theorem 4. *Under the assumptions of Theorem 1, let $(\mathbf{u}, \mathbf{p}, \boldsymbol{\zeta}, \varphi) \in (\mathbf{H}^{s_1+1}(\Omega) \cap \mathbf{V}_1) \times (H^{s_1}(\Omega) \cap Q_{b_1}) \times (\mathbf{H}^{s_2} \cap \mathbf{V}_2) \times (H^{s_2} \cap Q_{b_2})$ and $(\mathbf{u}_h, \mathbf{p}_h, \boldsymbol{\zeta}_h, \varphi_h) \in \mathbf{V}_1^{h,k_1} \times Q_1^{h,k_1} \times \mathbf{V}_2^{h,k_2} \times Q_2^{h,k_2}$ be the respective solutions of the continuous and discrete problems, with the data satisfying $\mathbf{f} \in \mathbf{H}^{s_1-1} \cap \mathbf{Q}_{b_1}$ and $\mathbf{g} \in H^{s_2}(\Omega) \cap Q_{b_2}$. If $\bar{C}_1 \sqrt{M} L_\ell + \bar{C}_2^2 \sqrt{M^3} L_M \sqrt{2\mu} (\|\varphi_D\|_{1/2, \Gamma_D} + \|\mathbf{g}\|_{0,\Omega}) < 1/2$, then, the total error $\bar{e}_h := \|(\mathbf{u} - \mathbf{u}_h, \mathbf{p} - \mathbf{p}_h, \boldsymbol{\zeta} - \boldsymbol{\zeta}_h, \varphi - \varphi_h)\|_{\mathbf{V}_1 \times Q_1 \times \mathbf{V}_2 \times Q_2}$ decays with the rate $s := \min\{s_1, s_2\}$ and*

$$\bar{e}_h \lesssim h^s (|\mathbf{f}|_{s_1-1, Q_{b_1}} + |\mathbf{u}|_{s_1+1, \mathbf{V}_1} + |\mathbf{p}|_{s_1, Q_{b_1}} + |\mathbf{g}|_{s_2, Q_{b_2}} + |\boldsymbol{\zeta}|_{s_2, \mathbf{V}_2} + |\varphi|_{s_2, Q_{b_2}}).$$

4 Numerical results

The simulations presented are implemented in VEM++ [4] for lowest case order ($k_1 = 2, k_2 = 1$). The fixed point algorithm based on the analysis

of Khot et al. [6] is optimised to ensure that, in each iteration, only the blocks containing non-linearities are reconstructed, improving the performance of the code. We recall that the computational error is computed as $\bar{e}_* := \|(\mathbf{u} - \bar{\mathbf{u}}_h, \mathbf{p} - \bar{\mathbf{p}}_h, \boldsymbol{\zeta} - \bar{\boldsymbol{\zeta}}_h, \varphi - \bar{\varphi}_h)\|_{\mathbf{V}_1 \times \mathbf{Q}_1 \times \mathbf{V}_2 \times \mathbf{Q}_2}$, and the fixed point tolerance is set to 10^{-5} .

Example 1. Let $\Omega = (0, 1)^3$ with $\Gamma_N = \{(x, y, z) \in \mathbb{R}^3 : x, y, z = 1\}$ and $\Gamma_D = \partial\Omega \setminus \Gamma_N$. We set the manufactured solutions as

$$\begin{aligned} \mathbf{u}(x, y, z) &= \frac{1}{5}[x^2 + x \cos(x) \sin(y), y^2 + x \cos(y) \sin(x), z^2 + x \cos(x) \cos(y)], \\ \varphi(x, y, z) &= \cos(\pi y) + \sin(\pi x) + x^2 + y^2 + z^2. \end{aligned}$$

The non-linearities are $\mathbb{M}(\boldsymbol{\varepsilon}(\mathbf{u}), \mathbf{p}) = 10^{-3}[e^{-10^{-4} \operatorname{tr}((2\boldsymbol{\mu}\boldsymbol{\varepsilon}(\mathbf{u}) - \mathbf{p})\mathbb{I})}]\mathbb{I}$ and $\ell(\varphi) = 1 + \varphi^2/(1 + \varphi^2)$, with the adimensional parameters $\boldsymbol{\mu} = 10^2$, $\lambda = 10^3$ and $\theta = 10^{-3}$, $\mathbf{M} = 2 \times 10$.

Figure 1 confirms the linear convergence rate predicted in Theorem 4 for a variety of meshes, thanks to the flexibility provided by the proposed VEM scheme.

Example 2. The lithiation process is configured in a perforated cylindrical particle of outer radius $5 \mu\text{m}$, inner radius of $1 \mu\text{m}$, and height of $5 \mu\text{m}$. The boundary conditions are clamped and zero lithium fluxes on the inner circumference, the maximum lithium concentration $\hat{\Omega} = 2.29 \times 10^{-14} \text{ mol}/\mu\text{m}^3$ is fixed on the outer circumference, and a traction of $-2 \times 10^{-4} \text{ N}/\mu\text{m}^2$ is applied on the outer circumference. The Young's modulus is given by $E = 1 \times 10^{-2} \text{ N}/\mu\text{m}^2$ and the Poisson ratio is $\nu = 0.3$. The diffusive source is zero and there is no body load force. The non-linear terms are $\mathbb{M}(\boldsymbol{\varepsilon}(\mathbf{u}), \mathbf{p}) = \mathbf{m}_0 [\mathbb{I} + \mathbf{m}_0 \mathbf{m}_1 ([2\boldsymbol{\mu}\boldsymbol{\varepsilon}(\mathbf{u}) - \mathbf{p}]\mathbb{I})^2]$ and $\ell(\varphi) = K_0 \varphi$, with $\mathbf{m}_0 = 1 \times 10^2 \mu\text{m}^2/\text{s}$, $\mathbf{m}_1 = 1 \times 10^3 \mu\text{m}^2/\text{N}$, $K_0 = \hat{\Omega}(2\boldsymbol{\mu} + 3\lambda)/3$ and the partial molar volume $\tilde{\Omega} = 3.497 \times 10^{12} \mu\text{m}^3/\text{mol}$. Finally, $\theta = \mathbf{M} = 1$. In this experiment, we check the behaviour of the solution when the top and bottom bases are unclamped (Figure 2) and clamped (Figure 3). The results coincide with the expected behaviour [9], confirming the applicability of the model.

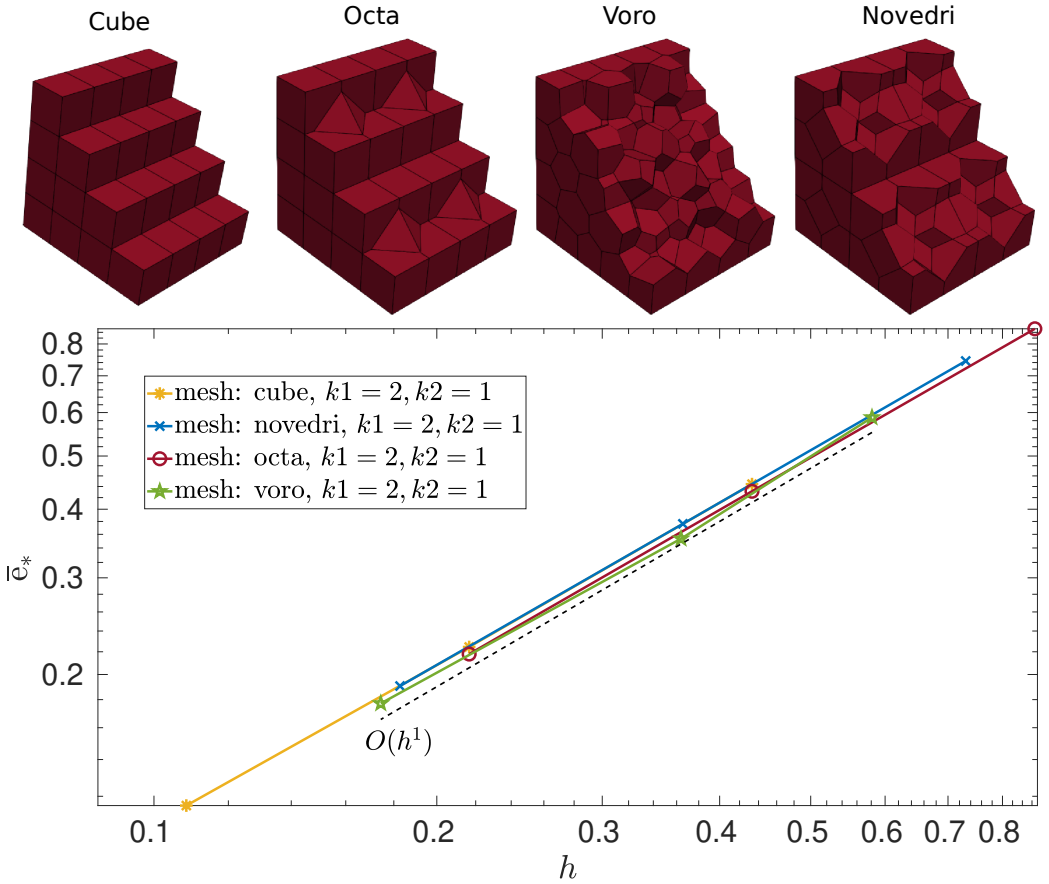


Figure 1: Example 1. (Top) An illustration of the distinct meshes used (top row), and (Bottom) the converge plot under uniform refinement.

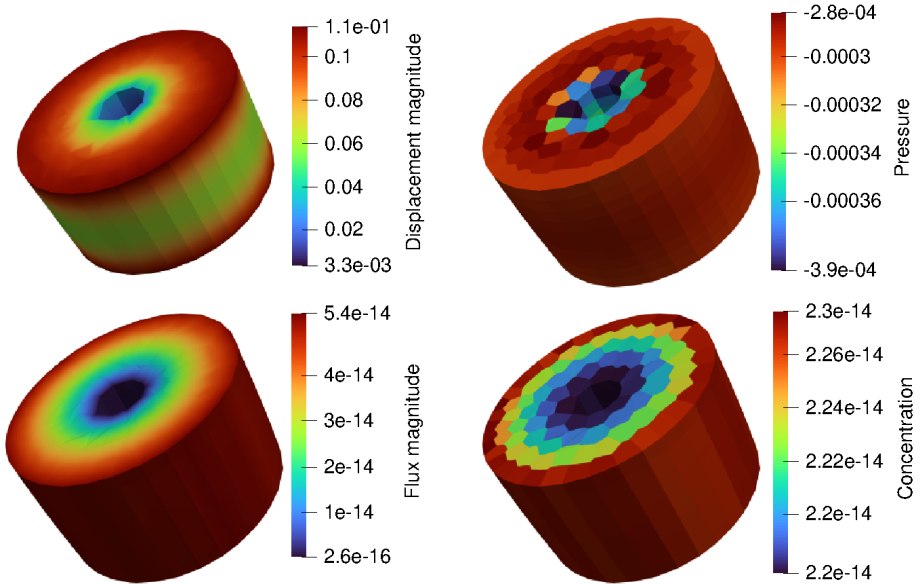


Figure 2: Example 2. Snapshots of the variables of interest in the reference configuration for the unclamped configuration: (top left) displacement; (top right) pressure; (bottom left) flux; and (bottom right) concentration.

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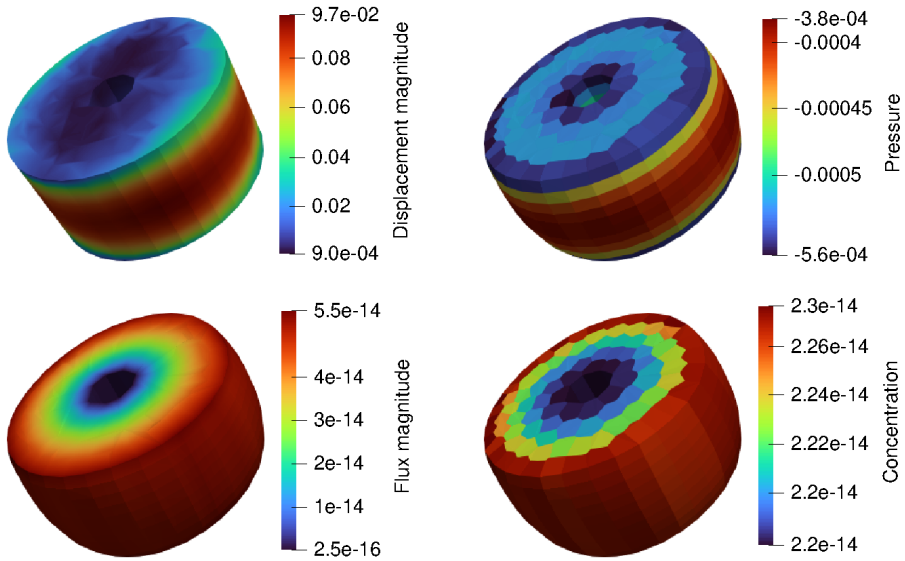


Figure 3: Example 2. Snapshots of the variables of interest in the reference configuration for the clamped configuration: (top left) displacement; (top right) pressure; (bottom left) flux; and (bottom right) concentration.

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